On the Dual Weighted Residual Method for Multiple Goal Functionals Applied to Nonlinear Problems

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What is the goal ?

- U, V Banach spaces (normed, complete)
- $J : U \mapsto \mathbb{R}$ and $J \in C^3(U, \mathbb{R})$
- $A : U \mapsto V^*$ and $A \in C^3(U, V^*)$

The Goal

Find $J(u) \in \mathbb{R}$ such that $u \in U$ solves

$$A(u)(v) = 0 \qquad \forall v \in V.$$

Typical example for A: p-Laplace

- The PDE (in strong form)

$$\begin{aligned} -\operatorname{div}\left(\left(\varepsilon^2 + |\nabla u(x)|^2\right)^{\frac{p-2}{2}} \nabla u(x)\right) &= f(x) \qquad && \forall x \in \Omega, \\ u(x) &= 0 && \forall x \in \partial\Omega. \end{aligned}$$

- The corresponding operator A is given by the identity

$$A(u)(v) := \int_\Omega \left[fv - \left(\varepsilon^2 + |\nabla u|^2\right)^{\frac{p-2}{2}} \nabla u \cdot \nabla v \right] dx,$$

for all $u \in U$ and $v \in V$.

Examples for J

- $J(u) = \int_{\Omega_1 \subset \Omega} u(x)\, dx$
- $J(u) = u(x_0)$ for some $x_0 \in \Omega$
- $J(u) = u(x_0)^3 u(x_1)$ for some $x_0, x_1 \in \Omega$
- $J(u) = \left(\int_{\Omega_1 \subset \Omega} (u(x) - u(x_0))\, dx \right)^2$ for some $x_0 \in \Omega$

Conforming discretization

- $U_h \subset U, V_h \subset V$ finite dimensional subspaces

The finite dimensional problem

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

$$A(u_h)(v_h) = 0 \qquad \forall v_h \in V_h.$$

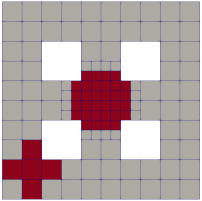
This leads to a system of nonlinear equations.
Here the exact solution of this system is approximated by $\tilde{u}_h$.
But $J(u) - J(\tilde{u}_h) =$?????.

We wish that

- the error $J(u) - J(\tilde{u}_h)$ is small,
- low computational cost.

Our Solution:

- adaptive refinement for our goal functional J.
  This means
  solve $\rightarrow$ *estimate* $\rightarrow$ *mark* $\rightarrow$ *refine.*



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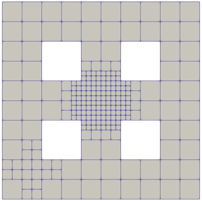

We employ the dual weigthed residual method [Becker & Rannacher (2001)]:

Adjoint problem

Find $z \in V$ such that

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

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

Error representation

- split in discretization and linearization error

Theorem (error representation); see [Rannacher & Vihharev 2013]

Let $\tilde{u} \in U, \tilde{z} \in V$. Then it holds:

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

where

$$\underline{e} := \max(\|u - \tilde{u}\|_U, \|z - \tilde{z}\|_V).$$

Error estimates

For approximations $\tilde{u}_h, \tilde{z}_h$ of u, z, it holds:

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

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

It turns out that

- η_h is related to the discretization error $|J(u) - J(u_h)|$.
- η_k is related to the linearization error $|J(u_h) - J(\tilde{u}_h)|$.
- $|\eta_k| \leq \gamma |\eta_h|$ with $\gamma \in (0, 1]$ can be used as stopping rule for the nonlinear solver.

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For approximations $\tilde{u}_h, \tilde{z}_h$ of u, z, it holds:

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

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

It turns out that

- $\eta_h^{(2)}$ is related to the discretization error $|J(u) - J(u_h)|$.
- η_k is related to the linearization error$|J(u_h) - J(\tilde{u}_h)|$.
- $|\eta_k| \leq \gamma|\eta_h^{(2)}|$ with $\gamma \in (0, 1]$ can be used as stopping rule for the nonlinear solver.

Localization

One localization approach is Partition of Unity (PU), which is presented in [T. Richter & T. Wick (2015)]. Let ψ_i be such that

$$\sum_i \psi_i \equiv 1.$$

We have the representation

$$J(u) - J(\tilde{u}_h) \approx \sum_i \eta_i^{PU},$$

with

$$\begin{aligned} \eta_i^{PU} := & -\frac{1}{2} A(\tilde{u}_h)((z_h^{(2)} - \tilde{z}_h)\psi_i) \\ & + \frac{1}{2}\left(J'(\tilde{u}_h)((u_h^{(2)} - \tilde{u}_h)\psi_i) - A'(\tilde{u}_h)((u_h^{(2)} - \tilde{u}_h)\psi_i, \tilde{z}_h)\right). \end{aligned}$$

Multiple goal approach

- up to now we considered only one functional $J(.)$
- now we consider N functionals $J_1, J_2, \ldots, J_N$
- refine until $|J_i(u) - J_i(u_h)| < TOL_i$

$\rightarrow$ but that means we have to solve **N** linear systems !

$\rightarrow$ try to combine the functionals

$\rightarrow$ Problem: error cancellation effects

Definition (error-weighting function)

We say that $\mathfrak{E} : (\mathbb{R}_0^+)^N \times M \subseteq \mathbb{R}^N \mapsto \mathbb{R}_0^+$ is an **error-weighting function** if

- $\mathfrak{E}(\cdot, m) \in C^3((\mathbb{R}_0^+)^N, \mathbb{R}_0^+)$
- $\mathfrak{E}(\cdot, m)$ strictly monotonically increasing in each component
- $\mathfrak{E}(0, m) = 0$ for all $m \in M$.

- $\vec{J}(v) := (J_1(v), J_2(v), \ldots, J_N(v))$
- $|x|_N := (|x_1|, |x_2|, \ldots, |x_N|)$

This allows us to define the **error functional** as follows

$$\tilde{J}_{\mathfrak{E}}(v) := \mathfrak{E}(|\vec{J}(u) - \vec{J}(v)|_N, \vec{J}(\tilde{u}_h)) \qquad \forall v \in \bigcap_{i=1}^{N} \mathcal{D}(J_i).$$

- This generalizes the approach of [Hartmann & Housten (2003)].

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This allows us to define the **error functional** as follows

$$J_{\mathfrak{E}}(v) := \mathfrak{E}(|\vec{J}(u_h^{(2)}) - \vec{J}(v)|_N, \vec{J}(\tilde{u}_h)) \qquad \forall v \in \bigcap_{i=1}^{N} \mathcal{D}(J_i).$$

- This generalizes the approach of [Hartmann & Housten (2003)].

Assumption (Saturation)

Let $u_h^{(2)} \in U_h^{(2)} \supset U_h$ be the solution of the primal problem on the spaces $U_h^{(2)}$ and $V_h^{(2)}$. Then

$$|J(u) - J(u_h^{(2)})| \leq b|J(u) - J(\tilde{u}_h)|,$$

for some $b \in (0, b_0)$ with $b_0 \in (0, 1)$.

From the saturation assumption follows that we have no error cancellation.

Adaptive Newton algorithm on level l

1: Start with some initial guess $u_h^{l,0} \in U_h^l$ and $k = 0$.

2: For $z_h^{l,0}$, solve

$$A'(u_h^{l,0})(v_h, z_h^{l,0}) = (J_{\mathfrak{E}}^{(0)})'(u_h^{l,0})(v_h) \quad \forall v_h \in V_h^l,$$

with $(J_{\mathfrak{E}}^{(0)})'$ constructed with $u_h^{l,(2)}$ and $u_h^{l,0}$.

3: **while** $|A(u_h^{l,k})(z_h^{l,k})| > 10^{-2}\eta_h^{l-1}$ **do**

4: For $\delta u_h^{l,k}$, solve

$$A'(u_h^{l,k})(\delta u_h^{l,k}, v_h) = -A(u_h^{l,k})(v_h) \quad \forall v_h \in V_h^l.$$

5: Update : $u_h^{l,k+1} = u_h^{l,k} + \alpha\delta u_h^{l,k}$ for some good choice $\alpha \in (0, 1]$.

6: $k = k + 1.$

7: For $z_h^{l,k}$, solve

$$A'(u_h^{l,k})(v_h, z_h^{l,k}) = (J_{\mathfrak{E}}^{(k)})'(u_h^{l,k})(v_h) \quad \forall v_h \in U_h^l,$$

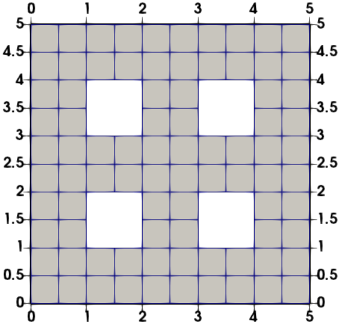
with $(J_{\mathfrak{E}}^{(k)})'$ constructed with $u_h^{l,(2)}$ and $u_h^{l,k}$.

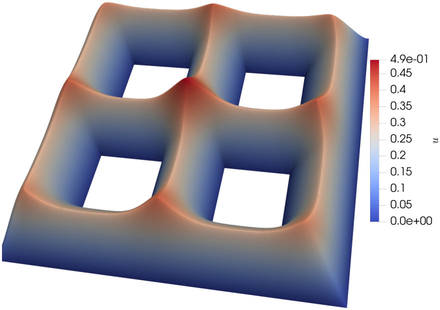
The final algorithm

1: Start with some initial guess $u_h^{0,(2)}$,u_h^0, set $l = 1$ and set $TOL_{dis} > 0$.
2: Solve $A(u_h^{l-1,(2)}) = 0$ for $u_h^{l,(2)}$ using Newton Algorithm with the initial guess $u_h^{l-1,(2)}$ on the discrete space $U_h^{l,(2)}$.
3: Solve $A(u_h^l) = 0$ and $A'(u_h^l)(\cdot, z_h^l) = (J_{\mathfrak{E}})'(u_h^l)(\cdot)$ using Adaptive Newton algorithm with the initial guess u_h^{l-1} on the discrete spaces U_h^l and V_h^l .
4: Construct the combined functional $J_{\mathfrak{E}}$.
5: Solve the adjoint problem $A'(u_h^{l-1,(2)})(\cdot, z_h^{l,(2)}) = (J_{\mathfrak{E}}^{(k)})'(u_h^{l,(2)})(\cdot)$ on $V_h^{l,(2)}$.
6: Construct the error estimator η_K by distributing η_i to the elements.
7: Mark elements with some refinement strategy.
8: Refine marked elements: $\mathcal{T}_h^l \mapsto \mathcal{T}_h^{l+1}$ and $l = l + 1$.
9: If $|\eta_h| < TOL_{dis}$ stop, else go to 2.

Numerical experiment: $p = 4$ and $\varepsilon = 10^{-10}$

$$-\operatorname{div}\left((\varepsilon^2 + |\nabla u|^2)^{\frac{p-2}{2}} \nabla u\right) = 1 \quad \forall x \in \Omega,$$
$$u(x) = 0 \quad \forall x \in \partial\Omega.$$





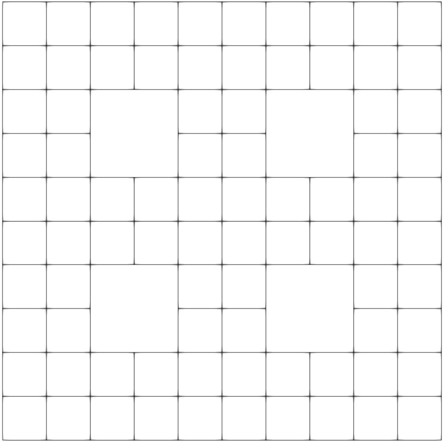
We are interested in the following functional evaluations

$$
\begin{aligned}
J_1(u) :=& (1 + u(2.9, 2.1))(1 + u(2.1, 2.9)),\\
J_2(u) :=& (\int_\Omega [u(x, y) - u(2.5, 2.5)] d(x, y))^2,\\
J_3(u) :=& \int_{(2,3)\times(2,3)} u(x, y) d(x, y),\\
J_4(u) :=& u(0.6, 0.6).
\end{aligned}
$$

The error weighting function is given by

$$
\mathfrak{E}(x, \vec{J}(\tilde{u}_h)) := \sum_{i=1}^{4} \frac{x_i}{|J_i(\tilde{u}_h)|}.
$$

Mesh



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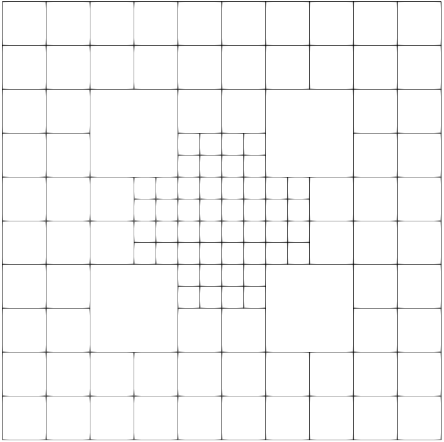

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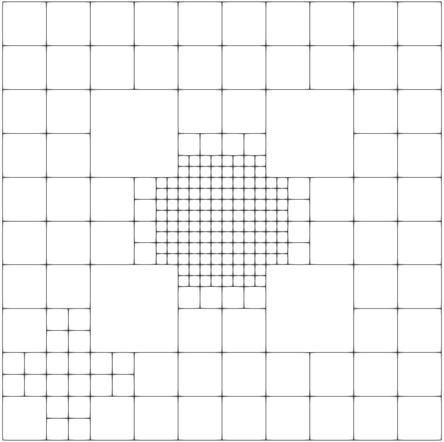

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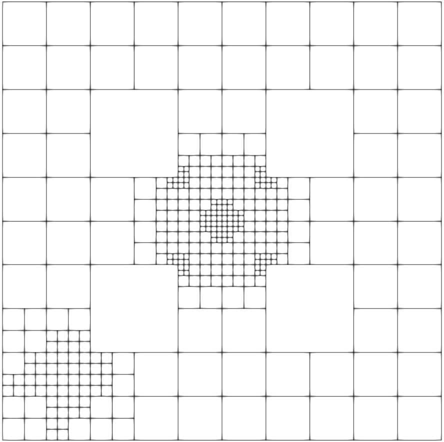

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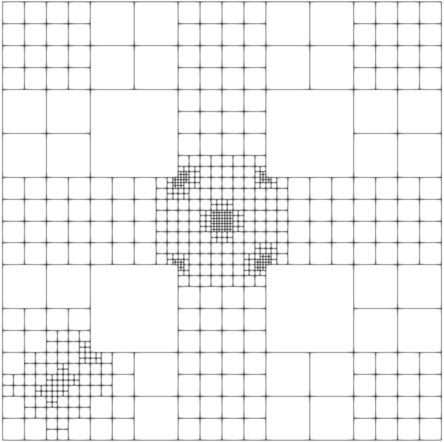

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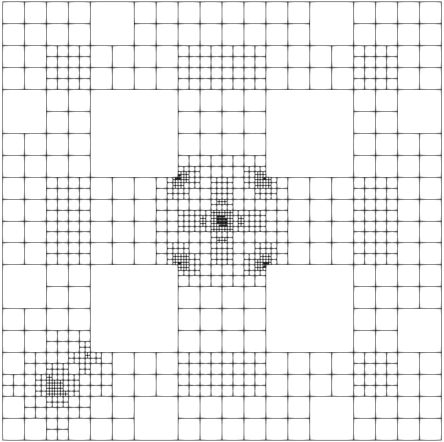

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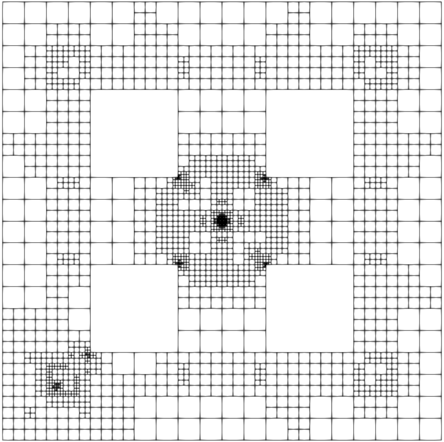

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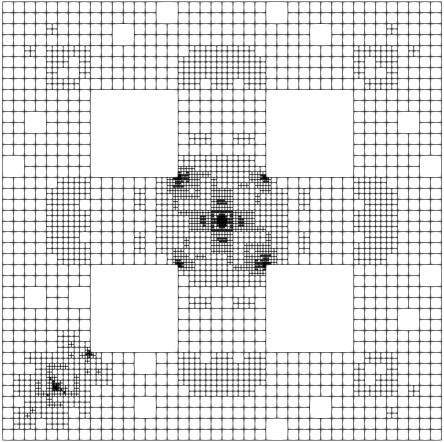

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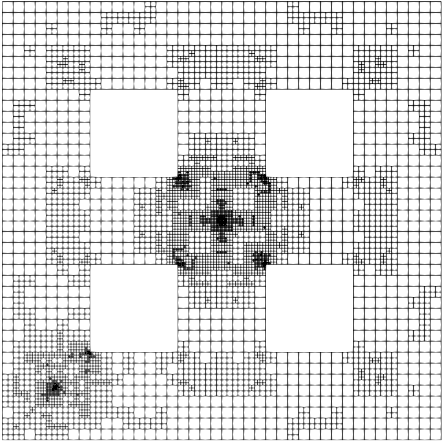

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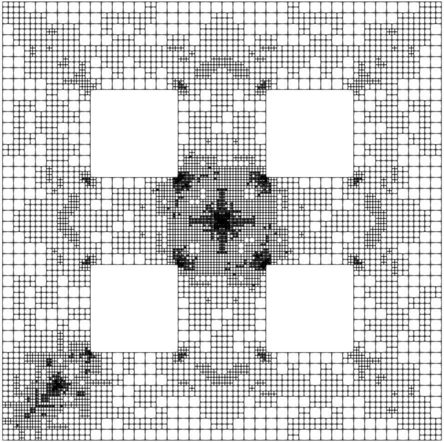

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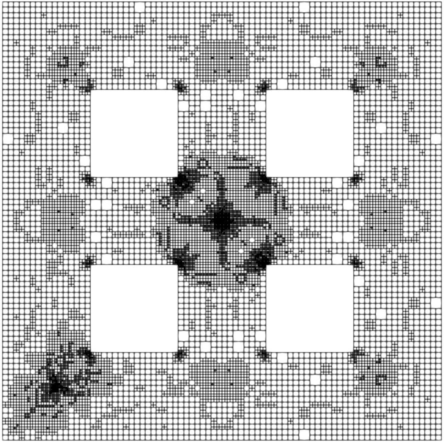

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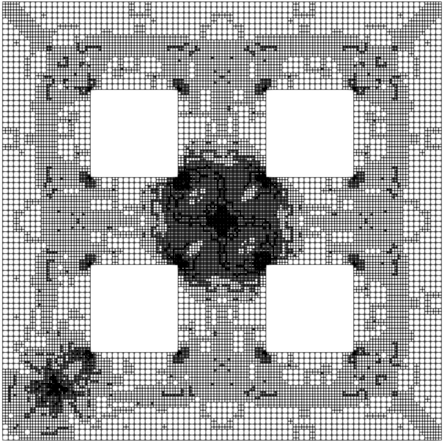

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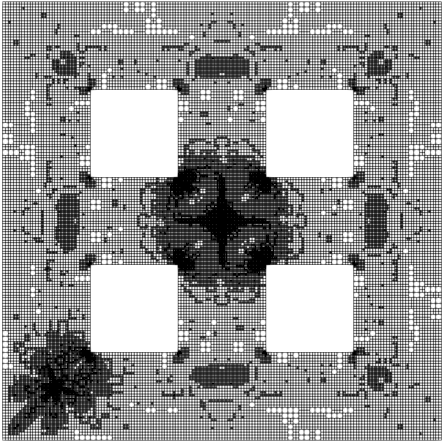

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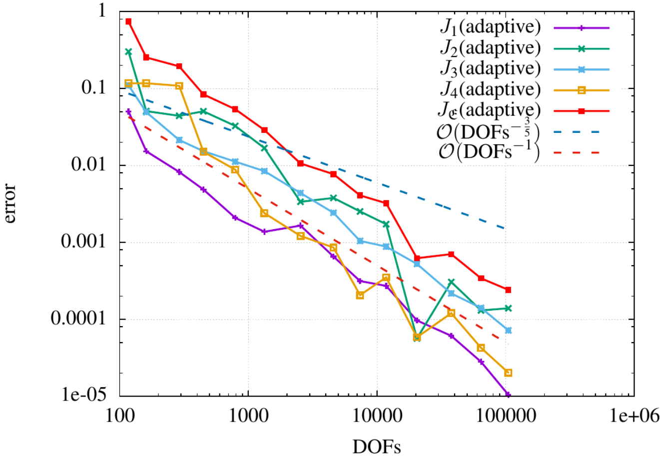
Effectivity indices

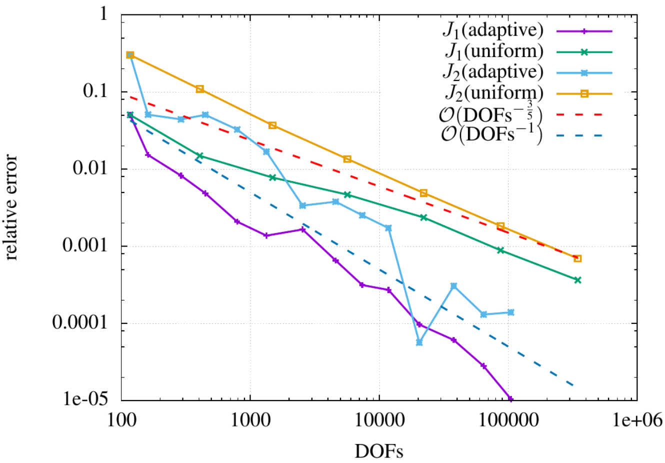
Rl.	*DOFs*	error in $J_{\mathfrak{E}}$	I_{eff}	I_{effp}	I_{effa}
0	117	7.43E-01	0.63	0.6	0.65
1	161	2.54E-01	0.53	0.27	0.79
2	290	1.94E-01	0.84	0.24	1.43
3	447	8.40E-02	0.81	0.28	1.34
4	791	5.39E-02	0.96	0.48	1.45
...	...	...	...	...	...
11	37 747	7.03E-04	1.87	0.66	3.07
12	64 316	3.41E-04	1.63	0.39	2.87
13	104 832	2.42E-04	1.44	0.5	2.38

$$I_{eff} := \frac{\eta_h}{|J(u) - J(u_h)|}, \qquad I_{effp} := \frac{|A(u_h)(z - z_h)|}{|J(u) - J(u_h)|}, \qquad I_{effa} := \frac{|J'(u_h)(u - u_h) - A'(u_h)(u - u_h, z_h)|}{|J(u) - J(u_h)|}.$$

Bounding the Errors



Error vs. DOFs



Recent results

Theorem

It holds:

$$|\eta_h^{(2)}| - \gamma(A, J, u_h^{(2)}, u, \tilde{u}) \leq |J(u) - J(\tilde{u})| \leq |\eta_h^{(2)}| + \gamma(A, J, u_h^{(2)}, u, \tilde{u}),$$

where

$$\gamma(A, J, u_h^{(2)}, u, \tilde{u}) = |J(u) - J(u_h^{(2)})| + |\mathcal{R}^{(3)} - \mathcal{R}^{(3)(2)}| + |\eta_k| + |\mathcal{R}^{(3)}|.$$

Under the Saturation assumption this shows efficiency and reliability with the constants $\underline{c} := \frac{1}{1+b}$, $\overline{c} := \frac{1}{1-b}$ up to some higher order terms.

Recent results

Lemma

It holds:

$$|J(\tilde{u}) - J(u_h^{(2)})| = |\eta_h^{(2)} + \eta_k + \eta_{\mathcal{R}}^{(2)}|,$$

and consequently

$$|J(u) - J(\tilde{u})| - |J(u) - J(u_h^{(2)})| \leq |\eta_h^{(2)} + \eta_k + \eta_{\mathcal{R}}^{(2)}| \leq |J(u) - J(\tilde{u})| + |J(u) - J(u_h^{(2)})|,$$

and

$$\frac{1}{1+b}|J(u) - J(\tilde{u})| \leq |\eta_h^{(2)} + \eta_k + \eta_{\mathcal{R}}^{(2)}| \leq \frac{1}{1-b}|J(u) - J(\tilde{u})|.$$

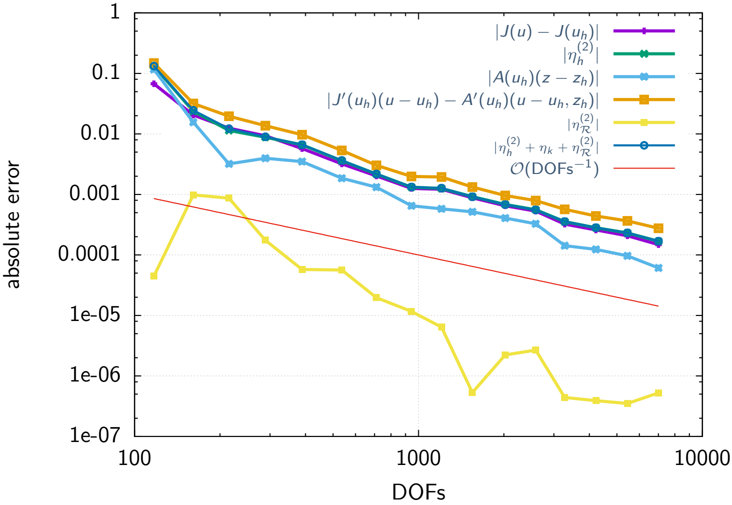
Under the Saturation assumption this shows efficiency and reliability.

Numerical experiment II (influence of $\mathcal{R}^{(3)}$)

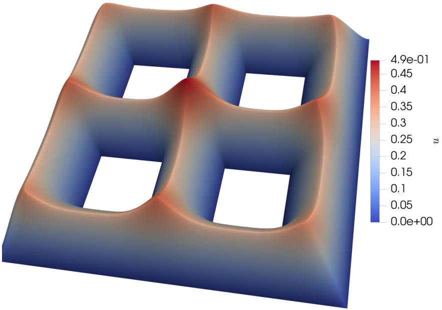
$$
\begin{aligned}
-\mathrm{div}((\varepsilon^2 + |\nabla u|^2)^{\frac{4-2}{2}} \nabla u) &= 1 \quad \forall x \in \Omega, \\
u(x) &= 0 \quad \forall x \in \partial\Omega.
\end{aligned}
$$

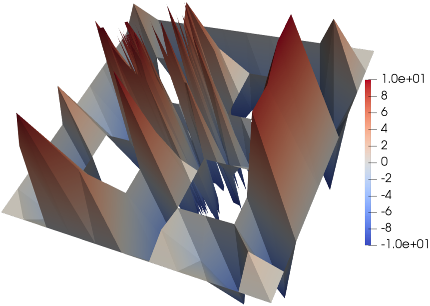
We are interested in the following functional evaluation:

$$
J_1(u) := (1 + u(2.9, 2.1))(1 + u(2.1, 2.9)).
$$


1
0.1
0.01
0.001
0.0001
1e-05
1e-06
1e-07
100
1000
10000
DOFs
absolute error
$|J(u) - J(u_h)|$
$|\eta_h^{(2)}|$
$|A(u_h)(z - z_h)|$
$|J'(u_h)(u - u_h) - A'(u_h)(u - u_h, z_h)|$
$|\eta_{\mathcal{R}}^{(2)}|$
$|\eta_h^{(2)} + \eta_k + \eta_{\mathcal{R}}^{(2)}|$
$\mathcal{O}(\mathrm{DOFs}^{-1})$

Poor(random) approximations





Error estimation for a 'random' solution

DOFs	I_{eff}	I_{effp}	I_{effa}	$\frac{\lvert\eta_h^{(2)}+\eta_k+\eta_{\mathcal{R}}^{(2)}\rvert}{\lvert J(u)-J(u_h)\rvert}$	$\lvert J(u_h^{(2)}) - J(\tilde{u}) - \eta_h^{(2)} - \eta_k - \eta_{\mathcal{R}}^{(2)}\rvert$
117	4.34E+02	8.67E+02	1.39E-01	**0.9646**	2.69E-13
151	8.38E+02	1.68E+03	2.26E-02	**0.9993**	3.04E-13
203	3.16E+02	6.31E+02	7.96E-04	**0.9999**	8.52E-12
277	2.40E+03	4.80E+03	2.47E-03	**0.9995**	1.04E-10
391	3.84E+03	7.68E+03	6.80E-03	**1.0004**	6.06E-10
...	...	...	...	...	...
7 132	3.87E+06	7.73E+06	4.02E-03	**1.0002**	1.98E-04
10 076	1.65E+06	3.30E+06	3.49E-03	**0.9997**	8.65E-03
14 221	4.97E+07	9.93E+07	5.11E-03	**0.9982**	2.32E-02

$$I_{eff} := \frac{|\eta_h|}{|J(u) - J(u_h)|}, \qquad I_{effp} := \frac{|A(u_h)(z - z_h)|}{|J(u) - J(u_h)|}, \qquad I_{effa} := \frac{|J'(u_h)(u - u_h) - A'(u_h)(u - u_h, z_h)|}{|J(u) - J(u_h)|}.$$

The largest error contribution in a single cell for 14 221 DOFs is given by $6.845e + 12$.

Main references

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Thanks for your attention

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Numerical Experiment: PDE-System

Find $u = (u_1, u_2, u_3)$ such that

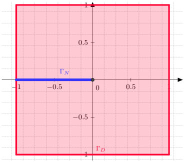
$$\begin{aligned} -\Delta u_1 + u_2 + u_3 &= 1, \quad \text{in } \Omega, \\ -\Delta u_2 + g_1(1 - u_2) - g_1(u_3) &= 0, \quad \text{in } \Omega, \\ -\operatorname{div}(g_2(u_1 + u_2)\nabla u_3) + g_1(u_3) - g_1(u_1) &= 0, \quad \text{in } \Omega, \end{aligned}$$

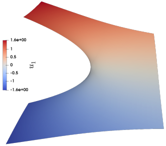
with

$$g_1(t) := e^t - \sin(t-1) \quad g_2(t) := e^{t^2 - t}$$

and

$$\begin{aligned} u_1(x,y) = 1 - u_2(x,y) = u_3(x,y) = \operatorname{sign}(y)\sqrt{\sqrt{x^2+y^2} - x} \quad &\text{on } \Gamma_D, \\ \nabla u_1.\vec{n} = \nabla u_2.\vec{n} = g_2(u_1+u_2)\nabla u_3.\vec{n} = 0 \qquad &\text{on } \Gamma_N. \end{aligned}$$





$$J_A(u) := u_3(-0.5, 0.01), \qquad J_B(u) := u_1(-0.01, 0.01), \qquad J_C(u) := \int_\Omega \Phi_C(x,y)\cdot u(x,y)\,d(x,y),$$

$$J_D(u) := \int_\Omega \Phi_D(x,y)\cdot u(x,y)\,d(x,y), \qquad J_E(u) := u_1(-0.9, -0.9), \qquad J_F(u) := u_2(-0.9, -0.1),$$

where $\Phi_C(x,y) := (0, 0, \chi_C(x,y))$ and

$$\Phi_D(x,y) := \left(-4\chi_D(x,y), \frac{2\chi_D(x,y)}{1-\operatorname{sign}(y)\sqrt{\sqrt{x^2+y^2}-x}}, 4\chi_D(x,y)\right),$$

with

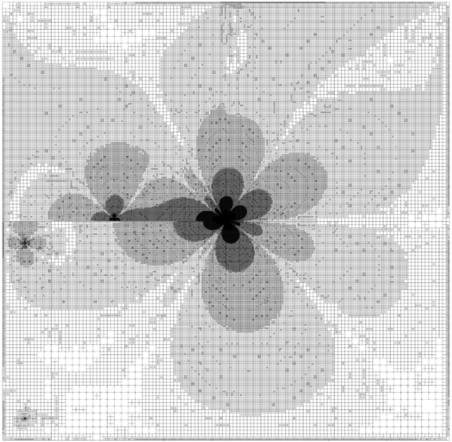
$$\chi_C(x,y) := \begin{cases} y-x & x<y \\ 0 & x \geq y \end{cases} \quad \text{and} \quad \chi_D(x,y) := \begin{cases} 1 & x,y>0 \\ 0 & \text{else} \end{cases}.$$

We are now interested in the six goal functionals

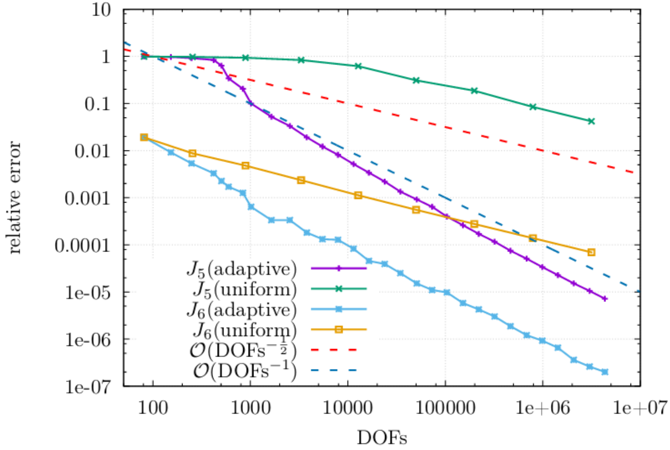
$$J_1(u) := J_B(u)J_D(u), \qquad J_2(u) := J_A(u)J_C(u), \qquad J_3(u) := J_A(u)J_C(u)J_F(u),$$

$$J_4(u) := J_B(u)J_E(u), \qquad J_5(u) := J_B^3(u)J_E(u), \qquad J_6(u) = J_C(u).$$

Mesh



Error vs. DOFs



Another Numerical Experiment: $p = 4$ and $\varepsilon = 10^{-10}$

$$
\begin{aligned}
-\mathrm{div}((\varepsilon^2 + |\nabla u|^2)^{\frac{p-2}{2}} \nabla u) &= 1 \quad \forall x \in \Omega, \\
u(x) &= 0 \quad \forall x \in \partial\Omega.
\end{aligned}
$$