New Approaches for Adjoint-Based Error Estimation and Mesh Adaptation in Stabilized Finite Element Methods with an Emphasis on Solid Mechanics Applications

Brian N. Granzow

Mechanical Engineering
Rensselaer Polytechnic Instutite
Troy, NY 12180 USA

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About this talk

- Review of adjoint-based *a posteriori* error estimation.
- An automated approach for adjoint-based analysis.
- Example applications of the automated approach.
- A non-uniform refinement approach for adjoint analysis.
- Goal-oriented analysis for variational multiscale methods.
- Summary and conclusions.

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?

Provides a useful analysis tool to:

- measure the accuracy of FEM approximations u^H.
- control errors in FEM approximations (e.g. mesh adaptation).

Traditional estimates:

- choose a norm: $\| \cdot \|$ (e.g. energy, L_2)
- approximate: $\mathcal{E} \approx \|e\|$.

Goal-oriented error estimates:

- choose a physically meaningful functional: $J(u)$.
- approximate: $\mathcal{E} \approx J(u) - J(u^H)$.

From a high level, adjoint-based error analysis follows the steps:

- Choose a physically meaningful functional quantity $J(u)$.
- Solve the PDE of interest approximately with the FEM $\rightarrow u^H$.
- Solve an auxiliary adjoint PDE with the FEM $\rightarrow z^H$.
- Determine an enriched representation of the dual solution z^h.
- Utilize u^H, z^H, and z^h to estimate $J(u) - J(u^H)$.
- Localize contributions to $J(u) - J(u^H)$ to mesh entities.
- Use localized error contributions to drive adaptation.

Key features:

- The adjoint PDE relates $J(u)$ to the original PDE of interest.
- $z \rightarrow$ sensitivity of the functional quantity of interest with respect to perturbations in the original PDE residual.

Primal $\boxed{\text{Find } u \in V \text{ such that } R_g(w;u) = 0 \quad \forall w \in V}$

FEM $\boxed{\text{Find } u^H \in V^H \text{ such that } R_g(w^H;u^H) + R_\tau(w^H;u^H) = 0 \quad \forall w^H \in V^H}$

Dual $\boxed{\text{Find } z \in V \text{ such that } R_g'[u^H](w,z) = J'[u^H](w) \quad \forall w \in V}$

Error $$J(u) - J(u^H) = \underbrace{-R_g(z - z^H;u^H) + R_\tau(z^H;u^H)}_{\text{discretization error}} + \underbrace{\mathcal{O}(e^2)}_{\text{linearization error}} \quad \forall w^H \in V^H$$

- $J'[u^H](w)$ - Fréchet linearization about u^H.
- $R'[u^H](w)$ - Fréchet linearization about u^H.
- Error representation obtained from functional relation to the primal PDE residual via the dual solution z.

Adjoint-based *a posteriori* error estimation
A two-level approach

Two discretization levels:
$V^H \subset V \rightarrow$ coarse space
$V^h \subset V \rightarrow$ fine space

Primal equation discretized by FEM:

$$\textcolor{blue}{Coarse} \quad \boxed{\boldsymbol{R}^H(\boldsymbol{u}^H) = \boldsymbol{0}}$$

$$\textcolor{blue}{Fine} \quad \boxed{\boldsymbol{R}^h(\boldsymbol{u}^h) = \boldsymbol{0}}$$

$\boldsymbol{R}^H : \mathbb{R}^N \rightarrow \mathbb{R}^N$
$\boldsymbol{R}^h : \mathbb{R}^n \rightarrow \mathbb{R}^n$

Functional discretized by FEM:
$J^H : \mathbb{R}^N \rightarrow \mathbb{R}$
$J^h : \mathbb{R}^n \rightarrow \mathbb{R}$

Let $\boldsymbol{u}_H^h : I_H^h \boldsymbol{u}^H$ be prolongation of u^H onto the fine space V^h, where $I_H^h : V^H \rightarrow V^H$.

Taylor expansions of fine space lead to:

$$J^h(\boldsymbol{u}^h) - J^H(\boldsymbol{u}^H) \approx -\boldsymbol{z}^h \cdot \boldsymbol{R}^h(\boldsymbol{u}_H^h)$$

where $\boldsymbol{z}^h$ is the solution to the adjoint problem on the fine space given by

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

My contributions

- A fully automated approach for adjoint-based error estimation.
- Applicable to stabilized finite element methods.
- Runs in parallel for solid mechanics applications.
- Applied to finite deformation solid mechanics.
- With complex three dimensional geometries.
- Non-uniform refinement approaches for adjoint solves.
- New adjoint-based error estimation for VMS methods.

Potential difficulties in goal oriented error estimation and mesh adaptation for modern engineers practitioners:

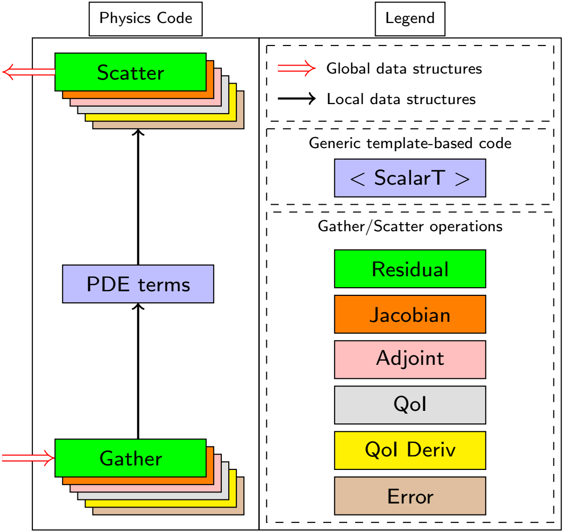
- Many components must be implemented $\rightarrow$ primal analysis, dual analysis, dual enrichment, error localization, mesh adaptation
- Residuals and functionals can be highly nonlinear $\rightarrow$ linearizations are required
- Problems of interest necessitate parallel analysis $\rightarrow$ scalable primal and dual mechanics analysis code is required.
- Fully unstructured parallel mesh adaptation $\rightarrow$ requires performant software tools.

A solution: I wrote a goal-oriented analysis library:

https://github.com/bgranzow/goal

- Utilizes performant software components (Trilinos and PUMI)
- Automates primal, dual, and error localization steps
- Allows for rapid implementation of new physics / QoIs
- Approach similar to Albany / Panzer (Sandia codes)

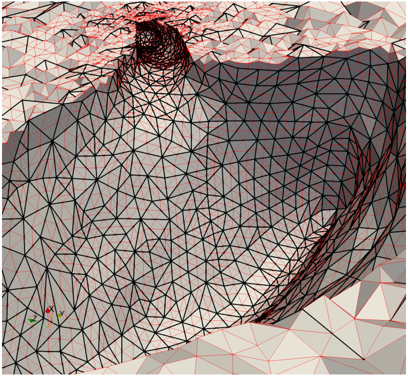
Template-based generic programming



- Residual : assembles residual vector, R^H
- Jacobian : assembles Jacobian matrix, $\frac{\partial R^H}{\partial u^H}$ or adjoint $[\frac{\partial R^H}{\partial u^H}]^T$
- QoI : computes functional, J^H, and assembles functional derivative, $\frac{\partial J^H}{\partial u^H}$
- Error localizes error, $\mathcal{E}_i = R_g((z^h - I^H z^h)\psi_i \; ; \; u^H) + R_\tau((I^H z^h)\psi_i \; ; \; u^H)$

- Allows rapid implementation of new physics, quantities of interest
- Avoids tedious / error-prone implementation of specialization-specific code.

⋆ Thomas Richter, and Thomas Wick. *Variational localizations of the dual weighted residual estimator*. Journal of Computational and Applied Mathematics 279 (2015): 192-208.



- Global higher order solve $\rightarrow$ greater accuracy
- Prefer over p-enrichment
  - Stabilized FEM $\rightarrow$ higher order terms difficult to implement
  - Higher order stabilized FEM $\rightarrow$ rarely used in practice

Balance of linear momentum residual

```
for (int elem = 0; elem < workset.size; ++elem) {
  for (int ip = 0; ip < num_ips; ++ip)
  for (int node = 0; node < num_nodes; ++node)
  for (int i = 0; i < num_dims; ++i)
  for (int j = 0; j < num_dims; ++j)
    resid[i](elem, node, i) +=
      stress(elem, ip, i, j) *
      grad_w(elem, node, ip, i, j) *
      wdv(elem, ip);
}
```

Primal problem: involves:

$$\frac{\partial R^H}{\partial u^H}\delta u^H = -R^H$$

Dual problem: solve

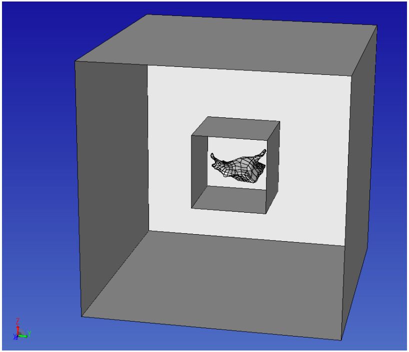
$$[\frac{\partial R^h}{\partial u^h}]^T z^h = [\frac{\partial J^h}{\partial u^h}]^T$$

Error localization:

$$\mathcal{E}_i = R_g^h((z^h - I^H z^h)\psi_i \,;\, u^H) + R_\tau^h((I^H z^h)\psi_i \,;\, u^H)$$

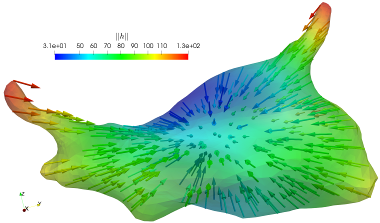
Key idea:
Evaluations share single implementation R

A cell embedded in a matrix : problem definition

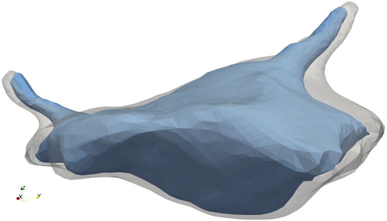


Geometry for the cell problem

Neohookean constitutive model:
$E = 600$ Pa
$\nu = 0.4999$
$J(u) = \int_{\mathcal{B}_0} \frac{1}{3}(u_x + u_y + u_z)\,\mathrm{d}V$



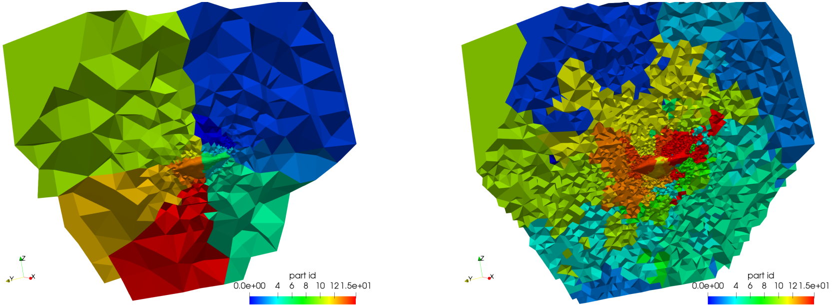
Applied tractions for the cell problem



Deformed cell membrane after tractions

A cell embedded in a matrix : parallelization

Problem run with 16 MPI ranks
ParMA $\rightarrow$ load balancing to ensure partition quality
10 solve / adapt cycles for the model problem

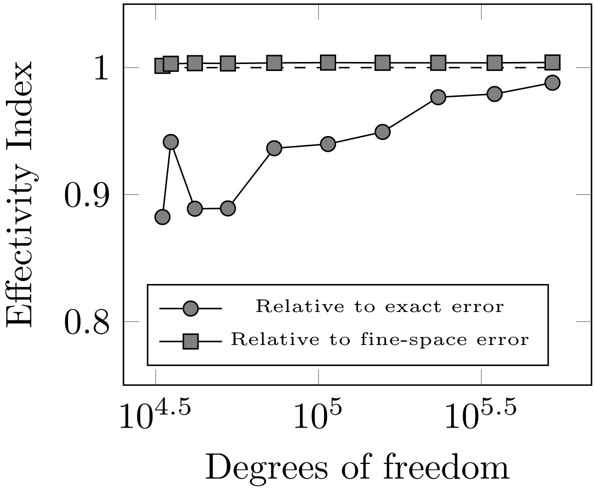


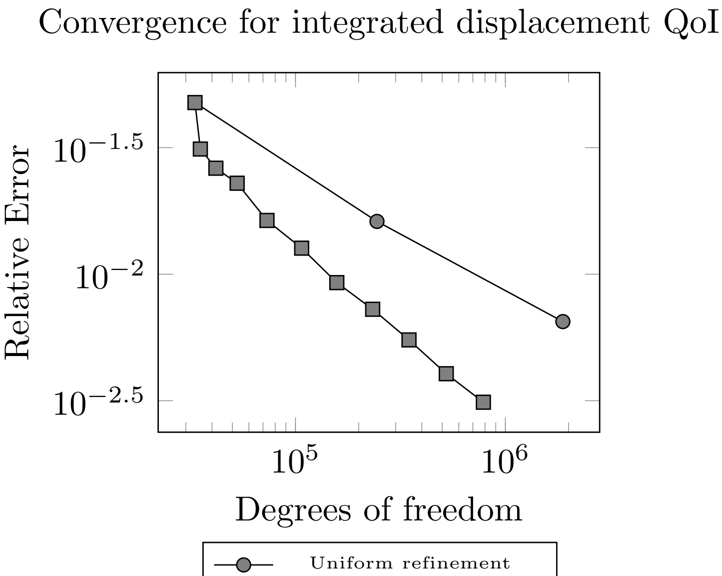
Initial mesh partitioning   Final mesh partitioning

Reference QoI value $J(u) = 527.1453$
using about 60 million degrees of freedom

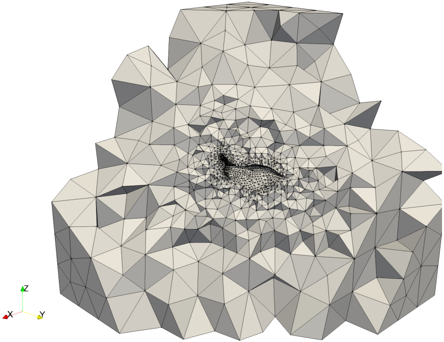
A cell embedded in a matrix : effectivities

Effectivities for integrated displacement QoI

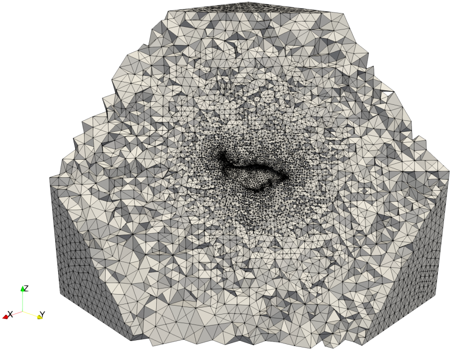



Convergence for integrated displacement QoI
Relative Error
$10^{-1.5}$
10^{-2}
$10^{-2.5}$
10^{5}
10^{6}
Degrees of freedom
Uniform refinement

A cell embedded in a matrix : adapted meshes

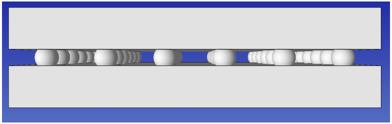


Initial mesh



Final adapted mesh

Elastoplasticity in an array of solder joints : problem definition

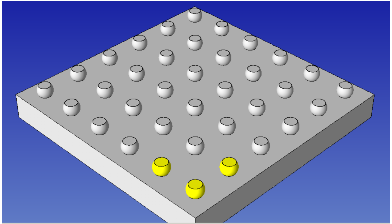


Domain geometry problem geometry

6×6 array of solder joints.
Between two dissimilar materials.
Cooled from $T_0 = 393K$ to $T_f = 318K$.

Elastoplastic constitutive model.

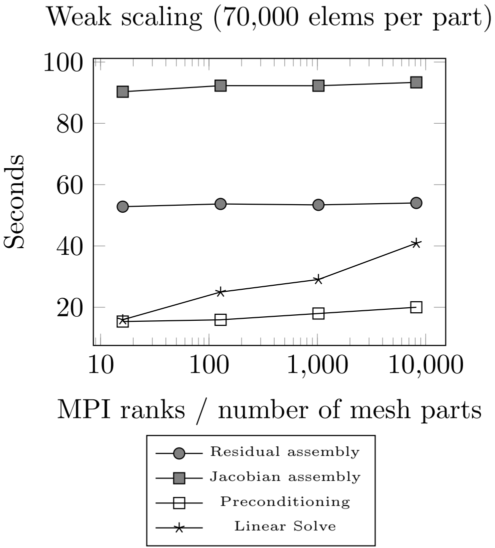
- von-Mises yield criterion
- Isotropic linear hardening
- Thermal correction



Solder joints defining the QoI

$J(u)$: average von-Mises stress over $\mathcal{B}_0$.
$\mathcal{B}_0$: defined by 3 solder joints
$\sigma_{vm} := \sqrt{\frac{3}{2}\boldsymbol{\sigma}' : \boldsymbol{\sigma}'}$
$\boldsymbol{\sigma}'$: deviatoric stress

Elastoplasticity in an array of solder joints : weak scaling



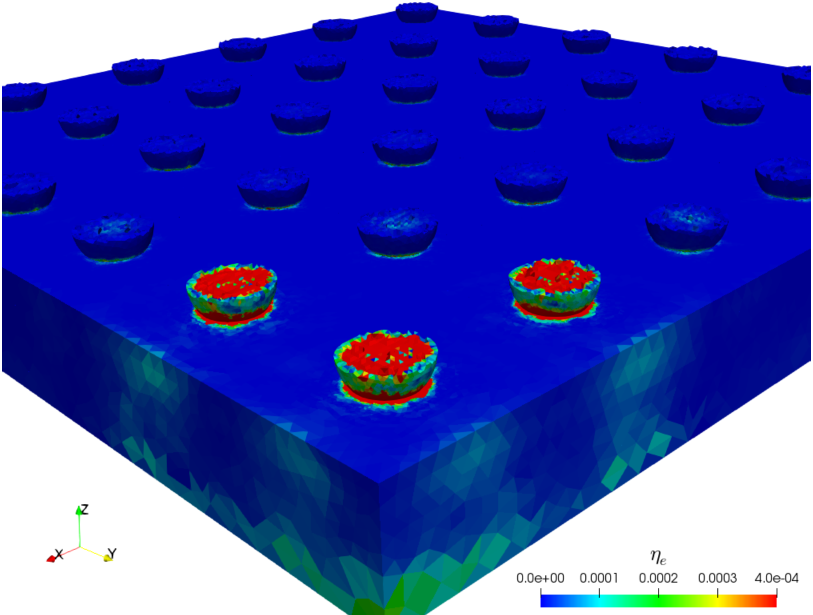
Richardson extrapolation:
Reference value:
$J(u) = 328.9$

Final solve:

- 8192 MPI ranks
- $> \frac{1}{2}$ billion elements

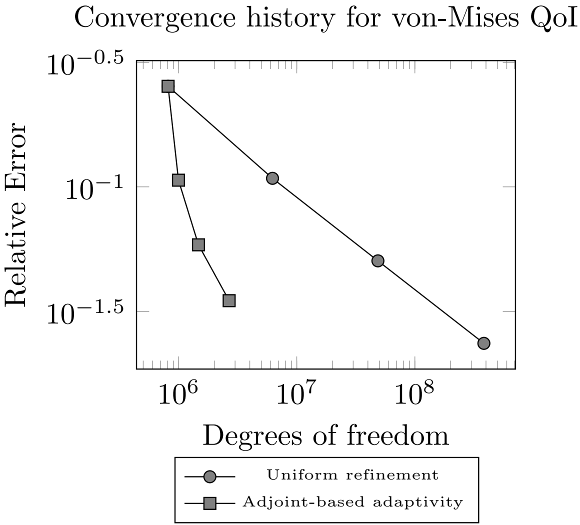
Applications to finite deformation mechanics

Elastoplasticity in an array of solder joints : errors



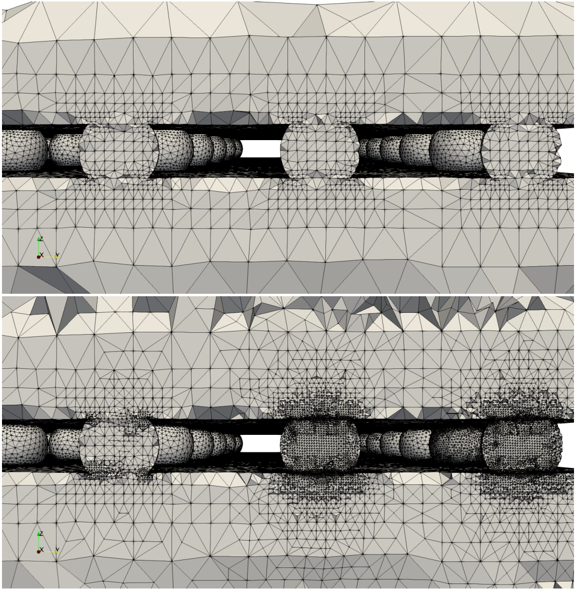
Elastoplasticity in an array of solder joints : convergence

$4\times$ Solve primal $\rightarrow$ Solve adjoint $\rightarrow$ Estimate error $\rightarrow$ Adapt mesh

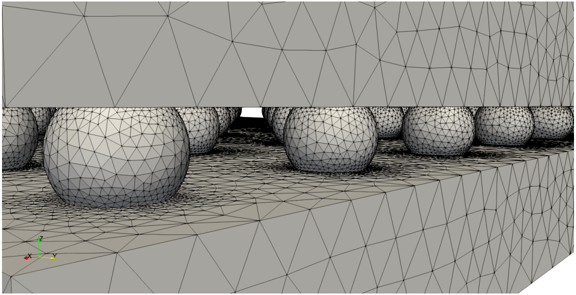


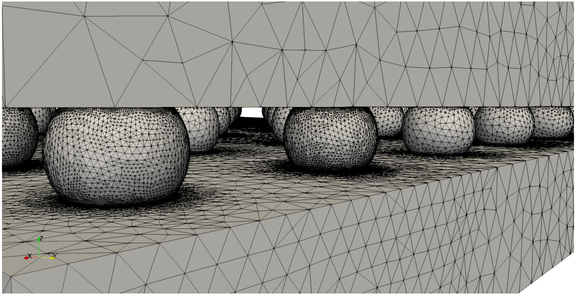
Applications to finite deformation mechanics

Elastoplasticity in an array of solder joints : adaptation



Elastoplasticity in an array of solder joints : adaptation





Adjoint solution must be represented in richer FEM space

Full global enriched adjoint solve

- Guaranteed more accurate adjoint approximation
- Expensive proposition

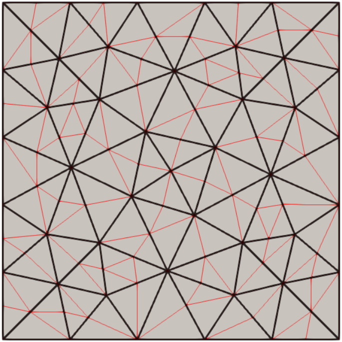
Reconstruction of adjoint problem in richer space

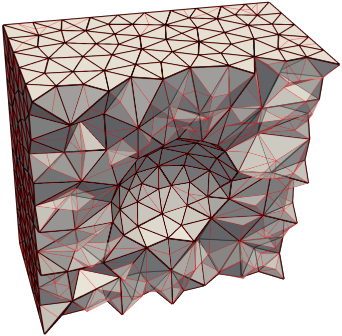
- More practical approach
- Not guaranteed to yield more accurate adjoint

Compromise? Solve adjoint globally on non-uniformly refined meshes

- Less computationally expensive
- Still maintains more accuracy in adjoint approximation

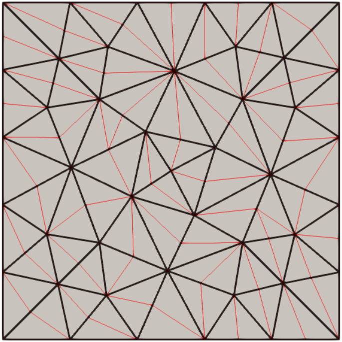
Mark longest edge in each element for refinement

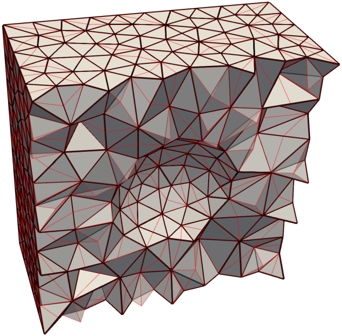




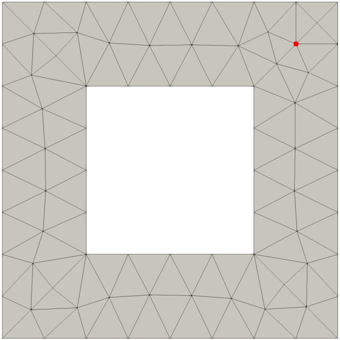
Single edge refinement

Attempt to mark only a single edge in each element for refinement





Application to Poisson's equation



Initial mesh and point-wise QoI location for the Poisson example problem

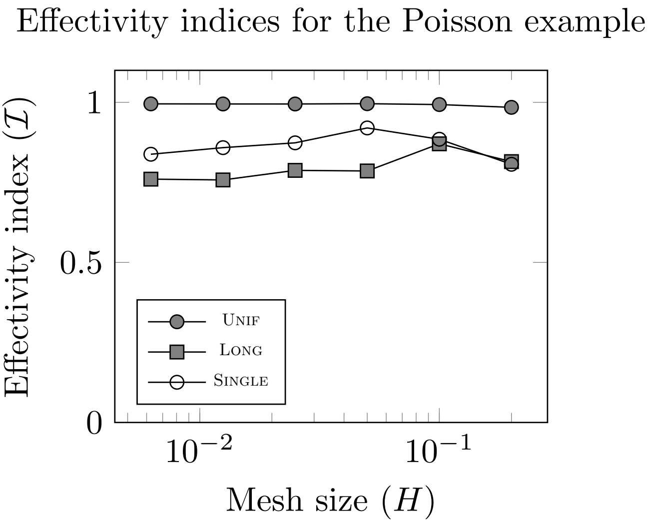
$$R(w, u) := (\nabla w, \nabla u) - (w, f)$$

$$f := 1$$

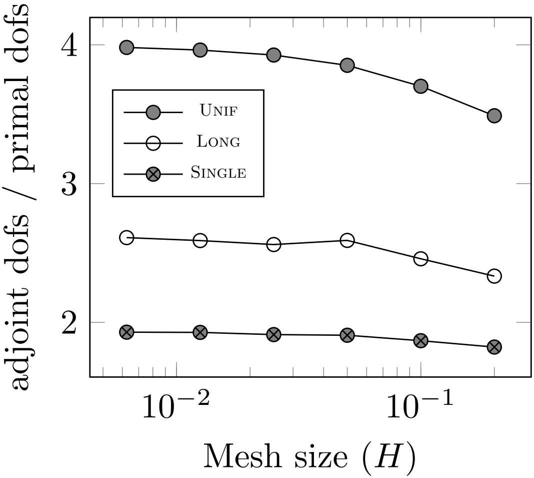
$$J(u) := u(0.75, 0.75)$$

Compare adjoint-based error estimation when solving the adjoint problem with meshes obtained with:

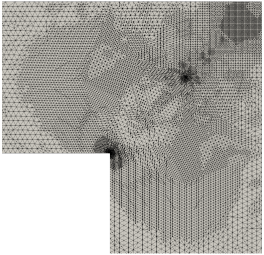
- Uniform refinement
- Long-edge refinement
- Single-edge refinement


Effectivity indices for the Poisson example
Effectivity index ($\mathcal{I}$)
1
0.5
0
10^{-2}
10^{-1}
Mesh size (H)
UNIF
LONG
SINGLE

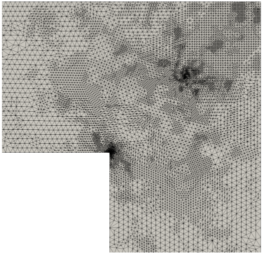
Effectivity indices for the Poisson example



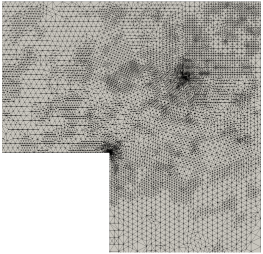
Final adapted meshes when adjoint problem solved with



Uniform



Long-edge



Single-edge

Main takeaway?

Goal application: extensible, usable for novel research.

VMS method : decompose solution, $u = u^h + u'$.
u^h : coarse scale component.
u' : fine scale components.

For linear variational problems: $\mathcal{L}u = f$,
Strong form residual: $\mathcal{R}u := f - \mathcal{L}u$,

$$B(w^h, u^h) + B(w^h, u') = (w^h, f) \quad \forall w^h \in V^h$$
$$B(w', u^h) + B(w', u') = (w', f) \quad \forall w' \in V'$$

Idea : solve or approximately u' analytically.
Solve for u^h numerically accounting for effect of u' on u^h.

Let $J(u) = \int_\Omega j(\boldsymbol{x}) u \, \mathrm{d}V$
Adjoint problem: $\mathcal{L}^* z = j$
Strong form adjoint residual: $\mathcal{R}^* z := j - \mathcal{L}^* z$

VMS method : immediately suggests two approaches for error estimation:

1. Use fine scale solution directly, $\eta_1 = J(u) - J(u^H) = J(u')$
2. Solve adjoint problem on same space as primal problem, but enrich it with VMS method $z = z^h + z'$.

$u' \approx \tau_e \mathcal{R} u^h$
$z' \approx \tau_e^* \mathcal{R}^* z^h$

Two error estimates:

$$\eta_1 = J(u) - J(u^h) \approx (j(\boldsymbol{x}), \tau_e \mathcal{R} u^h)$$

$$\eta_2 = J(u) - J(u^h) \approx -(\tau_e^* \mathcal{R}^* z^h, \mathcal{R} u^h) + (\mathcal{L}^* z^h, \tau_e \mathcal{R} u^h)$$

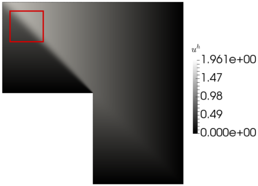
Remarkably, the two error estimates are identical
(when commonly used approximation for u', z' is used)

However, when decomposed into contributions at the element-level
The two error estimates have drastically different behavior

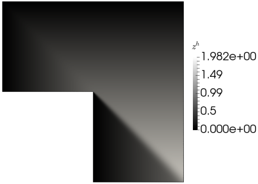
Advection diffusion in L-shaped domain:
$\kappa = 0.001$, $\boldsymbol{\alpha} = [-1, 1], f = 1$.

Two QoIS : $J_1(u) = \int_\Omega u \mathrm{d}V$, $J_2(u) = \int_\Omega q_2 u \mathrm{d}V$.

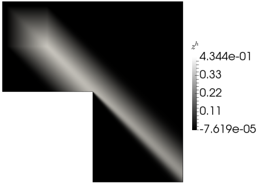
$q_2 := 1$ inside red square and 0 outside



Primal



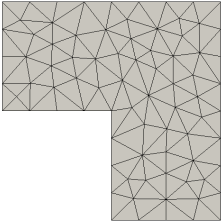
Adjoint ($J_1(u)$)



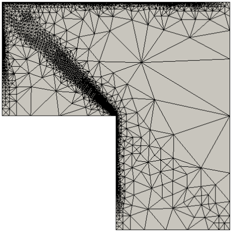
Adjoint ($J_2(u)$)

Application to advection diffusion : $J_1(u)$ meshes

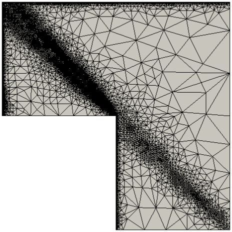
Initial mesh



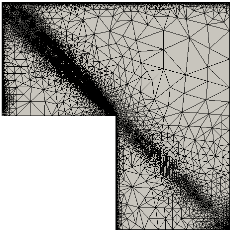
SPR



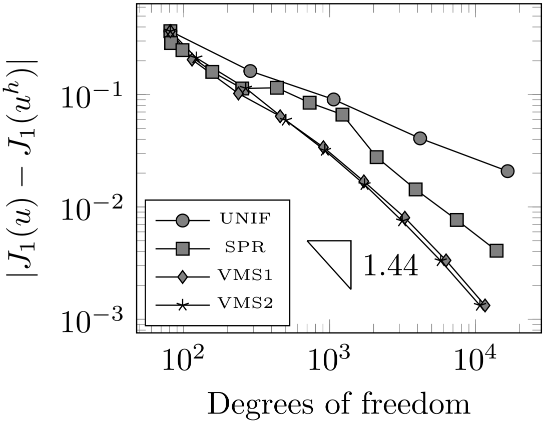
VMS (η_1)



VMS (η_2)

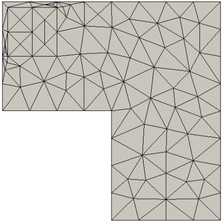


Application to advection diffusion : $J_1(u)$ convergence

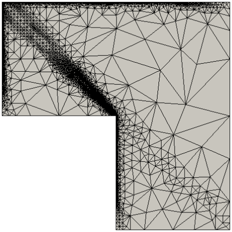


Application to advection diffusion : $J_2(u)$ meshes

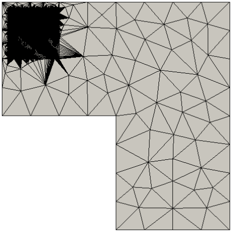
Initial mesh



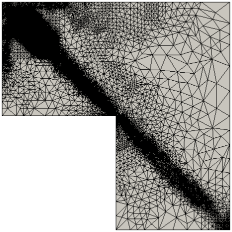
SPR



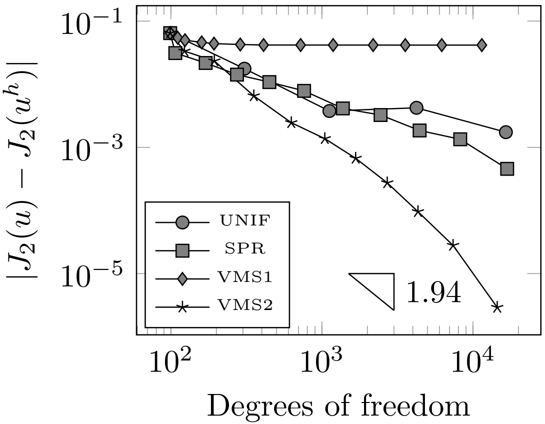
VMS (η_1)



VMS (η_2)



Application to advection diffusion : $J_2(u)$ convergence



Summary

- Developed automated approach for adjoint-based error estimation
- That is applicable to low-order stabilized FEM methods
- And we've applied to finite deformation solid mechanics
- And also used to investigate adjoint solves on non-uniformly refined meshes
- Novel investigation of adjoint error estimation in VMS methods

Future Work

- Extend automated approach to higher order FEM (Taylor-Hood elements)
- Consider load-stepping / truly dynamic behavior in solid mechanics
- Extend VMS method to non-linear variational problems / QoIs
- Wrap-in VMS method into the Goal application for solid mechanics

Questions? Thank you!