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Linearization Errors in Discrete Goal-Oriented Error Estimation

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BACKGROUND

The big picture:

- Partial differential equation (PDE) $\rightarrow$ exact solution u.
- PDE $\rightarrow$ analytic solution u is, in general, unknown.
- Finite element method (FEM) $\rightarrow$ approx. PDE solution u^H.
- FEM $\rightarrow$ error associated with the discretization, $e := u - u^H$.
- Analyst $\rightarrow$ how reliable/accurate is the solution u^H?

Goal-oriented error estimates:

- Choose physically meaningful functional: $\mathcal{J}(u)$.
- Functional referred to as a 'quantity of interest' (QoI).
- Approximate $\mathcal{E} := \mathcal{J}(u) - \mathcal{J}(u^H)$, discretization error in the QoI.

Presently, we consider nonlinear PDEs and nonlinear QoIs.

GOAL-ORIENTED ERROR ESTIMATION

Primal	Find $u \in \mathcal{V}$ such that $\mathcal{R}(w; u) = 0 \quad \forall w \in \mathcal{V}$
FEM	Find $u^H \in \mathcal{V}^H$ such that $\mathcal{R}(w^H; u^H) = 0 \quad \forall w^H \in \mathcal{V}^H$
Dual	Find $z \in \mathcal{V}$ such that $\mathcal{R}'[u^H](w, z) = \mathcal{J}'[u^H](w) \quad \forall w \in \mathcal{V}$
Error	$\mathcal{J}(u) - \mathcal{J}(u^H) = \underbrace{-\mathcal{R}(z - z^H; u^H)}_{\text{discretization error}} + \underbrace{\mathcal{O}(e^2)}_{\text{linearization error}} \quad \forall w^H \in \mathcal{V}^H$

- $J'[u^H](w)$ - Fréchet linearization about u^H.
- $R'[u^H](w)$ - Fréchet linearization about u^H.

DISCRETE GOAL-ORIENTED ERROR ESTIMATION

Primal PDE discretized by FEM on two spaces: $\mathcal{V}^H \subset \mathcal{V}^h \subset \mathcal{V}$ results in:

Coarse $\boxed{\boldsymbol{R}^H(\boldsymbol{u}^H) = \boldsymbol{0}}$ $\quad \boldsymbol{R}^H : \mathbb{R}^N \to \mathbb{R}^N,$

Fine $\boxed{\boldsymbol{R}^h(\boldsymbol{u}^h) = \boldsymbol{0}}$ $\quad \boldsymbol{R}^h : \mathbb{R}^n \to \mathbb{R}^n, \quad n > N,$

Let $\boldsymbol{u}_h^H := I_h^H \boldsymbol{u}^H$, where $I_h^H : \mathcal{V}^H \to \mathcal{V}^h$.
Let $\boldsymbol{e}^h := \boldsymbol{u}^h - \boldsymbol{u}^H$.
Talyor expansions about $\boldsymbol{u}_h^H$:

$$\cancelto{0}{\boldsymbol{R}^h(\boldsymbol{u}^h)} = \boldsymbol{R}^h(\boldsymbol{u}_h^H) + \left[\left. \frac{\partial \boldsymbol{R}^h}{\partial \boldsymbol{u}^h} \right|_{\boldsymbol{u}_h^H} \right] \boldsymbol{e}^h + \boldsymbol{E}_L^{\mathcal{R}},$$

$$\mathcal{J}^h(\boldsymbol{u}^h) = \mathcal{J}^h(\boldsymbol{u}_h^H) + \left[\left. \frac{\partial \mathcal{J}^h}{\partial \boldsymbol{u}^h} \right|_{\boldsymbol{u}_h^H} \right] \boldsymbol{e}^h + \mathcal{E}_L^{\mathcal{J}}.$$

Disregard $\mathcal{E}_L^{\mathcal{J}}$ and $\boldsymbol{E}_L^{\mathcal{R}}$ $\implies$

$$\begin{aligned} \mathcal{E} &:= \mathcal{J}(u) - \mathcal{J}(u^H), \\ &\approx \mathcal{J}(u^h) - \mathcal{J}(u^H), \\ &:= \mathcal{E}^h, \\ &\approx (\boldsymbol{z}^h - \boldsymbol{z}_H^h) \cdot \boldsymbol{R}^h(\boldsymbol{u}_h^H), \\ &:= \eta_1. \end{aligned}$$

$\boldsymbol{z}^h \to$ solution to *adjoint problem*

$$\left[\left. \frac{\partial \boldsymbol{R}^h}{\partial \boldsymbol{u}^h} \right|_{\boldsymbol{u}_h^H} \right]^T \boldsymbol{z}^h = \left[\left. \frac{\partial \mathcal{J}^h}{\partial \boldsymbol{u}^h} \right|_{\boldsymbol{u}_h^H} \right]^T.$$

$\boldsymbol{z}_H^h := I_H^h \boldsymbol{z}^h$, where $I_H^h : \mathcal{V}^h \to \mathcal{V}^H$.

A MOTIVATING EXAMPLE

A nonlinear Poisson's equation:

$$\begin{cases} -\nabla \cdot [(1 + \alpha u^2)\nabla u] = f, & \text{in } \Omega, \\ u = 0, & \text{on } \Gamma. \end{cases}$$

In weak form:

$$\mathcal{R}(w; u) := (f, w)_\Omega - ((1 + \alpha u^2)\nabla u, \nabla w)_\Omega = 0.$$

Consider functionals/manufactured solution:

$$\mathcal{J}_1(u) = \int_{\Omega_s} u^3 \, \mathrm{d}\Omega,$$

$$\mathcal{J}_2(u) = \int_{\Omega_s} \nabla u \cdot \nabla u \, \mathrm{d}\Omega,$$

$$u(x, y) = \sin(2\pi x)\sin(2\pi y)\exp(5/2(x + y)).$$

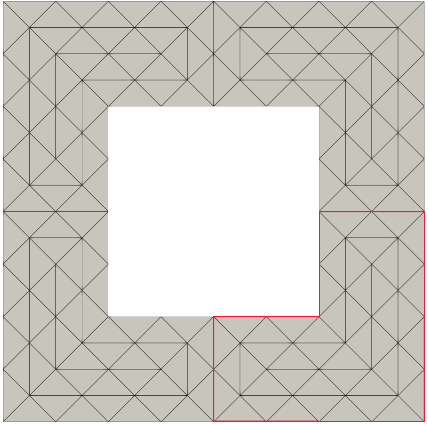
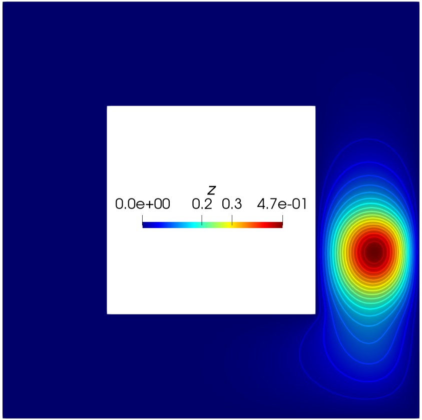
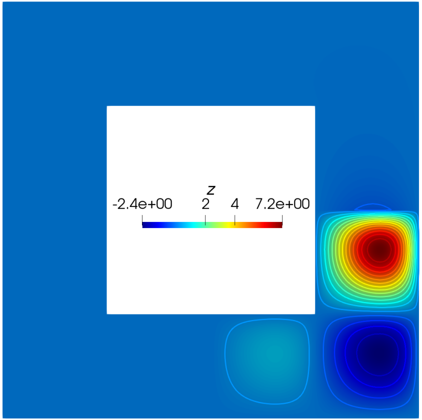


Figure: Example domain Ω and sub-domain Ω_s with an initial mesh occupying the space $[-1, 1]^2$.

A MOTIVATING EXAMPLE: ADJOINT SOLUTIONS

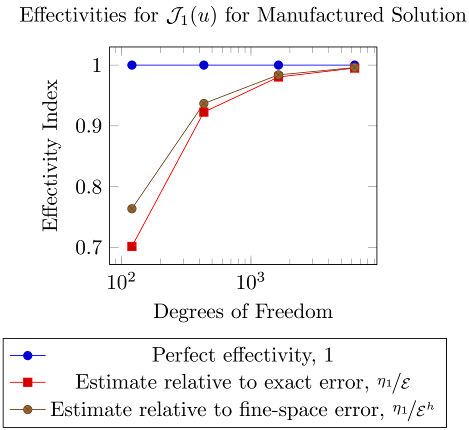


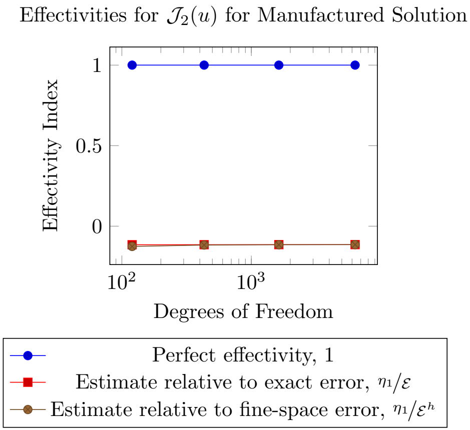
(a) Adjoint solution for QoI $\mathcal{J}_1(u)$



(b) Adjoint solution for QoI $\mathcal{J}_2(u)$

A MOTIVATING EXAMPLE: ESTIMATE EFFECTIVITY





A MOTIVATING EXAMPLE: WHAAAAAA?!?!?!

Consider the quadratic QoI:

$$\mathcal{J}(u) = \int_\Omega \nabla u \cdot \nabla u,$$

The discretization error in this functional can be exactly represented as:

$$\mathcal{J}(u) - \mathcal{J}(u^H) = 2\int_\Omega \nabla u^H \cdot \nabla e \, \mathrm{d}\Omega + \int_\Omega \nabla e \cdot \nabla e \, \mathrm{d}\Omega.$$

- First integral: linearization used for η_1
- Second integral: should $\to 0$ quickly since its $\mathcal{O}(e^2)$
- However, second integral is strictly positive
- First integral: might $\to 0$ quickly relatively due to subtractive cancellation.
- Neglecting linearization error: could significantly under-predict actual error.

A MODIFIED ERROR ESTIMATE

From mean value $\exists$ a $\boldsymbol{u}^*$ such that $\mathcal{E}_L^{\mathcal{J}}$ vanishes:

$$\mathcal{J}^h(\boldsymbol{u}^h) = \mathcal{J}^h(\boldsymbol{u}_h^H) + \left[\frac{\partial \mathcal{J}^h}{\partial \boldsymbol{u}^h}\bigg|_{\boldsymbol{u}^*} \right] \boldsymbol{e}^h.$$

$\boldsymbol{u}^*$: point on linear path between $\boldsymbol{u}_h^H$ and $\boldsymbol{u}^h$

$$\boldsymbol{u}^*(\theta) = \boldsymbol{u}_h^H + \theta \boldsymbol{e}^h, \quad \theta \in [0,1].$$

Finding $\boldsymbol{u}^*$: solve nonlinear scalar equation:

$$f(\theta) := \mathcal{E}^h - \left[\frac{\partial \mathcal{J}^h}{\partial \boldsymbol{u}^h}\bigg|_{\boldsymbol{u}^*(\theta)} \right] \boldsymbol{e}^h = 0.$$

Introduce *modified adjoint problem*:

$$\left[\frac{\partial \boldsymbol{R}^h}{\partial \boldsymbol{u}^h}\bigg|_{\boldsymbol{u}_h^H} \right]^T \boldsymbol{z}^* = \left[\frac{\partial \mathcal{J}^h}{\partial \boldsymbol{u}^h}\bigg|_{\boldsymbol{u}^*} \right]^T.$$

No mean-value analogue for vector-valued functions.

$\boldsymbol{E}_L^{\mathcal{R}}$ must be accounted for in different manner.

Introduce:

$$\boldsymbol{z}^{**} = \boldsymbol{z}^* + \frac{\boldsymbol{z}^* \cdot \boldsymbol{E}_L^{\mathcal{R}}}{\boldsymbol{R}^h(\boldsymbol{u}_h^H) \cdot \boldsymbol{R}^h(\boldsymbol{u}_h^H)} \boldsymbol{R}^h(\boldsymbol{u}_h^H),$$

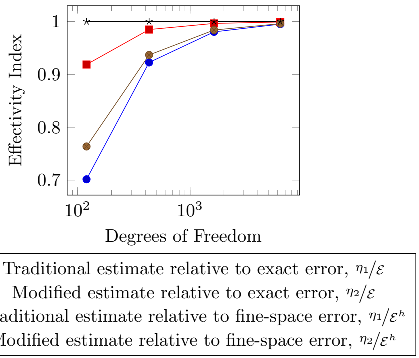
QoI error between the two spaces:

$$\mathcal{E}^h = \eta_2 := -\boldsymbol{z}^{**} \cdot \boldsymbol{R}^h(\boldsymbol{u}_h^H).$$

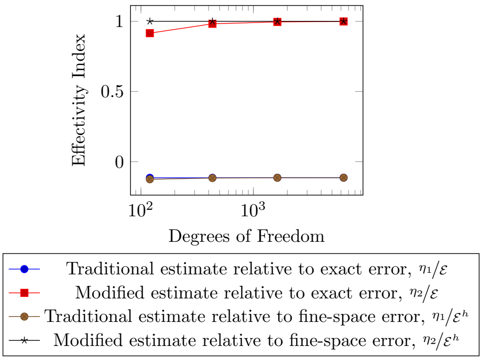
- con: Requires primal solve on the fine space.
- pro: Including linearization errors in error *localization* $\rightarrow$ might lead to better meshes.
- pro: Can be used to safeguard termination criteria at coarse mesh resolutions in adaptive iterations when η_1 may under-predict error.

A MOTIVATING EXAMPLE: ERROR EFFECTIVITY REVISITED

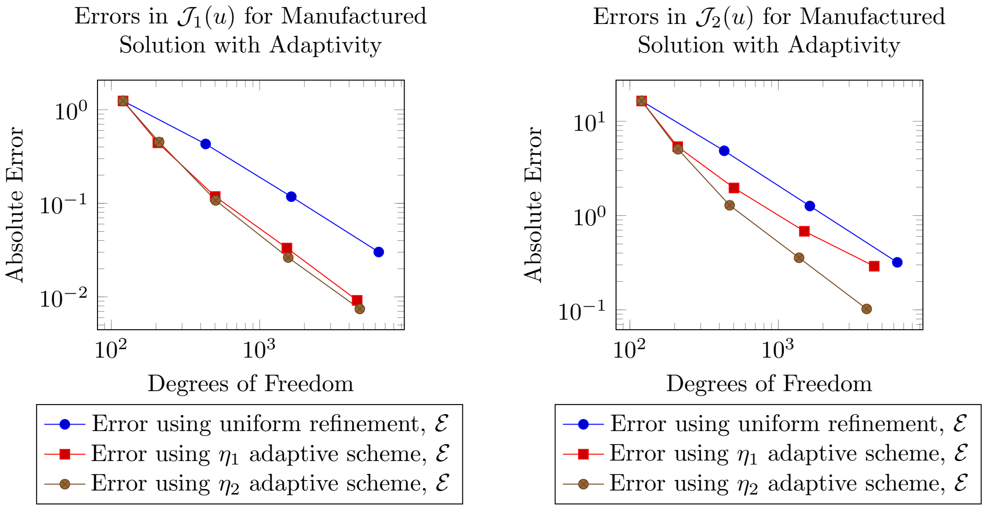
Effectivities for $\mathcal{J}_1(u)$ for Manufactured Solution



Effectivities for $\mathcal{J}_2(u)$ for Manufactured Solution



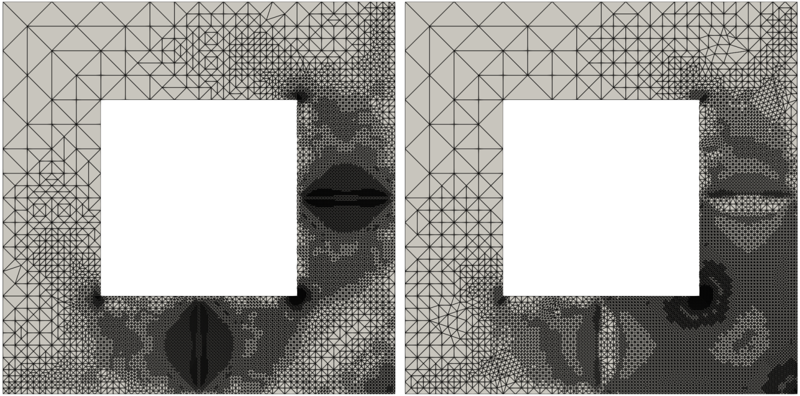
A MOTIVATING EXAMPLE: MESH ADAPTIVITY



A PROBLEM WITH GRADIENT SINGULARITIES

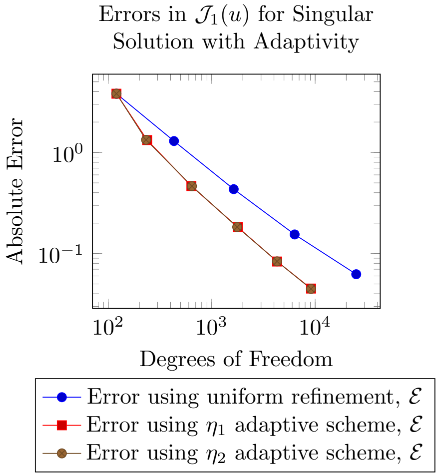
If instead we choose $f = 1$ in forcing function:

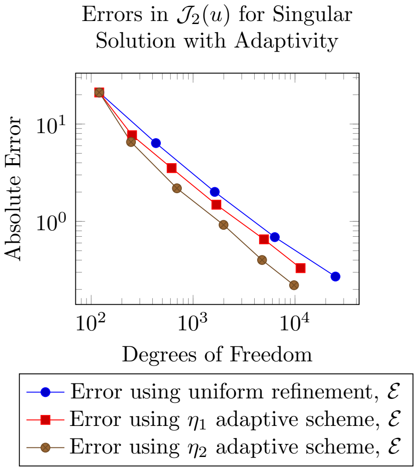
- $\mathcal{J}_1(u)$: Adapting based on η_1 or η_2 $\rightarrow$ nearly identical meshes
- $\mathcal{J}_2(u)$: Adapting based on η_1 or η_2 $\rightarrow$ very distinct meshes



(a) $\mathcal{J}_2(u)$: Mesh obtained using η_1. (b) $\mathcal{J}_2(u)$: Mesh obtained using η_2.

A PROBLEM WITH GRADIENT SINGULARITIES





NONLINEAR ELASTICITY: DESCRIPTION

Balance of linear momentum:

$$\begin{cases} -\nabla \cdot \boldsymbol{P} = \boldsymbol{0}, & \boldsymbol{X} \in \Omega, \\ \boldsymbol{u} = \boldsymbol{G}, & \boldsymbol{X} \in \Gamma_G, \\ \boldsymbol{P} \cdot \boldsymbol{N} = \boldsymbol{0}, & \boldsymbol{X} \in \Gamma_H. \end{cases}$$

A neo-Hookean material model

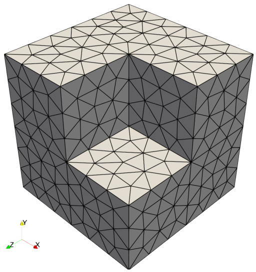
$$\boldsymbol{\sigma} = \mu J^{-5/3} \mathrm{dev}(\boldsymbol{F}\boldsymbol{F}^T) + \frac{\kappa}{2}(J - 1/J)\boldsymbol{I},$$

Weak form:

$$\mathcal{R}(\boldsymbol{w}; \boldsymbol{u}) := -\int_\Omega \boldsymbol{P}(\boldsymbol{u}) : \nabla \boldsymbol{w} \, \mathrm{d}\Omega,$$

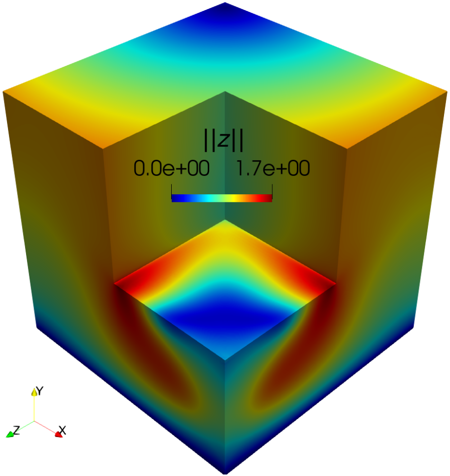
QoI: von Mises stress integrated over domain:

$$\mathcal{J}_{vm}(\boldsymbol{u}) := \int_\Omega \sigma_{vm}(\boldsymbol{u}) \, \mathrm{d}\Omega,$$

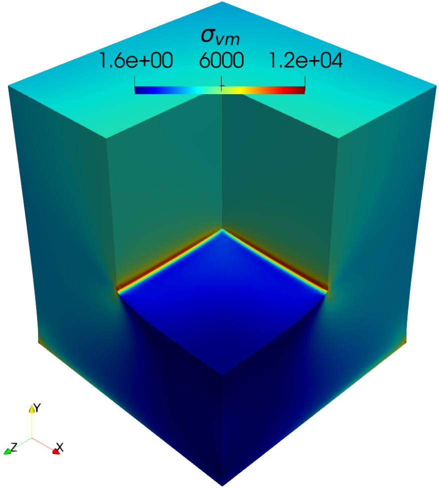


- Domain: 5mm × 5mm × 5mm.
- Elastic modulus: $E = 192.7$ GPa.
- Poisson's ratio: $\nu = 0.27$.
- $u_x, u_y, u_z = 0$ on minimal y face.
- $u_y = 0.1$ on maximal y face.
- About 2% strain in y-direction.

NONLINEAR ELASTICITY: SOLUTIONS

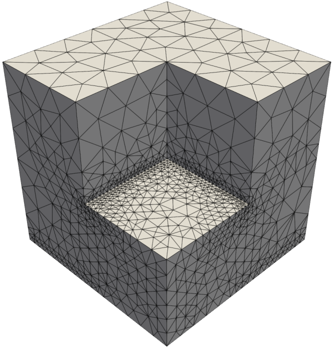


(a) Norm of the adjoint solution z.

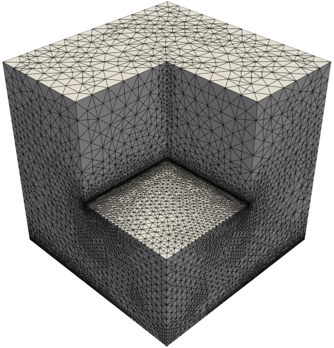


(b) von Mises stress plotted over the domain.

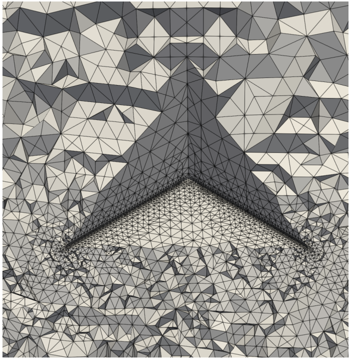
NONLINEAR ELASTICITY: MESH ADAPTIVITY



(a) Mesh after 5 adaptive iterations.

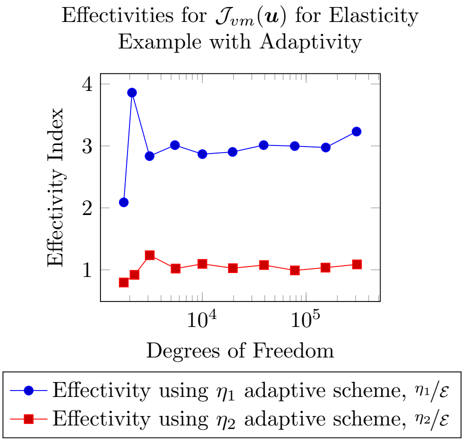


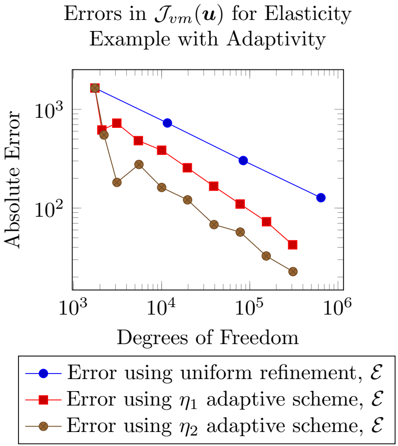
(b) Mesh after 10 adaptive iterations.



(c) Cut-away of mesh after 10 adaptive iterations.

NONLINEAR ELASTICITY: ESTIMATE BEHAVIOR





CONCLUSIONS

- Considered *a posteriori* goal-oriented error estimation for Galerkin FEM.
- Traditional adjoint-weighted residual estimate η_1 incurs linearization errors.
- Developed novel estimate η_2 that accounts for discrete linearization errors.
- η_2 can be more *effective* than η_1 in certain contexts.
- Localization of η_2 can lead to better meshes in certain contexts.
    - Reduced errors with fewer DOFs when considering mesh adaptivity.
- Full details can be found at `https://arxiv.org/abs/2305.15285`.
- Thank you!