

# Adaptive regularization, linearization, and discretization for the two-phase Stefan problem

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*joint work with D. A. Di Pietro and S. Yousef*

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# Outline

- 1 Introduction
- 2 Error estimates for the dual norm of the residual
  - Residual and its dual norm
  - A posteriori error estimate
  - Error components identification and adaptivity
  - Efficiency
- 3 Energy error estimates
- 4 Numerical results
- 5 Conclusions and future directions

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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
- $\beta$ :  $L_\beta$ -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

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

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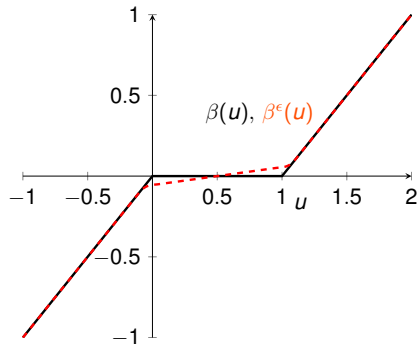
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# Numerical practice: regularization

## Regularization of $\beta$ with a parameter $\epsilon$



# 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  $\|u|_{I_n} - u_{h\tau}^{n,\epsilon,k,i}\|$  on time step  $n$ , space mesh  $\mathcal{K}^n$ , 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), guaranteed estimates
- 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
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## Degenerate parabolic problems

- Nchetto, Schmidt, Verdi (2000), Stefan problem
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# Weak formulation

## Functional spaces

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

## Weak formulation

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

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

$$\langle \partial_t u, \varphi \rangle(s) + (\nabla \beta(u), \nabla \varphi)(s) = (f, \varphi)(s) \quad \forall \varphi \in H_0^1(\Omega) \\ \text{a.e. } s \in (0, T)$$



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# Residual and its dual norm

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

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

$$\varphi \in X$$

**Dual norm of the residual**

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

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# Time-localization of the dual norm of the residual

**Time interval**  $I_n$

$$X_n := L^2(I_n; H_0^1(\Omega))$$

$$\begin{aligned} \|\mathcal{R}(u_{h\tau})\|_{X'_n} := & \sup_{\varphi \in X_n, \|\varphi\|_{X_n}=1} \int_{I_n} \{ \langle \partial_t(u - u_{h\tau}), \varphi \rangle \\ & + (\nabla\beta(u) - \nabla\beta(u_{h\tau}), \nabla\varphi) \}(\mathbf{s}) \, d\mathbf{s} \end{aligned}$$

$L^2$  in time ...

$$\|\mathcal{R}(u_{h\tau})\|_{X'}^2 = \sum_{1 \leq n \leq N} \|\mathcal{R}(u_{h\tau})\|_{X'_n}^2$$

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# Assumptions

## Assumption A (Approximate solution)

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

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

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

## Assumption B (Equilibrated flux reconstruction)

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

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

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

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

with

$$\begin{aligned} \eta_{R,K}^n &:= C_{P,K} h_K \|f^n - \partial_t u_{h\tau}^n - \nabla \cdot \mathbf{t}_h^n\|_K, \\ \eta_{F,K}^n(t) &:= \|\nabla \beta(u_{h\tau}(t)) + \mathbf{t}_h^n\|_K, \\ \eta_{IC} &:= \|u_0 - u_{h\tau}(\cdot, 0)\|_{H^{-1}(\Omega)}. \end{aligned}$$

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# Sketch of the proof

- $\varphi \in X$  with  $\|\varphi\|_X = 1$  given ( $f$  pw constant in time)
- adding and subtracting  $(\mathbf{t}_{h\tau}, \nabla\varphi)$ , Green theorem:

$$\langle \mathcal{R}(\mathbf{u}_{h\tau}), \varphi \rangle_{X', X} = \mathfrak{T}_1 + \mathfrak{T}_2$$

$$:= \int_0^T \{ (f - \partial_t \mathbf{u}_{h\tau} - \nabla \cdot \mathbf{t}_{h\tau}, \varphi) - (\mathbf{t}_{h\tau} + \nabla \beta(\mathbf{u}_{h\tau}), \nabla \varphi) \}(\mathbf{s}) ds$$

- 

$$\mathfrak{T}_1 = \sum_{n=1}^N \int_{I_n} \sum_{K \in \mathcal{K}^n} (f^n - \partial_t \mathbf{u}_{h\tau}^n - \nabla \cdot \mathbf{t}_h^n, \varphi - \Pi_0^n \varphi)_K(\mathbf{s}) ds$$

$$\leq \sum_{n=1}^N \int_{I_n} \sum_{K \in \mathcal{K}^n} \underbrace{C_{P,K} h_K \|f^n - \partial_t \mathbf{u}_{h\tau}^n - \nabla \cdot \mathbf{t}_h^n\|_K}_{\eta_{R,K}^n} \|\nabla \varphi\|_K(\mathbf{s}) ds$$

- 

$$\mathfrak{T}_2 \leq \sum_{n=1}^N \int_{I_n} \sum_{K \in \mathcal{K}^n} \underbrace{\|\mathbf{t}_h^n + \nabla \beta(\mathbf{u}_{h\tau})\|_K}_{\eta_{E,K}^n} \|\nabla \varphi\|_K(\mathbf{s}) ds$$

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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

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

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

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

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

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

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

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# Adaptive algorithm

## Goal

$$\frac{\sum_{n=1}^N \|\mathcal{R}(u_{h\tau}^{n,\epsilon,k})\|_{X'_n}^2}{\sum_{n=1}^N \|u_h^{n,\epsilon,k}\|_{L^2(I_n; L^2(\Omega))}^2} \leq \zeta^2$$

## Computer resources limitations

$$\min_{K \in \mathcal{K}^n} h_K \geq \underline{h}, \quad \tau^n \geq \underline{\tau}$$

### Algorithm (Adaptive algorithm, initialization)

Choose an initial mesh  $\mathcal{K}^0$ , regularization parameter  $\epsilon_0$ , and a tolerance  $\zeta_{IC} > 0$

**repeat** {Initial mesh and regularization parameter adaptation}

    Compute  $\eta_{IC}$ , adapt  $\mathcal{K}^0$ , and adjust  $\epsilon_0$ .

**until**  $\eta_{IC} \leq \zeta_{IC} \|\nabla(\beta_{\epsilon_0}(u_h^0))\|$

Choose an initial time step  $\tau^0$ ,  $\epsilon \leftarrow \epsilon_0$ ,  $t^0 \leftarrow 0$ ,  $n \leftarrow 0$



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```

while  $t^n \leq T$  do {Time loop}
   $n \leftarrow n + 1$ ,  $\mathcal{K}^n \leftarrow \mathcal{K}^{n-1}$ ,  $\tau^n \leftarrow \tau^{n-1}$ ,  $u_h^{n,\epsilon,0} \leftarrow u_h^{n-1}$ 
  repeat {Space refinement}
    repeat {Space and time error balancing}
      repeat {Regularization}
         $k \leftarrow 0$ 
        repeat {Nonlinear solver}
           $k \leftarrow k + 1$ ;  $u_h^{n,\epsilon,k} = \Psi(u_h^{n,\epsilon,k-1}, \tau^n, \mathcal{K}^n)$ ; compute  $\eta_{sp}^{n,\epsilon,k}$ ,  $\eta_{tm}^{n,\epsilon,k}$ ,  $\eta_{reg}^{n,\epsilon,k}$ ,  $\eta_{lin}^{n,\epsilon,k}$ 
          until  $\eta_{lin}^{n,\epsilon,k} \leq \Gamma_{lin}(\eta_{sp}^{n,\epsilon,k} + \eta_{tm}^{n,\epsilon,k} + \eta_{reg}^{n,\epsilon,k})$ 
           $k_n \leftarrow k$ 
          if  $\eta_{reg}^{n,\epsilon,k_n} \leq \Gamma_{reg}(\eta_{sp}^{n,\epsilon,k_n} + \eta_{tm}^{n,\epsilon,k_n})$  does not hold then
             $\epsilon \leftarrow \epsilon/2$ 
          end if
          until  $\eta_{reg}^{n,\epsilon,k_n} \leq \Gamma_{reg}(\eta_{sp}^{n,\epsilon,k_n} + \eta_{tm}^{n,\epsilon,k_n})$ 
           $\epsilon_n \leftarrow \epsilon$ 
          if  $\eta_{tm}^{n,\epsilon_n,k_n} < \gamma_{tm}\eta_{sp}^{n,\epsilon_n,k_n}$  then
             $\tau^n \leftarrow 2\tau^n$ 
          else if  $\eta_{tm}^{n,\epsilon_n,k_n} > \Gamma_{tm}\eta_{sp}^{n,\epsilon_n,k_n}$  and  $\tau^n \geq 2\tau$  then
             $\tau^n \leftarrow \tau^n/2$ 
          end if
          until  $\gamma_{tm}\eta_{sp}^{n,\epsilon_n,k_n} \leq \eta_{tm}^{n,\epsilon_n,k_n} \leq \Gamma_{tm}\eta_{sp}^{n,\epsilon_n,k_n}$  or  $\tau^n = \tau$ 
          Refine the cells  $K \in \mathcal{K}^n$  such that  $\eta_{sp,K}^{n,\epsilon_n,k_n} \geq c_{ref} \max_{L \in \mathcal{K}^n} \eta_{sp,L}^{n,\epsilon_n,k_n}$ 
          until  $\eta_{sp}^{n,\epsilon_n,k_n} + \eta_{tm}^{n,\epsilon_n,k_n} + \eta_{reg}^{n,\epsilon_n,k_n} + \eta_{lin}^{n,\epsilon_n,k_n} \leq \zeta \|v_h^{n,\epsilon_n,k_n}\|_{L^2(J_n; L^2(\Omega))}$  or  $h_K = \underline{h}$  for all  $K$ 
          Derefine cells  $\eta_{sp,K}^{n,\epsilon_n,k_n} \leq c_{deref} \max_{L \in \mathcal{K}^n} \eta_{sp,L}^{n,\epsilon_n,k_n}$ ;  $u_h^n \leftarrow u_h^{n,\epsilon_n,k_n}$ ;  $t^n \leftarrow t^{n-1} + \tau^n$ ;  $\epsilon \leftarrow 2\epsilon$ 
        end while
      end repeat
    end repeat
  end repeat

```

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# Efficiency assumptions

## Assumption C (Technicalities)

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

## Residual estimators

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

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

## Assumption D (Approximation property)

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

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

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# Efficiency assumptions

## 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

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



# Sketch of the proof, part 1

- stopping and balancing criteria:

$$\eta_{\text{sp}}^{n,\epsilon_n,k_n} + \eta_{\text{tm}}^{n,\epsilon_n,k_n} + \eta_{\text{reg}}^{n,\epsilon_n,k_n} + \eta_{\text{lin}}^{n,\epsilon_n,k_n} \lesssim \eta_{\text{sp}}^{n,\epsilon_n,k_n}$$

- inverse inequality,  $K \in \mathcal{K}^n$ :

$$\eta_{\mathbb{R},K}^{n,\epsilon_n,k_n} \lesssim \left\{ \sum_{K' \in \mathcal{K}^{n-1,n}, K' \subset K} h_{K'}^2 \|f^n - \partial_t u_{h\tau}^{n,\epsilon_n,k_n} + \nabla \cdot \mathbf{l}_h^{n,\epsilon_n,k_n}\|_{K'}^2 \right\}^{\frac{1}{2}} \\ + \left\{ \sum_{K' \in \mathcal{K}^{n-1,n}, K' \subset K} \|\mathbf{l}_h^{n,\epsilon_n,k_n} + \mathbf{t}_h^{n,\epsilon_n,k_n}\|_{K'}^2 \right\}^{\frac{1}{2}}$$

- approximation property:

$$\eta_{\text{sp}}^{n,\epsilon_n,k_n} \lesssim \eta_{\text{res},1}^{n,\epsilon_n,k_n} + \eta_{\text{res},2}^{n,\epsilon_n,k_n}$$

# Sketch of the proof, part 2

- denote

$$\left(\eta_{\text{LRQT}}^{n,\epsilon_n,k_n}\right)^2 := \int_{I_n} \sum_{K \in \mathcal{K}^{n-1,n}} \|\nabla \beta(\mathbf{u}_{h\tau}^{n,\epsilon_n,k_n}(t)) - \mathbf{I}_h^{n,\epsilon_n,k_n}\|_K^2 dt$$

- element bubble function technique:

$$\eta_{\text{res},1}^{n,\epsilon_n,k_n} \lesssim \|\mathcal{R}(\mathbf{u}_{h\tau}^{n,\epsilon_n,k_n})\|_{X'_n} + \eta_{\text{LRQT}}^{n,\epsilon_n,k_n}$$

- face bubble function technique:

$$\eta_{\text{res},2}^{n,\epsilon_n,k_n} \lesssim \|\mathcal{R}(\mathbf{u}_{h\tau}^{n,\epsilon_n,k_n})\|_{X'_n} + \eta_{\text{LRQT}}^{n,\epsilon_n,k_n}$$

- thus:

$$\eta_{\text{sp}}^{n,\epsilon_n,k_n} \lesssim \|\mathcal{R}(\mathbf{u}_{h\tau}^{n,\epsilon_n,k_n})\|_{X'_n} + \eta_{\text{LRQT}}^{n,\epsilon_n,k_n}$$

- triangle inequality and stopping and balancing criteria:

$$\eta_{\text{LRQT}}^{n,\epsilon_n,k_n} \leq \eta_{\text{lin}}^{n,\epsilon_n,k_n} + \eta_{\text{reg}}^{n,\epsilon_n,k_n} + \eta_{\text{tm}}^{n,\epsilon_n,k_n} \leq C(\Gamma_{\text{lin}}, \Gamma_{\text{reg}}, \Gamma_{\text{tm}}) \eta_{\text{sp}}^{n,\epsilon_n,k_n}$$

- parameters  $\Gamma_{\text{lin}}, \Gamma_{\text{reg}}, \Gamma_{\text{tm}}$  small enough:

$$\eta_{\text{sp}}^{n,\epsilon_n,k_n} \lesssim \|\mathcal{R}(\mathbf{u}_{h\tau}^{n,\epsilon_n,k_n})\|_{X'_n}$$

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# Relation residual–energy norm

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

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

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

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

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# Sketch of the proof, part 1

## Lemma (Duality estimate)

Let  $u_{h\tau} \in Z$  be such that  $\beta(u_{h\tau}) \in X$ . Then, for a.e.  $t \in (0, T)$ ,

$$\begin{aligned} & \frac{2}{L_\beta} \|\beta(u) - \beta(u_{h\tau})\|_{Q_t}^2 + \|(u - u_{h\tau})(\cdot, t)\|_{H^{-1}(\Omega)}^2 \\ & \leq \|(u - u_{h\tau})(\cdot, 0)\|_{H^{-1}(\Omega)}^2 + \|\mathcal{R}(u_{h\tau})\|_{X'_t}^2 + \|u - u_{h\tau}\|_{X'_t}^2. \end{aligned}$$

- $W(\cdot, t) \in H_0^1(\Omega)$  the solution to

$$(\nabla W(\cdot, t), \nabla \psi) = ((u - u_{h\tau})(\cdot, t), \psi) \quad \forall \psi \in H_0^1(\Omega)$$

- duality:

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

- there holds

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

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# Sketch of the proof, part 2

- definition of the residual:

$$\begin{aligned} \langle \mathcal{R}(u_{h\tau}), W \rangle_{X'_t, X_t} &= \mathfrak{R}_1 + \mathfrak{R}_2 \\ &:= \int_0^t \langle \partial_t(u - u_{h\tau}), W \rangle(s) ds + \int_0^t (\nabla\beta(u) - \nabla\beta(u_{h\tau}), \nabla W)(s) ds \end{aligned}$$

- definition of  $W$  gives for  $\mathfrak{R}_1$ :

$$\begin{aligned} \int_0^t (\partial_t \nabla W, \nabla W)(s) ds &= \frac{1}{2} \left( \|\nabla W(\cdot, t)\|_{L^2(\Omega)}^2 - \|\nabla W(\cdot, 0)\|_{L^2(\Omega)}^2 \right) \\ &= \frac{1}{2} \left( \|(u - u_{h\tau})(\cdot, t)\|_{H^{-1}(\Omega)}^2 - \|u_0 - u_{h\tau}(\cdot, 0)\|_{H^{-1}(\Omega)}^2 \right) \end{aligned}$$

- definition of  $W$  and Lipschitz continuity of  $\beta$  gives for  $\mathfrak{R}_2$ :

$$\begin{aligned} &\int_0^t (u - u_{h\tau}, \beta(u) - \beta(u_{h\tau}))(s) ds \\ &\geq \frac{1}{L_\beta} \int_0^t (\beta(u) - \beta(u_{h\tau}), \beta(u) - \beta(u_{h\tau}))(s) ds = \frac{1}{L_\beta} \|\beta(u) - \beta(u_{h\tau})\|_{Q_t}^2 \end{aligned}$$



# As tight as possible employment of Gronwall lemma

## Gronwall lemma

$$\xi(t) \leq \alpha(t) + \int_0^t \xi(s) ds \implies \xi(t) \leq \alpha(t) + \int_0^t \alpha(s) e^{t-s} ds$$

Lemma (As tight as possible employment of Gronwall lemma)

*Additionally, there holds*

$$\begin{aligned} & \|u - u_{h\tau}\|_{X'}^2 \\ & \leq (e^T - 1) \|(u - u_{h\tau})(\cdot, 0)\|_{H^{-1}(\Omega)}^2 \\ & \quad + \int_0^T \left( \|\mathcal{R}(u_{h\tau})\|_{X'_t}^2 + \int_0^t \|\mathcal{R}(u_{h\tau})\|_{X'_s}^2 e^{t-s} ds \right) dt \\ & \quad - \frac{2}{L_\beta} \int_0^T \left( \|\beta(u) - \beta(u_{h\tau})\|_{Q_t}^2 + \int_0^t \|\beta(u) - \beta(u_{h\tau})\|_{Q_s}^2 e^{t-s} ds \right) dt. \end{aligned}$$

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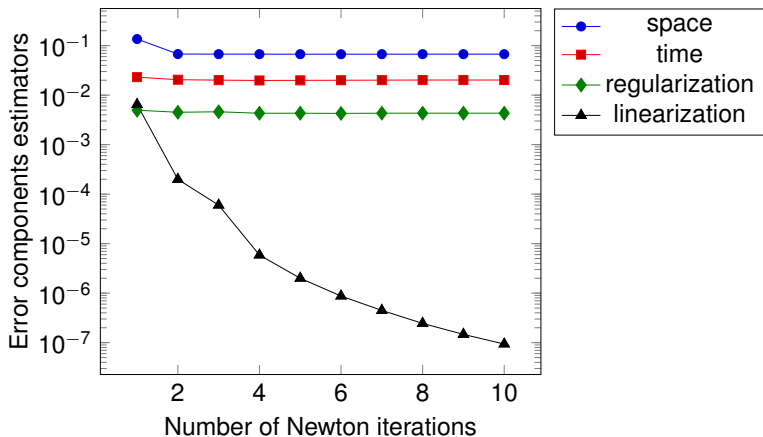
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# Linearization stopping criterion

## Linearization stopping criterion

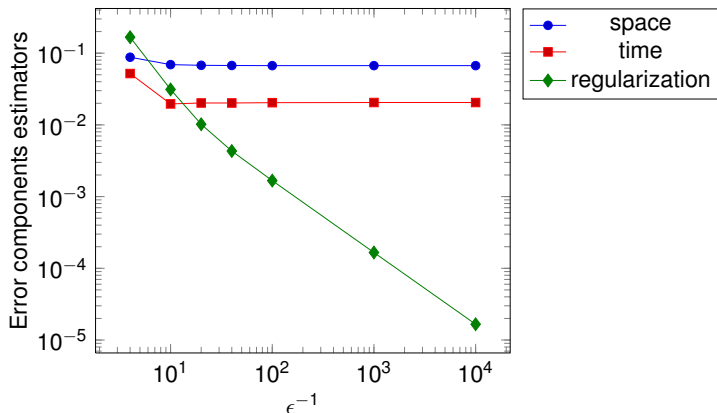
$$\eta_{\text{lin}}^{n,\epsilon,k} \leq \Gamma_{\text{lin}} (\eta_{\text{sp}}^{n,\epsilon,k} + \eta_{\text{tm}}^{n,\epsilon,k} + \eta_{\text{reg}}^{n,\epsilon,k})$$



# Regularization stopping criterion

## Regularization stopping criterion

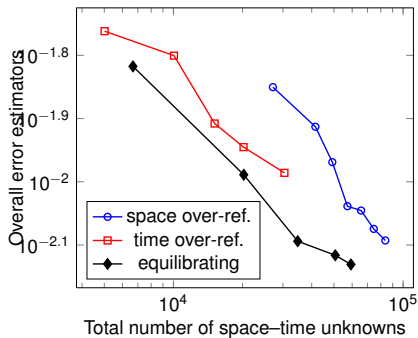
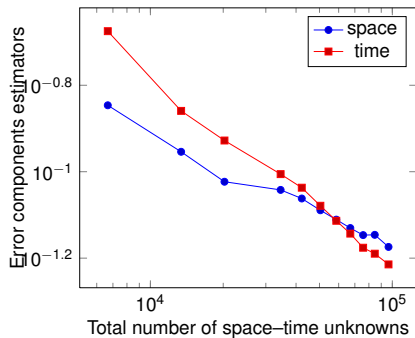
$$\eta_{\text{reg}}^{n,\epsilon,k_n} \leq \Gamma_{\text{reg}} (\eta_{\text{sp}}^{n,\epsilon,k_n} + \eta_{\text{tm}}^{n,\epsilon,k_n})$$



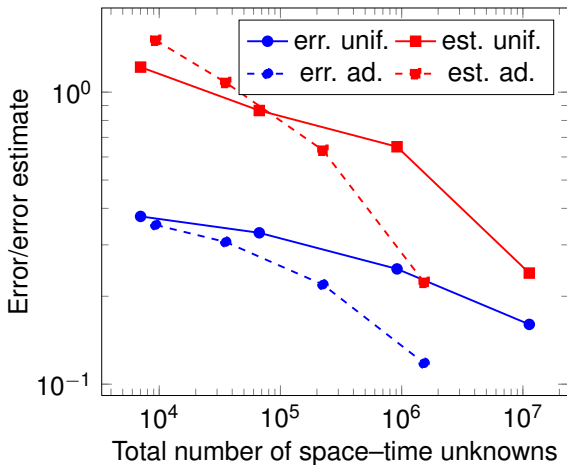
# Equilibrating time and space errors

## Equilibrating time and space errors

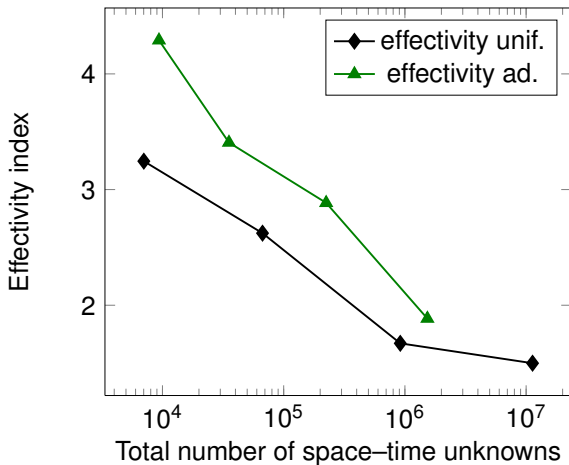
$$\gamma_{\text{tm}} \eta_{\text{sp}}^{n, \epsilon_n, k_n} \leq \eta_{\text{tm}}^{n, \epsilon_n, k_n} \leq \Gamma_{\text{tm}} \eta_{\text{sp}}^{n, \epsilon_n, k_n}$$



# Error and estimate (dual norm of the residual)

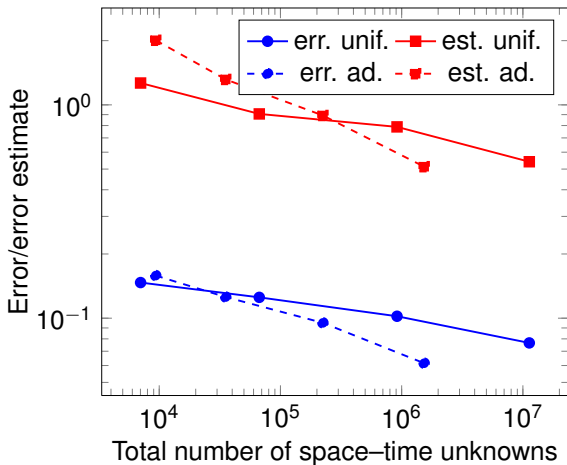


# Effectivity indices (dual norm of the residual)

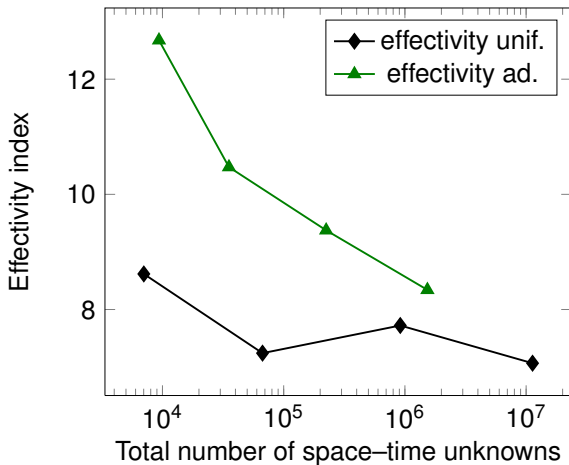




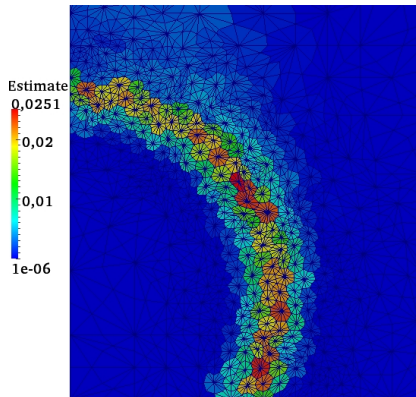
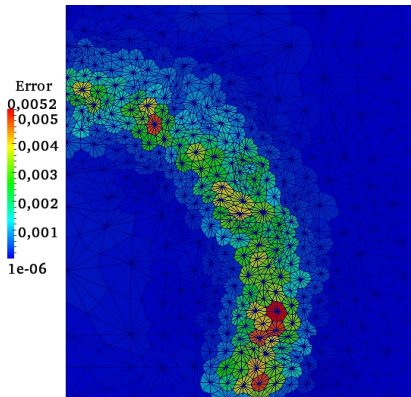
# Error and estimate (energy norm)



# Effectivity indices (energy norm)



# Actual and estimated error distribution



# Computational efficiency

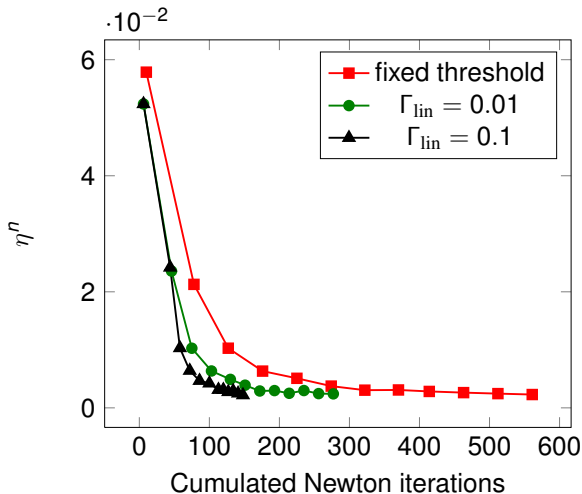


Figure: Number of cumulated Newton iterations vs. error estimate

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- 3 Energy error estimates
- 4 Numerical results
- 5 Conclusions and future directions

# Conclusions

## Complete adaptivity

- only a **necessary number** of **linearization iterations**
- **optimal** choice of the **regularization parameter**
- **space-time** mesh **adaptivity**
- **“smart online decisions”**: 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

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# Bibliography

- DI PIETRO D. A., VOHRALÍK M., YOUSEF S., Adaptive regularization, linearization, and discretization and a posteriori error control for the two-phase Stefan problem, HAL Preprint 00690862.

**Thank you for your attention!**