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

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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
Outline

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The Stefan problem

\[ \partial_t u - \Delta \beta(u) = f \quad \text{in } \Omega \times (0, T), \]
\[ u(\cdot, 0) = u_0 \quad \text{in } \Omega, \]
\[ \beta(u) = 0 \quad \text{on } \partial \Omega \times (0, T) \]

Nomenclature

- \( u \) enthalpy, \( \beta(u) \) temperature
- \( \beta \): \( L_\beta \)-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
The Stefan problem

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Numerical practice: regularization

Regularization of $\beta$, parameter $\epsilon$

\[
\beta(u), \beta^\epsilon(u)
\]
Questions

Discretization

- ...

Question (Stopping and balancing criteria)

- What is a good choice of the regularization parameter $\epsilon$?
- time step?
- space mesh?

- What is a good stopping criterion for the nonlinear solver?
- linear solver?

Question (Error)

- How big is the error $\| u |_{l_n} - u_{hT}^{n,\epsilon,k,i} \|$ on time step $n$, space mesh $K^n$, regularization parameter $\epsilon$, 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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Previous results – a posteriori error estimates

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

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

Degenerate parabolic problems
- Nochetto, Schmidt, Verdi (2000), Stefan problem
- Dolejší, Ern, Vohralík (2013), ADR, Richards, robustness in a space–time dual mesh-dependent norm
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- engineering literature, since 1950’s
- Becker, Johnson, and Rannacher (1995), multigrid stopping criterion
- Arioli (2000’s), comparison of the algebraic and discretization errors by a priori arguments

Adaptive inexact Newton method
- Bank and Rose (1982), combination with multigrid
- Hackbusch and Reusken (1989), damping and multigrid
- Deuflhard (1990’s, 2004 book), adaptive damping and multigrid

Model errors
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Multiphase flow in porous media

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The Stefan problem

Multiphase flow in porous media


Weak formulation

Functional spaces

\[ X := L^2(0, T; H^1_0(\Omega)), \quad Z := H^1(0, T; H^{-1}(\Omega)) \]

Weak formulation

\[ u \in Z \quad \text{with} \quad \beta(u) \in X \]

\[ u(\cdot, 0) = u_0 \quad \text{in} \quad \Omega \]

\[ \langle \partial_t u, \varphi \rangle(s) + (\nabla \beta(u), \nabla \varphi)(s) = (f, \varphi)(s) \quad \forall \varphi \in H^1_0(\Omega) \]

a.e. \( s \in (0, T) \)
Weak formulation

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\[ X := L^2(0, T; H^1_0(\Omega)), \quad Z := H^1(0, T; H^{-1}(\Omega)) \]

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\[ \langle \partial_t u, \varphi \rangle(s) + (\nabla \beta(u), \nabla \varphi)(s) = (f, \varphi)(s) \quad \forall \varphi \in H^1_0(\Omega) \quad \text{a.e.} \quad s \in (0, T) \]
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4 Conclusions and future directions
Assumptions

Assumption A (Approximate solution)

The function \( u_{h\tau} \) is such that

\[
\begin{align*}
    u_{h\tau} & \in Z, \\
    \partial_t u_{h\tau} & \in L^2(0, T; L^2(\Omega)), \\
    \beta(u_{h\tau}) & \in X, \\
    u_{h\tau} \Big|_{I_n} & \text{ is affine in time on } I_n \\
    \forall 1 \leq n \leq N.
\end{align*}
\]

Assumption B (Equilibrated flux reconstruction)

For all \( 1 \leq n \leq N \), there exists a vector field \( t^n_h \in H(\text{div}; \Omega) \) such that

\[
(\nabla \cdot t^n_h, 1)_K = (f^n, 1)_K - (\partial_t u^n_{h\tau}, 1)_K \\
\forall K \in K_n.
\]

We denote by \( t_{h\tau} \) the space–time function such that \( t_{h\tau} \Big|_{I_n} := t^n_h \).

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Adaptive regularization, linearization, and algebraic solution
Assumptions

Assumption A (Approximate solution)

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

$$u_{h\tau} \in Z, \quad \partial_t u_{h\tau} \in L^2(0, T; L^2(\Omega)), \quad \beta(u_{h\tau}) \in X,$$

$u_{h\tau}|_{I_n}$ is affine in time on $I_n$, $\forall 1 \leq n \leq N$.

Assumption B (Equilibrated flux reconstruction)

For all $1 \leq n \leq N$, there exists a vector field $t^n_h \in H(\text{div}; \Omega)$ such that

$$(\nabla \cdot t^n_h, 1)_K = (f^n, 1)_K - (\partial_t u^n_{h\tau}, 1)_K \quad \forall K \in \mathcal{K}^n.$$

We denote by $t_{h\tau}$ the space–time function such that $t_{h\tau}|_{I_n} := t^n_h$. 
Theorem (A posteriori error estimate)

Let Assumptions A and B hold. Then

\[
\| R(u_{h,T}) \|_{X'} + \| u_0 - u_{h,T} (\cdot, 0) \|_{H^{-1}(\Omega)} \leq \left\{ \sum_{n=1}^{N} \int_{I^n} \sum_{K \in K^n} \left( \eta_{R,K}^n + \eta_{F,K}^n(t) \right)^2 \, dt \right\}^{1/2} + \eta_{IC},
\]

with

\[
\eta_{R,K}^n := C_{P,K} h_K \| f^n - \partial_t u_{h,T}^n - \nabla \cdot t_h^n \|_K,
\]

\[
\eta_{F,K}^n(t) := \| \nabla \beta(u_{h,T}(t)) + t_h^n \|_K,
\]

\[
\eta_{IC} := \| u_0 - u_{h,T} (\cdot, 0) \|_{H^{-1}(\Omega)}.
\]
Theorem (A posteriori error estimate)

Let Assumptions A and B hold. Then

\[ \| \mathcal{R}(u_{hT}) \|_{X'} + \| u_0 - u_{hT}(\cdot, 0) \|_{H^{-1}(\Omega)} \leq \left\{ \sum_{n=1}^{N} \int_{l_n} \sum_{K \in K^n} \left( \eta^n_{R,K} + \eta^n_{F,K}(t) \right)^2 \, dt \right\}^{\frac{1}{2}} + \eta_{IC}, \]

with

\[ \eta^n_{R,K} := C_{P,K} h_K \left\| f^n - \partial_t u^n_{hT} - \nabla \cdot t^n_h \right\|_K, \]
\[ \eta^n_{F,K}(t) := \| \nabla \beta(u_{hT}(t)) + t^n_h \|_K, \]
\[ \eta_{IC} := \| u_0 - u_{hT}(\cdot, 0) \|_{H^{-1}(\Omega)}. \]
Theorem (A posteriori error estimate)

Let Assumptions A and B hold. Then

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

with

$$\eta^n_{R,K} := C_{P,K} h_K \| f^n - \partial_t u^n_{h\tau} - \nabla \cdot t^n_h \|_{K},$$

$$\eta^n_{F,K}(t) := \| \nabla \beta(u_{h\tau}(t)) + t^n_h \|_{K},$$

$$\eta_{IC} := \| u_0 - u_{h\tau}(\cdot, 0) \|_{H^{-1}(\Omega)}.$$
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Distinguishing different error components

Theorem (An estimate distinguishing the error components)

For time $n$, linearization $k$, and regularization $\epsilon$, there holds

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

- $I_{h}^{n,\epsilon,k}$ a scheme linearized flux (not $H(\text{div}, \Omega)$), $t_{h}^{n,\epsilon,k}$ reconstructed $H(\text{div}, \Omega)$ flux, $\Pi^n$ interpolation op.

$$(\eta^{n,\epsilon,k}_{sp})^2 := \tau^n \sum_{K \in K^n} \left( \eta^{n,\epsilon,k}_{R,K} + \| I_{h}^{n,\epsilon,k} + t_{h}^{n,\epsilon,k} \|_K \right)^2,$$

$$(\eta^{n,\epsilon,k}_{tm})^2 := \int_{I^n} \sum_{K \in K^n} \| \nabla \Pi^n \beta(u_{h_{\tau}}^{n,\epsilon,k})(t) - \nabla \Pi^n \beta(u_{h_{\tau}}^{n,\epsilon,k})(t^n) \|_K^2 \, dt,$$

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

$$(\eta^{n,\epsilon,k}_{lin})^2 := \tau^n \sum_{K \in K^n} \| \nabla \Pi^n \beta_\epsilon(u_{h_{\tau}}^{n,\epsilon,k})(t^n) - I_{h}^{n,\epsilon,k} \|_K^2.$$
Distinguishing different error components

Theorem (An estimate distinguishing the error components)

For time \(n\), linearization \(k\), and regularization \(\epsilon\), there holds

\[
\| R(u^{n,\epsilon,k}_{h\tau}) \|_{X_n} \leq \eta_{sp}^{n,\epsilon,k} + \eta_{tm}^{n,\epsilon,k} + \eta_{reg}^{n,\epsilon,k} + \eta_{lin}^{n,\epsilon,k}.
\]

- \( I_h^{n,\epsilon,k} \) a scheme linearized flux (not \( H(\text{div}, \Omega) \)), \( t_h^{n,\epsilon,k} \) reconstructed \( H(\text{div}, \Omega) \) flux, \( \Pi^n \) interpolation op.

\[
(\eta_{sp}^{n,\epsilon,k})^2 := \tau^n \sum_{K \in \mathcal{K}_n} \left( \eta_{R,K}^{n,\epsilon,k} + \| I_h^{n,\epsilon,k} + t_h^{n,\epsilon,k} \|_K \right)^2,
\]

\[
(\eta_{tm}^{n,\epsilon,k})^2 := \int_{I^n} \sum_{K \in \mathcal{K}_n} \| \nabla^n \beta(u^{n,\epsilon,k}_{h\tau})(t) - \nabla^n \beta(u^{n,\epsilon,k}_{h\tau})(t^n) \|_K^2 \, dt,
\]

\[
(\eta_{reg}^{n,\epsilon,k})^2 := \tau^n \sum_{K \in \mathcal{K}_n} \| \nabla^n \beta(\epsilon u^{n,\epsilon,k}_{h\tau})(t^n) - \nabla^n \beta(\epsilon u^{n,\epsilon,k}_{h\tau})(t^n) \|_K^2,
\]

\[
(\eta_{lin}^{n,\epsilon,k})^2 := \tau^n \sum_{K \in \mathcal{K}_n} \| \nabla^n \beta(\epsilon u^{n,\epsilon,k}_{h\tau})(t^n) - I_h^{n,\epsilon,k} \|_K^2.
\]
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Adaptive regularization, linearization, and algebraic solution
Efficiency assumptions

Assumption C (Technicalities)

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

Residual estimators

\[
\left( \eta_{\text{res,1}}^{n,\epsilon_n, k_n} \right)^2 := \tau^n \sum_{K \in K^{n-1,n}} h_K^2 \left\| f^n - \partial_t u_{hT}^{n,\epsilon_n, k_n} + \nabla \cdot I_h^{n,\epsilon_n, k_n} \right\|_K^2,
\]

\[
\left( \eta_{\text{res,2}}^{n,\epsilon_n, k_n} \right)^2 := \tau^n \sum_{F \in F^{i,n-1,n}} h_F \left\| [I_h^{n,\epsilon_n, k_n}] \cdot n_F \right\|_F^2.
\]

Assumption D (Approximation property)

For all \(1 \leq n \leq N\), there holds

\[
\tau^n \sum_{K \in K^{n-1,n}} \left\| I_h^{n,\epsilon_n, k_n} + t_h^{n,\epsilon_n, k_n} \right\|_K^2 \leq C \left( \left( \eta_{\text{res,1}}^{n,\epsilon_n, k_n} \right)^2 + \left( \eta_{\text{res,2}}^{n,\epsilon_n, k_n} \right)^2 \right).
\]
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\]

\[
\left( \eta_{\text{res},2}^{n,\epsilon_n,k_n} \right)^2 := \tau^n \sum_{F \in \mathcal{F}^{i,n-1,n}} h_F \| [l_h^{n,\epsilon_n,k_n}] \cdot n_F \|_F^2
\]

Assumption D (Approximation property)

For all \( 1 \leq n \leq N \), there holds

\[
\tau^n \sum_{K \in \mathcal{K}^{n-1,n}} \| l_h^{n,\epsilon_n,k_n} + t_h^{n,\epsilon_n,k_n} \|_K^2 \leq C \left( \left( \eta_{\text{res},1}^{n,\epsilon_n,k_n} \right)^2 + \left( \eta_{\text{res},2}^{n,\epsilon_n,k_n} \right)^2 \right).
\]
Theorem (Efficiency)

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

$$\eta_{\text{sp}}^{n,\epsilon_n,k_n} + \eta_{\text{tm}}^{n,\epsilon_n,k_n} + \eta_{\text{reg}}^{n,\epsilon_n,k_n} + \eta_{\text{lin}}^{n,\epsilon_n,k_n} \lesssim \|\mathcal{R}(u_{hT}^{n,\epsilon_n,k_n})\|_{X'_n}.$$
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Relation residual–energy norm

**Energy estimate** (by the Gronwall lemma)

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

**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

\[
\frac{L\beta}{2} \| u - u_{h \tau} \|^2_{X'} + \frac{L\beta}{2} \| (u - u_{h \tau})(\cdot, T) \|^2_{H^{-1}(\Omega)} + \| \beta(u) - \beta(u_{h \tau}) \|^2_{Q_T} \\
+ 2 \int_0^T \left( \| \beta(u) - \beta(u_{h \tau}) \|^2_{Q_t} + \int_0^t \| \beta(u) - \beta(u_{h \tau}) \|^2_{Q_s} e^{t-s} \, ds \right) \, dt \\
\leq \frac{L\beta}{2} \left\{ \left(2e^T - 1\right) \| (u - u_{h \tau})(\cdot, 0) \|^2_{H^{-1}(\Omega)} + \| R(u_{h \tau}) \|^2_{X'} \right\} \\
+ 2 \int_0^T \left( \| R(u_{h \tau}) \|^2_{X'_t} + \int_0^t \| R(u_{h \tau}) \|^2_{X'_s} e^{t-s} \, ds \right) \, dt 
\]
Relation residual–energy norm

Energy estimate (by the Gronwall lemma)

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

Theorem (Temperature and enthalpy errors, tight Gronwall)

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

\[
\frac{L_\beta}{2} \| u - u_{h_T} \|^2_{X'} + \frac{L_\beta}{2} \| (u - u_{h_T}) (\cdot, T) \|^2_{H^{-1}(\Omega)} + \| \beta(u) - \beta(u_{h_T}) \|^2_{Q_T} \\
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\leq \frac{L_\beta}{2} \left\{ (2e^T - 1) \| (u - u_{h_T}) (\cdot, 0) \|^2_{H^{-1}(\Omega)} + \| \mathcal{R}(u_{h_T}) \|^2_{X'} \right. \\
+ 2 \int_0^T \left( \| \mathcal{R}(u_{h_T}) \|^2_{X'_t} + \int_0^t \| \mathcal{R}(u_{h_T}) \|^2_{X'_s} e^{t-s} \, ds \right) \, dt \left\}.
\]
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Linearization stopping criterion

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

Number of Newton iterations

Error components estimators

- space
- time
- regularization
- linearization

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Adaptive regularization, linearization, and algebraic solution
Regularization stopping criterion

\[ \eta_{reg,n,\epsilon,k_n} \leq \Gamma_{reg}(\eta_{sp,n,\epsilon,k_n} + \eta_{tm,n,\epsilon,k_n}) \]
Equilibrating time and space errors

\[ \gamma_{tm} \eta_{sp}^{n,\epsilon_n,k_n} \leq \eta_{tm}^{n,\epsilon_n,k_n} \leq \Gamma_{tm} \eta_{sp}^{n,\epsilon_n,k_n} \]

Error components estimators

- **Space**
- **Time**

Total number of space–time unknowns

Overall error estimators

- **Space over-ref.**
- **Time over-ref.**
- **Equilibrating**
Error and estimate (dual norm of the residual)

![Graph showing error and error estimate vs. total number of space–time unknowns]

- **err. unif.** - Error uniform
- **est. unif.** - Estimate uniform
- **err. ad.** - Error adaptive
- **est. ad.** - Estimate adaptive

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Effectivity indices (dual norm of the residual)

![Graph showing effectivity indices](image)

- Effectivity index vs. Total number of space–time unknowns
  - Black diamond: Effectivity unif.
  - Green triangle: Effectivity ad.

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Adaptive regularization, linearization, and algebraic solution
Error and estimate (energy norm)

![Graph showing error and estimate (energy norm)]

- **Error and estimate (energy norm)**
  - **Error**
    - error. unif.
    - err. ad.
  - **Estimate**
    - est. unif.
    - est. ad.

**Total number of space–time unknowns**

- $10^4$
- $10^5$
- $10^6$
- $10^7$

- **Error/error estimate**
  - $10^0$
  - $10^{-1}$

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Adaptive regularization, linearization, and algebraic solution
<table>
<thead>
<tr>
<th>Total number of space–time unknowns</th>
<th>Effectivity index</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^4$</td>
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<tr>
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<tr>
<td>$10^6$</td>
<td>8</td>
</tr>
<tr>
<td>$10^7$</td>
<td>8</td>
</tr>
</tbody>
</table>

- **Effectivity indices (energy norm)**
  - M. Vohralík
  - Adaptive regularization, linearization, and algebraic solution
Actual and estimated error distribution
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Multiphase compositional flows

Governing *partial differential* equations

- conservation of mass for *components*
  \[ \partial_t l_c + \nabla \cdot \Phi_c = q_c, \quad \forall c \in C \]
- + boundary & initial conditions

Constitutive laws

- *phase* pressures – reference pressure – capillary pressure
  \[ P_p := P + P_{cp}(S) \]
- Darcy's law
  \[ v_p(P_p, C_p) := -\Lambda (\nabla P_p - \rho_p(P_p, C_p)g) \]
- component fluxes
  \[ \Phi_c := \sum_{p\in P_c} \Phi_{p,c}, \quad \Phi_{p,c} := v_p(P_p, S, C_p)C_{p,c}v_p(P_p, C_p) \]
- amount of moles of component *c* per unit volume
  \[ l_c := \phi \sum_{p\in P_c} \zeta_p(P_p, C_p)S_p C_{p,c} \]
Multiphase compositional flows

**Governing partial differential equations**
- conservation of mass for components
  \[ \partial_t l_c + \nabla \cdot \Phi_c = q_c, \quad \forall c \in C \]
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Closure algebraic equations

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

Mathematical issues

- coupled system
- unsteady, nonlinear
- elliptic–parabolic degenerate type
- dominant advection
Closure **algebraic equations**

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**Mathematical issues**

- coupled system
- unsteady, nonlinear
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Weak solution

Energy spaces

\[ X := L^2((0, t_F); H^1(\Omega)), \]
\[ Y := H^1((0, t_F); L^2(\Omega)) \]

Definition (Weak solution)

Find \((P, (S_p)_{p \in P}, (C_p, c)_{p \in P, c \in C_p})\) such that

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

the initial condition holds,
the algebraic closure equations hold.
Weak solution

Energy spaces

\[
X := L^2((0, t_F); H^1(\Omega)), \\
Y := H^1((0, t_F); L^2(\Omega))
\]

Definition (Weak solution)

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

- \(l_c \in Y \forall c \in \mathcal{C}\),
- \(P_p(P, S) \in X \forall p \in \mathcal{P}\),
- \(\Phi_c \in [L^2((0, t_F); L^2(\Omega))]^d \forall c \in \mathcal{C}\),
- \[\int_0^{t_F} \left\{ (\partial_t l_c, \varphi)(t) - (\Phi_c, \nabla \varphi)(t) \right\} \, dt = \int_0^{t_F} (q_c, \varphi)(t) \, dt \quad \forall \varphi \in X, \forall c \in \mathcal{C},\]

the initial condition holds,

the algebraic closure equations hold.
Estimate distinguishing different error components

Consider

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

and the corresponding approximations. Then

$$(\text{dual error + nonconformity})_{ln} \leq \eta_{sp,\alpha}^{n,k,i} + \eta_{tm,\alpha}^{n,k,i} + \eta_{lin,\alpha}^{n,k,i} + \eta_{alg,\alpha}^{n,k,i}.$$

**Error components**

- $\eta_{sp,\alpha}^{n,k,i}$: spatial discretization
- $\eta_{tm,\alpha}^{n,k,i}$: temporal discretization
- $\eta_{lin,\alpha}^{n,k,i}$: linearization
- $\eta_{alg,\alpha}^{n,k,i}$: algebraic solver
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Estimate distinguishing different error components

Theorem (Estimate distinguishing different error components)

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Error components

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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
Test case and numerical setting

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Discretization and resolution
- fully implicit cell-centered finite volumes
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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 number of Newton iterations

Cumulated

Time

Classical

Adaptive

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Adaptive regularization, linearization, and algebraic solution
GMRes iterations

Per time and Newton step

Cumulated number of GMRes iterations

- Classical
- Adaptive

Cumulated

54067 iterations

5110 iterations
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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
- convergence and optimality
Conclusions

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Thank you for your attention!