An application of the Grönwall lemma avoiding exponential of the final time: a posteriori error estimates for the Stefan and Richards problems

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Outline

The heat equation

The Grönwall lemma

3 The Stefan equation

- A posteriori error estimates
- Numerical experiments
- Wrap up
- 4 The Richards equation
 - A posteriori error estimates
 - Numerical experiments
 - Wrap up
- 5 Two-phase porous media flows
- 6 Conclusions

The heat equation $(f \in L^2(0, T; L^2(\Omega)), u_0 \in L^2(\Omega))$

The heat equation

$$\partial_t u - \Delta u = f$$
 in $\Omega \times (0, T)$,
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Spaces

$$\begin{aligned} \mathbf{X} &:= L^2(0, T; H_0^1(\Omega)), \|\mathbf{v}\|_X^2 := \int_0^T \|\nabla \mathbf{v}\|^2 \, \mathrm{d}t, \\ \mathbf{Y} &:= L^2(0, T; H_0^1(\Omega)) \cap H^1(0, T; H^{-1}(\Omega)), \|\mathbf{v}\|_Y^2 := \int_0^T \|\partial_t \mathbf{v}\|_{H^{-1}(\Omega)}^2 + \|\nabla \mathbf{v}\|^2 \, \mathrm{d}t + \|\mathbf{v}(T)\|^2 \end{aligned}$$

Y norm error characterization, $u_{h au} \in X$

$$\|u-u_{h\tau}\|_{Y}^{2} = \sup_{v \in X, \|v\|_{X}=1} \left[\int_{0}^{T} (f,v) - \langle \partial_{t}u_{h\tau}, v \rangle - (\nabla u_{h\tau}, \nabla v) dt \right]^{2} + \underbrace{\|u_{0} - u_{h\tau}(0)\|^{2}}_{\text{initial condition}}$$

dual norm of the residual

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Grönwall lemma avoiding e^T: a posteriori error estimates for the Stefan & Richards problems 2/32

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Guaranteed error upper bound (reliability) ($u_{h\tau}$ FE in space, DG in time approx.)

$$\underbrace{\||u-u_{h\tau}||}_{\mathcal{H}} \leq \underbrace{\eta}$$

unknown error

computable estimator

• C_{eff} a generic constant independent of Ω , u, $u_{h\tau}$, h, p, τ , q,

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Time dependency, nonsymmetry

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- Details in Ern, Smears, and Vohralík, SINUM (2017)

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- gives rise to time-integrated and exponentially weighted norms

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Modelling problems with evolving interfaces and phase changes

The Stefan equation

Find $u: \Omega \times (0, T) \rightarrow \mathbb{R}$ such that $\partial_t u - \Delta \beta(u) = f \quad \text{in } \Omega \times (0, T),$ $\beta(u) = 0 \quad \text{on } \partial \Omega \times (0, T),$ $u(0) = u_0 \quad \text{in } \Omega.$

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Setting

- *u*: enthalpy
- $\beta(u)$: temperature
- $\Omega \subset \mathbb{R}^d$, $1 \le d \le 3$, open polytope with Lipschitz boundary $\partial \Omega$
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- source term $f \in L^2(0, T; L^2(\Omega))$, initial enthalpy $u_0 \in L^2(\Omega)$
- **nonlinear (degenerate) function** β : L_{β} -Lipschitz continuous, $\beta(s) = 0$ in (0, 1), strictly increasing otherwise



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Grönwall lemma avoiding e^{t} : a posteriori error estimates for the Stefan & Bichards problems

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Weak formulation

Spaces

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

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Residual $\mathcal{R}(u_{h\tau}) \in X'$, for $u_{h\tau} \in Z$ such that $\beta(u_{h\tau}) \in X$

$$\langle \mathcal{R}(u_{h\tau}), v \rangle_{X',X} := \int_0^T \{(f, v) - \langle \partial_t u_{h\tau}, v \rangle - (\nabla \beta(u_{h\tau}), \nabla v)\}(s) \,\mathrm{d}s \qquad v \in X$$

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Duality estimate

Lemma (Duality estimate)

Let
$$u_{h\tau} \in Z$$
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 $\frac{2}{L_{\beta}} \|\beta(u) - \beta(u_{h\tau})\|_{Q_{t}}^{2} + \|(u - u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2}$
 $\leq \|(u - u_{h\tau})(0)\|_{H^{-1}(\Omega)}^{2} + \|\mathcal{R}(u_{h\tau})\|_{X_{t}'}^{2} + \|u - u_{h\tau}\|_{X_{t}'}^{2}.$

• $W(t) \in H_0^1(\Omega)$ the solution to:

$$(\nabla W(t), \nabla \psi) = ((u - u_{h\tau})(t), \psi) \qquad \forall \psi \in H^1_0(\Omega)$$

• duality:

$$\|\nabla W(t)\| = \|(u - u_{h\tau})(t)\|_{H^{-1}(\Omega)}$$

• there holds

$$\langle \mathcal{R}(u_{h\tau}), W \rangle_{X'_t, X_t} \leq \frac{1}{2} \| \mathcal{R}(u_{h\tau}) \|_{X'_t}^2 + \frac{1}{2} \| u - u_{h\tau} \|_X^2$$

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 $\leq \|(u - u_{h\tau})(0)\|_{H^{-1}(\Omega)}^{2} + \|\mathcal{R}(u_{h\tau})\|_{X_{t}'}^{2} + \|u - u_{h\tau}\|_{X_{t}'}^{2}$

• $W(t) \in H_0^1(\Omega)$ the solution to:

$$(\nabla W(t), \nabla \psi) = ((u - u_{h\tau})(t), \psi) \qquad \forall \psi \in H^1_0(\Omega)$$

• duality:

$$\|
abla W(t)\| = \|(u - u_{h\tau})(t)\|_{H^{-1}(\Omega)}$$

• there holds

$$\langle \mathcal{R}(u_{h au}), W
angle_{X'_t, X_t} \leq rac{1}{2} \| \mathcal{R}(u_{h au}) \|^2_{X'_t} + rac{1}{2} \| u - u_{h au} \|^2_{X'_t}$$

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Duality estimate

• definition of the residual:

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$$\langle \mathcal{R}(u_{h\tau}), W \rangle_{X'_t, X_t} = \underbrace{\int_0^t \langle \partial_t(u - u_{h\tau}), W \rangle(s) \mathrm{d}s}_{\mathfrak{R}_1} + \underbrace{\int_0^t (\nabla \beta(u) - \nabla \beta(u_{h\tau}), \nabla W)(s) \mathrm{d}s}_{\mathfrak{R}_2}$$

• definition of W:

$$\mathfrak{R}_{1} = \int_{0}^{t} (\partial_{t} \nabla W, \nabla W)(s) \mathrm{d}s = \frac{1}{2} \left(\|\nabla W(t)\|_{L^{2}(\Omega)}^{2} - \|\nabla W(0)\|_{L^{2}(\Omega)}^{2} \right)$$
$$= \frac{1}{2} \left(\|(u - u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2} - \|u_{0} - u_{h\tau}(0)\|_{H^{-1}(\Omega)}^{2} \right)$$

• definition of *W* and Lipschitz continuity of β :

$$\mathfrak{R}_{2} = \int_{0}^{t} (u - u_{h\tau}, \beta(u) - \beta(u_{h\tau}))(s) \mathrm{d}s$$
$$\geq \frac{1}{L_{\beta}} \int_{0}^{t} (\beta(u) - \beta(u_{h\tau}), \beta(u) - \beta(u_{h\tau}))(s) \mathrm{d}s = \frac{1}{L_{\beta}} \|\beta(u) - \beta(u_{h\tau})\|_{\mathcal{Q}_{t}}^{2}$$

Relation error – residual featuring e^{T} , 1st component

Recall

$$egin{aligned} & rac{2}{L_eta} \|eta(u) - eta(u_{h au})\|^2_{Q_t} + \|(u-u_{h au})(t)\|^2_{H^{-1}(\Omega)} \ & \leq & \|(u-u_{h au})(0)\|^2_{H^{-1}(\Omega)} + \|\mathcal{R}(u_{h au})\|^2_{X'_t} + \int_0^t & \|u-u_{h au}\|^2_{X'_s} \mathrm{d}s \end{aligned}$$

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Relation error – residual featuring e^{T} , 1st component

Recall

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$$\frac{\frac{2}{L_{\beta}}\|\beta(u)-\beta(u_{h\tau})\|_{Q_{t}}^{2}}{\leq} \underbrace{\|(u-u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2}}_{\xi(t)} + \underbrace{\|(u-u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2}}_{\alpha(t)} + \frac{\|\mathcal{R}(u_{h\tau})\|_{X_{t}'}^{2}}{\leq} + \int_{0}^{t} \underbrace{\|u-u_{h\tau}\|_{X_{s}'}^{2}}_{\xi(s)} ds$$

A posteriori error estimates Numerical experiments Wrap up

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I Grönwall Stefan Richards Two-phase flow C A posteriori error estimates Numerical experiments Wrap up Relation error – residual featuring e^{T} , 1st component

Recall

$$\frac{\frac{2}{L_{\beta}}\|\beta(u)-\beta(u_{h\tau})\|_{Q_{t}}^{2}}{\leq} \underbrace{\|(u-u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2}}_{\alpha(t)} + \frac{\|(u-u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2}}{(u-u_{h\tau})\|_{X_{t}'}^{2}} + \int_{0}^{t} \underbrace{\|u-u_{h\tau}\|_{X_{s}'}^{2}}_{\xi(s)} ds$$

The Grönwall lemma (common form, $\alpha \ge 0$ nondecreasing)

$$\xi(t) \leq lpha(t) + \int_0^t \xi(s) \mathrm{d}s \Longrightarrow \xi(t) \leq e^t lpha(t)$$

Relation error – residual featuring e^{T} , 1st component

Recall

$$\frac{\frac{2}{L_{\beta}}\|\beta(u)-\beta(u_{h\tau})\|_{Q_{t}}^{2}}{\leq} \underbrace{\|(u-u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2}}_{\alpha(t)} + \frac{\|(u-u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2}}{(u-u_{h\tau})\|_{X_{t}'}^{2}} + \int_{0}^{t} \underbrace{\|u-u_{h\tau}\|_{X_{s}'}^{2}}_{\xi(s)} ds$$

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Thus

$$\|(u-u_{h\tau})(t)\|_{H^{-1}(\Omega)}^2 \leq e^t \big(\|(u-u_{h\tau})(0)\|_{H^{-1}(\Omega)}^2 + \|\mathcal{R}(u_{h\tau})\|_{X_s'}^2\big)$$

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Recall

$$\frac{\frac{2}{L_{\beta}}\|\beta(u)-\beta(u_{h\tau})\|_{Q_{t}}^{2}}{\leq} \underbrace{\|(u-u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2}}_{\alpha(t)} + \frac{\|(u-u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2}}{\xi(t)} + \int_{0}^{t} \underbrace{\|u-u_{h\tau}\|_{X_{s}'}^{2}}_{\xi(s)} ds$$

The Grönwall lemma (common form, $\alpha \ge 0$ nondecreasing)

$$\xi(t) \leq \alpha(t) + \int_0^t \xi(s) \mathrm{d}s \Longrightarrow \xi(t) \leq e^t \alpha(t)$$

Thus

$$\begin{aligned} \|(u-u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2} &\leq e^{t} \big(\|(u-u_{h\tau})(0)\|_{H^{-1}(\Omega)}^{2} + \|\mathcal{R}(u_{h\tau})\|_{X'_{s}}^{2} \big) \\ \implies \|u-u_{h\tau}\|_{X'}^{2} &\leq (e^{T}-1) \big(\|(u-u_{h\tau})(0)\|_{H^{-1}(\Omega)}^{2} + \|\mathcal{R}(u_{h\tau})\|_{X'}^{2} \big) \end{aligned}$$

Relation error – residual featuring e^{T} , 2nd component

Recall

$$\begin{split} & \frac{2}{L_{\beta}} \|\beta(u) - \beta(u_{h\tau})\|_{Q_{t}}^{2} + \|(u - u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2} \\ & \leq \|(u - u_{h\tau})(0)\|_{H^{-1}(\Omega)}^{2} + \|\mathcal{R}(u_{h\tau})\|_{X_{t}'}^{2} + \int_{0}^{t} \|u - u_{h\tau}\|_{X_{s}'}^{2} \mathsf{d}s \end{split}$$

Relation error – residual featuring e^{T} , 2nd component

Recall

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$$\underbrace{\frac{2}{L_{\beta}}\|\beta(u) - \beta(u_{h\tau})\|_{Q_{t}}^{2} + \|(u - u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2}}_{\xi(t)}}_{\alpha(t)} \leq \underbrace{\frac{\|(u - u_{h\tau})(0)\|_{H^{-1}(\Omega)}^{2} + \|\mathcal{R}(u_{h\tau})\|_{X_{t}'}^{2}}_{\alpha(t)} + \int_{0}^{t} \underbrace{\left(\frac{2}{L_{\beta}}\|\beta(u) - \beta(u_{h\tau})\|_{Q_{s}}^{2} + \|u - u_{h\tau}\|_{X_{s}'}^{2}\right)}_{\xi(s)} ds}_{\xi(s)}$$

A posteriori error estimates Numerical experiments Wrap up

I Grönwall Stefan Richards Two-phase flow C A posteriori error estimates Numerical experiments Wrap up Relation error – residual featuring e^{T} , 2nd component

Recall

$$\underbrace{\frac{2}{L_{\beta}}\|\beta(u) - \beta(u_{h\tau})\|_{Q_{t}}^{2} + \|(u - u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2}}_{\xi(t)}}_{\alpha(t)} \leq \underbrace{\frac{\|(u - u_{h\tau})(0)\|_{H^{-1}(\Omega)}^{2} + \|\mathcal{R}(u_{h\tau})\|_{X_{t}'}^{2}}_{\alpha(t)} + \int_{0}^{t} \underbrace{\left(\frac{2}{L_{\beta}}\|\beta(u) - \beta(u_{h\tau})\|_{Q_{s}}^{2} + \|u - u_{h\tau}\|_{X_{s}'}^{2}\right)}_{\xi(s)} ds}_{\xi(s)}$$

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$$\underbrace{\frac{2}{L_{\beta}}\|\beta(u) - \beta(u_{h\tau})\|_{Q_{t}}^{2} + \|(u - u_{h\tau})(t)\|_{H^{-1}(\Omega)}^{2}}_{\xi(t)}}_{\alpha(t)} \leq \underbrace{\frac{\|(u - u_{h\tau})(0)\|_{H^{-1}(\Omega)}^{2} + \|\mathcal{R}(u_{h\tau})\|_{X_{t}'}^{2}}_{\alpha(t)} + \int_{0}^{t} \underbrace{\left(\frac{2}{L_{\beta}}\|\beta(u) - \beta(u_{h\tau})\|_{Q_{s}}^{2} + \|u - u_{h\tau}\|_{X_{s}'}^{2}\right)}_{\xi(s)} ds}_{\xi(s)}$$

A posteriori error estimates Numerical experiments Wrap up

The Grönwall lemma (common form, $\alpha \ge 0$ nondecreasing)

$$\xi(t) \leq lpha(t) + \int_0^t \xi(s) \mathrm{d}s \Longrightarrow \xi(t) \leq e^t lpha(t)$$

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

Relation error – residual featuring e^{T} , altogether

Lemma (Relation error – residual featuring e^{T})

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

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

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Relation error – residual without e^{T} by the sharp Grönwall

Lemma (Relation error – residual without e^{T})

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

$$\begin{split} & \frac{L_{\beta}}{2} \| u - u_{h\tau} \|_{X'}^{2} + \frac{L_{\beta}}{2} \| (u - u_{h\tau})(\cdot, T) \|_{H^{-1}(\Omega)}^{2} + \| \beta(u) - \beta(u_{h\tau}) \|_{Q_{T}}^{2} \\ & + 2 \int_{0}^{T} \left(\| \beta(u) - \beta(u_{h\tau}) \|_{Q_{t}}^{2} + \int_{0}^{t} \| \beta(u) - \beta(u_{h\tau}) \|_{Q_{s}}^{2} e^{t-s} \, \mathrm{d}s \right) \, \mathrm{d}t \\ & \leq \frac{L_{\beta}}{2} \bigg\{ (2e^{T} - 1) \| (u - u_{h\tau})(\cdot, 0) \|_{H^{-1}(\Omega)}^{2} + \| \mathcal{R}(u_{h\tau}) \|_{X'}^{2} \\ & + 2 \int_{0}^{T} \left(\| \mathcal{R}(u_{h\tau}) \|_{X'_{t}}^{2} + \int_{0}^{t} \| \mathcal{R}(u_{h\tau}) \|_{X'_{s}}^{2} e^{t-s} \, \mathrm{d}s \right) \, \mathrm{d}t \bigg\}. \end{split}$$



Outline

- The heat equation
- 2 The Grönwall lemma

3 The Stefan equation

• A posteriori error estimates

Numerical experiments

Wrap up

4 The Richards equation

- A posteriori error estimates
- Numerical experiments
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- 5 Two-phase porous media flows
- 6 Conclusions

How large is the error? (Effectivity indices)



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Where (in space and time) is the error localized?



How large are the error components? (Linearization)

Linearization stopping criterion



M. Vohralík

How large are the error components? (Regularization)

Regularization stopping criterion



How large are the error components? (Time and space)

Equilibrating time and space errors



Outline

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- treatment of time-dependent nonlinearity: sharp Grönwall lemma not neglecting the integral terms
- avoids the appearance of e^T but gives rise to time-integrated and exponentially-weighted norms



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- Details in D. Pietro, M. Vohralík, and S. Yousef, Math. Comp. (2015)

Outline

- The heat equation
- 2 The Grönwall lemma
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Modelling flow of water and air through soil

The Richards equation

Find $u : \Omega \times (0, T) \to \mathbb{R}$ such that $\partial_t S(u) - \nabla \cdot [\mathbf{K} \kappa(S(u))(\nabla u + \mathbf{g})] = f(S(u)) \quad \text{in } \Omega \times (0, T),$ $u = 0 \quad \text{on } \partial\Omega \times (0, T),$ $(S(u))(0) = s_0 \quad \text{in } \Omega.$

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Setting

- U: pressure
- S(u): saturation
- $\Omega \subset \mathbb{R}^d$, $1 \le d \le 3$, open polytope with Lipschitz boundary $\partial \Omega$
- T: final time
- diffusion tensor *K*, source term *f* ∈ *C*¹([0, 1] × Ω × ℝ), gravity *g*, initial saturation *s*₀ ∈ *L*[∞](Ω), 0 ≤ *s*₀ ≤ 1
- nonlinear (degenerate) functions S and κ

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Nonlinear (degenerate) functions S and κ



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Weak formulation

Spaces

 $\boldsymbol{X} := L^2(0, T; H^1_0(\Omega)),$

$$\boldsymbol{Z} := \boldsymbol{H}^{1}(\boldsymbol{0}, \boldsymbol{T}; \boldsymbol{H}^{-1}(\Omega))$$

Total pressure (Kirchhoff transform)

$$\mathcal{K}(p) := egin{cases} \int_0^p \kappa(S(arrho)) \, \mathrm{d}arrho & ext{for } p \leq p_{\mathsf{M}}, \ P_{\mathsf{M}} + \kappa(1)(p - p_{\mathsf{M}}) & ext{for } p > p_{\mathsf{M}}, \end{cases}, \qquad heta \, \circ \, \mathcal{K} = S$$

Weak formulation

$$\Psi \in X \quad \text{with } s := \theta(\Psi) \in Z, \quad s(0) = s_0 \quad \text{in } \Omega,$$

$$\int_0^T \langle \partial_t \theta(\Psi), v \rangle + \int_0^T (\mathcal{K}(\nabla \Psi + \mathcal{g}\kappa(\theta(\Psi))), \nabla v) = \int_0^T (f(\theta(\Psi)), v) \quad \forall v \in X$$

Residual $\mathcal{R}(\Psi_{h\tau}) \in X'$, for $\Psi_{h\tau} \in X$ such that $s_{h\tau} := \theta(\Psi_{h\tau}) \in Z$
$$\langle \mathcal{R}(\Psi_{h\tau}), v \rangle_{X',X} := \int_0^T \{(f(\theta(\Psi_{h\tau})), v) - \langle \partial_t \theta(\Psi_{h\tau}), v \rangle - (\mathcal{K}(\nabla \Psi_{h\tau} + \mathcal{g}\kappa(\theta(\Psi_{h\tau}))), \nabla v)\}(s) ds$$

Dual norm of the residual

 $\|\mathcal{R}(u_{h\tau})\|_{X'} := \sup_{v \in X, v \in V} \langle \mathcal{R}(u_{h\tau}), v \rangle_{X', X'}$

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 $Z := H^1(0, T; H^{-1}(\Omega))$

Weak formulation

Spaces

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Grönwall Stefan Richards Two-phase flow C

 $Z := H^1(0, T; H^{-1}(\Omega))$

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 $\langle \mathcal{R}(\Psi_{h\tau}), v \rangle_{X',X} := \int_0 \{ (f(\theta(\Psi_{h\tau})), v) - \langle \partial_t \theta(\Psi_{h\tau}), v \rangle - (\mathbf{K}(\nabla \Psi_{h\tau} + \mathbf{g}\kappa(\theta(\Psi_{h\tau}))), \nabla v) \} (s) ds$ Dual norm of the residual

$$\|\mathcal{R}(u_{h\tau})\|_{X'} := \sup_{v \in X, \, \|v\|_X = 1} \langle \mathcal{R}(u_{h\tau}), v \rangle_{X', X}$$

Weak formulation

Spaces

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Dual norm of the residual

$$\|\mathcal{R}(u_{h au})\|_{X'} := \sup_{v\in X, \|v\|_X=1} \langle \mathcal{R}(u_{h au}), v
angle_{X', X}$$

Weak formulation

Spaces

 $X := L^2(0, T; H^1_0(\Omega)), \qquad Z := H^1(0, T; H^{-1}(\Omega))$ Total pressure (Kirchhoff transform)

$$\mathcal{K}(\boldsymbol{p}) := egin{cases} \int_0^{\boldsymbol{p}} \kappa(\mathcal{S}(\varrho)) \, \mathrm{d} \varrho & ext{for } \boldsymbol{p} \leq \boldsymbol{p}_\mathsf{M}, \ \mathcal{P}_\mathsf{M} + \kappa(1)(\boldsymbol{p} - \boldsymbol{p}_\mathsf{M}) & ext{for } \boldsymbol{p} > \boldsymbol{p}_\mathsf{M}, \end{cases}, \qquad heta \, \circ \, \mathcal{K} = \mathsf{S}$$

Weak formulation

$$\begin{split} \Psi \in X & \text{with } \boldsymbol{s} := \theta(\Psi) \in Z, \qquad \boldsymbol{s}(0) = \boldsymbol{s}_0 \quad \text{in } \Omega, \\ \int_0^T \langle \partial_t \theta(\Psi), \boldsymbol{v} \rangle + \int_0^T (\boldsymbol{K}(\nabla \Psi + \boldsymbol{g}\kappa(\theta(\Psi))), \nabla \boldsymbol{v}) = \int_0^T (f(\theta(\Psi)), \boldsymbol{v}) & \forall \boldsymbol{v} \in X \\ \text{Residual } \mathcal{R}(\Psi_{h\tau}) \in X', \text{ for } \Psi_{h\tau} \in X \text{ such that } \boldsymbol{s}_{h\tau} := \theta(\Psi_{h\tau}) \in Z \\ \langle \mathcal{R}(\Psi_{h\tau}), \boldsymbol{v} \rangle_{X',X} := \int_0^T \{(f(\theta(\Psi_{h\tau})), \boldsymbol{v}) - \langle \partial_t \theta(\Psi_{h\tau}), \boldsymbol{v} \rangle - (\boldsymbol{K}(\nabla \Psi_{h\tau} + \boldsymbol{g}\kappa(\theta(\Psi_{h\tau}))), \nabla \boldsymbol{v})\}(\boldsymbol{s}) d\boldsymbol{s} \\ \text{Dual norm of the residual} \end{split}$$

$$\|\mathcal{R}(u_{h\tau})\|_{X'} := \sup_{v \in \mathcal{X}, \, \|v\|_X = 1} \langle \mathcal{R}(u_{h\tau}), v \rangle_{X', X}$$

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Time-integration functionals based on the sharp Grönwall lemma

Time-integration functionals, $\alpha : [0, T] \rightarrow [0, \infty)$

$$\mathcal{J}_{\alpha}: L^{2}([0, T]) \to [0, \infty),$$
$$\mathcal{J}_{\alpha}(\varrho) := \left[\exp\left(-\int_{0}^{T} \alpha\right) \int_{0}^{T} \left(\varrho^{2}(t) + \alpha(t) \exp\left(\int_{t}^{T} \alpha\right) \int_{0}^{t} \varrho^{2} \right) \mathrm{d}t \right]^{\frac{1}{2}}$$

• define norm on $L^2([0, T])$

• actually equivalent to the L²([0, T]) norm

$$\exp\left(-\frac{1}{2}\int_{0}^{T}\alpha\right)\|\varrho\|_{L^{2}([0,T])} \leq \mathcal{J}_{\alpha}(\varrho) \leq \|\varrho\|_{L^{2}([0,T])}$$

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• define norm on $L^2([0, T])$

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Relation error – residual without e^{T} by the sharp Grönwall lemma

Lemma (Relation error – residual without e^{T})

Let $\Psi_{h\tau} \in X$ such that $s_{h\tau} := \theta(\Psi_{h\tau}) \in Z$. Then

$$\begin{split} & e^{-\int_0^T (\lambda+\mathfrak{C}_1)} \|(s-s_{h\tau})(T)\|_{H^{-1}(\Omega)}^2 + \mathcal{J}_{\lambda+\mathfrak{C}_1} \left(\theta_{\partial,\mathsf{M}}^{-\frac{1}{2}} \|s-s_{h\tau}\|\right)^2 \\ &\leq \|s_0-s_{h\tau}(0)\|_{H^{-1}(\Omega)}^2 + \mathcal{J}_{\lambda+\mathfrak{C}_1} (\lambda^{-\frac{1}{2}} \|\mathcal{R}(\Psi_{h\tau})\|_{H^{-1}(\Omega)})^2, \end{split}$$

$$\begin{split} & e^{-\int_0^T \mathfrak{C}_2} \| (s-s_{h\tau})(T) \|^2 + \frac{1}{2} \mathcal{J}_{\mathfrak{C}_2} \left(\left\| D(s)^{-\frac{1}{2}} \mathcal{K}^{\frac{1}{2}} \nabla (\Psi - \Psi_{h\tau}) \right\| \right)^2 \\ & \leq \| s_0 - s_{h\tau}(0) \|^2 + \mathcal{J}_{\mathfrak{C}_2} \left(\eta^{\mathsf{deg}} \right)^2 + 4 \, \mathcal{J}_{\mathfrak{C}_2} \left(D_{\mathsf{m}}^{-\frac{1}{2}} \| \mathcal{R}(\Psi_{h\tau}) \|_{H^{-1}(\Omega)} \right)^2, \end{split}$$

$$\begin{aligned} & \mathcal{J}_{\lambda}(\|\partial_{t}(s-s_{h\tau})\|_{H^{-1}(\Omega)})^{2} \\ & \leq 3\left[\mathcal{J}_{\lambda}(\|\Psi-\Psi_{h\tau}\|_{H^{-1}(\Omega)})^{2} + \mathfrak{C}_{3}(\mathcal{T})\mathcal{J}_{\lambda}\left(\|s-s_{h\tau}\|\right)^{2} + \mathcal{J}_{\lambda}(\|\mathcal{R}(\Psi_{h\tau})\|_{H^{-1}(\Omega)})^{2}\right] \end{aligned}$$

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How large is the error? Robustness wrt the final time (known sol.)



K. Mitra, M. Vohralík, preprint (2022)

Where (in space and time) is the error **localized**? (benchmark case)





Exact local error

K. Mitra, M. Vohralík, preprint (2022)

Estimated local error

Grönwall lemma avoiding e^{T} : a posteriori error estimates for the Stefan & Richards problems 24 / 32

Realistic case

Setting

- unit square $\Omega = (0, 1)^2$
- *T* = 1
- $f(\mathbf{x}, u) = 0$, heterogeneous and anisotropic \mathbf{K} , $\mathbf{g} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
- Brooks-Corey-type saturation and permeability laws

$$S(u) := egin{cases} rac{1}{(2-u)^{rac{1}{3}}} & ext{if } u < 1, \ 1 & ext{if } u \geq 1 \end{cases}, \quad \kappa(s) := s^3$$

• $(h, \tau) = (h_0, \tau_0)/\ell$ with $\ell \in \{1, 2, 4\}$, $h_0 = 0.2$, and $\tau_0 = 0.04$

Realistic case





Numerical saturation for $\ell = 2$ at t = 1

Where (in space and time) is the error **localized**? (realistic test case)



Estimated local error

Exact local error

K. Mitra, M. Vohralík, preprint (2022)

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A posteriori error estimates for the Richards equation

Time dependency, nonsymmetry, nonlinearity, double degeneracy

treatment of time-dependent nonlinearity: combined energy & negative norms together with weighted time-integration functionals (~ sharp Grönwall lemma)



A posteriori error estimates for the Richards equation

- treatment of time-dependent nonlinearity: combined energy & negative norms together with weighted time-integration functionals (~ sharp Grönwall lemma)
- guaranteed error upper bound (reliability)
- Iocal in space and in time efficiency

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- Details in K. Mitra, M. Vohralík, Math. Comp. (2024)

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I Grönwall Stefan Richards Two-phase flow C

Two-phase flow, water saturation



M. Vohralík, M. Wheeler, Computational Geosciences (2013)

I Grönwall Stefan Richards Two-phase flow C

Where (in space and time) is the error **localized**? (two-phase flow)



M. Vohralík, M. Wheeler, Computational Geosciences (2013)

All error components (two-phase flow)



M. Vohralík, M. Wheeler, Computational Geosciences (2013)

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• a posteriori error certification for unsteady, nonlinear, & degenerate pbs

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Conclusions

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Thank you for your attention!



Grönwall lemma avoiding e^T: a posteriori error estimates for the Stefan & Richards problems 32 / 3









Partition of unity





Grönwall lemma avoiding e^{T} : a posteriori error estimates for the Stefan & Richards problems 33 / 32

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Equilibrated flux reconstruction Destuynder and Métivet (1998), Braess & Schöberl (2008), Ern & Vohralik (2013)



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Equilibrated flux reconstruction Destuynder and Métivet (1998), Braess & Schöberl (2008), Ern & Vohralik (2013)

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Outline







Two-phase flow, water saturation



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Recovering mass balance: two-phase flow (inexact solver, water)



original mass balance misfit (m²s⁻¹)

Setting

- fully implicit discretization of a two-phase oil-water flow
- cell-centered finite volumes on a square mesh
- time step 260, 1st Newton linearization, GMRes iteration 195

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

Grönwall lemma avoiding e^T: a posteriori error estimates for the Stefan & Richards problems 36 / 32

corrected mass balance misfit $(m^2 s^{-1})$

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