Goal-oriented adaptive space-time FEMs for regularized parabolic p-Laplace problems

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joint work with
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Outline

Outline

Intro: Regularized parabolic p-Laplace equation

We consider the regularized parabolic p-Laplace initial-boundary value problem (IBVP)

$$\partial_t u - \mathrm{div}_x((|\nabla_x u|^2 + \varepsilon^2)^{\frac{p-2}{2}} \nabla_x u) = f \text{ in } Q = \Omega \times (0, T),$$
$$u = u_D := 0 \text{ on } \Sigma = \partial\Omega \times (0, T),$$
$$u = u_0 := 0 \text{ on } \overline{\Sigma}_0 = \overline{\Omega} \times \{0\},$$

with $p \in (1, \infty)$, $\varepsilon > 0$, and $\Omega \subset \mathbb{R}^d$ denotes some bounded spatial domain with Lipschitz boundary $\Gamma = \partial\Omega$, $d = 1, 2, 3$.

Note

Alternatively, $\partial_t u - \mathrm{div}_x((|\nabla_x u| + \varepsilon)^{p-2} \nabla_x u) = f$.

Intro: ST FEM + QoI + DWR + PU + A ST FEM

- STFEM based on fully unstructured simplicial meshes for Q
- $u \longmapsto$ QoI represented by some functional $J(u) \in \mathbb{R}$
- DWR = Dual Weighted Residual technique requires the solution of adjoint linear problems providing the sensitivities for mesh refinement
- PU = Partion of Unity providing localization of the error
- **A**STFEM based on Dörfler's marking using localized errors

Intro: References

The talk is based on our papers

- B. Endtmayer, U. Langer, and A. Schafelner,
  Goal-Oriented Adaptive Space-Time Finite Element Methods for Regularized Parabolic p-Laplace Problems,
  Computers and Mathematics with Applications, 167:286–297, 2024.

- B. Endtmayer, U. Langer, T. Richter, A. Schafelner, and T. Wick,
  A Posteriori Single- and Multi-Goal Error Control and Adaptivity for Partial Differential Equation,
  In F. Chouly, S.P.A. Bordas, R. Becker, and P. Omnes, editors, Error Control, Adaptive Discretizations, and Applications, Part 2, volume 59 of Advances in Applied Mechanics, pages 19–108. Elsevier, 2024.

Outline

STVF: The variational (weak) formulation

Find $u \in U := \{v \in V : \partial_t v \in V^*, v = 0 \text{ on } \Sigma_0\}$ such that

$$\langle \partial_t u, v\rangle + ((|\nabla_x u|^2 + \varepsilon^2)^{\frac{p-2}{2}} \nabla_x u, \nabla_x v) = \langle f, v\rangle \quad \forall\, v \in V,$$

with $V := L_p((0,T); \mathring{W}^1_p(\Omega))$, $V^* := L_q((0,T); W^{-1}_q(\Omega))$,
$q = p/(p-1)$, $\langle \cdot,\cdot\rangle : V^* \times V \to \mathbb{R}$, $(\cdot,\cdot) := (\cdot,\cdot)_{L_2(Q)}$, $f \in V^*$.

Existence, Uniqueness, Regularity, ...

- This VF has a unique solution $u \in U \cap C([0,T]; L_2(\Omega))$.
- **If** $f \in L_2(Q)$ and $u_0 \in \mathring{W}^1_p(\Omega)$, **then** $u \in L_\infty((0,T); \mathring{W}^1_p(\Omega))$, $\partial_t u \in L_2(Q)$ and $|\nabla_x u|^{p-2} \nabla_x u \in L_2((0,T); W^1_2(\Omega))$, **i.e.** the p-Laplace equation holds in the strong sense in $L_2(Q)$.

Ref.: [Lions, 1069], [Zeidler, 1990], [Roubičk, 2013] ...; [CianchiMazya, 2020]

STVF: Reformulation as operator equation in V^*

Find $u \in U$ such that

$$\mathcal{A}(u) := \partial_t u + A(u) - f = 0 \quad \text{in } V^*,$$

where

$$\mathcal{A}(u)(v) = \langle \mathcal{A}(u), v \rangle := \langle \partial_t u, v \rangle + \langle A(u), v \rangle - \langle f, v \rangle \quad \forall\, v \in V,\ \forall\, u \in U,$$

with $\langle A(u), v \rangle := ((|\nabla_x u|^2 + \varepsilon^2)^{\frac{p-2}{2}} \nabla_x u, \nabla_x v)$.

Outline

STFEM: Space-time finite element spaces

- Decompose Q into *shape-regular* elements $\Delta \in \mathcal{T}_h = \{\Delta\}$
- Define conforming finite element spaces

$$U_h = V_h := \{v_h \in S_h^k(\overline{Q}) : v_h = 0 \text{ on } \overline{\Sigma} \cup \overline{\Sigma}_0\} \subset U \subset V$$

of polynomial degree k, with

$$S_h^k(\overline{Q}) := \{v_h \in C(\overline{Q}) : v_h \circ x_\Delta \in \mathbb{P}_k(\widehat{\Delta}), \forall \Delta \in \mathcal{T}_h\},$$

where $x_\Delta : \widehat{\Delta} \to \Delta$ - reference-to-physical element map.

STFEM: Space-time Galerkin finite element scheme

Find $u_h \in U_h$ such that

$$\mathcal{A}(u_h)(v_h) \equiv \langle \partial_t u_h, v_h \rangle + \langle A(u_h), v_h \rangle - \langle f, v_h \rangle = 0.$$

for all $v_h \in V_h = U_h$.

The Existence and Uniqueness is guaranteed by Browder-Minty's theorem and the strict monotonicity of A.

STFEM: The nonlinear system of fe equations

Let $U_h = V_h = \text{span}\{\varphi_j : j = 1, \ldots, N_h\}$. Then the fe solution

$$U_h \ni u_h = \sum_{j=1}^{N_h} u_j \varphi_j \longleftrightarrow \mathbf{u}_h = (u_1, \ldots, u_{N_h})^\top \in \mathbb{R}^{N_h}$$

can be defined by solving the non-linear system of fe equations

$$\mathcal{A}_h(\mathbf{u}_h) = T_h \mathbf{u}_h + \widehat{A}_h(\mathbf{u}_h)\mathbf{u}_h - \mathbf{f}_h = \mathbf{0}_h \quad \text{in } \mathbb{R}^{N_h},$$

where the $N_h \times N_h$ matrices T_h and $\widehat{A}_h(\mathbf{u}_h)$ are defined by

$$(T_h \mathbf{w}_h, \mathbf{v}_h) = \langle \partial_t w_h, v_h \rangle \text{ and } (\widehat{A}_h(\mathbf{u}_h)\mathbf{w}_h, \mathbf{v}_h) = ((|\nabla_x u_h|^2 + \varepsilon^2)^{\frac{p-2}{2}} \nabla_x w_h, \nabla_x v_h)$$

for all $w_h, v_h \leftrightarrow \mathbf{w}_h, \mathbf{v}_h$, respectively, and $\mathbf{f}_h = (\langle f, \varphi_i \rangle)_{i=1}^{N_h} \in \mathbb{R}^{N_h}$.

STFEM: Newton's method

For given initial guess $\mathbf{u}_h^0 \in \mathbb{R}^{N_h}$, find $\mathbf{u}_h^{n+1} = \mathbf{u}_h^n + \mathbf{w}_h^{n+1}$ via the Newton correction $\mathbf{w}_h^{n+1} \in \mathbb{R}^{N_h}$ that is nothing but the unique solution of the linear system

$$\mathcal{A}_h'(\mathbf{u}_h^n)\mathbf{w}_h^{n+1} = -\mathcal{A}_h(\mathbf{u}_h^n),$$

with the Jacobian $\mathcal{A}_h'(\mathbf{u}_h^n) = T_h + \widehat{A}_h(\mathbf{u}_h^n) + \widehat{A}_h'(\mathbf{u}_h^n)$, $n = 0, 1, \ldots$.

Remark

The Jacobian $\mathcal{A}_h'(\mathbf{u}_h^n)$ is positive definite: Indeed, we have

$$(\mathcal{A}_h'(\mathbf{u}_h^n)\mathbf{w}_h, \mathbf{w}_h) \geq c(p,\varepsilon)\, ch^{d+1}(\mathbf{w}_h, \mathbf{w}_h)\ \forall \mathbf{w}_h \in \mathbb{R}^{N_h},$$

with $c(p,\varepsilon) = (p-1)\varepsilon^{p-2}$ for $p \in (1,2)$, and $c(p,\varepsilon) = \varepsilon^{p-2}$ for $p \in [2,\infty)$.

Outline

GO-ASTFEM: Main ideas

- We are not (primarily) interested in the solution u, but in some Quantity of Interest (QoI), which can be represented by some (possibly nonlinear) functional $J(u)$ at u.
  Examples: $J(u) = \int_{Q_I \subset Q} u(x,t)dxdt$, $J(u) = \int_{\Omega} u(x,T)dx$,
  $J(u) = \int_{Q_I \subset Q} |\nabla u(x,t)|^p dxdt$
  $J(u) = u(x_0,t_0)$, $J(u) = (u(x_0,t_0))^3 u(x_1,t_1)$
- Construction of error estimator η_h such that
  $$\eta_h \approx J(u) - J(u_h)$$
- Adaptivity is driven by the QoI J using
  - the Dual Weighted Residual (DWR) technique[1] and
  - the Partion of Unity (PU) localization[2].

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[1] [BeckerRannacher, 1998, 2001], [RannacherVihharev, 2013]
[2] [WickRichter, 2015]

GO-ASTFEM: DWR [BeckerRannacher]

Adjoint problem

Find $z \in V$ such that

$$\mathcal{A}'(u)(v, z) = J'(u)(v) \qquad \forall v \in U,$$

for $u \in U$ solving $\mathcal{A}(u) = 0$.

The Discrete (FE) Adjoint problem

Find $z_h \in V_h$ such that

$$\mathcal{A}'(u_h)(v_h, z_h) = J'(u_h)(v_h) \qquad \forall v_h \in U_h,$$

for $u_h \in U_h$ solving $\mathcal{A}(u_h)(v_h) = 0 \ \forall v_h \in V_h$.

In practice, we can just use the transposed of the Newton Matrix

GO-ASTFEM: Error representation

Theorem ([RannacherVihharev, 2013])

Let $\mathcal{A}, J \in \mathcal{C}^3$, and let $\tilde{u}$ and $\tilde{z}$ arbitrary elements from U and V, respectively. Then the error representation

$$J(u) - J(\tilde{u}) = \frac{1}{2}\left[-\mathcal{A}(\tilde{u})(z-\tilde{z}) + J'(\tilde{u})(u-\tilde{u}) - \mathcal{A}'(\tilde{u})(u-\tilde{u},\tilde{z})\right] + \mathcal{A}(\tilde{u})(\tilde{z}) + \mathcal{R}^{(3)},$$

holds, where $\mathcal{R}^{(3)} = \mathcal{O}(\underline{e}^3)$ with $\underline{e} := \max(\|u-\tilde{u}\|_U, \|z-\tilde{z}\|_V)$.

Note that $\mathcal{A}(u_h)(z_h) = 0$!

GO-ASTFEM: Non-computable errore estimates

For approximations $\tilde{u}_h, \tilde{z}_h$ to u_h, z_h to u, z, we have

$$J(u) - J(\tilde{u}_h) = \underbrace{\frac{1}{2}\left[-\mathcal{A}(\tilde{u}_h)(z - \tilde{z}_h) + J'(\tilde{u}_h)(u - \tilde{u}_h) - \mathcal{A}'(\tilde{u})(u - \tilde{u}_h, \tilde{z}_h)\right]}_{\eta_h}$$

$$+ \underbrace{\mathcal{A}(\tilde{u}_h)(\tilde{z}_h)}_{\eta_{it}} + \underbrace{\mathcal{R}^{(3)}}_{\eta_{\mathcal{R}}}.$$

- η_h: **discretization** error $\left|J(u) - J(u_h)\right|$
- η_{it}: **iteration** error $\left|J(u_h) - J(\tilde{u}_h)\right|$
- $\eta_{\mathcal{R}}$: **higher order**
- stopping rule for Newton's iteration: $|\eta_{it}| \leq \gamma|\eta_h|$, $\gamma \in (0, 1]$

Unfortunately, η_h is not computable because u and z are unknown !

GO-ASTFEM: Hierachical approach to computability

Let $U_h \subset U_h^{(2)} \subset U$ and $V_h \subset V_h^{(2)} \subset V$ enriched fe spaces.

The enriched discrete primal (non-linear) problem

Find $J(u_h^{(2)}) \in \mathbb{R}$ such that $u_h^{(2)} \in U_h^{(2)}$ solves

$$\mathcal{A}(u_h^{(2)})(v_h^{(2)}) = 0 \qquad \forall v_h^{(2)} \in V_h^{(2)}.$$

The enriched discrete adjoint (linear)problem

Find $z_h^{(2)} \in V_h^{(2)}$ such that

$$\mathcal{A}'(u_h^{(2)})(v_h^{(2)}, z_h^{(2)}) = J'(u_h^{(2)})(v_h^{(2)}) \qquad \forall v_h^{(2)} \in U_h^{(2)},$$

for $u_h^{(2)} \in U_h^{(2)}$ solving $\mathcal{A}(u_h^{(2)})(v_h^{(2)}) = 0 \quad \forall v_h^{(2)} \in V_h^{(2)}$.

GO-ASTFEM: Non-computable error representation

For approximations $\tilde{u}_h, \tilde{z}_h$ to u_h, z_h to u, z, we have

$$J(u) - J(\tilde{u}_h) = \underbrace{\frac{1}{2}\left[-\mathcal{A}(\tilde{u}_h)(z - \tilde{z}_h) + J'(\tilde{u}_h)(u - \tilde{u}_h) - \mathcal{A}'(\tilde{u})(u - \tilde{u}_h, \tilde{z}_h)\right]}_{\eta_h}$$

$$+ \underbrace{\mathcal{A}(\tilde{u}_h)(\tilde{z}_h)}_{\eta_{it}} + \underbrace{\mathcal{R}^{(3)}}_{\eta_{\mathcal{R}}}.$$

GO-ASTFEM: Computable error representation

For approximations $\tilde{u}_h, \tilde{z}_h$ to u_h, z_h to u, z, we have

$$J(u) - J(\tilde{u}_h) \approx \underbrace{\frac{1}{2}\left[\overbrace{-\mathcal{A}(\tilde{u}_h)(z_h^{(2)} - \tilde{z}_h)}^{\eta_{h,p}^{(2)}} + \overbrace{J'(\tilde{u}_h)(u_h^{(2)} - \tilde{u}_h) - \mathcal{A}'(\tilde{u})(u_h^{(2)} - \tilde{u}_h, \tilde{z}_h)}^{\eta_{h,a}^{(2)}}\right]}_{\eta_h^{(2)}}$$

$$+ \underbrace{\mathcal{A}(\tilde{u}_h)(\tilde{z}_h)}_{\eta_{it}} + \underbrace{\mathcal{R}^{(3)(2)}}_{\eta_{\mathcal{R}}^{(2)}}.$$

GO-ASTFEM: Saturation assumption

Saturation assumption for the goal functional

Let $u_h^{(2)}$ be the solution on an enriched discrete space, and $\tilde{u}_h$ be some approximation.
We now assume that the inequality

$$|J(u) - J(u_h^{(2)})| < b_h |J(u) - J(\tilde{u}_h)|$$

holds for some $b_h < b_0$ with some fixed $b_0 \in (0, 1)$.

GO-ASTFEM: Efficency and reliability

Theorem ([EndmayerLangerWick, 2020])

If the saturation assumption is fulfilled, then the full error indicator

$$\eta^{(2)} := \eta_h^{(2)} + \eta_{it} + \eta_{\mathcal{R}}^{(2)}$$

satisfies the efficiency and reliability estimates

$$\underline{c}|\eta^{(2)}| \leq |J(u) - J(\tilde{u}_h)| \leq \overline{c}|\eta^{(2)}|,$$

with the positive constants $\underline{c} := 1/(1 + b_0)$, *and* $\overline{c} := 1/(1 - b_0)$.

GO-ASTFEM: Strenghtened saturation assumption

Strengthened saturation assumption for the goal functional

Let $u_h^{(2)}$ be the solution on an enriched discrete space, and $\tilde{u}_h$ be some approximation.
We now assume that the inequality

$$|J(u) - J(u_h^{(2)})| + |\mathcal{R}^{(3)} - \mathcal{R}^{(3)(2)}| + |\mathcal{R}^{(3)}| + |\eta_{it}| < b_{h,st}|J(u) - J(\tilde{u}_h)|$$

holds for some $b_{h,st} < b_{0,st}$ with some fixed $b_{0,st} \in (0,1)$.

- higher order terms
- controlled by the nonlinear solver

GO-ASTFEM: Efficency and reliability

Theorem ([EndmayerLangerWick, 2020])

If the strengthened saturation assumption is fulfilled, then the discretization part $\eta_h^{(2)}$ *of the full error indicator*

$$\eta^{(2)} := \eta_h^{(2)} + \eta_{it} + \eta_{\mathcal{R}}^{(2)}$$

satisfies the efficiency and reliability estimates

$$\underline{c}_{st}|\eta_h^{(2)}| \le |J(u) - J(\tilde{u}_h)| \le \overline{c}_{st}|\eta_h^{(2)}|,$$

with positive constants $\underline{c}_{st} := 1/(1 + b_{0,st})$, $\overline{c}_{st} := 1/(1 - b_{0,st})$.

Remark: We get similar results for **interpolations** to enriched spaces instead of **solution** on enriched spaces [EndmayerLangerWick2021CMAM].

GO-ASTFEM: Relaxed differentiability of $\mathcal{A}$

$\mathcal{A}_h \in \mathcal{C}^3$, but not $\mathcal{A}$ as for the p-Laplace !

We get the same results for **efficiency and reliability** with different higher order terms provided that

- $\mathcal{A}$ and J are **smooth** on the **discrete** spaces only.

GO-ASTFEM: PU localization [RichterWick, 2015]

Global discretization error estimator

$$\eta_h^{(2)} = \frac{1}{2}\left(\eta_{h,p}^{(2)} + \eta_{h,a}^{(2)}\right)$$

can be localized via the PU technique:

Let $\{\psi_i\}_{i=1}^{N_{PU}}$ be a localizing PU system of basis function such that $\sum_{i=1}^{N_{PU}} \psi_i \equiv 1$, e.g., Courant's basis functions from $S_h^1(\overline{Q})$. Then

$$\eta_\Delta = \sum_{j \in V(\Delta)} \frac{\eta_j^{PU}}{|\mathcal{N}_j|}, \quad \Delta \in \mathcal{T}_h,$$

where

$\eta_j^{PU} = -\frac{1}{2}\mathcal{A}(\tilde{u}_h)((z_h^{(2)} - \tilde{z}_h)\psi_j) + \frac{1}{2}[J'(\tilde{u}_h)((u_h^{(2)} - \tilde{u}_h)\psi_i) - \mathcal{A}'(\tilde{u}_h)((u_h^{(2)} - \tilde{u}_h)\psi_j, \tilde{z}_h)]$,

$V(\Delta)$ denotes all vertices of the fe $\Delta \in \mathcal{T}_h$, and $\mathcal{N}_j = \{\Delta \in \mathcal{T}_h; v_j \in \overline{\Delta}\}$.

Note: $\sum_{\Delta \in \mathcal{T}_h} \eta_\Delta = \sum_{j=1}^{N_{PU}} \eta_j^{PU} = \eta_h^{(2)}$.

GO-ASTFEM: Adaptive space-time algorithm

Algorithm

1: **repeat**
2: solve the primal problem by Newton's method
3: solve the adjoint problem
4: solve the enriched primal problem using Newton's method
5: solve the enriched adjoint problem
6: compute the elementwise contributions by PU technique
7: select a set $\mathcal{M}_\ell$ of marked elements using Dörfler marking
8: $\mathcal{T}_{\ell+1} \leftarrow \texttt{REFINE}(\mathcal{T}_\ell, \mathcal{M}_\ell)$
9: $\ell \leftarrow \ell + 1$
10: **until** some stopping criterion is fulfilled.

Complexity in terms of DOFs: $\widetilde{N}_{\ell+1} = 2^{d+1} N_\ell = 2^{d+1} q_\ell N_{\ell-1} = q_\ell 2^{d+1} N_{\ell-1} = q_\ell \widetilde{N}_\ell$

$\widetilde{N}_{\ell+1} = q_\ell \widetilde{N}_\ell = q_\ell q_{\ell-1} \ldots q_1 \widetilde{N}_0 = q^{10} \widetilde{N}_0 = 2.59 \widetilde{N}_0$ for $\ell = 10$, $q_j = q = 1.1$ forall $j = 1, 2, \ldots, \ell$

Outline

NumExp: Implementation details

- implemented with MFEM[3]
- linear solvers by *hypre*[4] / PETSC[5]
- parallel computers:
  - `Quartz` (LLNL)
  - `Radon1` (RICAM)
  - `MUSICA` (JKU)
- Linear solvers
  - GMRES preconditioned by (1,1) V-cycle AMG precoditioner (relative tolerance 10^{-8})
  - sparse direct solver MUMPS

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[3] https://mfem.org, Thanks to LLNL for hosting Andreas Schafelner
[4] https://www.llnl.gov/casc/hypre/
[5] https://petsc.org

NumExp: Solver details

AMG parameters (experimental / “best practice”)

- Falgout coarsening
- ℓ_1-hybrid SGS / ℓ_1-Jacobi relaxation
- multipass/classical interpolation
- strong threshold 0.75

Nested Newton’s method

- ℓ_2-residual based stopping criterion
  - coarsest level: absolute, i.e. stop when error is below 10^{-8}
  - otherwise: relative reduction by 10^{-2}
- initial guess
  - coarsest level: (scaled) random vector
  - otherwise: prolongated solution from the previous level
- ℓ_2-residual based damping

NumExp: Efficiency Indices (EIs)

Total EI:

$$\mathrm{I}_{\mathrm{eff},h} := \frac{\eta_h}{J(u) - J(u_h)}.$$

Primal and adjoint EIs:

$$\mathrm{I}_{\mathrm{eff},p} := \frac{\eta_{h,p}}{J(u) - J(u_h)}, \quad \text{and} \quad \mathrm{I}_{\mathrm{eff},a} := \frac{\eta_{h,a}}{J(u) - J(u_h)}.$$

NumExp1 = Example 1: Smooth solution

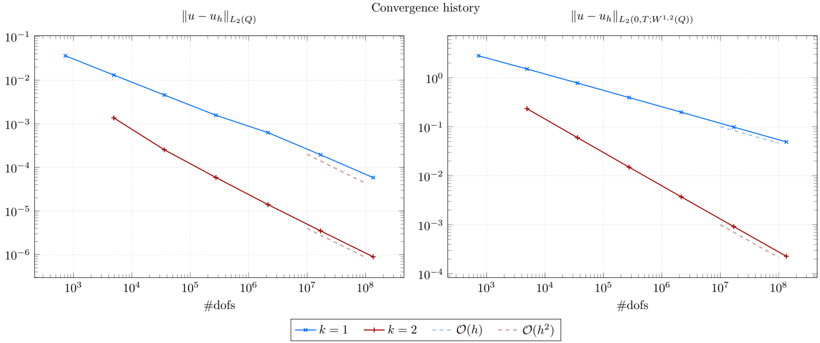
Consider ε-reg. parabolic p-Laplace in $Q = (0,1)^{d+1}$, $d = 2, 3$, with $p = 4$ and $\varepsilon \in \{1, 10^{-5}, 10^{-10}\}$, and the

manufactured solution

$$u(x,t) = t^2\, e^t \prod_{i=1}^{d} \sin(x_i\, \pi)$$

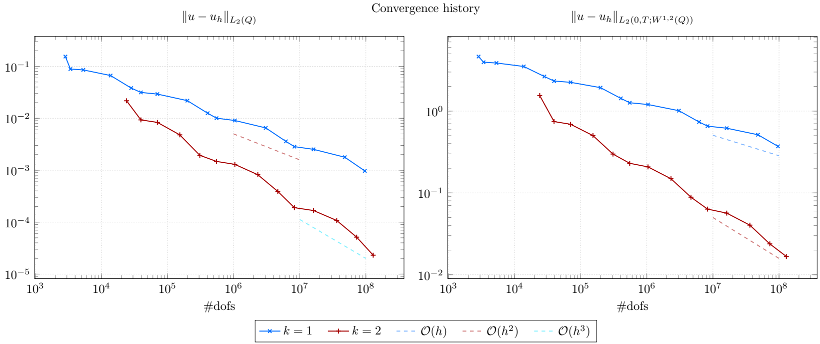
RHS computed accordingly (i.e. $f = f_{p,\varepsilon}$)

NumExp1: Convergence studies for $d = 2$



Convergence history of the discretization errors in different norms for linear ($k = 1$) and quadratic ($k = 2$) shape functions, using uniform tetrahedral refinement via octasection (MFEM).

NumExp1: Convergence studies for $d = 3$



Convergence history of the discretization errors in different norms for linear $(k = 1)$ and quadratic $(k = 2)$ shape functions, using uniform pentatopial refinement via Stevenson's bisection.

NumExp1: Solver performance for $d = 2$

		$\varepsilon = 1$		$\varepsilon = 10^{-5}$		$\varepsilon = 10^{-10}$	
ℓ	#dofs	GMRES	MUMPS	GMRES	MUMPS	GMRES	MUMPs
0	4 913	16 (46)	13	22 (127)	20	22 (127)	20
1	35 937	4 (11)	3	3 (22)	3	3 (22)	3
2	274 625	4 (11)	2	3 (37)	2	3 (37)	2
3	2 146 689	3 (12)	–	3 (60)	–	3 (60)	–
4	16 974 593	3 (16)	–	3 (98)	–	3 (111)	–
5	135 005 697	2 (12)	–	3 (199)	–	3 (216)	–

Scaling of the (damped) Newton solver with total number of inner solves in $(\cdot)$, for $d + 1 = 3$ and $k = 1$; using 288 cores of quartz.

NumExp1: GO-AFEM driven by a linear functional

Consider parameters from before and the linear goal functional

$$J_{linear}(u) = \int_\Omega u(\,.\,, T)\,\mathrm{d}\Omega = \frac{4\,e}{\pi^2} \approx 1.10167812933171,$$

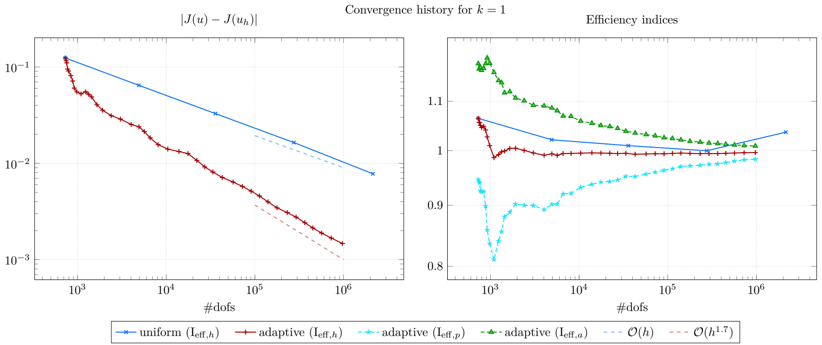
with $\Omega = (0,1)^d$.

Here and in the following examples, we use

- $U_h = V_h := \{v_h \in S_h^{k=1}(\overline{Q}) : v_h = 0 \text{ on } \overline{\Sigma} \cup \overline{\Sigma}_0\}$and
- $U_h^{(2)} = V_h^{(2)} := \{v_h \in S_h^{k=2}(\overline{Q}) : v_h = 0 \text{ on } \overline{\Sigma} \cup \overline{\Sigma}_0\}$

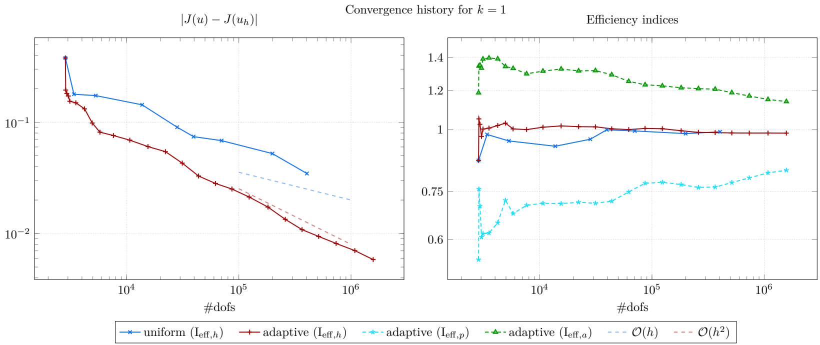
for the original and enriched FE spaces, respectively.

NumExp1: Convergence studies for $d = 2$



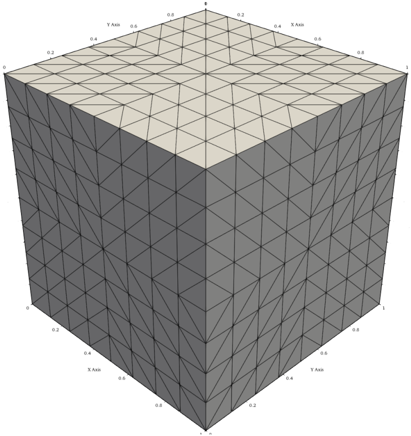
Convergence history of the error in the functional as well as efficiency plots, with the efficiency of the primal and adjoint parts.

NumExp1: Convergence studies for $d = 3$

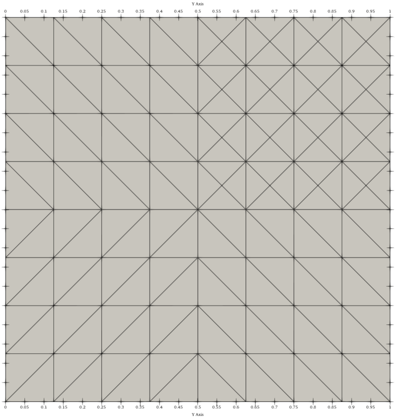


Convergence history of the error in the functional as well as efficiency plots, with the efficiency of the primal and adjoint parts.

NumExp1: $d = 2$: Initial mesh

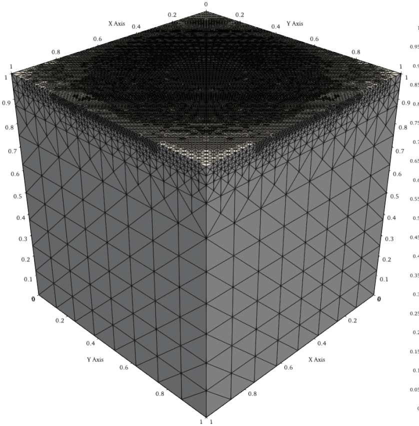


Initial space-time mesh

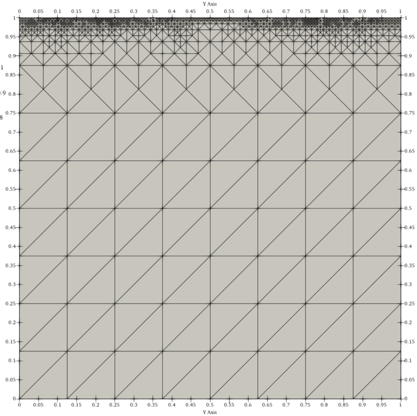


(x_2, t)-plane at $x_1 = 0.5$

NumExp1: $d = 2$: Mesh after 9 adaptive refs



Initial space-time mesh



(x_2, t)-plane at $x_1 = 0.5$

NumExp1: Solver performance

ℓ	#dofs	$\varepsilon = 1$ GMRES	MUMPS	$\varepsilon = 10^{-5}$ GMRES	MUMPS	$\varepsilon = 10^{-10}$ GMRES	MUMPs
0	729	11 (178)	11	17 (374)	17	17 (127)	17
4	$\sim$ 4 860	3 (96)	3	3 (141)	3	3 (141)	3
7	$\sim$ 52 000	2 (130)	2	2 (168)	2	2 (168)	2
9	$\sim$ 270 000	2 (200)	2	2 (200)	2	2 (200)	2
11	$\sim$ 1 300 000	2 (200)	2	3 (200)	3	3 (200)	3

GO-ASTFEM for linear functional J_{linear}: Scaling of the (damped) Newton solver with total number of inner GMRES solves in parentheses $(\,\cdot\,)$, for $d+1=3$ and $k=1$.

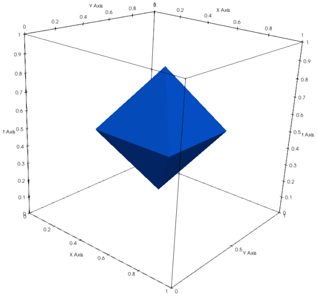
E.g., $\sim$ 1 300 000: 1 304 463 1 312 007 1 312 007

NumExp1: GO-AFEM with non-linear functional

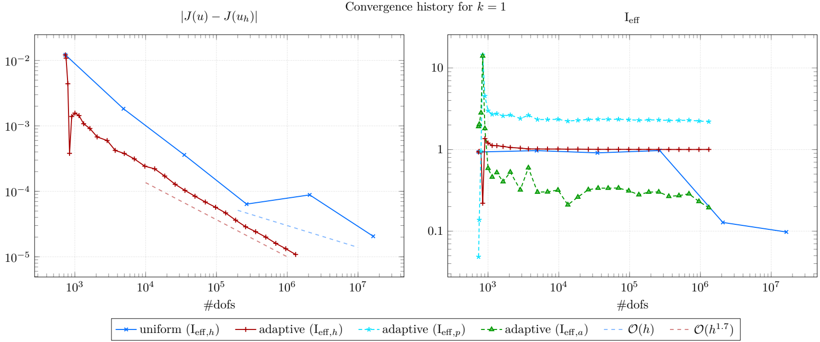
Consider parameters from before and the non-linear goal functional

$$J_{nonlinear}(u) = \int_{Q_I} |\nabla_x u|^{p=4} \, dQ \approx 0.0193712506056641 9,$$

where Q_I is the blue octahedron:

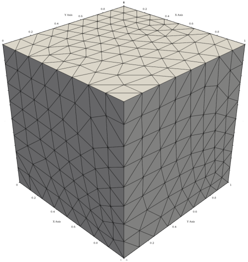


NumExp1: Convergence studies

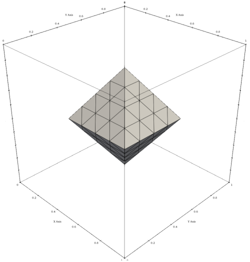


Convergence history of the error in the functional as well as efficiency plots, with the efficiency of the primal and adjoint parts for $d + 1 = 3$.

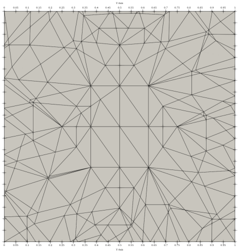
NumExp1: $d = 2$: Initial mesh



on ∂Q

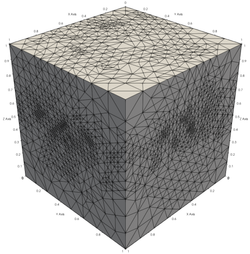


on ∂Q_I

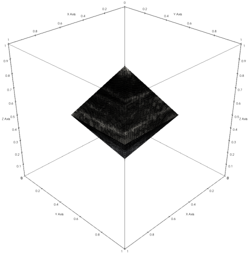


in the (x_2, t)-plane at $x_1 = 0.5$

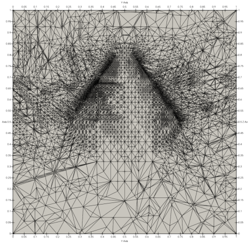
NumExp1: $d = 2$: Mesh after 8 adaptive refs



on ∂Q



on ∂Q_I



in the (x_2, t)-plane at $x_1 = 0.5$

NumExp1: Solver performance

		$\varepsilon = 1$		$\varepsilon = 10^{-5}$		$\varepsilon = 10^{-10}$	
ℓ	#dofs	GMRES	MUMPS	GMRES	MUMPS	GMRES	MUMPs
0	735	11 (213)	11	17 (355)	17	17 (355)	17
3	∼ 5 675	3 (79)	3	3 (107)	3	3 (107)	3
5	∼ 35 000	3 (107)	3	3 (142)	3	3 (142)	3
7	∼ 200 000	2 (114)	2	2 (170)	2	2 (170)	2
9	∼1 000 000	2 (173)	2	3 (300)	3	3 (300)	3

GO-ASTFEM for the non-linear functional $J_{nonlinear}$: Scaling of the (damped) Newton solver with total number of inner GMRES solves $(\,\cdot\,)$, for $d+1=3$ and $k=1$.

NumExp2 = Example 2 (L-shaped): Singular solution

Consider the ε-regularized parabolic p-Laplace in $Q = \Omega \times (0,1)$, with the L-shaped spatial domain $\Omega = (-1,1)^2 \setminus \{[0,1) \times (-1,0]\}$, $p = 4$, $\varepsilon = 10^{-2}$, and the

manufactured solution

$$u(x_1, x_2, t) = \frac{3}{2}(1 - x_1)^2(1 - x_2)^2 r^{2/3} \sin(\frac{2}{3}\theta) \sin(t),$$

where (r, θ) denote the polar representation of the spatial coordinates (x_1, x_2). The right-hand side is computed accordingly.

NumExp2: Goal functionals

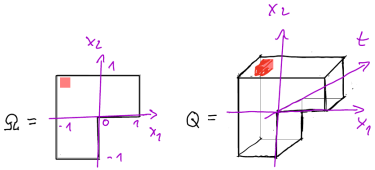
We consider the following two goal functionals

$$J_1(u) := \int_{0.5}^{0.75} \int_{\Omega_I} |\nabla u(x,t)|^4 \,\mathrm{d}x\mathrm{d}t \quad \text{and} \quad J_2(u) = \int_{\Omega} u(x,T)\,\mathrm{d}x,$$

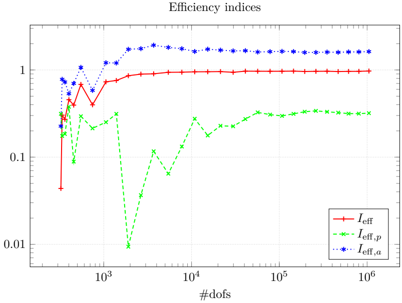
and the combined goal functional

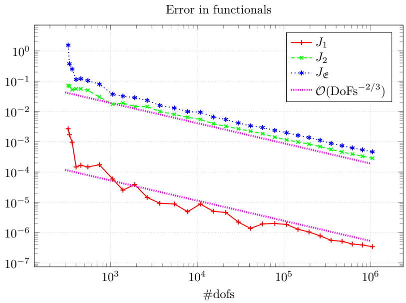
$$J_{12}(v) = \frac{|J_1(u_h^{(2)}) - J_1(v)|}{J_1(u_h)} + \frac{|J_2(u_h^{(2)}) - J_2(v)|}{J_2(u_h)},$$

where $\Omega_I := (-15/16, -11/16) \times (11/16, 15/16) \subset \Omega \subset \mathbb{R}^{d=2}$



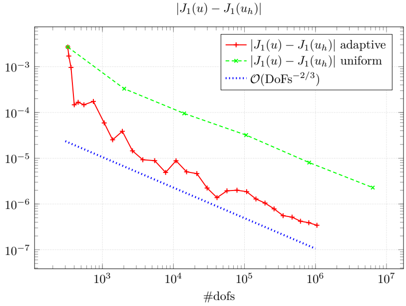
NumExp2: Convergence studies for L-shaped domain

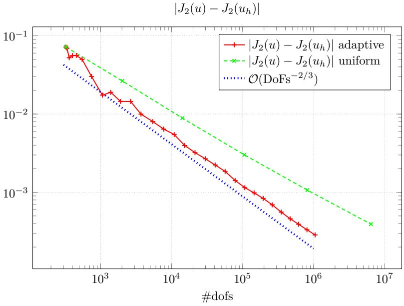




Efficiency indices and convergence of the functionals for $k = 1$.

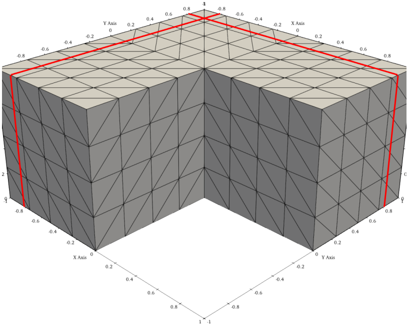
NumExp2: Convergence studies for L-shaped domain

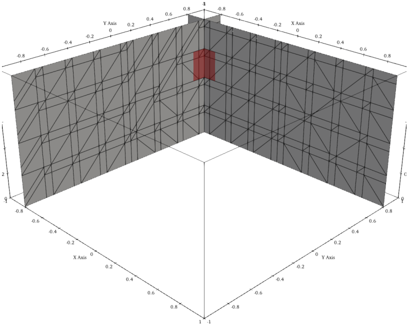




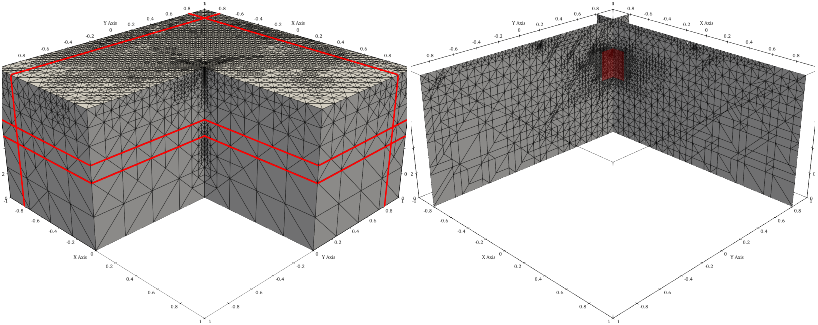
Comparison of adaptive and uniform refinements for $k = 1$.

NumExp2: Initial mesh

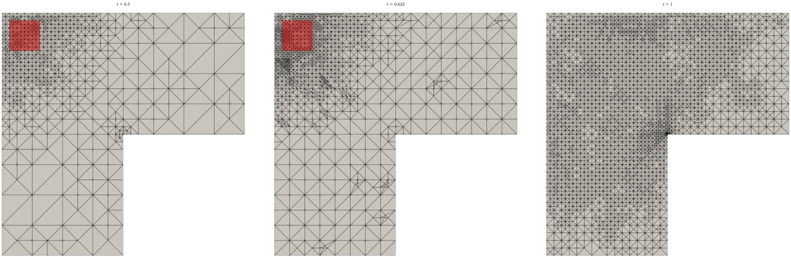




NumExp2: Mesh after 18 adaptive refinements



NumExp2: Mesh cuts at $t = 0.5$, $t = 0.625$, $t = 1$



NumExp3 = Example 3 (Fichera): Singular solution

Consider the ε-regularized parabolic p-Laplace in $Q = \Omega \times (0,1)$, with the Fichera corner $\Omega = (-1,1)^3 \setminus (-1,0]^3$ as spatial domain, $p = 4$, $\varepsilon = 10^{-2}$, and the

the right-hand side [6]

$$f(x,t) = \frac{\sin(t)}{\sqrt{x_1^2 + x_2^2 + x_3^3}}.$$

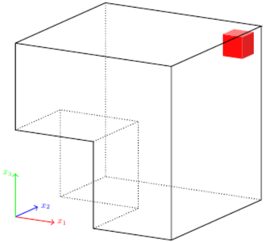
[6] see https://math.nist.gov/amr-benchmark/index.html

NumExp3: Goal functionals

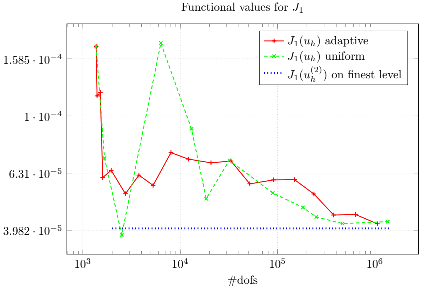
We consider the following two goal functionals

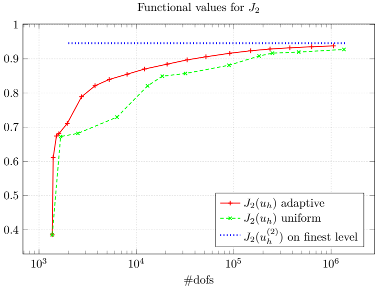
$$J_1(u) := \int_{0.5}^{0.75} \int_{\Omega_I} |\nabla u(x,t)|^4 \, \mathrm{d}x\mathrm{d}t \text{ and } J_2(u) = \int_{\Omega} u(x,T) \, \mathrm{d}x,$$

where $\Omega_I := (11/16, 15/16)^3 \subset \Omega \subset \mathbb{R}^{d=3}$



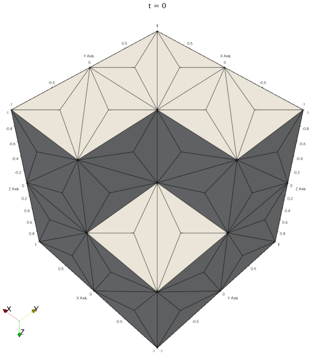
NumExp3: Convergence history of functional values



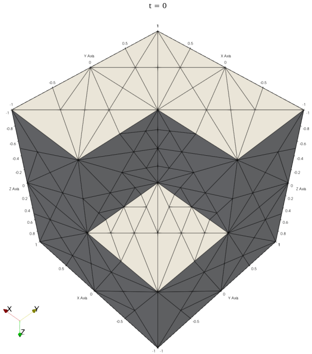


NumExp3: Meshes at cut $t = 0$

Initial mesh

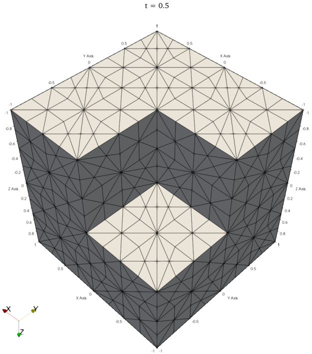


Mesh after 18 adaptive refinements

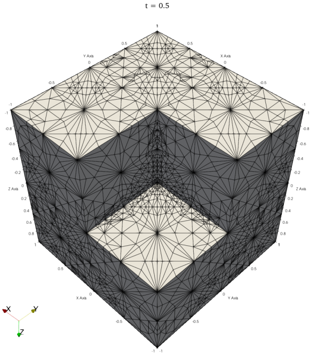


NumExp3: Meshes at cut $t = 0.5$

Initial mesh

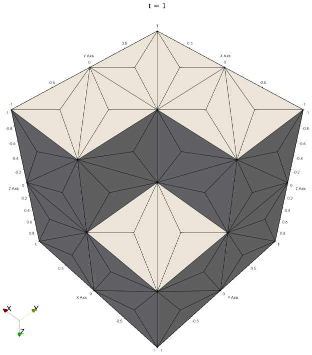


Mesh after 18 adaptive refinements

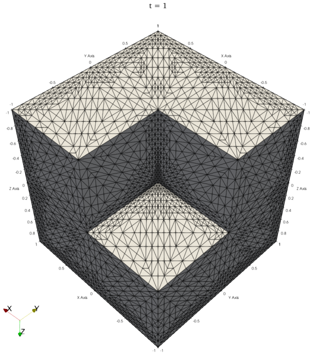


NumExp3: Meshes at cut $t = 1$

Initial mesh



Mesh after 18 adaptive refinements



Outline

ConOut: **Conclusions** & Outlook

- New GO ASTFEM 4 regularized parabolic p-Laplace IBVPs
- Adaptivity is based on DWR technique and PU localization
- Efficiency indices are close to 1 in our numerical examples
- From single-goal to multi-goal[7]

[7] [LangerEndtmayerWick, 2019], [Endtmayer, 2021, PhD], ...

ConOut: Conclusions & **Outlook**

- A priori discretization error estimates[8]
- Convergence analysis of the adaptive process[9]
- Convergence of the Newton solver
- Improvement of the linear solver
- Adaption of the inner its to the convergence of Newton
- Simultaneous parallelization in space and time
- More complex practical applications like non-Newtonian flow[10]
- Optimal Control Problems (OCPs) [11]

8 [Toulopoulos, 2022]

9 [BeckerInnerbergerPraetorius, 2021, CMAM]

10 [Toulopoulos, 2023]

11 [BeuchlerEndtmayerLangerSchafelnerWick, 2025, work in progress]

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ConOut: Optimal Control of Carreau Flow

Let us consider the parabolic p–Laplace–like OCP: Find the state $y_\varrho \in Y$ and the control $u_\varrho \in U$ minimizing the cost functional

$$J_\varrho(y,u) := \frac{1}{2}\|y_d - y\|^2_{L_2(Q)} + \frac{\varrho}{2}\|u\|^2_{U:=L_2(Q)}$$

subject to a simplified Carreau flow model[12]

$$\partial_t y - \mathrm{div}_x\big(\big(1 + c|\nabla_x y|^2\big)^{\frac{n-1}{2}}\nabla_x y\big) = u \;\text{ in } Q = \Omega \times (0,T) \subset \mathbb{R}^4,$$
$$y = 0 \;\text{ on } \Sigma := \Omega \times (0,T),\; y = 0 \;\text{ on } \overline{\Sigma}_0 := \overline{\Omega} \times \{0\},$$

where $n = p - 1 > 0$ ($n \leq 1$ - dilatant, $n > 1$ - pseudoplastic fluids), $c > 0$, $\varrho > 0$ - regularization resp. cost parameter, $y_d \in L_2(Q)$ - target.

[12] [Kennedy, 2005], [AliHouFengZahidRanaSouayeh, 2023]

ConOut: OC of Carreau Flow: KKT

The first-order optimality (Karush-Kuhn-Tucker = KKT) system of the OCP reads as follows: Find the state $y_\varrho \in Y$, the control $u_\varrho \in U$, and the adjoint $p_\varrho \in P$ such that

$$L'(y_\varrho, u_\varrho, p_\varrho)(y, u, p) = 0 \quad \forall (y, u, p) \in Y \times U \times P$$

with the Lagrangian $L(y, u, p) := J_\varrho(y, u) - A(y, u)(p)$, where

$$A(y, u)(p) := B(y)(p) - (u, p)_{L_2(Q)}, \text{ with}$$

$$B(y)(p) := (\partial_t y, p)_{L_2(Q)} + \left(\left(1 + c|\nabla_x y|^2\right)^{\frac{n-1}{2}} \nabla_x y, \nabla_x p\right)_{L_2(Q)}$$

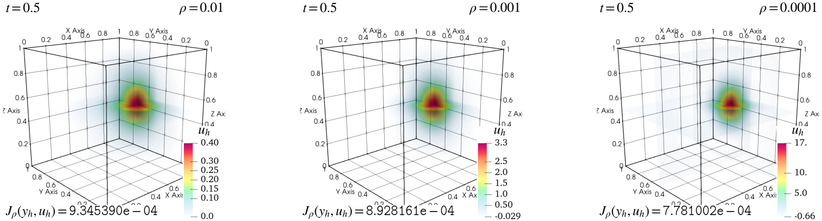
After the Space-Time contP_1 FE discretisation, and after the elimination of the control $\mathbf{u}_h$ via gradient equation $(\varrho u + p = 0)$, we have to solve the reduced nonlinear FE OS

$$\begin{bmatrix} \frac{1}{\varrho}\mathbf{M}_h & \mathbf{B}_h(\mathbf{y}_h) \\ \mathbf{B}^*_{y,h}(\mathbf{y}_h) & -\mathbf{I}_h \end{bmatrix} \begin{bmatrix} \mathbf{p}_h \\ \mathbf{y}_h \end{bmatrix} = \begin{bmatrix} \mathbf{0}_h \\ -\mathbf{y}_{dh} \end{bmatrix},$$

e.g., by Newton + AMG Block-Diagonal-Preconditioned GMRES.

ConOut: OC of Carreau Flow: NumExperiments

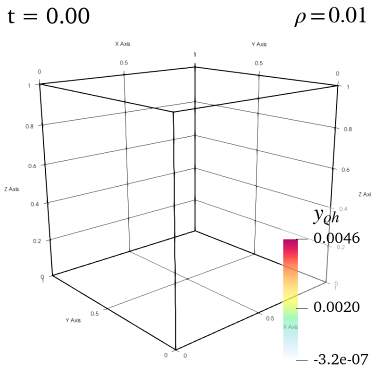
- Target: $y_d(x,t) := \exp(-100\,\|x - (\frac{1}{2} + \frac{1}{4}\sin(\pi t), \frac{1}{2} + \frac{1}{4}\cos(\pi t), t)\|_2^2)$
- Data: $Q = \Omega x(0,T) = (0,1)^4 \subset \mathbb{R}^4$, $\Omega = (0,1)^3$, $T = 1$, $c = 1$, $n = 6$
- Regular Space-Time Mesh: $\approx 480x10^6$ pentatopal elements ($h = 1/24$)
- Space-Time contP_1 FEM: $2x31x10^6$ state and co-state (adjoint) DoFs
- Solver for reduced OS: Newton (10^{-6}) + AMG-BDPGMRES (10^{-2}) [13]

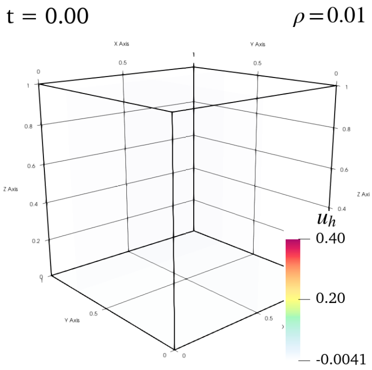


[13] 5 Newtonian its, 52 inner its in total, 380 s on MUSICA with 190 cores

ConOut: OC of Carreau Flow: Animation

state $y_{\varrho h}(x, t_j)$ control $u_{\varrho h}(x, t_j)$





ConOut: OC of Carreau Flow: Discussion

1. We refer to [1] for more details.
2. GO ASTFEM; see [2] for the elliptic case.
3. Parallel Smart Nested Solver:
   For $n = 1$, i.e. $p = 2$ (linear parabolic IBVP), we refer to [3].
4. References:

[1] S. Beuchler, B. Endtmayer, U. Langer, A. Schafelner, and T. Wick: 5d concept for space-time optimal control problems with application to simplified Carreau flow. *arXiv:2511.09086*, 2025.

[2] B. Endtmayer, U. Langer, I. Neitzel, W. Wollner, and T. Wick: Multigoal-oriented optimal control problems with nonlinear PDE constraints. *Comput. Math. Appl.*, 79(10): 3001–3026, 2020.

[3] U. Langer, O. Steinbach, and H. Yang: Robust space-time finite element error estimates for parabolic distributed optimal control problems with energy regularization. *Adv. Comput. Math.*, 50:24, 2024.

PinT 2026

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