Adaptive discretization, regularization, linearization, and algebraic solution in unsteady nonlinear problems

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INRIA Paris-Rocquencourt

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Outline

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The Stefan problem

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$$\begin{aligned} \partial_t u - \Delta\beta(u) &= f && \text{in } \Omega \times (0,T), \\ u(\cdot,0) &= u_0 && \text{in } \Omega, \\ \beta(u) &= 0 && \text{on } \partial\Omega \times (0,T) \end{aligned}$$

Nomenclature

- u enthalpy, $\beta(u)$ temperature
- β: L_β-Lipschitz continuous, $\beta(s) = 0$ in $(0,1)$, strictly increasing otherwise
- phase change, degenerate parabolic problem
- $u_0 \in L^2(\Omega)$, $f \in L^2(0,T;L^2(\Omega))$

Context

- Ph.D. thesis of Soleiman Yousef
- collaboration with IFP Energies Nouvelles

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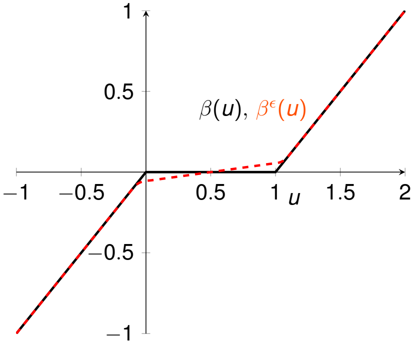
Numerical practice: regularization

Regularization of β, parameter ϵ



Questions

Discretization

- . . .

Question (Stopping and balancing criteria)

- *What is a good choice of the*
  - *regularization parameter ϵ?*
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  - *space mesh?*
- *What is a good stopping criterion for the*
  - *nonlinear solver?*
  - *linear solver?*

Question (Error)

- *How big is the error $\|u|_{I_n} - u_{h\tau}^{n,\epsilon,k,i}\|$ on time step n, space mesh $\mathcal{K}^n$, regularization parameter ϵ, linearization step k, and algebraic solver step i? How big are the individual components? How is error distributed in time and space?*

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Nonlinear steady problems

- Ladevèze (since 1990's), guaranteed upper bound
- Verfürth (1994), residual estimates
- Carstensen and Klose (2003), p-Laplacian
- Chaillou and Suri (2006, 2007), linearization errors
- Kim (2007), guaranteed estimates, loc. cons. methods

Linear unsteady problems

- Bieterman and Babuška (1982), introduction
- Verfürth (2003), efficiency, robustness wrt the final time

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- Verfürth (1998), framework for energy norm control
- Ohlberger (2001), non energy-norm estimates

Degenerate parabolic problems

- Nochetto, Schmidt, Verdi (2000), Stefan problem
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Adaptive inexact Newton method

- Bank and Rose (1982), combination with multigrid
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Model errors

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Weak formulation

Functional spaces

$$X := L^2(0,T;H_0^1(\Omega)), \qquad Z := H^1(0,T;H^{-1}(\Omega))$$

Weak formulation

$$u \in Z \qquad \text{with } \beta(u) \in X$$
$$u(\cdot,0) = u_0 \qquad \text{in } \Omega$$
$$\langle \partial_t u, \varphi\rangle(s) + (\nabla \beta(u), \nabla\varphi)(s) = (f,\varphi)(s) \qquad \forall \varphi \in H_0^1(\Omega)$$
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Outline

Assumptions

Assumption A (Approximate solution)

The function $u_{h\tau}$ *is such that*

$$u_{h\tau} \in Z, \qquad \partial_t u_{h\tau} \in L^2(0,T;L^2(\Omega)), \qquad \beta(u_{h\tau}) \in X,$$
$$u_{h\tau}|_{I_n} \text{ is affine in time on } I_n \qquad \forall 1 \le n \le N.$$

Assumption B (Equilibrated flux reconstruction)

For all $1 \le n \le N$*, there exists a vector field* $\mathbf{t}_h^n \in \mathbf{H}(\mathrm{div};\Omega)$ *such that*

$$(\nabla\cdot\mathbf{t}_h^n, 1)_K = (f^n, 1)_K - (\partial_t u_{h\tau}^n, 1)_K \qquad \forall K \in \mathcal{K}^n.$$

We denote by $\mathbf{t}_{h\tau}$ *the space–time function such that* $\mathbf{t}_{h\tau}|_{I_n} := \mathbf{t}_h^n$.

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A posteriori error estimate

Theorem (A posteriori error estimate)

Let Assumptions A and B hold. Then

$$\|\mathcal{R}(u_{h\tau})\|_{X'} + \|u_0 - u_{h\tau}(\cdot,0)\|_{H^{-1}(\Omega)}$$
$$\leq \left\{ \sum_{n=1}^{N} \int_{I_n} \sum_{K\in\mathcal{K}^n} \left(\eta_{\mathrm{R},K}^n + \eta_{\mathrm{F},K}^n(t)\right)^2 \,\mathrm{d}t \right\}^{\frac{1}{2}} + \eta_{\mathrm{IC}},$$

with

$$\eta_{\mathrm{R},K}^n := C_{\mathrm{P},K} h_K \|f^n - \partial_t u_{h\tau}^n - \nabla\cdot\mathbf{t}_h^n\|_K,$$
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Residual $\mathcal{R}(u_{h\tau}) \in X'$, defined for $\varphi \in X$, and its dual norm

$$\langle\mathcal{R}(u_{h\tau}),\varphi\rangle_{X',X} = \int_0^T \{\langle\partial_t(u-u_{h\tau}),\varphi\rangle + (\nabla\beta(u)-\nabla\beta(u_{h\tau}),\nabla\varphi)\}(s)\,\mathrm{d}s$$

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Distinguishing different error components

Theorem (An estimate distinguishing the error components)

For time n, linearization k, and regularization ϵ, there holds

$$\|\mathcal{R}(u_{h\tau}^{n,\epsilon,k})\|_{X_n'} \leq \eta_{\mathrm{sp}}^{n,\epsilon,k} + \eta_{\mathrm{tm}}^{n,\epsilon,k} + \eta_{\mathrm{reg}}^{n,\epsilon,k} + \eta_{\mathrm{lin}}^{n,\epsilon,k}.$$

- $\mathbf{l}_h^{n,\epsilon,k}$ a scheme linearized flux (not $\mathbf{H}(\mathrm{div},\Omega)$), $\mathbf{t}_h^{n,\epsilon,k}$ reconstructed $\mathbf{H}(\mathrm{div},\Omega)$ flux, Π^n interpolation op.

$$(\eta_{\mathrm{sp}}^{n,\epsilon,k})^2 := \tau^n \sum_{K\in\mathcal{K}^n} \left(\eta_{\mathrm{R},K}^{n,\epsilon,k} + \|\mathbf{l}_h^{n,\epsilon,k} + \mathbf{t}_h^{n,\epsilon,k}\|_K\right)^2,$$

$$(\eta_{\mathrm{tm}}^{n,\epsilon,k})^2 := \int_{I_n} \sum_{K\in\mathcal{K}^n} \|\nabla\Pi^n\beta(u_{h\tau}^{n,\epsilon,k})(t) - \nabla\Pi^n\beta(u_{h\tau}^{n,\epsilon,k})(t^n)\|_K^2 \,\mathrm{d}t,$$

$$(\eta_{\mathrm{reg}}^{n,\epsilon,k})^2 := \tau^n \sum_{K\in\mathcal{K}^n} \|\nabla\Pi^n\beta(u_{h\tau}^{n,\epsilon,k})(t^n) - \nabla\Pi^n\beta_\epsilon(u_{h\tau}^{n,\epsilon,k})(t^n)\|_K^2,$$

$$(\eta_{\mathrm{lin}}^{n,\epsilon,k})^2 := \tau^n \sum_{K\in\mathcal{K}^n} \|\nabla\Pi^n\beta_\epsilon(u_{h\tau}^{n,\epsilon,k})(t^n) - \mathbf{l}_h^{n,\epsilon,k}\|_K^2$$

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Efficiency assumptions

Assumption C (Technicalities)

All the meshes are shape-regular and all the approximations are piecewise polynomial.

Residual estimators

$$\left(\eta_{\mathrm{res},1}^{n,\epsilon_n,k_n}\right)^2 := \tau^n \sum_{K\in\mathcal{K}^{n-1,n}} h_K^2 \|f^n - \partial_t u_{h\tau}^{n,\epsilon_n,k_n} + \nabla\cdot\mathbf{l}_h^{n,\epsilon_n,k_n}\|_K^2,$$

$$\left(\eta_{\mathrm{res},2}^{n,\epsilon_n,k_n}\right)^2 := \tau^n \sum_{F\in\mathcal{F}^{\mathrm{i},n-1,n}} h_F \|[\![\mathbf{l}_h^{n,\epsilon_n,k_n}]\!]\cdot\mathbf{n}_F\|_F^2$$

Assumption D (Approximation property)

For all $1 \le n \le N$, there holds

$$\tau^n \sum_{K\in\mathcal{K}^{n-1,n}} \|\mathbf{l}_h^{n,\epsilon_n,k_n} + \mathbf{t}_h^{n,\epsilon_n,k_n}\|_K^2 \le C\left(\left(\eta_{\mathrm{res},1}^{n,\epsilon_n,k_n}\right)^2 + \left(\eta_{\mathrm{res},2}^{n,\epsilon_n,k_n}\right)^2\right).$$

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Efficiency assumptions

Theorem (Efficiency)

Let, for all $1 \leq n \leq N$, the stopping and balancing criteria be satisfied with the parameters $\Gamma_{\rm lin}$, $\Gamma_{\rm reg}$, and $\Gamma_{\rm tm}$ small enough. Let Assumptions C and D hold. Then

$$\eta_{\rm sp}^{n,\epsilon_n,k_n} + \eta_{\rm tm}^{n,\epsilon_n,k_n} + \eta_{\rm reg}^{n,\epsilon_n,k_n} + \eta_{\rm lin}^{n,\epsilon_n,k_n} \lesssim \|\mathcal{R}(u_{h\tau}^{n,\epsilon_n,k_n})\|_{X_n'}.$$

Outline

Relation residual–energy norm

Energy estimate (by the Gronwall lemma)

$$\frac{L_\beta}{2}\|u-u_{h\tau}\|_{X'}^2+\frac{L_\beta}{2}\|(u-u_{h\tau})(\cdot,T)\|_{H^{-1}(\Omega)}^2+\|\beta(u)-\beta(u_{h\tau})\|_{Q_T}^2$$
$$\leq\frac{L_\beta}{2}(2e^T-1)\left(\|\mathcal{R}(u_{h\tau})\|_{X'}^2+\|(u-u_{h\tau})(\cdot,0)\|_{H^{-1}(\Omega)}^2\right)$$

Theorem (Temperature and enthalpy errors, tight Gronwall)

Let $u_{h\tau}\in Z$ such that $\beta(u_{h\tau})\in X$ be arbitrary. There holds

$$\frac{L_\beta}{2}\|u-u_{h\tau}\|_{X'}^2+\frac{L_\beta}{2}\|(u-u_{h\tau})(\cdot,T)\|_{H^{-1}(\Omega)}^2+\|\beta(u)-\beta(u_{h\tau})\|_{Q_T}^2$$
$$+2\int_0^T\left(\|\beta(u)-\beta(u_{h\tau})\|_{Q_t}^2+\int_0^t\|\beta(u)-\beta(u_{h\tau})\|_{Q_s}^2e^{t-s}\,\mathrm{d}s\right)\mathrm{d}t$$
$$\leq\frac{L_\beta}{2}\Bigg\{(2e^T-1)\|(u-u_{h\tau})(\cdot,0)\|_{H^{-1}(\Omega)}^2+\|\mathcal{R}(u_{h\tau})\|_{X'}^2$$
$$+2\int_0^T\left(\|\mathcal{R}(u_{h\tau})\|_{X_t'}^2+\int_0^t\|\mathcal{R}(u_{h\tau})\|_{X_s'}^2e^{t-s}\,\mathrm{d}s\right)\mathrm{d}t\Bigg\}.$$

Relation residual–energy norm

Energy estimate (by the Gronwall lemma)

$$\frac{L_\beta}{2}\|u-u_{h\tau}\|^2_{X'}+\frac{L_\beta}{2}\|(u-u_{h\tau})(\cdot,T)\|^2_{H^{-1}(\Omega)}+\|\beta(u)-\beta(u_{h\tau})\|^2_{Q_T}$$
$$\leq\frac{L_\beta}{2}(2e^T-1)\left(\|\mathcal{R}(u_{h\tau})\|^2_{X'}+\|(u-u_{h\tau})(\cdot,0)\|^2_{H^{-1}(\Omega)}\right)$$

Theorem (Temperature and enthalpy errors, tight Gronwall)

Let $u_{h\tau}\in Z$ such that $\beta(u_{h\tau})\in X$ be arbitrary. There holds

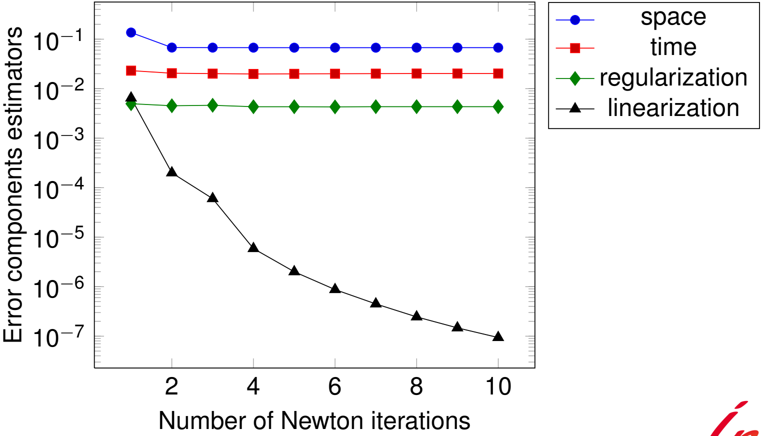
$$\frac{L_\beta}{2}\|u-u_{h\tau}\|^2_{X'}+\frac{L_\beta}{2}\|(u-u_{h\tau})(\cdot,T)\|^2_{H^{-1}(\Omega)}+\|\beta(u)-\beta(u_{h\tau})\|^2_{Q_T}$$
$$+2\int_0^T\left(\|\beta(u)-\beta(u_{h\tau})\|^2_{Q_t}+\int_0^t\|\beta(u)-\beta(u_{h\tau})\|^2_{Q_s}e^{t-s}\,\mathrm{d}s\right)\mathrm{d}t$$
$$\leq\frac{L_\beta}{2}\Bigg\{(2e^T-1)\|(u-u_{h\tau})(\cdot,0)\|^2_{H^{-1}(\Omega)}+\|\mathcal{R}(u_{h\tau})\|^2_{X'}$$
$$+2\int_0^T\left(\|\mathcal{R}(u_{h\tau})\|^2_{X'_t}+\int_0^t\|\mathcal{R}(u_{h\tau})\|^2_{X'_s}e^{t-s}\,\mathrm{d}s\right)\mathrm{d}t\Bigg\}.$$

Outline

Linearization stopping criterion

Linearization stopping criterion

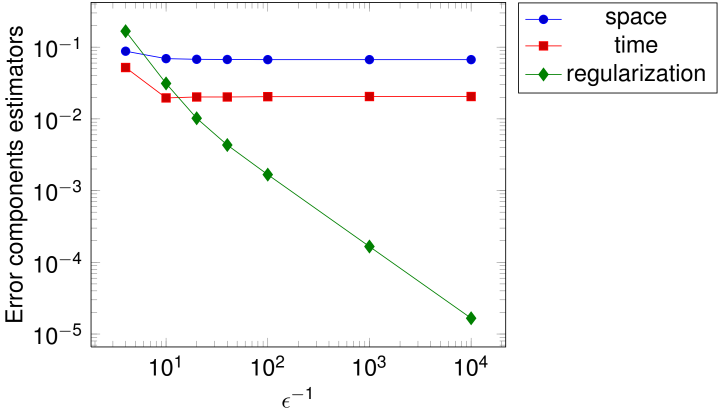
$$\eta_{\mathrm{lin}}^{n,\epsilon,k} \leq \Gamma_{\mathrm{lin}}\left(\eta_{\mathrm{sp}}^{n,\epsilon,k} + \eta_{\mathrm{tm}}^{n,\epsilon,k} + \eta_{\mathrm{reg}}^{n,\epsilon,k}\right)$$



Regularization stopping criterion

Regularization stopping criterion

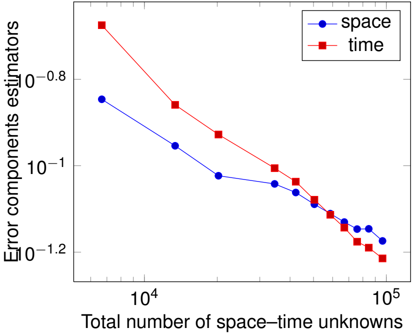
$$\eta_{\mathrm{reg}}^{n,\epsilon,k_n} \leq \Gamma_{\mathrm{reg}} \left(\eta_{\mathrm{sp}}^{n,\epsilon,k_n} + \eta_{\mathrm{tm}}^{n,\epsilon,k_n} \right)$$

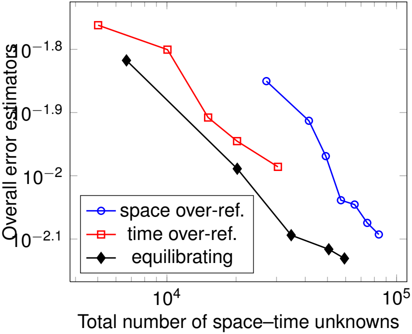


Equilibrating time and space errors

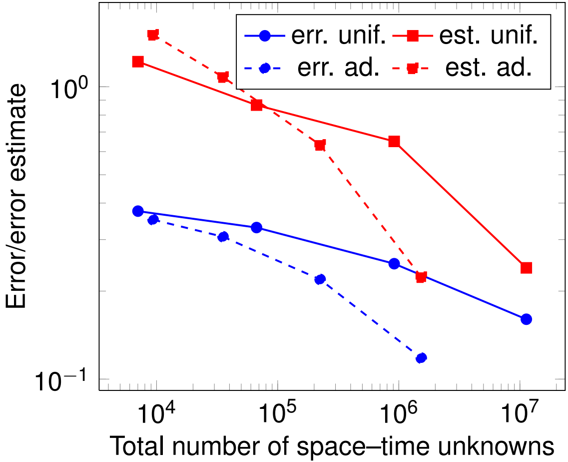
Equilibrating time and space errors

$$\gamma_{\rm tm}\eta_{\rm sp}^{n,\epsilon_n,k_n} \leq \eta_{\rm tm}^{n,\epsilon_n,k_n} \leq \Gamma_{\rm tm}\eta_{\rm sp}^{n,\epsilon_n,k_n}$$

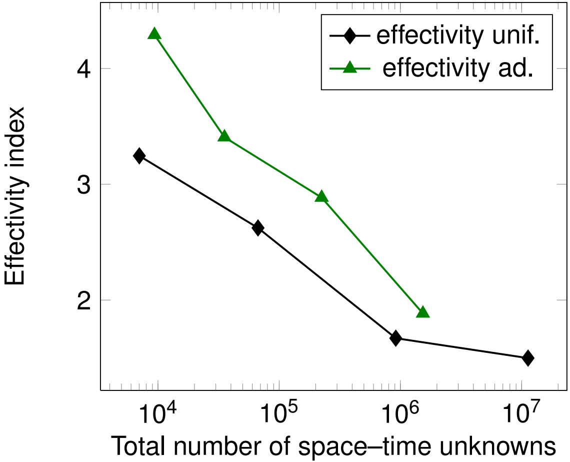




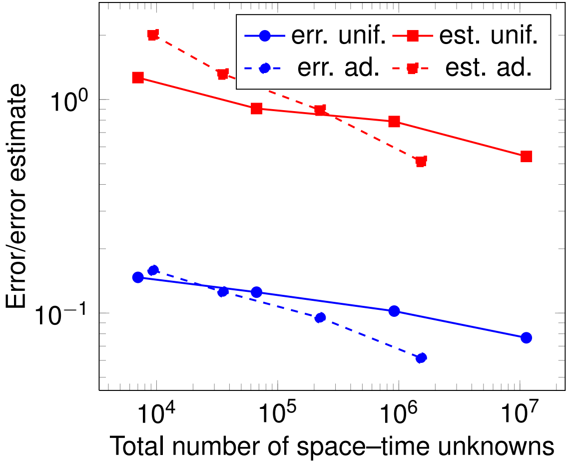
Error and estimate (dual norm of the residual)



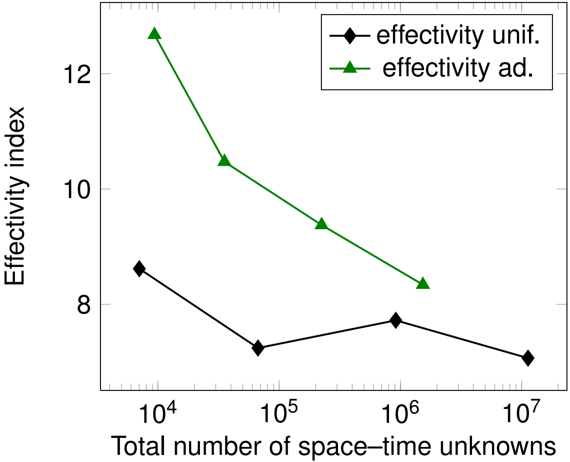
Effectivity indices (dual norm of the residual)



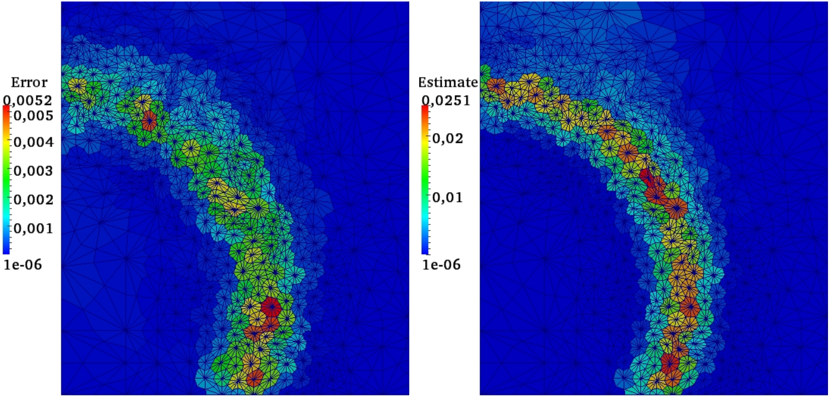
Error and estimate (energy norm)



Effectivity indices (energy norm)



Actual and estimated error distribution



Outline

Multiphase compositional flows

Governing partial differential equations

- conservation of mass for components

$$\partial_t l_c + \nabla \cdot \mathbf{\Phi}_c = q_c, \qquad \forall c \in \mathcal{C}$$

- + boundary & initial conditions

Constitutive laws

- phase pressures – reference pressure – capillary pressure

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

- Darcy's law

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

- component fluxes

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

- amount of moles of component c per unit volume

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

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- conservation of pore volume: $\sum_{p\in\mathcal{P}} S_p = 1$
- conservation of the quantity of the matter: $\sum_{c\in\mathcal{C}_p} C_{p,c} = 1$ for all $p \in \mathcal{P}$
- thermodynamic equilibrium

Mathematical issues

- coupled system
- unsteady, nonlinear
- elliptic–parabolic degenerate type
- dominant advection

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Outline

Weak solution

Energy spaces

$$X := L^2((0, t_\mathrm{F}); H^1(\Omega)),$$
$$Y := H^1((0, t_\mathrm{F}); L^2(\Omega))$$

Definition (Weak solution)

Find $(P, (S_p)_{p\in\mathcal{P}}, (C_{p,c})_{p\in\mathcal{P},c\in\mathcal{C}_p}$ such that

$$l_c \in Y \qquad \forall c \in \mathcal{C},$$
$$P_p(P, \mathbf{S}) \in X \qquad \forall p \in \mathcal{P},$$
$$\Phi_c \in [L^2((0, t_\mathrm{F}); L^2(\Omega))]^d \qquad \forall c \in \mathcal{C},$$
$$\int_0^{t_\mathrm{F}} \{(\partial_t l_c, \varphi)(t) - (\Phi_c, \nabla\varphi)(t)\}\,\mathrm{d}t = \int_0^{t_\mathrm{F}} (q_c, \varphi)(t)\mathrm{d}t \quad \forall \varphi \in X, \forall c \in \mathcal{C},$$

the initial condition holds,

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Estimate distinguishing different error components

Theorem (Estimate distinguishing different error components)

Consider

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

and the corresponding approximations. Then

$$(\textit{dual error + nonconformity})_{I_n} \leq \eta^{n,k,i}_{\mathrm{sp},\alpha} + \eta^{n,k,i}_{\mathrm{tm},\alpha} + \eta^{n,k,i}_{\mathrm{lin},\alpha} + \eta^{n,k,i}_{\mathrm{alg},\alpha}.$$

Error components

- $\eta^{n,k,i}_{\mathrm{sp},\alpha}$: spatial discretization
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Outline

Test case and numerical setting

Test case

- two-spot setting
- two phases and three components
- homogeneous/heterogeneous permeability distribution

Discretization and resolution

- fully implicit cell-centered finite volumes
- Newton linearization
- GMRes with ILU0 preconditioning algebraic solver

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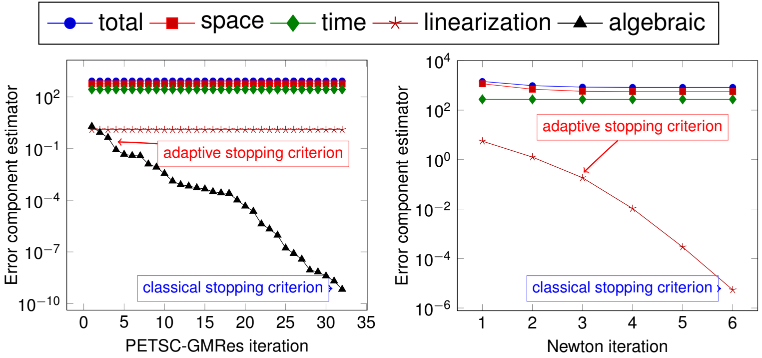
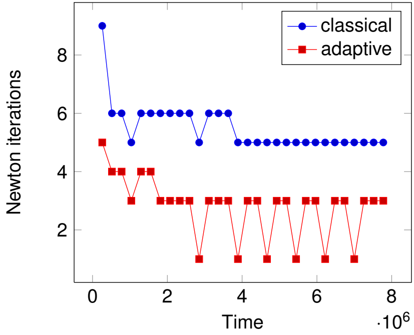
Estimators and stopping criteria

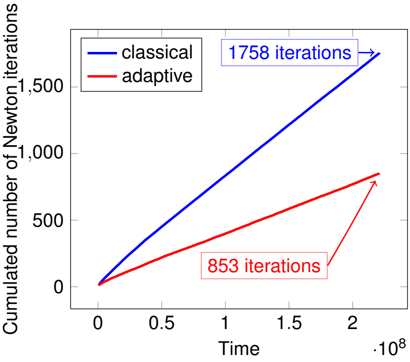


Estimators w.r.t. GMRes iterations Estimators w.r.t. Newton iterations

Newton iterations

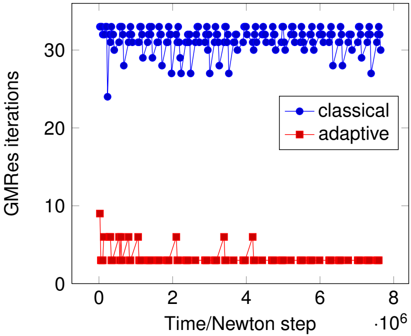


Per time step

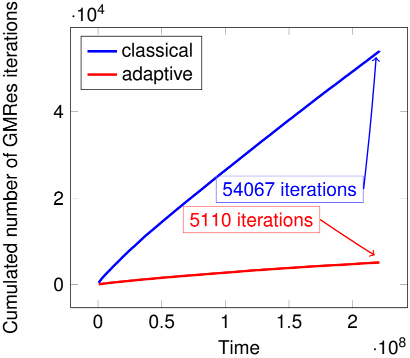


Cumulated

GMRes iterations



Per time and Newton step



Cumulated

Outline

1. Introduction
2. The Stefan problem
   - A posteriori estimate of the dual norm of the residual
   - Error components identification and adaptivity
   - Efficiency
   - Energy error a posteriori estimate
   - Numerical results
3. Multiphase flow in porous media
   - Weak solution & estimates
   - Numerical experiments
4. Conclusions and future directions

Conclusions

Complete adaptivity

- only a necessary number of algebraic solver / linearization iterations, optimal choice of the regularization parameter
- **"smart online decisions"**: algebraic solver step / linearization step / regularization / time step refinement / space mesh refinement
- important **computational savings**
- guaranteed upper bound via **a posteriori error estimates**

Future directions

- other coupled nonlinear systems
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- DI PIETRO D. A., FLAURAUD E., VOHRALÍK M., AND YOUSEF S., A posteriori error estimates, stopping criteria, and adaptivity for multiphase compositional Darcy flows in porous media, *J. Comput. Phys.* (2014), DOI 10.1016/j.jcp.2014.06.061.

Thank you for your attention!