Minimum Residual & Least-Squares Finite Element Methods

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Applications of a space-time first-order system least-squares formulation for parabolic PDEs

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joint work with

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Convergence

General second-order parabolic PDE

- Lipschitz domain $\Omega \subset \mathbb{R}^d$, $Q := (0,T) \times \Omega$, $\Sigma := (0,T) \times \partial\Omega$

$$\begin{aligned} \partial_t u - \operatorname{div}_{\mathbf{x}}(\mathbf{A}\nabla_{\mathbf{x}} u) + \mathbf{b} \cdot \nabla_{\mathbf{x}} u + cu &= f + \operatorname{div}_{\mathbf{x}} \mathbf{g} && \text{in } Q \\ u &= 0 && \text{on } \Sigma \\ u(0,\cdot) &= u_0 && \text{in } \Omega \end{aligned}$$

- $\mathbf{A} \in L^\infty(Q)^{d\times d}$ positive definite, $\mathbf{b} \in L^\infty(Q)$, $c \in L^\infty(Q)$
- $f \in L^2(Q), \mathbf{g} \in L^2(Q)^d, u_0 \in L^2(\Omega)$

General second-order parabolic PDE

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- $\mathbf{A} \in L^\infty(Q)^{d\times d}$ positive definite, $\mathbf{b} \in L^\infty(Q)$, $c \in L^\infty(Q)$
- $f \in L^2(Q), \mathbf{g} \in L^2(Q)^d, u_0 \in L^2(\Omega)$
- substitute $\boldsymbol{\sigma} := -\mathbf{A}\nabla_{\mathbf{x}} u - \mathbf{g}$

$$\begin{aligned} \partial_t u + \operatorname{div}_{\mathbf{x}} \boldsymbol{\sigma} + \mathbf{b}\cdot\nabla_{\mathbf{x}} u + cu &= f \\ u|_\Sigma &= 0 \\ u(0,\cdot) &= u_0 \end{aligned}$$

$\Longrightarrow$ find $\mathbf{u} = (u, \boldsymbol{\sigma})$ with $u|_\Sigma = 0$ s.t.

$$\begin{aligned} -\boldsymbol{\sigma} - \mathbf{A}\nabla_{\mathbf{x}} u &= \mathbf{g} \\ \underbrace{\operatorname{div} \mathbf{u}}_{\partial_t u + \operatorname{div}_{\mathbf{x}} \boldsymbol{\sigma}} + \mathbf{b}\cdot\nabla_{\mathbf{x}} u + cu &= f \\ u(0,\cdot) &= u_0 \end{aligned}$$

First-order system 2/2

- find $\mathbf{u} = (u, \boldsymbol{\sigma})$ with $u|_\Sigma = 0$ s.t.

$$G\mathbf{u} := \begin{cases} -\boldsymbol{\sigma} - \mathbf{A}\nabla_{\mathbf{x}} u &= \mathbf{g} \\ \operatorname{div} \mathbf{u} + \mathbf{b} \cdot \nabla_{\mathbf{x}} u + cu &= f \\ u(0, \cdot) &= u_0 \end{cases}$$

- domain of G

$$\underbrace{\left\{\mathbf{u} = (u, \boldsymbol{\sigma}) \in L^2(Q)^{d+1} \;:\; \operatorname{div} \mathbf{u} \in L^2(Q), \nabla_{\mathbf{x}} u \in L^2(Q)^d, u|_\Sigma = 0\right\}}_{=:U}$$

- U is Hilbert space with norm

$$\|\mathbf{u}\|_U^2 := \|\mathbf{u}\|_{L^2(Q)^{d+1}}^2 + \|\operatorname{div} \mathbf{u}\|_{L^2(Q)}^2 + \|\nabla_{\mathbf{x}} u\|_{L^2(Q)}^2$$

Theorem (Führer, Karkulik '21 + G., Stevenson '21)

- G is continuous linear isomorphism from U to $L^2(Q)^d \times L^2(Q) \times L^2(\Omega)$

Führer, Karkulik: CAMWA (2021) — cont. for diff. norm on U, injectivity

Gantner, Stevenson: M2AN (2021) — norms are equivalent, surjectivity

Normal equations

- find $\mathbf{u} \in U$ s.t. $G\mathbf{u} = (\mathbf{g}, f, u_0)$
- normal equations: $G^*G\mathbf{u} = G^*(\mathbf{g}, f, u_0)$, equivalent to

$$\langle G\mathbf{u}\,,\, G\mathbf{v}\rangle_{L^2} = \langle(\mathbf{g}, f, u_0)\,,\, G\mathbf{v}\rangle_{L^2} \quad \text{for all } \mathbf{v} \in U$$

Corollary

- $(\mathbf{u}, \mathbf{v}) \mapsto \langle G\mathbf{u}\,,\, G\mathbf{v}\rangle_{L^2}$ is bounded and coercive bilinear form on U

$\Longrightarrow$ for all $U_\delta \subset U$ ex. unique Galerkin approximation $\mathbf{u}_\delta = (u_\delta, \boldsymbol{\sigma}_\delta)$ s.t.

$$\langle G\mathbf{u}_\delta\,,\, G\mathbf{v}_\delta\rangle_{L^2} = \langle(\mathbf{g}, f, u_0)\,,\, G\mathbf{v}_\delta\rangle_{L^2} \quad \text{for all } \mathbf{v} \in U_\delta$$

$\Longrightarrow$ approximation is quasi-optimal: $\|\mathbf{u} - \mathbf{u}_\delta\|_U \lesssim \min_{\mathbf{v}_\delta \in U_\delta} \|\mathbf{u} - \mathbf{v}_\delta\|_U$

A posteriori error estimator

- G linear isomorphism from U to $L^2(Q)^d \times L^2(Q) \times L^2(\Omega)$

$\Longrightarrow$ a posteriori error estimator for arbitrary $\mathbf{u}_\delta$

$$\eta_\delta := \|G\mathbf{u}_\delta - (\mathbf{g}, f, u_0)\|_{L^2} = \|G(\mathbf{u}_\delta - \mathbf{u})\|_{L^2} \eqsim \|\mathbf{u}_\delta - \mathbf{u}\|_U$$

- local error indicators for elements of space-time mesh $\mathcal{T}$ of Q

$$\begin{aligned}
&\|G\mathbf{u}_\delta - (\mathbf{g}, f, u_0)\|_{L^2}^2 \\
&= \|(G\mathbf{u}_\delta)_1 - \mathbf{g}\|_{L^2(Q)^d}^2 + \|(G\mathbf{u}_\delta)_2 - f\|_{L^2(Q)}^2 + \|(G\mathbf{u}_\delta)_3 - u_0\|_{L^2(\Omega)}^2 \\
&= \sum_{K \in \mathcal{T}} \underbrace{\|(G\mathbf{u}_\delta)_1 - \mathbf{g}\|_{L^2(K)^d}^2 + \|(G\mathbf{u}_\delta)_2 - f\|_{L^2(K)}^2 + \|(G\mathbf{u}_\delta)_3 - u_0\|_{L^2(K_0)}^2}_{=:\eta_\delta(K)^2}
\end{aligned}$$

- $K_0 := K \cap \big(\{0\} \times \Omega\big)$

Adaptive algorithm

- initial mesh $\mathcal{T}_0$ of Q into simplices and polynomial degree p
- initial trial space $U_0 := \big\{(u, \boldsymbol{\sigma}) \in S^p(\mathcal{T}_0) \times S^p(\mathcal{T}_0)^d \,:\, u|_\Sigma = 0\big\}$ $\subset U = \big\{(u, \boldsymbol{\sigma}) \in H(\mathrm{div}\,; Q) \,:\, \nabla_{\mathbf{x}} u \in L^2(Q)^d \wedge u|_\Sigma = 0\big\}$
- adaptivity parameter $0 < \theta \leq 1$

Adaptive algorithm

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- adaptivity parameter $0 < \theta \le 1$

for $\ell = 0, 1, 2, \ldots$ do:

SOLVE: compute approximation $\mathbf{u}_\ell \in U_\ell$

ESTIMATE: compute indicators $\eta_\ell(K)$ for all $K \in \mathcal{T}_\ell$

MARK: find (minimal) set $\mathcal{M}_\ell \subseteq \mathcal{T}_\ell$ s.t.

$$\theta \sum_{K \in \mathcal{T}_\ell} \eta_\ell(K)^2 \le \sum_{K \in \mathcal{M}_\ell} \eta_\ell(K)^2$$

REFINE: bisect (at least) elements $K \in \mathcal{M}_\ell$ to obtain $\mathcal{T}_{\ell+1}$

Convergence

Theorem (G., Stevenson '21)

- estimator convergence: $\lim_{\ell\to\infty} \eta_\ell = 0$
- error convergence: $\lim_{\ell\to\infty} \|\mathbf{u} - \mathbf{u}_\ell\|_U = 0$

- proof: abstract framework
- also applicable for other least-squares problems:
  - Poisson+Helmholtz
  - linear elasticity
  - Stokes
- BUT: convergence rates for space-time can be poor for $p = 1$

Gantner, Stevenson: M2AN (2021)

Siebert: IMAJNA (2011) — abstract framework

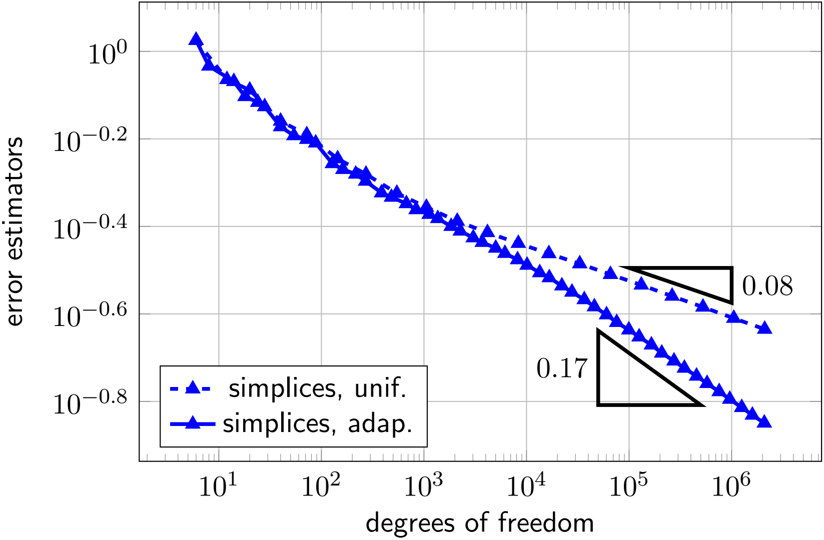
Führer, Praetorius: CAMWA (2021) — other least-squares problems

Carstensen, Park, Bringmann: NuMa (2017) — linear convergence for Poisson if $\theta \gg 0$

Führer, Karkulik: CAMWA (2021) — numerical experiments

Convergence plot for $p = 1$

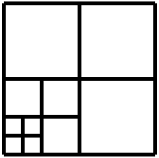
- heat equation on $\Omega = (0,1)$: $\partial_t u - \Delta_{\mathbf{x}} u = 2, \quad u|_\Sigma = 0, \quad u(0,\cdot) = 1$



Trial spaces

$\Longrightarrow$ remedy: different discrete trial space

- $U = \{\mathbf{u} = (u, \boldsymbol{\sigma}) \in L^2(Q)^{d+1} : \underbrace{\operatorname{div} \mathbf{u}}_{\partial_t u + \operatorname{div}_{\mathbf{x}} \boldsymbol{\sigma}}, \nabla_{\mathbf{x}} u \in L^2(Q) \wedge u|_\Sigma = 0\}$
- $U_\ell = \{(u, \boldsymbol{\sigma}) \in S^1(\mathcal{T}_\ell) \times S^1(\mathcal{T}_\ell)^d : u|_\Sigma = 0\} \subset H^1(Q)^{d+1}$
- prismatic mesh $\mathcal{P}_\ell$ of Q with elements $J \times K$, $J \subset I$ and $K \subset \Omega$



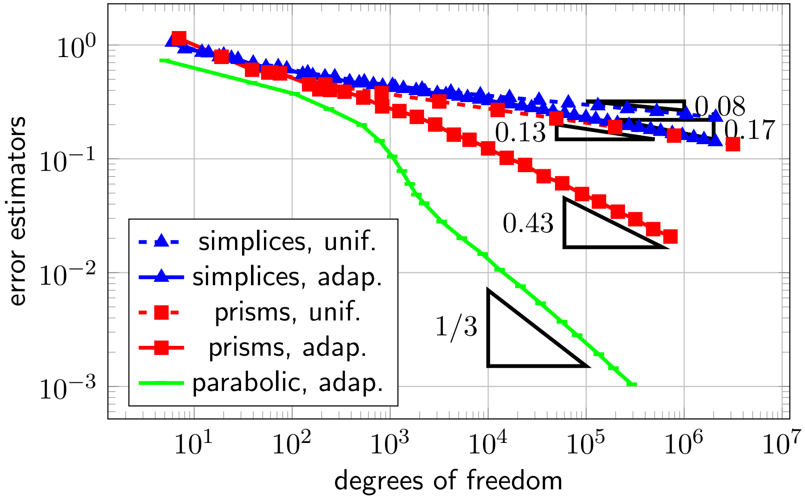
- $\widetilde{U}_\ell := \{(u, \boldsymbol{\sigma}) \in L^2(Q)^{d+1} : \partial_t u, \nabla_{\mathbf{x}} u, \operatorname{div}_{\mathbf{x}} \boldsymbol{\sigma} \in L^2(Q) \wedge u|_\Sigma = 0 \wedge u|_{J \times K} \in P^1(J) \otimes P^1(K) \wedge \boldsymbol{\sigma}|_{J \times K} \in P^0(J) \otimes RT^1(K) \ \forall (J \times K) \in \mathcal{P}_\ell\}$

Theorem (G., Stevenson '22)

- $\widetilde{U}_\ell$ has "better" approximation properties than U_ℓ and $\lim_{\ell \to \infty} \|\mathbf{u} - \widetilde{\mathbf{u}}_\ell\|_U = 0$

Gantner, Stevenson: arXiv (2022)

Convergence plot



- local parabolic scaling $h_t \eqsim h_{\mathbf{x}}^2$ with increased spatial poly. degrees

Diening, Storn: CAMWA (2022) parabolic scaling

Reduced basis method

Parameter dependence

$$\begin{aligned} \partial_t u - \mathrm{div}_{\mathbf{x}}(\mathbf{A}\nabla_{\mathbf{x}} u) + \mathbf{b}\cdot\nabla_{\mathbf{x}} u + cu &= f + \mathrm{div}_{\mathbf{x}}\,\mathbf{g} && \text{in } Q \\ u &= 0 && \text{on } \Sigma \\ u(0,\cdot) &= u_0 && \text{in } \Omega \end{aligned}$$

- $\mathbb{P} \subset \mathbb{R}^m$ compact parameter set
- $\mathbf{A} = \mathbf{A}[\boldsymbol{\mu}]$, $\mathbf{b} = \mathbf{b}[\boldsymbol{\mu}]$, $c = c[\boldsymbol{\mu}]$ for $\boldsymbol{\mu} \in \mathbb{P}$
- $f = f[\boldsymbol{\mu}]$, $\mathbf{g} = \mathbf{g}[\boldsymbol{\mu}]$, $u_0 = u_0[\boldsymbol{\mu}]$ for $\boldsymbol{\mu} \in \mathbb{P}$
- suppose parameter separability, e.g., for $\mathbf{A}$

$$\mathbf{A}[\boldsymbol{\mu}] = \sum_j \phi_j^{\mathbf{A}}(\boldsymbol{\mu})\mathbf{A}_j, \quad \phi_j^{\mathbf{A}} : \mathbb{P} \to \mathbb{R} \quad \mathbf{A}_j \in L^\infty(Q)^{d\times d}$$

- goal: after expensive offline phase compute in fast online phase

$$\mathbf{u} = (u, \boldsymbol{\sigma}) = (u[\boldsymbol{\mu}], \boldsymbol{\sigma}[\boldsymbol{\mu}]) = \mathbf{u}[\boldsymbol{\mu}]$$

Reduced basis method

- offline phase:
  - fix high-dimensional approximation space U_δ
  - choose parameters $\boldsymbol{\mu}^{(1)}, \ldots, \boldsymbol{\mu}^{(N)} \in \mathbb{P}$ with $N \ll \dim(U_\delta)$
  - compute approximation $\mathbf{u}_\delta[\boldsymbol{\mu}^{(i)}]$ of $\mathbf{u}[\boldsymbol{\mu}^{(i)}]$ in high.-dim. U_δ
  - computational effort depends on $\dim(U_\delta)$
- online phase:
  - given $\boldsymbol{\mu} \in \mathbb{P}$, compute $\mathbf{u}_N[\boldsymbol{\mu}]$ as approximation of $\mathbf{u}[\boldsymbol{\mu}]$ in

$$\operatorname{span}\{\mathbf{u}_\delta[\boldsymbol{\mu}^{(i)}] \,:\, i = 1, \ldots, N\}$$

  - Lax–Milgram setting guarantees unique Galerkin approximation!
  - computational effort depends on $N \ll \dim(U_\delta)$

Greedy algorithm

- how to choose $\boldsymbol{\mu}^{(i)}$?
- fix sufficiently large finite training set $\mathbb{P}_{\mathrm{train}} \subset \mathbb{P}$ and tolerance $\epsilon > 0$
- set $N := 0$ and $\mathbf{u}_0[\boldsymbol{\mu}] := 0$
- recall estimator for all $\mathbf{v} \in U$

$$\|\mathbf{u}[\boldsymbol{\mu}] - \mathbf{v}\|_U \eqsim \|G[\boldsymbol{\mu}](\mathbf{u}[\boldsymbol{\mu}] - \mathbf{v})\|_{L^2} = \underbrace{\|(\mathbf{g}[\boldsymbol{\mu}], f[\boldsymbol{\mu}], u_0[\boldsymbol{\mu}]) - G[\boldsymbol{\mu}]\mathbf{v}\|_{L^2}}_{=:\eta[\boldsymbol{\mu}](\mathbf{v})}$$

while $\max_{\boldsymbol{\mu} \in \mathbb{P}_{\mathrm{train}}} \eta[\boldsymbol{\mu}](\mathbf{u}_N[\boldsymbol{\mu}]) > \epsilon$ do:

- compute $\mathbf{u}_N[\boldsymbol{\mu}]$ in $\mathrm{span}\{\mathbf{u}_\delta[\boldsymbol{\mu}^{(i)}] : i = 1, \ldots, N\}$ for all $\boldsymbol{\mu} \in \mathbb{P}_{\mathrm{train}}$
- compute $\eta[\boldsymbol{\mu}](\mathbf{u}_N[\boldsymbol{\mu}])$ for all $\boldsymbol{\mu} \in \mathbb{P}_{\mathrm{train}}$
- determine $\boldsymbol{\mu}^{(N+1)} := \mathrm{argmax}_{\boldsymbol{\mu} \in \mathbb{P}_{\mathrm{train}}} \eta[\boldsymbol{\mu}](\mathbf{u}_N[\boldsymbol{\mu}])$
- add $\mathbf{u}_\delta[\boldsymbol{\mu}^{(N+1)}]$ to reduced basis $\{\mathbf{u}_\delta[\boldsymbol{\mu}^{(i)}] : i = 1, \ldots, N\}$
- update $N \rightsquigarrow N + 1$

Numerical experiment in 1+1D

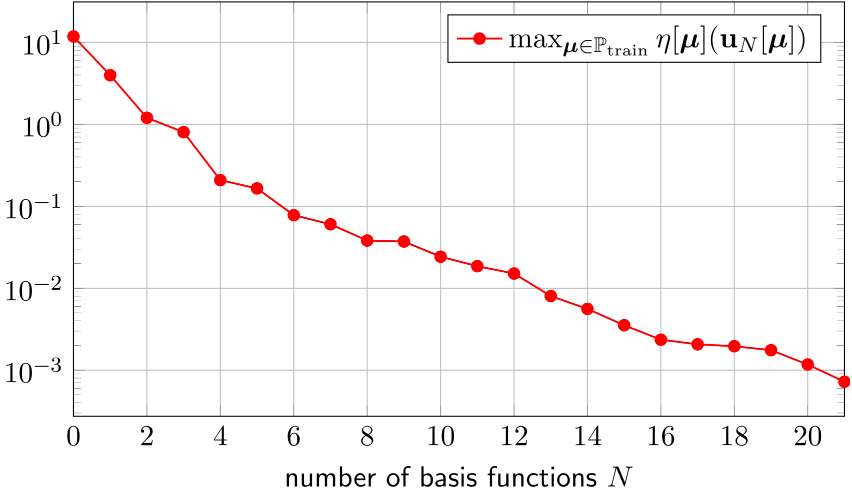
- $\Omega := (0, 1)$ and $T := 0.3$
- $\mathbb{P} := [0.5, 1.5] \times [0, 1] \times [0, 1]$

$$\begin{aligned} \partial_t u - \mu_1 \partial_x^2 u + \mu_2 \partial_x u + \mu_3 u &= f && \text{in } Q \\ u &= 0 && \text{on } \Sigma \\ u(0, \cdot) &= u_0 && \text{in } \Omega \end{aligned}$$

- choose f and u_0 s.t. $u[(1, 0.5, 0.5)] = \sin(2\pi x)\cos(4\pi t)$
- fix U_δ pw. poly. of degree $p = 3$ on tensor-mesh of Q (64 intervals)
- for $\mathbb{P}_{\text{train}}$ replace intervals $[0.5, 1.5]$, $[0, 1]$, $[0, 1]$ by 17 equidist. points
- tolerance $\epsilon = 10^{-3}$

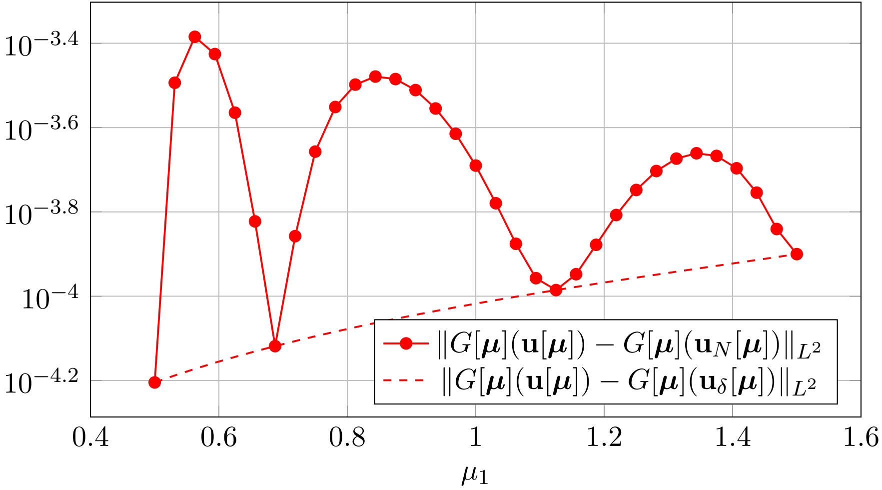
Glas, Mayerhofer, Urban: Model Reduction of Parametrized Systems (2017) inf-sup

Offline phase



- exponential convergence, parameter-dependence is smooth!

Online phase



- $\boldsymbol{\mu} = (\mu_1, 0, 0)$ with $\mu_1 \in [0.5, 1.5]$

Optimal control problems

Minimization problem

$$\begin{aligned} \partial_t u - \mathrm{div}_{\mathbf{x}}(\mathbf{A}\nabla_{\mathbf{x}} u) + \mathbf{b}\cdot\nabla_{\mathbf{x}} u + cu &= f + \mathrm{div}_{\mathbf{x}}\,\mathbf{g} && \text{in } Q \\ u &= 0 && \text{on } \Sigma \\ u(0,\cdot) &= u_0 && \text{in } \Omega \end{aligned}$$

$\Longleftrightarrow$ $\mathbf{u} = (u, \boldsymbol{\sigma}) \in U$ with $G\mathbf{u} = (\mathbf{g}, f, u_0) =: \mathbf{z}$

- control space $Z \hookrightarrow L^2$ and parameter $\varrho > 0$
- W Hilbert space, $w \in W$, $F : U \to W$ linear & bounded
- minimize

$$J(\mathbf{u}, \mathbf{z}) := \frac{1}{2}\|F\mathbf{u} - w\|_W^2 + \frac{\varrho}{2}\|\mathbf{z}\|_Z^2$$

over

$$\{(\mathbf{u}, \mathbf{z}) \in U \times Z \, : \, G\mathbf{u} = \mathbf{z}\}$$

Formulation as saddle-point problem

$\Longleftrightarrow$ saddle-point problem with Lagrange multiplier $\mathbf{p} \in U$

Theorem (Führer, Karkulik '22 + G., Stevenson '22)

- inf-sup stability depending on boundedness & coercivity

- inf-sup stability depending on bd. & coer. for all $U_\delta \times Z_\delta \times U_\delta$

$\Longrightarrow$ ex. unique Galerkin approximation $(\mathbf{u}_\delta, \mathbf{z}_\delta, \mathbf{p}_\delta)$

$\Longrightarrow$ approximation is quasi-optimal:

$$\|\mathbf{u} - \mathbf{u}_\delta\|_U + \|\mathbf{z} - \mathbf{z}_\delta\|_Z + \|\mathbf{p} - \mathbf{p}_\delta\|_U \lesssim \min_{(\widetilde{\mathbf{u}},\widetilde{\mathbf{z}},\widetilde{\mathbf{p}}) \in U_\delta \times Z_\delta \times U_\delta} \|\mathbf{u} - \mathbf{u}_\delta\|_U + \|\mathbf{z} - \mathbf{z}_\delta\|_Z + \|\mathbf{p} - \mathbf{p}_\delta\|_U$$

- a posteriori error estimator (involving solution of adjoint problem)

Führer, Karkulik: arXiv (2022)

Gantner, Stevenson: arXiv (2022)

Negative norms

$$\begin{aligned} \partial_t u - \mathrm{div}_{\mathbf{x}}(\mathbf{A}\nabla_{\mathbf{x}} u) + \mathbf{b}\cdot\nabla_{\mathbf{x}} u + cu &= f + \mathrm{div}_{\mathbf{x}}\,\mathbf{g} && \text{in } Q \\ u &= 0 && \text{on } \Sigma \qquad (*) \\ u(0,\cdot) &= u_0 && \text{in } \Omega \end{aligned}$$

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- control space $Z := L^2(Q)^d \times L^2(Q) \times Z_0 \hookrightarrow L^2$ and parameter $\varrho > 0$
- W Hilbert space, $w \in W$, $F = \widetilde{F} \circ (\mathbf{u} \mapsto u)$ linear & bounded
- minim. $\frac{1}{2}\|F\mathbf{u} - w\|_W^2 + \frac{\varrho}{2}\|\mathbf{z}\|_Z^2$ over $\{(\mathbf{u}, \mathbf{z}) \in U \times Z \,:\, G\mathbf{u} = \mathbf{z}\}$

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$\Longleftrightarrow$ minimize

$$\frac{1}{2}\|\widetilde{F}u - w\|_W^2 + \frac{\varrho}{2}\left(\|z\|^2_{L^2(I;H^{-1}(\Omega))} + \|u_0\|^2_{Z_0}\right)$$

over

$$\left\{(u, z, u_0) \in X \times L^2(I; H^{-1}(\Omega)) \times Z_0 \,:\, (*) \text{ with RHS } z\right\}$$

$\Longrightarrow$ optimal $z = f + \mathrm{div}_{\mathbf{x}}\,\mathbf{g}$, optimal u_0 coincide

$\Longleftarrow$ optimal f is Riesz lift of z: $f - \Delta_{\mathbf{x}} f = z$ and $f|_\Sigma = 0$, $\mathbf{g} = -\nabla_{\mathbf{x}} f$

Conclusion & further results

Conclusion & further results

Conclusion

- convergence of adaptive algorithm
- trial space with better convergence rates
- reduced basis method for parameter-dependent problems
- optimal control problems (including negative Sobolev norm)

Further results

- moving spatial domains possible
- other boundary conditions possible (involve fractional norms on Σ)
- similar least-squares method for instationary Stokes problem

Thank you for your attention!

- Gantner and Stevenson: Further results on a space-time FOSLS formulation of parabolic PDEs, M2AN 55 (2021)
- Gantner and Stevenson: Improved rates for a space-time FOSLS of parabolic PDEs, arXiv:2208.10824 (2022)
- Gantner and Stevenson: Applications of a space-time FOSLS formulation for parabolic PDEs, arXiv:2208.09616 (2022)
- Gantner and Stevenson: A well-posed first order system least squares formulation of the instationary Stokes equations, SINUM 60 (2022)

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