A posteriori error estimates, stopping criteria, and adaptivity for two-phase flows

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joint work with C. Cancès, I. S. Pop, and M. F. Wheeler

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Outline



Introduction

- Setting
 - The two-phase flow model
 - Global and complementary pressures
 - Weak formulation
 - Error measure
- 3 A posteriori estimates
 - Pressure and phase velocities reconstructions
 - Basic a posteriori error estimate
 - Estimate distinguishing different error components
- 4 Applications and numerical experiments
 - Fully implicit cell-centered finite volumes
 - Iteratively coupled implicit pressure—explicit saturation vertex-centered finite volumes
 - Extension to multiphase compositional flows
 - Conclusions and future directions



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Multiphase porous media flows

- highly nonlinear (degenerate) systems of PDEs
- involve phase transitions
- feature evolving sharp fronts
- different time and space scales
- highly contrasted, discontinuous coefficients
- unstructured and nonmatching grids

- derive fully computable a posteriori error upper bounds
- distinguish different error components
 - time step choice & mesh adaptivity
 - stopping criteria for linear and nonlinear solvers



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Previous results

Model analysis

- Kröner & Luckhaus (1984)
- Chavent & Jaffré (1986)
- Antontsev, Kazhikhov, & Monakhov (1990)
- Arbogast (1992)
- Chen (2001)
- lately: van Duijn, Mikelić, & Pop; Cancès, Gallouët, & Porretta; Khalil & Saad; Amaziane, Jurak, & Keko ...

Convergence and a priori estimates

- Chen & Ewing (2001)
- Michel (2003)
- Eymard, Herbin, & Michel (2003)
- lately: Enchéry, Eymard; & Michel, Epshteyn & Rivière; Cancès . . .

A posteriori indicators

- Chen & Ewing (2003)
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The model Darcy velocity \mathbf{u}_{α} $\partial_t(\phi s_{\alpha}) + \nabla \cdot \left(-\frac{k_{\mathrm{r},\alpha}(s_{\mathrm{w}})}{\mu_{\alpha}}\underline{\mathbf{K}}(\nabla p_{\alpha} + \rho_{\alpha}g\nabla z)\right) = q_{\alpha}, \quad \alpha \in \{\mathrm{n},\mathrm{w}\},$ $s_{\mathrm{n}} + s_{\mathrm{w}} = 1,$ $p_{\mathrm{n}} - p_{\mathrm{w}} = p_{\mathrm{c}}(s_{\mathrm{w}})$

- two immiscible, incompressible fluids
- space–time domain $\Omega \times (0, T)$
- + initial & boundary conditions
- p_n , p_w : unknown nonwetting and wetting phase pressures
- s_n , s_w : unknown nonwetting and wetting phase saturations
- $p_{c}(\cdot)$: the nonlinear capillary pressure
- $k_{r,\alpha}(\cdot)$: the nonlinear relative permeability
- φ porosity; <u>K</u> permeability tensor; μ_α, ρ_α, q_α: viscosities, densities, sources; *z* vertical coordinate; *g* gravity

The model $\partial_t(\phi s_{\alpha}) + \nabla \cdot \left(\overbrace{-\frac{k_{r,\alpha}(s_w)}{\mu_{\alpha}} \underline{\mathbf{K}}(\nabla \rho_{\alpha} + \rho_{\alpha} g \nabla z)}^{\text{Darcy velocity } \mathbf{u}_{\alpha}} \right) = q_{\alpha}, \qquad \alpha \in \{n, w\},$ $s_n + s_w = 1,$ $\rho_n - \rho_w = \rho_c(s_w)$

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Setting A posteriori estimates Applications & exps. C Two-phase fl. Pressures Weak formulation Error measure

Global and complementary pressures

Global pressure

$$\mathfrak{p}(s_{\mathrm{w}},
ho_{\mathrm{w}}) :=
ho_{\mathrm{w}} + \int_{0}^{s_{\mathrm{w}}} rac{\lambda_{\mathrm{n}}(a)}{\lambda_{\mathrm{w}}(a) + \lambda_{\mathrm{n}}(a)}
ho_{\mathrm{c}}'(a) \mathrm{d}a$$

Complementary pressure

$$\mathfrak{q}(s_{\mathrm{w}}):=-\int_{0}^{s_{\mathrm{w}}}rac{\lambda_{\mathrm{w}}(a)\lambda_{\mathrm{n}}(a)}{\lambda_{\mathrm{w}}(a)+\lambda_{\mathrm{n}}(a)}p_{\mathrm{c}}'(a)\mathrm{d}a$$

Comments

- phase mobilities $\lambda_{\alpha}(a) := k_{r,\alpha}(a)/\mu_{\alpha}, \alpha \in \{n, w\}$
- necessary for the correct definition of the weak solution
- equivalent Darcy velocities expressions

$$\begin{split} \mathbf{v}_{\mathrm{w}}(s_{\mathrm{w}}, \rho_{\mathrm{w}}) &:= -\underline{\mathbf{K}} \big(\lambda_{\mathrm{w}}(s_{\mathrm{w}}) \nabla \mathfrak{p}(s_{\mathrm{w}}, \rho_{\mathrm{w}}) + \nabla \mathfrak{q}(s_{\mathrm{w}}) + \lambda_{\mathrm{w}}(s_{\mathrm{w}}) \rho_{\mathrm{w}} g \nabla z \big), \\ \mathbf{v}_{\mathrm{n}}(s_{\mathrm{w}}, \rho_{\mathrm{w}}) &:= -\underline{\mathbf{K}} \big(\lambda_{\mathrm{n}}(s_{\mathrm{w}}) \nabla \mathfrak{p}(s_{\mathrm{w}}, \rho_{\mathrm{w}}) - \nabla \mathfrak{q}(s_{\mathrm{w}}) + \lambda_{\mathrm{n}}(s_{\mathrm{w}}) \rho_{\mathrm{n}} g \nabla z \big) \end{split}$$

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Global and complementary pressures

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$$\mathfrak{p}(s_{\mathrm{w}}, p_{\mathrm{w}}) := p_{\mathrm{w}} + \int_{0}^{s_{\mathrm{w}}} rac{\lambda_{\mathrm{n}}(a)}{\lambda_{\mathrm{w}}(a) + \lambda_{\mathrm{n}}(a)} p_{\mathrm{c}}'(a) \mathrm{d}a$$

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Weak formulation

Energy space

 $X:=L^2((0,\,T);\,H^1_{\rm D}(\Omega))$

```
\int_0^t \left\{ \langle \partial_t(\phi s_\alpha), \varphi \rangle - (\mathbf{v}_\alpha(s_{\mathrm{w}}, p_{\mathrm{w}}), \nabla \varphi) - (q_\alpha, \varphi) \right\} \mathrm{d}t = \mathbf{0}
```



Weak formulation

Energy space

$$X := L^2((0,T); H^1_{\mathrm{D}}(\Omega))$$

Definition (Weak solution (Chen 2001)) Find (s_w, p_w) such that, with $s_n := 1 - s_w$, $s_{w} \in C([0, T]; L^{2}(\Omega)), s_{w}(\cdot, 0) = s_{w}^{0},$ $\partial_t \mathbf{s}_{\mathrm{w}} \in L^2((0, T); (H^1_{\mathrm{D}}(\Omega))'),$ $\mathfrak{p}(s_w, p_w) \in X.$ $\mathfrak{q}(\mathbf{s}_{w}) \in X.$ $\int_0^t \left\{ \langle \partial_t(\phi \boldsymbol{s}_\alpha), \varphi \rangle - (\boldsymbol{v}_\alpha(\boldsymbol{s}_{\mathrm{w}}, \boldsymbol{\rho}_{\mathrm{w}}), \nabla \varphi) - (\boldsymbol{q}_\alpha, \varphi) \right\} \mathrm{d}t = \boldsymbol{0}$ $\forall \varphi \in \mathbf{X}, \ \alpha \in \{\mathbf{n}, \mathbf{w}\}.$



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Error measure

Error measure
$$|||(\mathbf{s}_{w} - \mathbf{s}_{w,h\tau}, \mathbf{p}_{w} - \mathbf{p}_{w,h\tau})|||$$

$$\left\{\sum_{\alpha \in \{n,w\}} \left\{\sup_{\varphi \in X, \|\varphi\|_{X}=1} \int_{0}^{T} \left\{ \langle \partial_{t}(\phi \mathbf{s}_{\alpha}) - \partial_{t}(\phi \mathbf{s}_{\alpha,h\tau}), \varphi \rangle - (\mathbf{v}_{\alpha}(\mathbf{s}_{w}, \mathbf{p}_{w}) - \mathbf{v}_{\alpha}(\mathbf{s}_{w,h\tau}, \mathbf{p}_{w,h\tau}), \nabla \varphi) \right\} dt \right\}^{2} \right\}^{\frac{1}{2}}$$

$$+ \left\{\inf_{\hat{\mathfrak{p}} \in X} \int_{0}^{T} ||\mathbf{K}(\lambda_{w}(\mathbf{s}_{w,h\tau}) + \lambda_{n}(\mathbf{s}_{w,h\tau})) \nabla(\mathfrak{p}(\mathbf{s}_{w,h\tau}, \mathbf{p}_{w,h\tau}) - \hat{\mathfrak{p}})||^{2} dt \right\}^{\frac{1}{2}}$$

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Comments

- dual norm of the residual
- $\mathfrak{p}(s_{w,h\tau}, p_{w,h\tau}) \notin X \Rightarrow$ global pressure nonconformity

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• $q(s_{w,h\tau}) \notin X \Rightarrow$ complementary pressure nonconformity

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Chinatics mathematics

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M. Vohralík A posteriori estimates and stopping criteria for two-phase flows

Link to functional spaces error measure

Theorem (Link to energy-type error (Cancès, Pop, V. 2013))

Let (s_w, p_w) be the weak solution. Let $(s_{w,h\tau}, p_{w,h\tau})$ be arbitrary but such that $\mathfrak{p}(s_{w,h\tau}, p_{w,h\tau}) \in X$ and $\mathfrak{q}(s_{w,h\tau}) \in X + IC$. Then

$$\begin{split} \| \boldsymbol{s}_{w} - \boldsymbol{s}_{w,h\tau} \|_{L^{2}((0,T);(H_{D}^{1}(\Omega))')} + \| \boldsymbol{\mathfrak{q}}(\boldsymbol{s}_{w}) - \boldsymbol{\mathfrak{q}}(\boldsymbol{s}_{w,h\tau}) \|_{L^{2}(\Omega \times (0,T))} \\ + \| \boldsymbol{\mathfrak{p}}(\boldsymbol{s}_{w},\boldsymbol{p}_{w}) - \boldsymbol{\mathfrak{p}}(\boldsymbol{s}_{w,h\tau},\boldsymbol{p}_{w,h\tau}) \|_{L^{2}((0,T);H_{D}^{1}(\Omega))} \\ &\leq C \bigg\{ \sum_{\alpha \in \{n,w\}} \bigg\{ \sup_{\varphi \in X, \, \|\varphi\|_{X} = 1} \int_{0}^{T} \big\{ \langle \partial_{t}(\phi \boldsymbol{s}_{\alpha}) - \partial_{t}(\phi \boldsymbol{s}_{\alpha,h\tau}), \varphi \rangle \\ - (\boldsymbol{v}_{e}(\boldsymbol{s}_{w},\boldsymbol{p}_{w}) - \boldsymbol{v}_{e}(\boldsymbol{s}_{w},\boldsymbol{p}_{w},\boldsymbol{p}_{w}), \, \nabla_{t} \varphi) \big\} dt \bigg\}^{2} \bigg\}^{\frac{1}{2}} \end{split}$$

Comments

 conforming approximations: energy-type error controlled by the dual norm of the residual

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A posteriori estimates and stopping criteria for two-phase flows

Link to functional spaces error measure

Theorem (Link to energy-type error (Cancès, Pop, V. 2013))

Let (s_w, p_w) be the weak solution. Let $(s_{w,h\tau}, p_{w,h\tau})$ be arbitrary but such that $\mathfrak{p}(s_{w,h\tau}, p_{w,h\tau}) \in X$ and $\mathfrak{q}(s_{w,h\tau}) \in X + IC$. Then

$$\begin{split} \|\boldsymbol{s}_{w} - \boldsymbol{s}_{w,h\tau}\|_{L^{2}((0,T);(H_{D}^{1}(\Omega))')} + \|\boldsymbol{\mathfrak{q}}(\boldsymbol{s}_{w}) - \boldsymbol{\mathfrak{q}}(\boldsymbol{s}_{w,h\tau})\|_{L^{2}(\Omega\times(0,T))} \\ + \|\boldsymbol{\mathfrak{p}}(\boldsymbol{s}_{w},\boldsymbol{p}_{w}) - \boldsymbol{\mathfrak{p}}(\boldsymbol{s}_{w,h\tau},\boldsymbol{p}_{w,h\tau})\|_{L^{2}((0,T);H_{D}^{1}(\Omega))} \\ &\leq C \bigg\{ \sum_{\alpha \in \{n,w\}} \bigg\{ \sup_{\varphi \in X, \|\varphi\|_{X}=1} \int_{0}^{T} \big\{ \langle \partial_{t}(\phi \boldsymbol{s}_{\alpha}) - \partial_{t}(\phi \boldsymbol{s}_{\alpha,h\tau}), \varphi \rangle \\ - (\boldsymbol{v}_{\alpha}(\boldsymbol{s}_{w},\boldsymbol{p}_{w}) - \boldsymbol{v}_{\alpha}(\boldsymbol{s}_{w,h\tau},\boldsymbol{p}_{w,h\tau}), \nabla\varphi) \big\} \mathrm{d}t \bigg\}^{2} \bigg\}^{\frac{1}{2}} \end{split}$$

Comments

 conforming approximations: energy-type error controlled by the dual norm of the residual

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A posteriori estimates and stopping criteria for two-phase flows

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Pressure reconstructions

Definition (Global & complementary pressure reconstructions)

Piecewise affine-in-time scalar fields such that

 $\hat{\mathfrak{p}}_{h\tau} \in X, \ \hat{\mathfrak{q}}_{h\tau} \in X.$

- $\hat{\mathfrak{p}}_{h\tau}$: global pressure reconstruction if $\mathfrak{p}(s_{w,h\tau}, p_{w,h\tau}) \notin X$
- $\hat{\mathfrak{q}}_{h\tau}$: complementary pressure reconstruction if $\mathfrak{q}(s_{w,h\tau}) \notin X$
- continuity of traces as for the exact solution
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Phase velocities reconstructions

Definition (Equilibrated phase velocities reconstructions)

Piecewise constant-in-time vector fields such that, for all $1 \le n \le N$ and $\alpha \in \{n, w\}$,

$$\mathbf{u}_{lpha,h au}|_{I_n}\in \mathbf{H}(\mathrm{div},\Omega)$$

and such that

$$(q_{\alpha}^n - \partial_t(\phi s_{\alpha,h\tau}|_{I_n}) - \nabla \cdot \mathbf{u}_{\alpha,h\tau}|_{I_n}, \mathbf{1})_{\mathcal{K}} = \mathbf{0} \qquad \forall \mathcal{K} \in \mathcal{T}_h^n.$$

Comments

- **u**_{n,hτ}: nonwetting phase velocity reconstruction
- $\mathbf{u}_{w,h\tau}$: wetting phase velocity reconstruction
- continuity of normal traces and local conservation as for the exact Darcy velocities **u**_α
- practice: discrete fields in Raviart–Thomas–Nédélec spaces

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Theorem (Basic a posteriori error estimate)

Let (s_w, p_w) be the weak solution. Let $(s_{w,h\tau}, p_{w,h\tau})$ be arbitrary (satisfying BC+IC). Let $\hat{\mathfrak{p}}_{h\tau}$, $\hat{\mathfrak{q}}_{h\tau}$, and $\mathbf{u}_{\alpha,h\tau}$, $\alpha \in \{n,w\}$, be the pressure and phase velocities reconstructions. Then

$$\|\|(\boldsymbol{s}_{\mathrm{w}}-\boldsymbol{s}_{\mathrm{w},h au},\boldsymbol{p}_{\mathrm{w}}-\boldsymbol{p}_{\mathrm{w},h au})\|\|$$

$$\leq \left\{ \sum_{n=1}^{N} \sum_{K \in \mathcal{T}_{h}^{n}} \left(\eta_{K}^{n}(\boldsymbol{s}_{\mathrm{w},h\tau},\boldsymbol{p}_{\mathrm{w},h\tau},\hat{\mathfrak{p}}_{h\tau},\hat{\mathfrak{q}}_{h\tau},\boldsymbol{\mathsf{u}}_{\mathrm{n},h\tau},\boldsymbol{\mathsf{u}}_{\mathrm{w},h\tau}) \right)^{2} \right\}$$

- overall error control
- a posteriori error estimators η_K^n fully computable



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$$|||(s_{w} - s_{w,h\tau}, p_{w} - p_{w,h\tau})|||$$

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Estimate distinguishing different error components

Theorem (Distinguishing different error components)

Consider

- time step n,
- Inearization step k.
- iterative algebraic solver step i,

and the corresponding approximations $s_{w,b_{\tau}}^{n,k,i}$ and $p_{w,b_{\tau}}^{n,k,i}$. Then

$$\|\|(\boldsymbol{s}_{\mathrm{w}}-\boldsymbol{s}_{\mathrm{w},h au}^{n,k,i},\boldsymbol{
ho}_{\mathrm{w}}-\boldsymbol{
ho}_{\mathrm{w},h au}^{n,k,i})\|\|_{I_n}\leq\eta_{\mathrm{sp}}^{n,k,i}+\eta_{\mathrm{tm}}^{n,k,i}+\eta_{\mathrm{lin}}^{n,k,i}+\eta_{\mathrm{alg}}^{n,k,i}.$$

- $\eta_{sp}^{n,k,i}$: spatial discretization
- $\eta_{tm}^{n,k,i}$: temporal discretization
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Model problem

Horizontal flow

$$egin{aligned} \partial_t(\phi oldsymbol{s}_lpha) -
abla \cdot \left(rac{k_{\mathrm{r},lpha}(oldsymbol{s}_\mathrm{w})}{\mu_lpha} rac{\mathbf{K}
abla oldsymbol{
ho}_lpha}{oldsymbol{s}_\mathrm{n} + oldsymbol{s}_\mathrm{w}} &= \mathbf{0}, \ oldsymbol{s}_\mathrm{n} + oldsymbol{s}_\mathrm{w} &= \mathbf{1}, \ oldsymbol{
ho}_\mathrm{n} - oldsymbol{
ho}_\mathrm{w} &= oldsymbol{
ho}_\mathrm{c}(oldsymbol{s}_\mathrm{w}) \end{aligned}$$

Brooks–Corey model

• relative permeabilities

$$k_{r,w}(s_w) = s_e^4, \quad k_{r,n}(s_w) = (1 - s_e)^2 (1 - s_e^2)$$

• capillary pressure

$$p_{\rm c}(\boldsymbol{s}_{\rm w}) = \boldsymbol{p}_{\rm d} \boldsymbol{s}_{\rm e}^{-\frac{1}{2}}$$

$$s_{\mathrm{e}} := rac{s_{\mathrm{w}} - s_{\mathrm{rw}}}{1 - s_{\mathrm{rw}} - s_{\mathrm{rn}}}$$



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Setting A posteriori estimates Applications & exps. C Fully implicit CCFV Iteratively coupled IMPES VCFV Exts

Fully implicit cell-centered finite volume scheme

Fully implicit cell-centered two-point finite volumes For all $1 \le n \le N$, look for $s_{w,h}^n, \bar{p}_{w,h}^n$ such that

$$\phi \frac{\mathbf{s}_{\mathbf{w},K}^{n} - \mathbf{s}_{\mathbf{w},K}^{n-1}}{\tau^{n}} |\mathbf{K}| + \sum_{\mathbf{e}_{KL} \in \mathcal{E}_{K}^{\text{int}}} F_{\mathbf{w},\mathbf{e}_{KL}}(\mathbf{s}_{\mathbf{w},h}^{n}, \bar{p}_{\mathbf{w},h}^{n}) = 0,$$
$$\mathbf{s}_{\mathbf{w},K}^{n} - \mathbf{s}_{\mathbf{w},K}^{n-1} + \sum_{\mathbf{e}_{KL} \in \mathcal{E}_{K}^{\text{int}}} F_{\mathbf{w},\mathbf{e}_{KL}}(\mathbf{s}_{\mathbf{w},h}^{n}, \bar{p}_{\mathbf{w},h}^{n}) = 0,$$

$$-\phi \frac{s_{\mathrm{w},\mathrm{K}} - s_{\mathrm{w},\mathrm{K}}}{\tau^n} |\mathrm{K}| + \sum_{e_{\mathrm{KL}} \in \mathcal{E}_{\mathrm{K}}^{\mathrm{int}}} F_{\mathrm{n},e_{\mathrm{KL}}}(s_{\mathrm{w},\mathrm{h}}^n,\bar{\mathrm{p}}_{\mathrm{w},\mathrm{h}}^n) = 0,$$

where the normal fluxes are given by

$$\begin{split} F_{\mathrm{w},e_{\mathrm{KL}}}(s_{\mathrm{w},h}^{n},\bar{p}_{\mathrm{w},h}^{n}) &:= -\frac{\lambda_{\mathrm{r},\mathrm{w}}(s_{\mathrm{w},\mathrm{K}}^{n}) + \lambda_{\mathrm{r},\mathrm{w}}(s_{\mathrm{w},L}^{n})}{2} |\underline{\mathbf{K}}| \frac{\bar{p}_{\mathrm{w},L}^{n} - \bar{p}_{\mathrm{w},\mathrm{K}}^{n}}{|\mathbf{x}_{\mathrm{K}} - \mathbf{x}_{L}|} |e_{\mathrm{KL}}|, \\ F_{\mathrm{n},e_{\mathrm{KL}}}(s_{\mathrm{w},h}^{n},\bar{p}_{\mathrm{w},h}^{n}) &:= -\frac{\lambda_{\mathrm{r},\mathrm{n}}(s_{\mathrm{w},\mathrm{K}}^{n}) + \lambda_{\mathrm{r},\mathrm{n}}(s_{\mathrm{w},L}^{n})}{2} |\underline{\mathbf{K}}| \\ \times \frac{\bar{p}_{\mathrm{w},L}^{n} + p_{\mathrm{c}}(s_{\mathrm{w},L}^{n}) - (\bar{p}_{\mathrm{w},\mathrm{K}}^{n} + p_{\mathrm{c}}(s_{\mathrm{w},\mathrm{K}}^{n}))}{|\mathbf{x}_{\mathrm{K}} - \mathbf{x}_{\mathrm{L}}|} \end{split}$$

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$$-\phi \frac{\boldsymbol{s}_{\mathrm{w},K}^{n} - \boldsymbol{s}_{\mathrm{w},K}^{n-1}}{\tau^{n}} |\boldsymbol{K}| + \sum_{\boldsymbol{e}_{\boldsymbol{K}\boldsymbol{L}} \in \mathcal{E}_{\boldsymbol{K}}^{\mathrm{int}}} \boldsymbol{F}_{\mathrm{n},\boldsymbol{e}_{\boldsymbol{K}\boldsymbol{L}}}(\boldsymbol{s}_{\mathrm{w},h}^{n}, \bar{\boldsymbol{p}}_{\mathrm{w},h}^{n}) = \boldsymbol{0},$$

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$$egin{aligned} & F_{ ext{w},m{e}_{\mathcal{K}\mathcal{L}}}(m{s}_{ ext{w},h}^n,ar{p}_{ ext{w},h}^n) &\coloneqq & -rac{\lambda_{ ext{r,w}}(m{s}_{ ext{w},\mathcal{K}}^n)+\lambda_{ ext{r,w}}(m{s}_{ ext{w},L}^n)}{2}|\mathbf{\underline{K}}|rac{ar{p}_{ ext{w},\mathcal{L}}^n-ar{p}_{ ext{w},\mathcal{K}}^n}{|m{x}_{\mathcal{K}}-m{x}_{\mathcal{L}}|}|m{e}_{\mathcal{K}\mathcal{L}}|, \ & F_{ ext{n},m{e}_{\mathcal{K}\mathcal{L}}}(m{s}_{ ext{w},h}^n,ar{p}_{ ext{w},h}^n) &\coloneqq & -rac{\lambda_{ ext{r,n}}(m{s}_{ ext{w},\mathcal{K}}^n)+\lambda_{ ext{r,n}}(m{s}_{ ext{w},L}^n)}{2}|\mathbf{\underline{K}}| \ & imes rac{ar{p}_{ ext{w},\mathcal{K}}^n+m{p}_{ ext{c}}(m{s}_{ ext{w},L}^n)-ar{(ar{p}_{ ext{w},\mathcal{K}}^n+m{p}_{ ext{c}}(m{s}_{ ext{w},\mathcal{K}}^n))}{|m{x}_{\mathcal{K}}-m{x}_{\mathcal{L}}|} egin{aligned} & egin{aligned} &$$

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Linearization and algebraic solution



$$\begin{split} F_{\alpha,e_{KL}}^{k-1}(s_{w,h}^{n,k,i},\bar{p}_{w,h}^{n,k,i}) &:= F_{\alpha,e_{KL}}(s_{w,h}^{n,k-1},\bar{p}_{w,h}^{n,k-1}) \\ &+ \sum_{M \in \{K,L\}} \frac{\partial F_{\alpha,e_{KL}}}{\partial s_{w,M}}(s_{w,h}^{n,k-1},\bar{p}_{w,h}^{n,k-1}) \cdot (s_{w,M}^{n,k,i} - s_{w,M}^{n,k-1}) \\ &+ \sum_{M \in \{K,L\}} \frac{\partial F_{\alpha,e_{KL}}}{\partial \bar{p}_{w,M}}(s_{w,h}^{n,k-1},\bar{p}_{w,h}^{n,k-1}) \cdot (\bar{p}_{w,M}^{n,k,i} - \bar{p}_{w,M}^{n,k-1}) \cdot (\bar{p}_{w,M}^{n,k-1} - \bar{p}_{w,M}^{n,k-1} - \bar{p}_{w,M}^{n,k-1}) \cdot (\bar{p}_{w,M}^{n,k-1} - \bar{p}_{w,M}^{n,k-1} - \bar{p}_{w,M}^{n,k-1} - \bar{p}_{w,M}^{n,k-1}) \cdot (\bar{p}_{w,M}^{n,k-1} - \bar{p}_{w,M}^{n,k-1} - \bar{p}_{w,M}^{n$$

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Linearization and algebraic solution

Linearization step k and algebraic step i Couple $s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}$ such that $\phi \frac{s_{w,K}^{n,k,i} - s_{w,K}^{n-1}}{\tau^n} |K| + \sum F_{w,e_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) = -R_{w,K}^{n,k,i},$ e_{KI} ∈ E^{int} $-\phi \frac{s_{w,K}^{n,\kappa,i}-s_{w,K}^{n-1}}{\tau^n} |K| + \sum F_{n,e_{KL}}^{k-1}(s_{w,h}^{n,k,i},\bar{p}_{w,h}^{n,k,i}) = -R_{n,K}^{n,k,i},$ eki ∈ E^{int}

where the linearized normal fluxes are given by

$$\begin{aligned} F_{\alpha,e_{KL}}^{k-1}(s_{w,h}^{n,k,i},\bar{p}_{w,h}^{n,k,i}) &:= F_{\alpha,e_{KL}}(s_{w,h}^{n,k-1},\bar{p}_{w,h}^{n,k-1}) \\ &+ \sum_{M \in \{K,L\}} \frac{\partial F_{\alpha,e_{KL}}}{\partial s_{w,M}}(s_{w,h}^{n,k-1},\bar{p}_{w,h}^{n,k-1}) \cdot (s_{w,M}^{n,k,i} - s_{w,M}^{n,k-1}) \\ &+ \sum_{M \in \{K,L\}} \frac{\partial F_{\alpha,e_{KL}}}{\partial \bar{p}_{w,M}}(s_{w,h}^{n,k-1},\bar{p}_{w,h}^{n,k-1}) \cdot (\bar{p}_{w,M}^{n,k,i} - \bar{p}_{w,M}^{n,k-1}) \cdot (\bar{p}_{w,M}^{n,k-1} - \bar{p}_{w,M}^{n,k-1} - \bar{p}_{w,M}^{n,k-1}) \cdot (\bar{p}_{w,M}^{n,k-1} - \bar{p}_{w,$$

Velocities reconstructions

Velocities reconstructions

$$\begin{aligned} (\mathbf{d}_{\alpha,h}^{n,k,i} \cdot \mathbf{n}_{K}, 1)_{\boldsymbol{e}_{KL}} &:= F_{\alpha, \boldsymbol{e}_{KL}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k,i}, \bar{\boldsymbol{p}}_{\mathrm{w},h}^{n,k,i}), \\ ((\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{I}_{\alpha,h}^{n,k,i}) \cdot \mathbf{n}_{K}, 1)_{\boldsymbol{e}_{KL}} &:= F_{\alpha, \boldsymbol{e}_{KL}}^{k-1}(\boldsymbol{s}_{\mathrm{w},h}^{n,k,i}, \bar{\boldsymbol{p}}_{\mathrm{w},h}^{n,k,i}), \\ \mathbf{a}_{\alpha,h}^{n,k,i} &:= \mathbf{d}_{\alpha,h}^{n,k,i+\nu} + \mathbf{I}_{\alpha,h}^{n,k,i+\nu} - (\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{I}_{\alpha,h}^{n,k,i}) \end{aligned}$$

Comments

 phase velocities reconstructions: u^{n,k,i}_{α,h} := d^{n,k,i}_{α,h} + l^{n,k,i}_{α,h} + a^{n,k,i}_{α,h}

 d^{n,k,i}_{α,h}, l^{n,k,i}_{α,h}, a^{n,k,i}_{α,h} used to identify error components



Velocities reconstructions

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 phase velocities reconstructions: u^{n,k,i}_{α,h} := d^{n,k,i}_{α,h} + l^{n,k,i}_{α,h} + a^{n,k,i}_{α,h}

 d^{n,k,i}_{α,h}, l^{n,k,i}_{α,h}, a^{n,k,i}_{α,h} used to identify error components



Global and complementary pressure reconstructions

Global and complementary pressures reconstructions

• piecewise quadratic global and complementary pressures:

$$-(\lambda_{w}(\boldsymbol{s}_{w,K}^{n,k,i}) + \lambda_{n}(\boldsymbol{s}_{w,K}^{n,k,i}))\underline{\mathbf{K}}\nabla(\boldsymbol{\mathfrak{p}}_{h}^{n,k,i}|_{K}) = (\mathbf{d}_{w,h}^{n,k,i} + \mathbf{d}_{n,h}^{n,k,i})|_{K},$$
$$\boldsymbol{\mathfrak{p}}_{h}^{n,k,i}(\mathbf{x}_{K}) = \boldsymbol{\mathfrak{p}}(\bar{\boldsymbol{p}}_{w,K}^{n,k,i}, \boldsymbol{s}_{w,K}^{n,k,i}),$$
$$\underline{\mathbf{K}}\nabla(\boldsymbol{\mathfrak{q}}_{h}^{n,k,i}|_{K}) = \lambda_{n}(\boldsymbol{s}_{w,K}^{n,k,i})\underline{\mathbf{K}}\nabla(\boldsymbol{\mathfrak{p}}_{h}^{n,k,i}|_{K}) + \mathbf{d}_{n,h}^{n,k,i}|_{K},$$
$$\boldsymbol{\mathfrak{q}}_{h}^{n,k,i}(\mathbf{x}_{K}) = \boldsymbol{\mathfrak{q}}(\boldsymbol{s}_{w,K}^{n,k,i})$$

reconstructions:

$$\hat{\mathfrak{p}}_h^{n,k,i} := \mathcal{I}_{\mathrm{av}}(\mathfrak{p}_h^{n,k,i}), \\ \hat{\mathfrak{q}}_h^{n,k,i} := \mathcal{I}_{\mathrm{av}}(\mathfrak{q}_h^{n,k,i})$$



Global pressure reconstructions





Approximate global pressure $\mathfrak{p}(s_{\mathrm{w},h\tau},p_{\mathrm{w},h\tau}) \not\in X$

Averaged approximate global pressure $\hat{\mathfrak{p}}_{h\tau} \in X$



Data from Klieber & Rivière (2006)

Data

$$\begin{split} \Omega &= (0, 300) \mathsf{m} \times (0, 300) \mathsf{m}, \quad \mathcal{T} = 4 \cdot 10^6 \mathsf{s}, \\ \phi &= 0.2, \quad \underline{\mathsf{K}} = 10^{-11} \underline{\mathsf{I}} \, \mathsf{m}^2, \\ \mu_{\mathrm{w}} &= 5 \cdot 10^{-4} \mathsf{kg} \, \mathsf{m}^{-1} \mathsf{s}^{-1}, \quad \mu_{\mathrm{n}} = 2 \cdot 10^{-3} \mathsf{kg} \, \mathsf{m}^{-1} \mathsf{s}^{-1}, \\ s_{\mathrm{rw}} &= s_{\mathrm{rn}} = 0, \quad p_{\mathrm{d}} = 5 \cdot 10^3 \mathsf{kg} \, \mathsf{m}^{-1} \mathsf{s}^{-2} \end{split}$$

Initial condition (\overline{K} 18m × 18m lower left corner block)

$$egin{aligned} & m{s}_{\mathrm{w}}^{\mathrm{0}} = 0.2 ext{ on } K \in \mathcal{T}_h, \, K
ot\in \widetilde{K}, \ & m{s}_{\mathrm{w}}^{\mathrm{0}} = 0.95 ext{ on } K \in \mathcal{T}_h, \, K \in \widetilde{K} \end{aligned}$$

Boundary conditions (\hat{K} 18m × 18m upper right corner block)

- no flow Neumann boundary conditions everywhere except of $\partial \widetilde{K} \cap \partial \Omega$ and $\partial \widehat{K} \cap \partial \Omega$
- \tilde{K} injection well: $s_{\rm w} = 0.95$, $p_{\rm w} = 3.45 \cdot 10^6$ kg m⁻¹s⁻²
- \widehat{K} production well: $s_w = 0.2$, $p_w = 2.41 \cdot 10^6$ kg m⁻¹

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Initial condition (\tilde{K} 18m × 18m lower left corner block)

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Water saturation/estimators evolution



Estimators and stopping criteria





GMRes relative residual/Newton iterations





GMRes iterations





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Iteratively coupled vertex-centered finite volumes

Implicit pressure equation on step k

$$\begin{split} &-\big(\big(\lambda_{\mathrm{r,w}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1})+\lambda_{\mathrm{r,n}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1})\big)\underline{\mathsf{K}}\nabla\boldsymbol{\rho}_{\mathrm{w},h}^{n,k}\cdot\boldsymbol{\mathsf{n}}_{D}\\ &+\lambda_{\mathrm{r,n}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1})\underline{\mathsf{K}}\nabla\overline{\boldsymbol{\rho}}_{\mathrm{c}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1})\cdot\boldsymbol{\mathsf{n}}_{D},1\big)_{\partial D\setminus\partial\Omega}=0 \quad \forall D\in\mathcal{D}_{h}^{\mathrm{int},n} \end{split}$$

$$\boldsymbol{s}_{\mathrm{w},D}^{n,k} := \frac{\tau^n}{\phi|D|} \big(\lambda_{\mathrm{r},\mathrm{w}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1}) \underline{\mathsf{K}} \nabla \boldsymbol{p}_{\mathrm{w},h}^{n,k} \cdot \mathbf{n}_D, 1 \big)_{\partial D \setminus \partial \Omega} + \boldsymbol{s}_{\mathrm{w},D}^{n-1} \quad \forall D \in \mathcal{D}_h^{\mathrm{int},n}$$



Iteratively coupled vertex-centered finite volumes

Implicit pressure equation on step k

$$\begin{split} &-\big(\big(\lambda_{\mathrm{r,w}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1}) + \lambda_{\mathrm{r,n}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1})\big)\underline{\mathbf{K}}\nabla\boldsymbol{\rho}_{\mathrm{w},h}^{n,k}\cdot\mathbf{n}_{D} \\ &+\lambda_{\mathrm{r,n}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla\overline{\boldsymbol{\rho}}_{\mathrm{c}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1})\cdot\mathbf{n}_{D},1\big)_{\partial D\setminus\partial\Omega} = \mathbf{0} \quad \forall D\in\mathcal{D}_{h}^{\mathrm{int},n} \end{split}$$

Explicit saturation equation on step k

$$\boldsymbol{s}_{\mathrm{w},D}^{n,k} := \frac{\tau^n}{\phi |\boldsymbol{D}|} \big(\lambda_{\mathrm{r},\mathrm{w}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1}) \underline{\mathbf{K}} \nabla \boldsymbol{\rho}_{\mathrm{w},h}^{n,k} \cdot \mathbf{n}_D, 1 \big)_{\partial D \setminus \partial \Omega} + \boldsymbol{s}_{\mathrm{w},D}^{n-1} \quad \forall \boldsymbol{D} \in \mathcal{D}_h^{\mathrm{int},n}$$



Linearization and algebraic solution

Iterative coupling step k and algebraic step i

$$-((\lambda_{\mathbf{r},\mathbf{w}}(\boldsymbol{s}_{\mathbf{w},h}^{n,k-1}) + \lambda_{\mathbf{r},\mathbf{n}}(\boldsymbol{s}_{\mathbf{w},h}^{n,k-1}))\underline{\mathbf{K}}\nabla\boldsymbol{p}_{\mathbf{w},h}^{n,k,i}\cdot\mathbf{n}_{D} \\ + \lambda_{\mathbf{r},\mathbf{n}}(\boldsymbol{s}_{\mathbf{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla\overline{\boldsymbol{p}}_{\mathbf{c}}(\boldsymbol{s}_{\mathbf{w},h}^{n,k-1})\cdot\mathbf{n}_{D},\mathbf{1})_{\partial D\setminus\partial\Omega} = -\boldsymbol{R}_{\mathbf{t},D}^{n,k,i} \quad \forall D \in \mathcal{D}_{h}^{\mathrm{int},n}$$

$$\boldsymbol{s}_{\mathrm{w},D}^{n,k,i} := \frac{\tau^n}{\phi|D|} \big(\lambda_{\mathrm{r},\mathrm{w}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1}) \underline{\mathbf{K}} \nabla \boldsymbol{p}_{\mathrm{w},h}^{n,k,i} \cdot \mathbf{n}_D, 1 \big)_{\partial D \setminus \partial \Omega} + \boldsymbol{s}_{\mathrm{w},D}^{n-1}$$



Linearization and algebraic solution

Iterative coupling step k and algebraic step i

$$-((\lambda_{\mathrm{r,w}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1}) + \lambda_{\mathrm{r,n}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1}))\underline{\mathbf{K}}\nabla\boldsymbol{p}_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_{D} \\ + \lambda_{\mathrm{r,n}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla\overline{\boldsymbol{p}}_{\mathrm{c}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1})\cdot\mathbf{n}_{D}, 1)_{\partial D\setminus\partial\Omega} = -\boldsymbol{R}_{\mathrm{t,D}}^{n,k,i} \quad \forall D \in \mathcal{D}_{h}^{\mathrm{int},n}$$

$$\boldsymbol{s}_{\mathrm{w},D}^{n,k,i} := \frac{\tau^n}{\phi |\boldsymbol{D}|} \big(\lambda_{\mathrm{r,w}}(\boldsymbol{s}_{\mathrm{w},h}^{n,k-1}) \underline{\mathbf{K}} \nabla \boldsymbol{p}_{\mathrm{w},h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1} \big)_{\partial D \setminus \partial \Omega} + \boldsymbol{s}_{\mathrm{w},D}^{n-1}$$



I Setting A posteriori estimates Applications & exps. C

Velocities reconstructions

Total velocities reconstructions

$$\begin{aligned} (\mathbf{d}_{t,h}^{n,k,i} \cdot \mathbf{n}_{D}, 1)_{e} &:= -\left(\left(\lambda_{r,w}(\boldsymbol{s}_{w,h}^{n,k,i}) + \lambda_{r,n}(\boldsymbol{s}_{w,h}^{n,k,i})\right)\underline{\mathbf{K}}\nabla \boldsymbol{p}_{w,h}^{n,k,i} \cdot \mathbf{n}_{D} \right. \\ &+ \lambda_{r,n}(\boldsymbol{s}_{w,h}^{n,k,i})\underline{\mathbf{K}}\nabla \overline{\boldsymbol{p}}_{c}(\boldsymbol{s}_{w,h}^{n,k,i}) \cdot \mathbf{n}_{D}, 1)_{e}, \\ (\mathbf{d}_{t,h}^{n,k,i} + \mathbf{l}_{t,h}^{n,k,i}) \cdot \mathbf{n}_{D}, 1)_{e} &:= -\left(\left(\lambda_{r,w}(\boldsymbol{s}_{w,h}^{n,k-1}) + \lambda_{r,n}(\boldsymbol{s}_{w,h}^{n,k-1})\right)\underline{\mathbf{K}}\nabla \boldsymbol{p}_{w,h}^{n,k,i} \cdot \mathbf{n}_{D} \right. \\ &+ \lambda_{r,n}(\boldsymbol{s}_{w,h}^{n,k-1})\underline{\mathbf{K}}\nabla \overline{\boldsymbol{p}}_{c}(\boldsymbol{s}_{w,h}^{n,k-1}) \cdot \mathbf{n}_{D}, 1)_{e}, \\ &+ \lambda_{r,n}(\boldsymbol{s}_{w,h}^{n,k,i+\nu} - \left(\mathbf{d}_{t,h}^{n,k,i} + \mathbf{l}_{t,h}^{n,k,i}\right) \end{aligned}$$

Wetting phase velocities reconstructions

$$\begin{aligned} (\mathbf{d}_{\mathbf{w},h}^{n,k,i} \cdot \mathbf{n}_{D}, 1)_{e} &:= - \left(\lambda_{\mathbf{r},\mathbf{w}}(\boldsymbol{s}_{\mathbf{w},h}^{n,k,i})\underline{\mathbf{K}}\nabla \boldsymbol{p}_{\mathbf{w},h}^{n,k,i} \cdot \mathbf{n}_{D}, 1\right)_{e}, \\ ((\mathbf{d}_{\mathbf{w},h}^{n,k,i} + \mathbf{l}_{\mathbf{w},h}^{n,k,i}) \cdot \mathbf{n}_{D}, 1)_{e} &:= - \left(\lambda_{\mathbf{r},\mathbf{w}}(\boldsymbol{s}_{\mathbf{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla \boldsymbol{p}_{\mathbf{w},h}^{n,k,i} \cdot \mathbf{n}_{D}, 1\right)_{e}, \\ \mathbf{a}_{\mathbf{w},h}^{n,k,i} &:= 0 \end{aligned}$$

Pressure reconstructions

conforming setting ⇒ no pressure reconstructions



I Setting A posteriori estimates Applications & exps. C

Velocities reconstructions

Total velocities reconstructions

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Pressure reconstructions

● conforming setting ⇒ no pressure reconstructions

M. Vohralík A posteriori estimates and stopping criteria for two-phase flows

Setting A posteriori estimates Applications & exps. C

Velocities reconstructions

Total velocities reconstructions

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Pressure reconstructions

• conforming setting \Rightarrow no pressure reconstructions /

Estimators and stopping criteria



GMRes iterations

iterative coupling iterations



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GMRes relative residual/iterative coupling iterations





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GMRes iterations





Space/time/nonlinear solver/linear solver adaptivity





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A posteriori estimates and stopping criteria for two-phase flows

Extension to multiphase compositional flows

Multiphase compositional flows

- $N_{\mathcal{P}}$ phases, $N_{\mathcal{C}}$ components
- miscible, compressible
- isothermal/thermal
- Ph.D. theses of Carole Heinry and Soleiman Yousef (Paris 6/IFPEN)

Discretization and resolution

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

Test case

- two phases and three components
- heterogeneous permeability distribution



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Newton iterations





GMRes iterations





M. Vohralík A posteriori estimates and stopping criteria for two-phase flows

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Conclusions

Complete adaptivity

- only a necessary number of algebraic solver iterations on each linearization step
- only a necessary number of linearization iterations
- space-time mesh adaptivity
- smart online decisions: algebraic step / linearization step / time step refinement / space mesh refinement
- important computational savings
- error upper bound via a posteriori error estimates

Future directions

- practical implementations
- other complex problems



Conclusions

Complete adaptivity

- only a necessary number of algebraic solver iterations on each linearization step
- only a necessary number of linearization iterations
- space-time mesh adaptivity
- smart online decisions: algebraic step / linearization step / time step refinement / space mesh refinement
- important computational savings
- error upper bound via a posteriori error estimates

Future directions

- practical implementations
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Thank you for your attention!

