An a posteriori-based fully adaptive algorithm for the two-phase Stefan problem

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The two-phase Stefan problem I

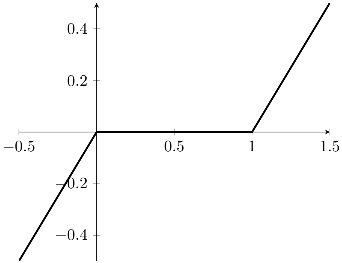

Figure: Enthalpy-temperature function β displaying latent phase-change heat

- Let $\beta \in \mathrm{Lip}(\mathbb{R};\mathbb{R})$ be strictly increasing in $\mathbb{R}^-$ and $\mathbb{R}^+\backslash(0,1)$
- Let $\Omega \subset \mathbb{R}^d$, $d \in \{2,3\}$. We seek the enthalpy $u : \Omega \to \mathbb{R}$ s.t.

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

The two-phase Stefan problem II

- Assume $u_0 \in L^2(\Omega)$ and $f \in L^2(0,T;L^2(\Omega))$, and define the spaces

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

- The weak formulation reads: Find $u \in Z$ with $\beta(u) \in X$ s.t.

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

and, for a.e. $s \in (0,T)$,

$$\boxed{\langle \partial_t u(\cdot,s), \varphi \rangle + (\nabla \beta(u(\cdot,s)), \nabla \varphi) = (f(\cdot,s), \varphi) \quad \forall \varphi \in H_0^1(\Omega)}$$

The two-phase Stefan problem III

- The quantity $\boldsymbol{\nabla}\beta(u)\cdot\boldsymbol{n}_{I(t)}$ may jump across the phase interface

$$I(t) := \{\mathbf{x} \in \Omega : \beta(u)(\mathbf{x}, t) = 0\}$$

- This can hinder the design and analysis of discretization methods
- Local time-step and mesh refinement needed to accurately track $I(t)$
- Lack of smoothness can prevent convergence of nonlinear iterations
- A common solution consists in considering a regularized problem

$$\boxed{\beta \leftarrow \beta_\epsilon \text{ with } \beta_\epsilon \in C^1(\mathbb{R}) \text{ and } \beta_\epsilon' \geqslant \epsilon > 0}$$

The two-phase Stefan problem IV

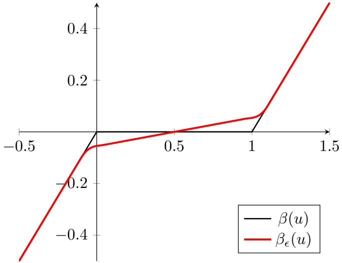

Figure: Example of regularized, strictly-increasing enthalpy-temperature function β_ϵ

The regularized problem reads: Find $u^\epsilon \in Z$ with $\beta_\epsilon(u^\epsilon) \in X$ s.t.

$$u^\epsilon(\cdot, 0) = \beta_\epsilon^{-1}(\beta(u_0)) \quad \text{in } \Omega,$$

and, for a.e. $s \in (0, T)$,

$$\boxed{\langle \partial_t u^\epsilon(\cdot, s), \varphi \rangle + (\boldsymbol{\nabla} \beta_\epsilon(u^\epsilon(\cdot, s)), \boldsymbol{\nabla} \varphi) = (f(\cdot, s), \varphi) \quad \forall \varphi \in H_0^1(\Omega)}$$

Numerical resolution

Fix $\mathcal{K}^0$ and τ_0. Set $\epsilon \leftarrow \epsilon_0$ $t^0 \leftarrow 0$, $n \leftarrow 0$, $u_h^0 \leftarrow \Pi^0(\beta_{\epsilon_0}^{-1}(\beta(u_0)))$
while $t^n \leqslant T$ **do**
    Set $n \leftarrow n+1$, $\mathcal{K}^n \leftarrow \mathcal{K}^{n-1}$, $\tau^n \leftarrow \tau^{n-1}$, $u_h^{n,\epsilon,0} \leftarrow u_h^{n-1}$
    repeat { Space refinement }
        repeat { Balancing the spatial and temporal errors }
            repeat { Regularization }
                Set $k \leftarrow 0$ and $u_h^{n,\epsilon,0} \leftarrow u_h^{n-1,\epsilon}$
                repeat { Nonlinear iterations }
                    Set $k \leftarrow k+1$ and update $u_h^{n,\epsilon,k} = \Psi(u_h^{n,\epsilon,k-1}, \tau^n, \mathcal{K}^n)$
                until Nonlinear iterations stopping criterion
                Adapt the regularization parameter ϵ
            until Regularization stopping criterion
            Adapt the time step τ^n
        until Time-space balancing criterion
        Locally adapt the space mesh $\mathcal{K}^n$
    until Space refinement criterion
    Set $u_h^n \leftarrow u_h^{n,\epsilon,k}$, and $t^n \leftarrow t^{n-1} + \tau^n$
end while

Quadrature adaptation could also be included

A few references

- Stefan: Residual-based estimates with space adaptivity [Picasso, 1995]
- Stefan: Adaptivity with space-time balancing [Nochetto et al., 1991]
- Rigorous a posteriori analysis for nondegenerate parabolic problems [Verfürth, 1998a, Verfürth, 1998b]
- Pioneering work on degenerate parabolic problems [Nochetto et al., 2000]
- A posteriori estimates by flux balancing [Prager and Synge, 1947]
- A posteriori-based adaptive stopping criteria [Jiránek et al., 2010]

DP, Vohralík, Yousef (2015).
Adaptive regularization, linearization, discretization, and a posteriori error control for the two-phase Stefan problem.
Math. Comp., 84(291):153–186.

Error measure

- Let $u_{h\tau} \in Z$ with $\beta(u_{h\tau}) \in X$, and let $\mathcal{R}(u_{h\tau}) \in X'$ be s.t., $\forall \varphi \in X$,

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

- The norm of the residual in the dual space X' is given by

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

- We consider the following problem-specific measure:

$$\boxed{\|\mathcal{R}(u_{h\tau})\|_{X'} + \|u_0 - u_{h\tau}(\cdot, 0)\|_{H^{-1}(\Omega)}}$$

General assumptions I

- Let $\{\tau^n\}_{1 \leqslant n \leqslant N} \subset \mathbb{R}_+^*$ be a sequence of time steps s.t.

$$t^0 := 0, \qquad t^n := \sum_{i=1}^{n} \tau^i \quad \forall 1 \leqslant n \leqslant N, \qquad T = t^N$$

- Let $\{\mathcal{K}^n\}_{0 \leqslant n \leqslant N}$ denote a family of matching simplicial space meshes
- The mesh $\mathcal{K}^n$ is used to march in time from t^{n-1} to t^n
- For the actual computation of the estimators, we will assume that

  for all $1 \leqslant n \leqslant N$, $\mathcal{K}^{n-1}$ and $\mathcal{K}^n$ share a common submesh $\mathcal{K}^{n-1,n}$

General assumptions II

Assumption (Approximate enthalpy)

The approximate enthalpy $u_{h\tau}$ *is s.t.*

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

and, for all $1 \leqslant n \leqslant N$, $u_{h\tau|I_n}$ *is affine in time on* $I_n := (t^{n-1}, t^n)$*.*

Assumption (Equilibrated flux reconstruction)

For all $1 \leqslant n \leqslant N$, *there is an equilibrated flux* $\mathbf{t}_h^n \in \boldsymbol{H}(\mathrm{div};\Omega)$ *s.t.*

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

We denote by $\mathbf{t}_{h\tau}$ *the piecewise affine in time space–time function s.t.*

$$\mathbf{t}_{h\tau|I_n} := \mathbf{t}_h^n \quad \forall 1 \leqslant n \leqslant N.$$

A basic a posteriori error estimate I

Theorem (Basic a posteriori error estimate)

Under the above assumptions, we have the fully computable bound

$$\boxed{\|\mathcal{R}(u_{h\tau})\|_{X'} + \|u_0 - u_{h\tau}(\cdot,0)\|_{H^{-1}(\Omega)} \leqslant \eta + \eta_{\mathrm{IC}},}$$

where, denoting by $\hat{f}$ the piecewise constant in time projection of f,

$$\eta := \left\{ \sum_{n=1}^{N} \int_{I_n} \sum_{K\in\mathcal{K}^n} \left(\eta_{\mathrm{R},K}^n + \eta_{\mathrm{F},K}^n(t)\right)^2 \mathrm{d}t \right\}^{\frac{1}{2}} + \|f - \hat{f}\|_{X'}.$$

with residual, flux and initial condition estimators given by ($C_{\mathrm{P},K} := \pi^{-1}$)

$$\begin{aligned} \eta_{\mathrm{R},K}^n &:= C_{\mathrm{P},K} h_K \|\hat{f}^n - \partial_t u_{h\tau}^n - \boldsymbol{\nabla}\cdot \mathbf{t}_h^n\|_{L^2(K)}, \\ \eta_{\mathrm{F},K}^n(t) &:= \|\mathbf{t}_h^n + \boldsymbol{\nabla}\beta(u_{h\tau}(\cdot,t))\|_{L^2(K)} \qquad t \in I_n, \\ \eta_{\mathrm{IC}} &:= \|u_0 - u_{h\tau}(\cdot,0)\|_{H^{-1}(\Omega)}. \end{aligned}$$

A basic a posteriori error estimate II

- Inserting $\pm\big((\hat{f},\varphi)+(\mathbf{t}_{h\tau},\boldsymbol{\nabla}\varphi)\big)$ and using Green's Theorem, we get

$$\langle \mathcal{R}(u_{h\tau}),\varphi\rangle_{X',X} = \int_0^T (f-\hat{f},\varphi) + \int_0^T \Big\{ \underbrace{(\hat{f}-\partial_t u_{h\tau} - \boldsymbol{\nabla}{\cdot}\mathbf{t}_{h\tau},\varphi)}_{:=\mathfrak{T}(t)} - (\mathbf{t}_{h\tau}+\boldsymbol{\nabla}\beta(u_{h\tau}),\boldsymbol{\nabla}\varphi)\Big\}(s)\mathrm{d}s$$

- Using the equilibrated flux property, we can estimate

$$\begin{aligned}\mathfrak{T}(t) &= \sum_{K\in\mathcal{K}^n} (\hat{f}^n - \partial_t u_{h\tau}^n - \boldsymbol{\nabla}{\cdot}\mathbf{t}_h^n,\varphi)_K \\ &= \sum_{K\in\mathcal{K}^n} (\hat{f}^n - \partial_t u_{h\tau}^n - \boldsymbol{\nabla}{\cdot}\mathbf{t}_h^n,\varphi - \Pi_0^n\varphi)_K \\ &\leqslant \sum_{K\in\mathcal{K}^n} \underbrace{C_{\mathrm{P},K} h_K \|\hat{f}^n - \partial_t u_{h\tau}^n - \boldsymbol{\nabla}{\cdot}\mathbf{t}_h^n\|_{L^2(K)}}_{=\eta_{\mathrm{R},K}^n} \|\boldsymbol{\nabla}\varphi\|_{L^2(K)}\end{aligned}$$

- Conclude using the definition of $\|\cdot\|_{X'}$ and the Cauchy–Schwarz inequality

Bounding the temperature and enthalpy errors I

- In practice, one may want to control more standard error measures
- Let $u_{h\tau} \in Z$ be s.t. $\beta(u_{h\tau}) \in X$. Classically, we have that

$$\frac{L_\beta}{2}\|(u-u_{h\tau})(\cdot,T)\|^2_{H^{-1}(\Omega)} + \|\beta(u)-\beta(u_{h\tau})\|^2_{L^2(0,T;L^2(\Omega))} \leqslant \frac{L_\beta}{2} e^T \left(\|\mathcal{R}(u_{h\tau})\|^2_{X'} + \|u_0 - u_{h\tau}(\cdot,0)\|^2_{H^{-1}(\Omega)}\right)$$

- An a posteriori estimate readily follows using the previous theorem
- Owing to the factor e^T, this estimate is not accurate for large T
- A sharper bound can be obtained by a finer analysis

Bounding the temperature and enthalpy errors II

Theorem (An improved bound for the temperature and enthalpy errors)

It holds for all $u_{h\tau} \in Z$ *s.t.* $\beta(u_{h\tau}) \in X$,

$$\frac{L_\beta}{2}\|(u-u_{h\tau})(\cdot,T)\|^2_{H^{-1}(\Omega)} + \|\beta(u)-\beta(u_{h\tau})\|^2_{L^2(0,T;L^2(\Omega))}$$
$$\leqslant \frac{L_\beta}{2}\Bigg\{(2e^T-1)\|u_0-u_{h\tau}(\cdot,0)\|^2_{H^{-1}(\Omega)} + \|\mathcal{R}(u_{h\tau})\|^2_{X'}$$
$$+ 2\int_0^T \left(\|\mathcal{R}(u_{h\tau})\|^2_{X_t'} + \int_0^t \|\mathcal{R}(u_{h\tau})\|^2_{X_s'} e^{t-s}\,\mathrm{d}s\right)\mathrm{d}t\Bigg\},$$

with, for $t \in [0,T]$, $X_t := L^2(0,t;H^1_0(\Omega))$.

Bounding the temperature and enthalpy errors III

Corollary (A posteriori estimate for the temperature and enthalpy errors)

It holds,

$$\frac{L_\beta}{2}\|(u-u_{h\tau})(\cdot,T)\|^2_{H^{-1}(\Omega)} + \|\beta(u)-\beta(u_{h\tau})\|^2_{L^2(0,T;L^2(\Omega))}$$
$$\leqslant \frac{L_\beta}{2}\left\{(2e^T-1)\eta_{\mathrm{IC}}^2 + \eta^2 + 2\left(\sum_{n=1}^N \tau^n \sum_{l=1}^n (\eta^l)^2 + \sum_{n=1}^N \sum_{l=1}^n J_{nl}\left\{\sum_{i=1}^l (\eta^i)^2\right\}\right)\right\},$$

with η_{IC} *and* η *as above and, for all* $1 \leqslant n \leqslant N$,

$$\eta^n := \left\{\int_{I_n} \sum_{K\in\mathcal{K}^n} (\eta^n_{\mathrm{R},K} + \eta^n_{\mathrm{F},K}(t))^2 \mathrm{d}t\right\}^{\frac{1}{2}} + \|f-\hat{f}\|_{X'_n},$$

where, for all $1 \leqslant l \leqslant N$, $J_{nl} := \int_{I_n}\int_{I_l} e^{t-s}\mathrm{d}s\mathrm{d}t$.

The term in red can be made as small as needed by refining $\mathcal{K}^0$!

Distinguishing the error components I

- For $1 \leqslant n \leqslant N$, let $I_n := (t^{n-1}, t^n)$ and set

$$X_n := L^2(I_n; H_0^1(\Omega)), \quad Z_n := H^1(I_n; H^{-1}(\Omega))$$

- We localize in time the dual norm of the residual setting

$$\|\mathcal{R}(u_{h\tau})\|_{X_n'} := \sup_{\varphi \in X_n,\, \|\varphi\|_{X_n}=1} \int_{I_n} \{\langle \partial_t (u - u_{h\tau}), \varphi\rangle + (\boldsymbol{\nabla}(\beta(u) - \beta(u_{h\tau})), \boldsymbol{\nabla}\varphi)\}(s)\mathrm{d}s$$

- Clearly, for any $u_{h\tau} \in Z$ with $\beta(u_{h\tau}) \in X$, it holds

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

Distinguishing the error components II

- Let $u_{h\tau}^{n,\epsilon,k}$ the current possibly nonconverged guess for $u_{h\tau}^{n}$
- The affine in time function $u_{h\tau}^{n,\epsilon,k}$ on $\Omega \times I_n$ is s.t.

$$u_{h\tau}^{n,\epsilon,k}(\cdot,t) = (1-\rho(t))u_h^{n-1} + \rho(t)u_h^{n,\epsilon,k}, \quad \rho(t) := \frac{t-t^{n-1}}{\tau^n}$$

- We estimate $\|\mathcal{R}(u_{h\tau}^{n,\epsilon,k})\|_{X_n'}$ distinguishing the various error sources

Distinguishing the error components III

Assumption (Adaptive setting)

For given $1 \leqslant n \leqslant N$, $\epsilon \geqslant 0$, *and* $k \geqslant 1$,

- *The approximate enthalpy* $u_{h\tau}^{n,\epsilon,k}$ *is s.t.*

$$u_{h\tau}^{n,\epsilon,k} \in Z_n \quad \partial_t u_{h\tau}^{n,\epsilon,k} \in L^2(I_n; L^2(\Omega)), \quad \beta(u_{h\tau}^{n,\epsilon,k}) \in X_n$$

- *There exists an equilibrated flux* $\mathbf{t}_h^{n,\epsilon,k} \in \boldsymbol{H}(\mathrm{div};\Omega)$ *s.t.*

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

- $\mathbf{l}_h^{n,\epsilon,k} \in [L^2(\Omega)]^d$ *is the available linearized approximation of the flux:*

$$\mathbf{l}_h^{n,\epsilon,k} \approx \boldsymbol{\nabla}\beta_\epsilon(u(\cdot,t^n))$$

- Π^n *is an operator used for interpolatory numerical integration.*

Distinguishing the error components IV

- To distinguish among error components, we split the flux estimator

$$\eta_{\mathrm{F},K}^{n,\epsilon,k}(t) = \|\mathbf{t}_h^n + \boldsymbol{\nabla}\beta(u_{h\tau}^{n,\epsilon,k})\|_{L^2(K)}$$

- We identify flux differences representative of each error component
- Other components could be estimated besides those considered here

Distinguishing the error components V

Theorem (A posteriori estimate distinguishing the error components)

Under the above assumption, it holds,

$$\boxed{\|\mathcal{R}(u_{h\tau}^{n,\epsilon,k})\|_{X_n'} \leqslant \eta_{\mathrm{sp}}^{n,\epsilon,k} + \eta_{\mathrm{tm}}^{n,\epsilon,k} + \eta_{\mathrm{qd}}^{n,\epsilon,k} + \eta_{\mathrm{reg}}^{n,\epsilon,k} + \eta_{\mathrm{lin}}^{n,\epsilon,k} + \|f - \hat{f}\|_{X_n'},}$$

where, for all $K \in \mathcal{K}^n$,

$$\begin{aligned}
\eta_{\mathrm{sp},K}^{n,\epsilon,k} &:= \eta_{\mathrm{R},K}^{n,\epsilon,k} + \|\mathbf{l}_h^{n,\epsilon,k} + \mathbf{t}_h^{n,\epsilon,k}\|_{L^2(K)},\\
\eta_{\mathrm{tm},K}^{n,\epsilon,k}(t) &:= \|\boldsymbol{\nabla}(\Pi^n \beta(u_{h\tau}^{n,\epsilon,k}(\cdot,t))) - \boldsymbol{\nabla}(\Pi^n \beta(u_h^{n,\epsilon,k}))\|_{L^2(K)}, \quad t \in I_n,\\
\eta_{\mathrm{qd},K}^{n,\epsilon,k}(t) &:= \|\boldsymbol{\nabla}(\beta(u_{h\tau}^{n,\epsilon,k}(\cdot,t))) - \boldsymbol{\nabla}(\Pi^n \beta(u_{h\tau}^{n,\epsilon,k}(\cdot,t)))\|_{L^2(K)}, \quad t \in I_n,\\
\eta_{\mathrm{reg},K}^{n,\epsilon,k} &:= \|\boldsymbol{\nabla}(\Pi^n \beta(u_h^{n,\epsilon,k})) - \boldsymbol{\nabla}(\Pi^n \beta_\epsilon(u_h^{n,\epsilon,k}))\|_{L^2(K)},\\
\eta_{\mathrm{lin},K}^{n,\epsilon,k} &:= \|\boldsymbol{\nabla}(\Pi^n \beta_\epsilon(u_h^{n,\epsilon,k})) - \mathbf{l}_h^{n,\epsilon,k}\|_{L^2(K)},
\end{aligned}$$

and the corresponding global versions are obtained setting

$$(\eta_{\bullet}^{n,\epsilon,k})^2 := \int_{I_n} \sum_{K \in \mathcal{K}^n} \left(\eta_{\bullet,K}^{n,\epsilon,k}(t)\right)^2 \mathrm{d}t.$$

An a posteriori-driven adaptive algorithm

Fix $\mathcal{K}^0$ and τ_0. Set $\epsilon \leftarrow \epsilon_0$ $t^0 \leftarrow 0$, $n \leftarrow 0$, $u_h^0 \leftarrow \Pi^0(\beta_{\epsilon_0}^{-1}(\beta(u_0)))$
while $t^n \leqslant T$ **do**
  Set $n \leftarrow n+1$, $\mathcal{K}^n \leftarrow \mathcal{K}^{n-1}$, $\tau^n \leftarrow \tau^{n-1}$, $u_h^{n,\epsilon,0} \leftarrow u_h^{n-1}$
  repeat { Space refinement }
    repeat { Balancing the spatial and temporal errors }
      repeat { Regularization }
        Set $k \leftarrow 0$ and $u_h^{n,\epsilon,0} \leftarrow u_h^{n-1,\epsilon}$
        repeat { Nonlinear iterations }
          Set $k \leftarrow k+1$ and update $u_h^{n,\epsilon,k} = \Psi(u_h^{n,\epsilon,k-1}, \tau^n, \mathcal{K}^n)$
          Compute $\eta_{\mathrm{sp}}^{n,\epsilon,k}$, $\eta_{\mathrm{tm}}^{n,\epsilon,k}$, $\eta_{\mathrm{reg}}^{n,\epsilon,k}$, $\eta_{\mathrm{lin}}^{n,\epsilon,k}$
        until
        Adapt the regularization parameter ϵ
      until
      Adapt the time step τ^n
    until
    Locally adapt the space mesh $\mathcal{K}^n$
  until
  Set $u_h^n \leftarrow u_h^{n,\epsilon,k}$, and $t^n \leftarrow t^{n-1} + \tau^n$
end while

An a posteriori-driven adaptive algorithm

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          Set $k \leftarrow k+1$ and update $u_h^{n,\epsilon,k} = \Psi(u_h^{n,\epsilon,k-1}, \tau^n, \mathcal{K}^n)$
          Compute $\eta_{\mathrm{sp}}^{n,\epsilon,k}$, $\eta_{\mathrm{tm}}^{n,\epsilon,k}$, $\eta_{\mathrm{reg}}^{n,\epsilon,k}$, $\eta_{\mathrm{lin}}^{n,\epsilon,k}$
        until $\eta_{\mathrm{lin}}^{n,\epsilon,k} \leqslant \Gamma_{\mathrm{lin}}\left(\eta_{\mathrm{sp}}^{n,\epsilon,k} + \eta_{\mathrm{tm}}^{n,\epsilon,k} + \eta_{\mathrm{qd}}^{n,\epsilon,k} + \eta_{\mathrm{reg}}^{n,\epsilon,k}\right)$
        Adapt the regularization parameter ϵ
      until
      Adapt the time step τ^n
    until
    Locally adapt the space mesh $\mathcal{K}^n$
  until
  Set $u_h^n \leftarrow u_h^{n,\epsilon,k}$, and $t^n \leftarrow t^{n-1} + \tau^n$
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          Compute $\eta_{\mathrm{sp}}^{n,\epsilon,k}$, $\eta_{\mathrm{tm}}^{n,\epsilon,k}$, $\eta_{\mathrm{reg}}^{n,\epsilon,k}$, $\eta_{\mathrm{lin}}^{n,\epsilon,k}$
        until $\eta_{\mathrm{lin}}^{n,\epsilon,k} \leqslant \Gamma_{\mathrm{lin}}(\eta_{\mathrm{sp}}^{n,\epsilon,k} + \eta_{\mathrm{tm}}^{n,\epsilon,k} + \eta_{\mathrm{qd}}^{n,\epsilon,k} + \eta_{\mathrm{reg}}^{n,\epsilon,k})$
        Adapt the regularization parameter ϵ
      until $\eta_{\mathrm{reg}}^{n,\epsilon,k} \leqslant \Gamma_{\mathrm{reg}}(\eta_{\mathrm{sp}}^{n,\epsilon,k} + \eta_{\mathrm{tm}}^{n,\epsilon,k} + \eta_{\mathrm{qd}}^{n,\epsilon,k})$
      Adapt the time step τ^n
    until
    Locally adapt the space mesh $\mathcal{K}^n$
  until
  Set $u_h^n \leftarrow u_h^{n,\epsilon,k}$, and $t^n \leftarrow t^{n-1} + \tau^n$
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          Compute $\eta_{\mathrm{sp}}^{n,\epsilon,k}$, $\eta_{\mathrm{tm}}^{n,\epsilon,k}$, $\eta_{\mathrm{reg}}^{n,\epsilon,k}$, $\eta_{\mathrm{lin}}^{n,\epsilon,k}$

        until $\eta_{\mathrm{lin}}^{n,\epsilon,k} \leqslant \Gamma_{\mathrm{lin}}(\eta_{\mathrm{sp}}^{n,\epsilon,k} + \eta_{\mathrm{tm}}^{n,\epsilon,k} + \eta_{\mathrm{qd}}^{n,\epsilon,k} + \eta_{\mathrm{reg}}^{n,\epsilon,k})$

        Adapt the regularization parameter ϵ

      until $\eta_{\mathrm{reg}}^{n,\epsilon,k} \leqslant \Gamma_{\mathrm{reg}}(\eta_{\mathrm{sp}}^{n,\epsilon,k} + \eta_{\mathrm{tm}}^{n,\epsilon,k} + \eta_{\mathrm{qd}}^{n,\epsilon,k})$

      Adapt the time step τ^n

    until $\gamma_{\mathrm{tm}}\eta_{\mathrm{sp}}^{n,\epsilon,k} \leqslant \eta_{\mathrm{tm}}^{n,\epsilon,k} \leqslant \Gamma_{\mathrm{tm}}\eta_{\mathrm{sp}}^{n,\epsilon,k}$

    Locally adapt the space mesh $\mathcal{K}^n$

  until

  Set $u_h^n \leftarrow u_h^{n,\epsilon,k}$, and $t^n \leftarrow t^{n-1} + \tau^n$

end while

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Fix $\mathcal{K}^0$ and τ_0. Set $\epsilon \leftarrow \epsilon_0$ $t^0 \leftarrow 0$, $n \leftarrow 0$, $u_h^0 \leftarrow \Pi^0(\beta_{\epsilon_0}^{-1}(\beta(u_0)))$

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repeat { Regularization }

Set $k \leftarrow 0$ and $u_h^{n,\epsilon,0} \leftarrow u_h^{n-1,\epsilon}$

repeat { Nonlinear iterations }

Set $k \leftarrow k+1$ and update $u_h^{n,\epsilon,k} = \Psi(u_h^{n,\epsilon,k-1}, \tau^n, \mathcal{K}^n)$

Compute $\eta_{\mathrm{sp}}^{n,\epsilon,k}$, $\eta_{\mathrm{tm}}^{n,\epsilon,k}$, $\eta_{\mathrm{reg}}^{n,\epsilon,k}$, $\eta_{\mathrm{lin}}^{n,\epsilon,k}$

until $\eta_{\mathrm{lin}}^{n,\epsilon,k} \leqslant \Gamma_{\mathrm{lin}}(\eta_{\mathrm{sp}}^{n,\epsilon,k} + \eta_{\mathrm{tm}}^{n,\epsilon,k} + \eta_{\mathrm{qd}}^{n,\epsilon,k} + \eta_{\mathrm{reg}}^{n,\epsilon,k})$

Adapt the regularization parameter ϵ

until $\eta_{\mathrm{reg}}^{n,\epsilon,k} \leqslant \Gamma_{\mathrm{reg}}(\eta_{\mathrm{sp}}^{n,\epsilon,k} + \eta_{\mathrm{tm}}^{n,\epsilon,k} + \eta_{\mathrm{qd}}^{n,\epsilon,k})$

Adapt the time step τ^n

until $\gamma_{\mathrm{tm}}\eta_{\mathrm{sp}}^{n,\epsilon,k} \leqslant \eta_{\mathrm{tm}}^{n,\epsilon,k} \leqslant \Gamma_{\mathrm{tm}}\eta_{\mathrm{sp}}^{n,\epsilon,k}$

Locally adapt the space mesh $\mathcal{K}^n$

until $\eta_{\mathrm{sp},K_1}^{n,\epsilon,k} \approx \eta_{\mathrm{sp},K_2}^{n,\epsilon,k}$ for all $K_1, K_2 \in \mathcal{K}^n$

Set $u_h^n \leftarrow u_h^{n,\epsilon,k}$, and $t^n \leftarrow t^{n-1} + \tau^n$

end while

Efficiency

Assumption (Polynomial potential and fluxes and approximation)

Assume

- $u_{h\tau}^{n,\epsilon,k}$ *piecewise affine in time, piecewise polynomial in space on* $\mathcal{K}^{n-1,n}$*;*
- $\mathbf{l}_h^{n,\epsilon,k}$ *and* $\mathbf{t}_h^{n,\epsilon,k}$ *piecewise polynomial in space on* $\mathcal{K}^{n-1,n}$*;*
- *With* $\eta_{\mathrm{res},1}^n$ *and* $\eta_{\mathrm{res},2}^n$ *classical residual-based estimators,*

$$\tau^n \sum_{K\in\mathcal{K}^{n-1,n}} \|\mathbf{l}_h^{n,\epsilon,k} + \mathbf{t}_h^{n,\epsilon,k}\|_{L^2(K)}^2 \lesssim \left(\eta_{\mathrm{res},1}^n\right)^2 + \left(\eta_{\mathrm{res},2}^n\right)^2.$$

Theorem (Global efficiency)

Then, under the above assumptions, it holds using the adaptive algorithm

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

Application to a FE-FV discretization I

- We apply our strategy to an implicit FE-FV discretization
- For $1 \leqslant n \leqslant N$, let $\mathcal{T}^n$ be a matching simplicial mesh of Ω and set

$$V_h^n := \left\{\varphi_h \in C^0(\overline{\Omega});\ \varphi_{h|T} \in \mathbb{P}_1(T) \quad \forall T \in \mathcal{T}^n\right\}$$

- We denote by Π^n the usual Lagrange interpolation operator on V_h^n
- Let $u_h^0 \in V_h^0$ be a suitable approximation of $\beta_\epsilon^{-1}(\beta(u_0))$, e.g.,

$$u_h^0 = \Pi^0(\beta_\epsilon^{-1}(\beta(u_0)))$$

Application to a FE-FV discretization II

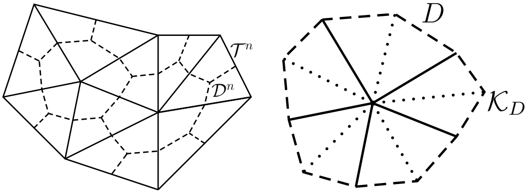


Figure: Primal mesh $\mathcal{T}^n$, dual mesh $\mathcal{D}^n$, dual element D and local tercial mesh $\mathcal{K}_D$

For all $1 \leqslant n \leqslant N$, given u_h^{n-1}, $\mathcal{T}^n$ and ϵ, we seek $u_h^{n,\epsilon} \in V_h^n$ s.t.

$$\boxed{\left(\frac{u_h^{n,\epsilon} - u_h^{n-1}}{\tau^n}, 1\right)_D - (\nabla \Pi^n(\beta_\epsilon(u_h^{n,\epsilon}))\cdot \mathbf{n}_D, 1)_{\partial D} = (\hat{f}^n, 1)_D \quad \forall D \in \mathcal{D}^{n,\mathrm{i}}}$$

Application to a FE-FV discretization III

- The above problem can be rewritten as the nonlinear AE system

$$\boxed{\mathbb{M}^n U^{n,\epsilon} - \tau^n \mathbb{K}^n \beta_\epsilon(U^{n,\epsilon}) = \tau^n F^n + G^{n-1} - H^{n,\epsilon},}$$

  where

  - F^n accounts for the forcing term
  - $(\mathbb{M}^n U^{n,\epsilon} - G^{n-1})/\tau^n$ is the discrete time derivative
  - $H^{n,\epsilon}$ accounts for boundary conditions

- To solve it, we linearize the second term and approximate

$$\beta_\epsilon(U^{n,\epsilon,k}) \approx \beta_\epsilon(U^{n,\epsilon,k-1}) + \beta'_\epsilon(U^{n,\epsilon,k-1})\big(U^{n,\epsilon,k} - U^{n,\epsilon,k-1}\big)$$

Application to a FE-FV discretization IV

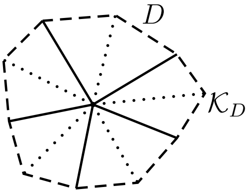
- The enthalpy appearing in the estimate (with $u_h^{\mathrm{b},n,\epsilon}$ BC lifting)

$$\boxed{u_h^{n,\epsilon,k} := \sum_{E \in D^{n,\mathrm{i}}} U_E^{n,\epsilon,k} \phi_E + u_h^{\mathrm{b},n,\epsilon},}$$

- The corresponding linearized flux is

$$\boxed{\mathbf{l}_h^{n,\epsilon,k} := \boldsymbol{\nabla} \sum_{E \in D^{n,\mathrm{i}}} \left\{ \beta_\epsilon(U_E^{n,\epsilon,k-1}) + \beta'_\epsilon(U_E^{n,\epsilon,k-1}) \big(U_E^{n,\epsilon,k} - U_E^{n,\epsilon,k-1}\big) \right\} \phi_E}$$

Application to a FE-FV discretization V



- Let D be an internal dual cell and set

$$\mathbf{RTN}_{\mathrm{N}}(\mathcal{K}_D) := \{\mathbf{v}_h \in \mathbf{RTN}(\mathcal{K}_D);\ \mathbf{v}_h{\cdot}\mathbf{n}_F = -\mathbf{l}_h^{n,\epsilon,k}{\cdot}\mathbf{n}_F \quad \forall F \in \partial\mathcal{K}_D^{\mathrm{i}}\}$$

- We seek $\mathbf{t}_h^{n,\epsilon,k} \in \mathbf{RTN}_{\mathrm{N}}(\mathcal{K}_D)$ and $q_h \in \mathbb{P}_0^*(\mathcal{K}_D)$ s.t.

$$\begin{aligned}
(\mathbf{t}_h^{n,\epsilon,k} + \mathbf{l}_h^{n,\epsilon,k}, \mathbf{v}_h)_D - (q_h, \boldsymbol{\nabla}{\cdot}\mathbf{v}_h)_D &= 0 \quad \forall \mathbf{v}_h \in \mathbf{RTN}_{\mathrm{N},0}(\mathcal{K}_D),\\
(\boldsymbol{\nabla}{\cdot}\mathbf{t}_h^{n,\epsilon,k}, \phi_h)_D - (\hat{f}^n - \partial_t u_{h\tau}^{n,\epsilon,k}, \phi_h)_D &= 0 \quad \forall \phi_h \in \mathbb{P}_0^*(\mathcal{K}_D)
\end{aligned}$$

- Compatible and well-posed problem (cf. [Boffi, Brezzi, Fortin, 2013])
- For boundary dual cells, we solve a Neumann–Dirichlet problem

Numerical examples: Stopping criteria I

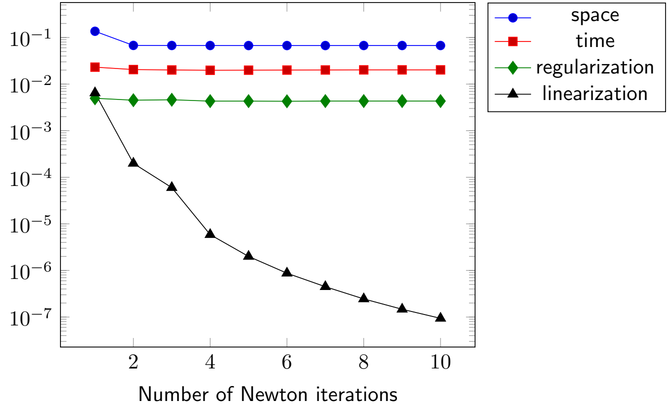


Figure: Spatial, temporal, regularization, and linearization error estimators vs. number of Newton iterations for a fixed mesh, time step, and regularization parameter

Numerical examples: Stopping criteria II

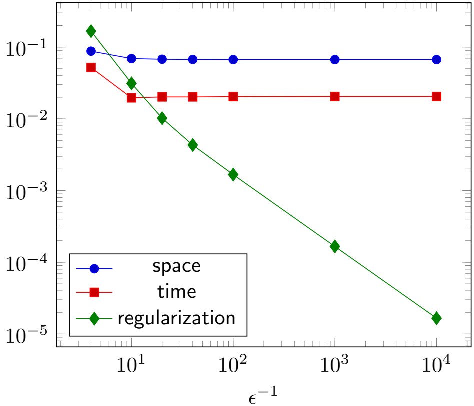


Figure: Spatial, temporal, and regularization error estimators vs. ϵ^{-1} for fixed mesh and time steps

Numerical examples: Balancing criteria I

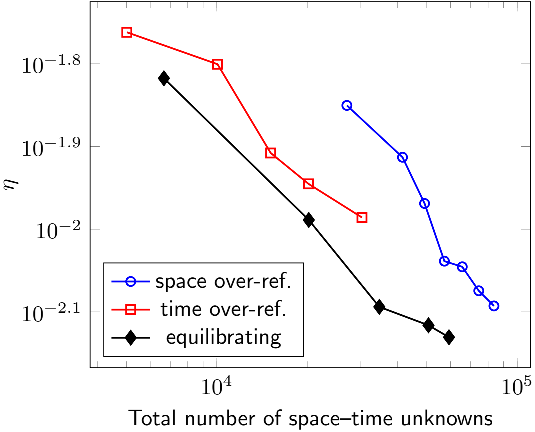


Figure: Space-time balancing errors vs. space/time overrefinement

Numerical examples: Balancing criteria II

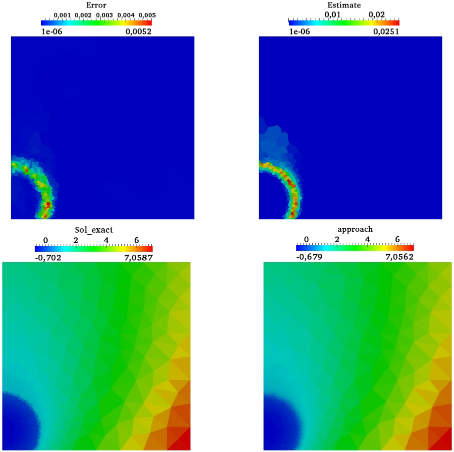


Figure: Top: error distribution. Bottom: enthalpy distribution. Left: actual. Right: estimated. User-depedent parameters for stopping criteria: $\Gamma_{\mathrm{lin}} = \Gamma_{\mathrm{reg}} = 0.1$

Numerical examples: Balancing criteria III

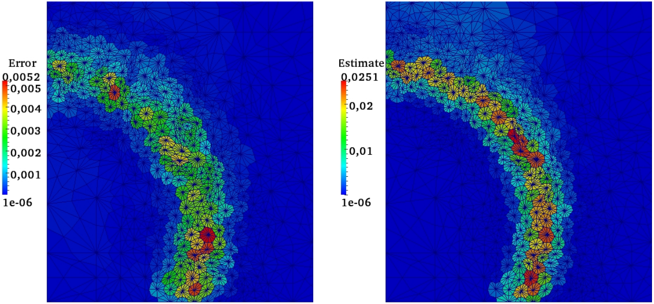


Figure: Error distribution for $\Gamma_{\rm lin} = \Gamma_{\rm reg} = 0.1$. Left: actual. Right: estimated

Numerical examples: Overall performance I

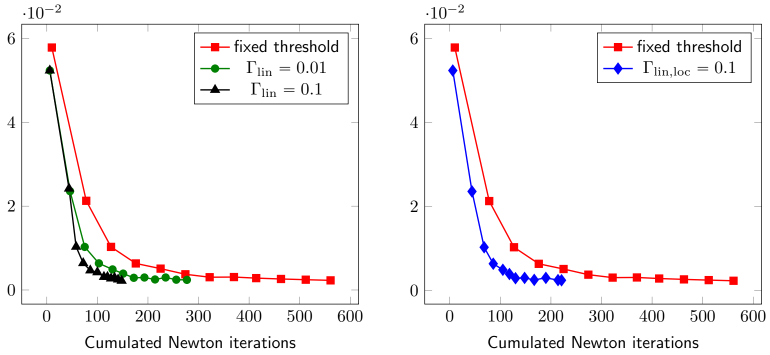


Figure: Error estimator η^n vs. cumulated Newton iterations at each time step (time steps are identified by markers). Left: global stopping criterion. Right: local stopping criterion

Numerical examples: Overall performance II

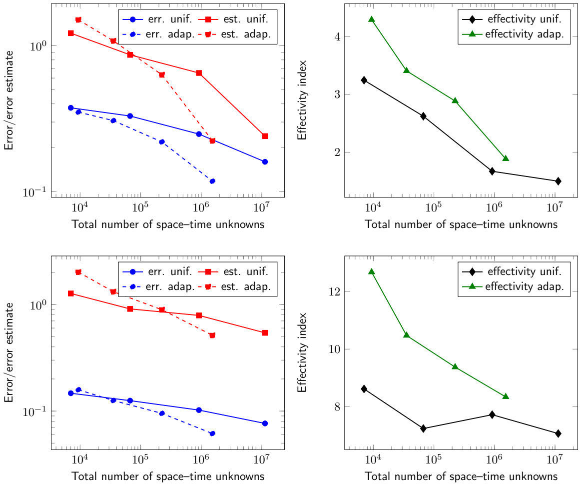


Figure: Adaptive vs. uniform refinement. Top: dual norm. Bottom: energy-norm. Left: error and estimators. Right: effectivity indices. Dual norms are approximated solving an auxiliary problem

A posteriori-driven algorithms for (multi-phase) flows I

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A posteriori-driven algorithms for (multi-phase) flows II

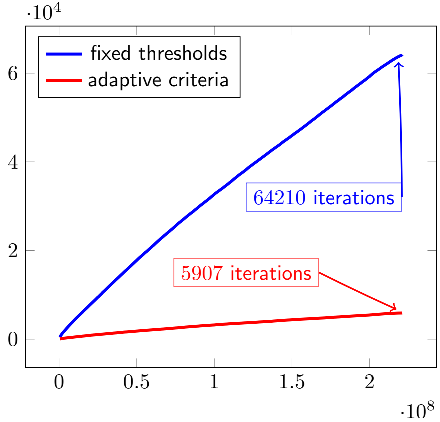

Figure: A posteriori-driven adaptive resolution for the compositional Darcy model. Cumulated linear solver iterations as a function of stopping criteria

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