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A Goal-oriented Approach to Model Form Error for Constitutive Models

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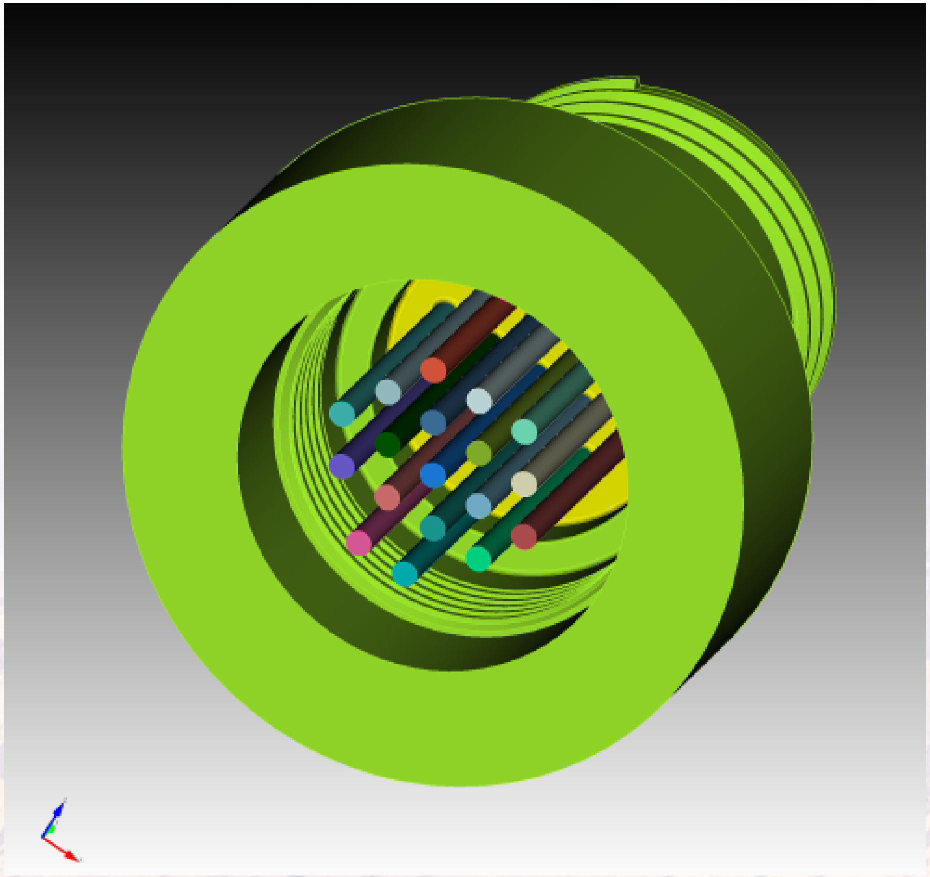
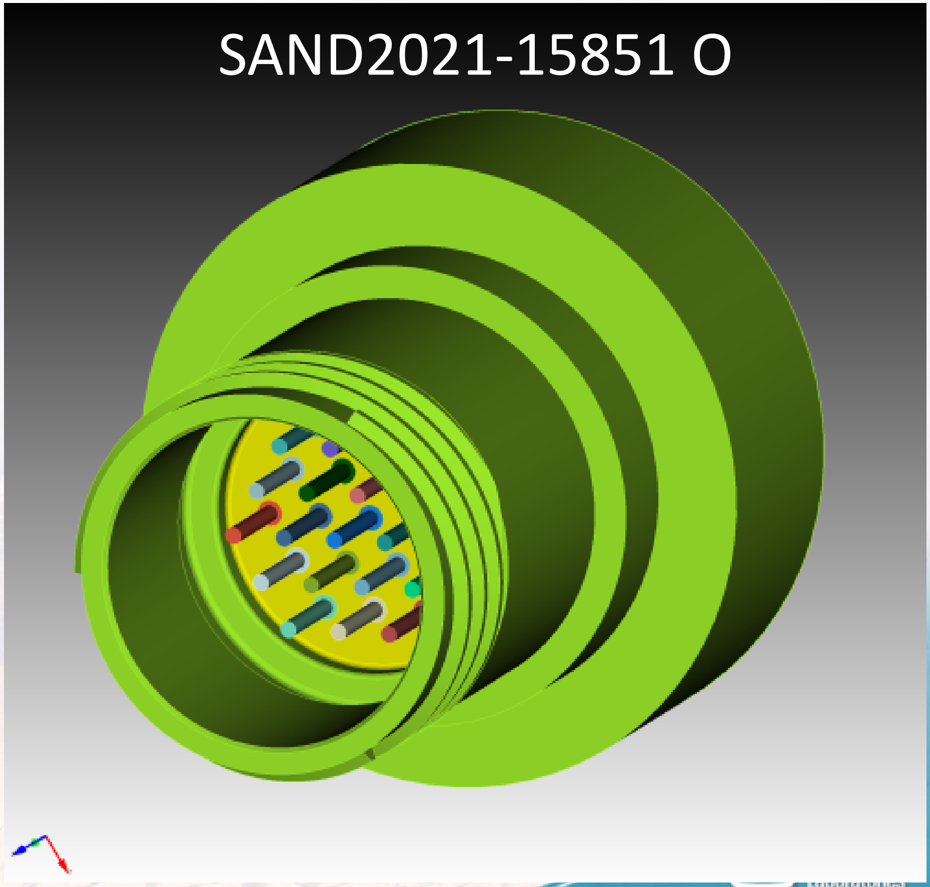
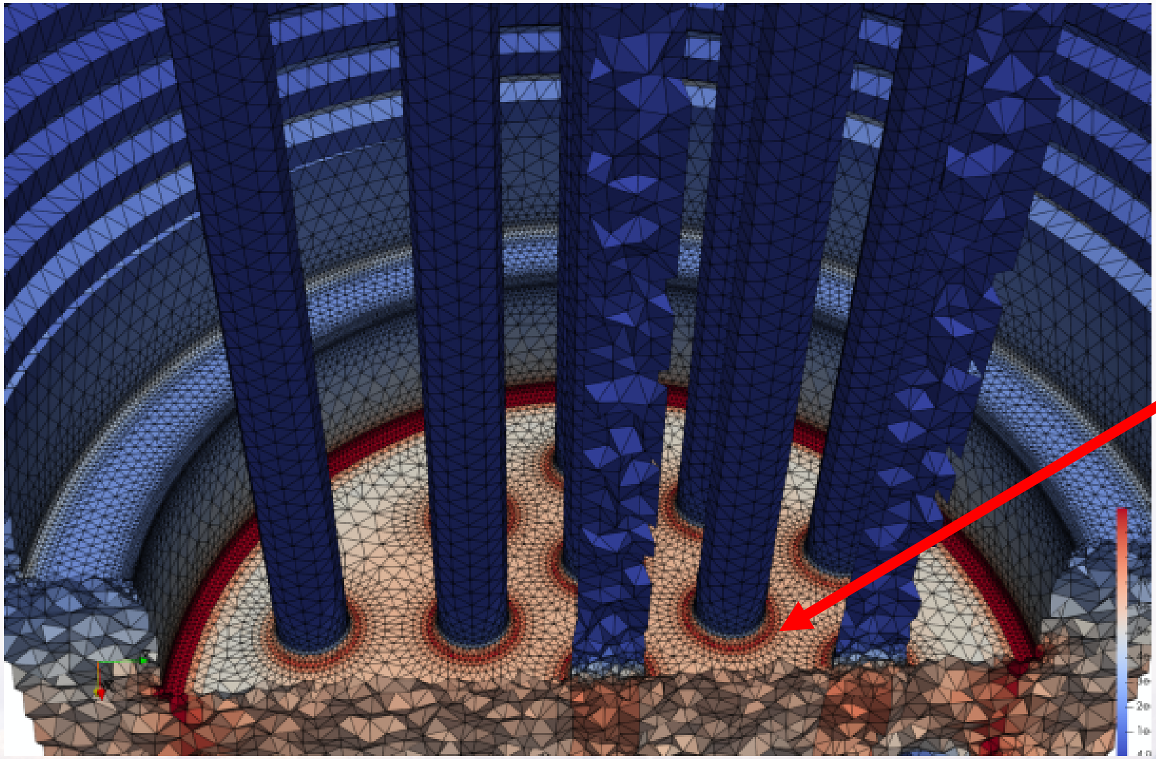
Motivating Application: Glass to Metal Seals

The connector is uniformly cooled from 600 ℃ to room temperature, which causes stresses to build up due to differing coefficients of thermal expansion.





Motivating Application: Glass to Metal Seals



"Interesting" phenomena at material interfaces

Several constitutive models with varying fidelities exist for the glass and metals.

How can we quantify the impact of this modeling choice?

Goal-oriented Error Estimation I

- Classical, *a priori* FEM error estimates are given in terms of solution norms:

$$\|\boldsymbol{u} - \boldsymbol{u}^h\| \leq c\, h^{\alpha} \|\boldsymbol{u}\|_r$$

- These are not computable because they require knowing the exact solution.

- Typically an analyst is interested in quantity of interest (QoI) that is some functional of the solution.

Goal-oriented Error Estimation II

- Goal-oriented error estimation provides computable estimates of error in a quantity of interest (QoI) and has most often been studied for discretization errors.

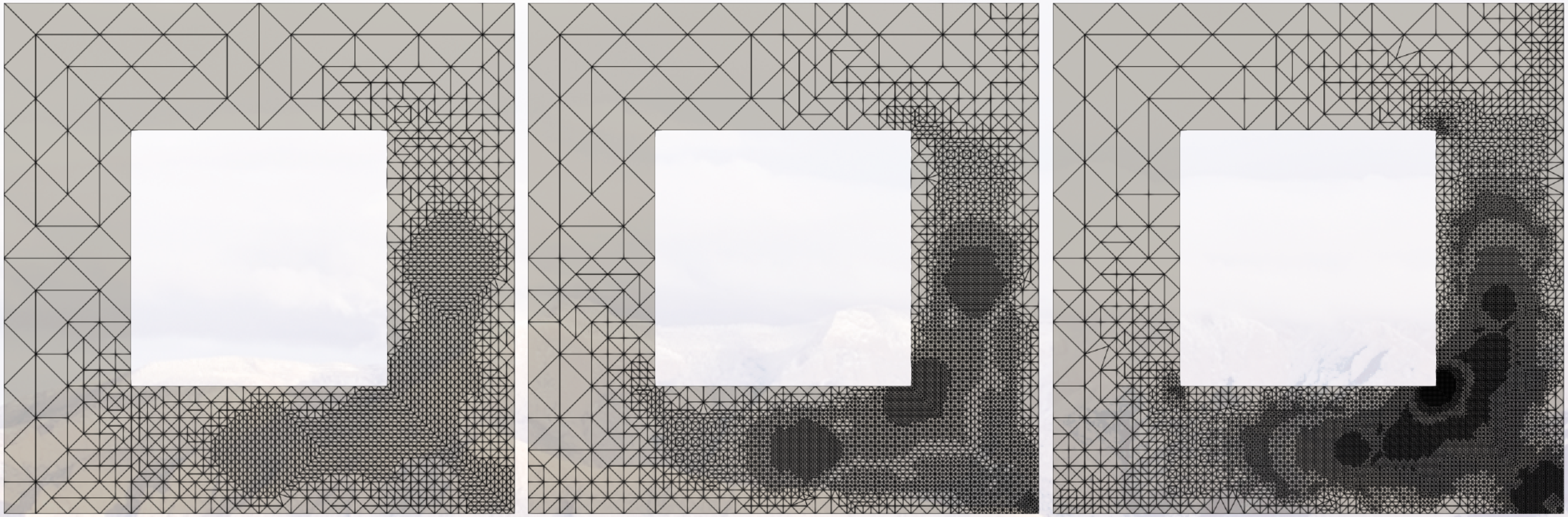


Figure 14: Sequence of meshes obtained for the example problem with gradient singularities for $\mathcal{J}_2(u)$ using either the estimate η_1 or η_2 at the third (left), fourth (center), and fifth (right) adaptive iterations.

https://arxiv.org/pdf/2305.15285.pdf

Goal-oriented Model Form Error Estimation for Constitutive Models

- Key idea: express the two physical models in terms of coupled residuals:

- Equilibrium PDE (nodes) and constitutive model evolution equations (quadrature points).
- Coarse scale (M):

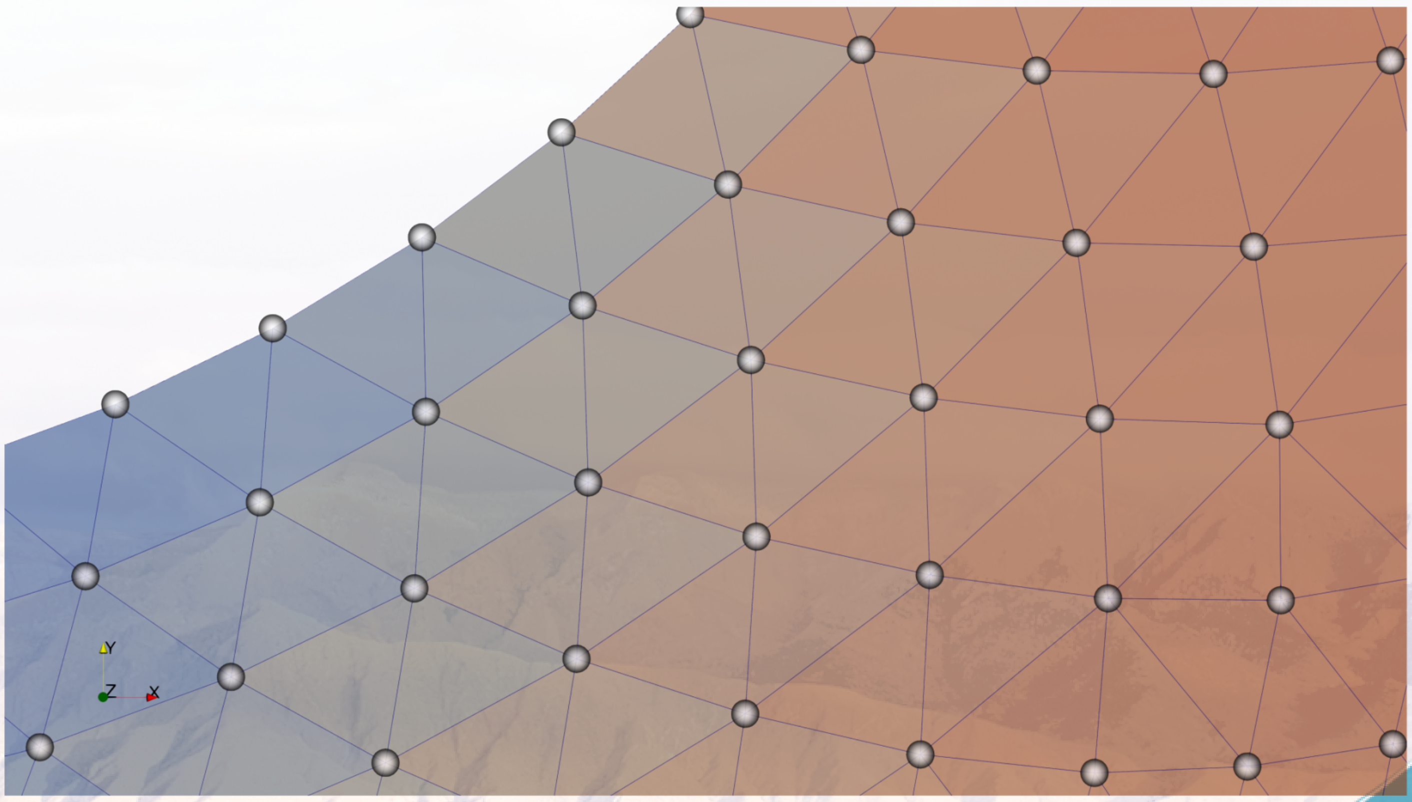
$$\boldsymbol{R}_n^M(\boldsymbol{U}_n^M, \xi_n^M) = \mathbf{0}, \qquad n = 1, 2, \ldots, N_L,$$
$$\boldsymbol{C}_n^M(\boldsymbol{U}_n^M, \xi_n^M, \boldsymbol{U}_{n-1}^M, \xi_{n-1}^M) = \mathbf{0}, \qquad n = 1, 2, \ldots, N_L.$$

- Fine scale (m):

$$\boldsymbol{R}_n^m(\boldsymbol{U}_n^m, \xi_n^m) = \mathbf{0}, \qquad n = 1, 2, \ldots, N_L,$$
$$\boldsymbol{C}_n^m(\boldsymbol{U}_n^m, \xi_n^m, \boldsymbol{U}_{n-1}^m, \xi_{n-1}^m) = \mathbf{0}, \qquad n = 1, 2, \ldots, N_L.$$

Goal-oriented Model Form Error Estimation for Constitutive Models

- Global state variables $\boldsymbol{U}$ live at nodes.
- Local state variables $\boldsymbol{\xi}$ live at quadrature points.



Error Estimate Math I

- Define prolongation operators (note the $'$):

$$\boldsymbol{U}'_n := [\boldsymbol{I}^m_M]^{\boldsymbol{U}} \boldsymbol{U}^M_n,$$
$$\boldsymbol{\xi}'_n := [\boldsymbol{I}^m_M]^{\boldsymbol{\xi}} \boldsymbol{\xi}^M_n.$$

- Fine scale quantity of interest (QoI):

$$\mathcal{Q}' = \sum_{n=1}^{N_L} \mathcal{Q}^m_n(\boldsymbol{U}'_m, \boldsymbol{\xi}'_m).$$

- Expand $\mathcal{Q}^m - \mathcal{Q}'$ in a Taylor series:

$$\mathcal{Q}^m - \mathcal{Q}' = \sum_{n=1}^{N_L} \left\{ \left(\frac{\partial \mathcal{Q}^m_n}{\partial \boldsymbol{U}^m_n}\right)' (\boldsymbol{U}^m_n - \boldsymbol{U}'_n) + \left(\frac{\partial \mathcal{Q}^m_n}{\partial \boldsymbol{\xi}^m_n}\right)' (\boldsymbol{\xi}^m_n - \boldsymbol{\xi}'_n) + E^{\mathcal{Q}_n}_L \right\}.$$

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Error Estimate Math II

- Expand the global and local constraints in Taylor series:

$$\boldsymbol{R}_n^m(\boldsymbol{U}_n^m, \xi_n^m) = \boldsymbol{R}'_n + \left(\frac{\partial \boldsymbol{R}_n^m}{\partial \boldsymbol{U}_n^m}\right)' (\boldsymbol{U}_n^m - \boldsymbol{U}'_n) + \left(\frac{\partial \boldsymbol{R}_n^m}{\partial \xi_n^m}\right)' (\xi_n^m - \xi'_n) + E_L^{\boldsymbol{R}_n},$$

$$\begin{aligned} \boldsymbol{C}_n^m(\boldsymbol{U}_n^m, \xi_n^m, \boldsymbol{U}_{n-1}^m, \xi_{n-1}^m) &= \boldsymbol{C}'_n + \left(\frac{\partial \boldsymbol{C}_n^m}{\partial \boldsymbol{U}_n^m}\right)' (\boldsymbol{U}_n^m - \boldsymbol{U}'_n) \\ &+ \left(\frac{\partial \boldsymbol{C}_n^m}{\partial \xi_n^m}\right)' (\xi_n^m - \xi'_n) + \left(\frac{\partial \boldsymbol{C}_n^m}{\partial \boldsymbol{U}_{n-1}^m}\right)' (\boldsymbol{U}_{n-1}^m - \boldsymbol{U}'_{n-1}) \\ &+ \left(\frac{\partial \boldsymbol{C}_n^m}{\partial \xi_{n-1}^m}\right)' (\xi_{n-1}^m - \xi'_{n-1}) + E_L^{\boldsymbol{C}_n}. \end{aligned}$$

Error Estimate Math III

- Adjoint system for a single (non-terminal) loadstep:

$$\left(\frac{\partial \boldsymbol{R}_n^m}{\partial \boldsymbol{U}_n^m}\right)^{T\prime} \boldsymbol{Z}_n^m + \left(\frac{\partial \boldsymbol{C}_n^m}{\partial \boldsymbol{U}_n^m}\right)^{T\prime} \phi_n^m = -\left(\frac{\partial \mathcal{Q}_n^m}{\partial \boldsymbol{U}_n^m}\right)' - \left(\frac{\partial \boldsymbol{C}_{n+1}^m}{\partial \boldsymbol{U}_n^m}\right)^{T\prime} \phi_{n+1}^m,$$

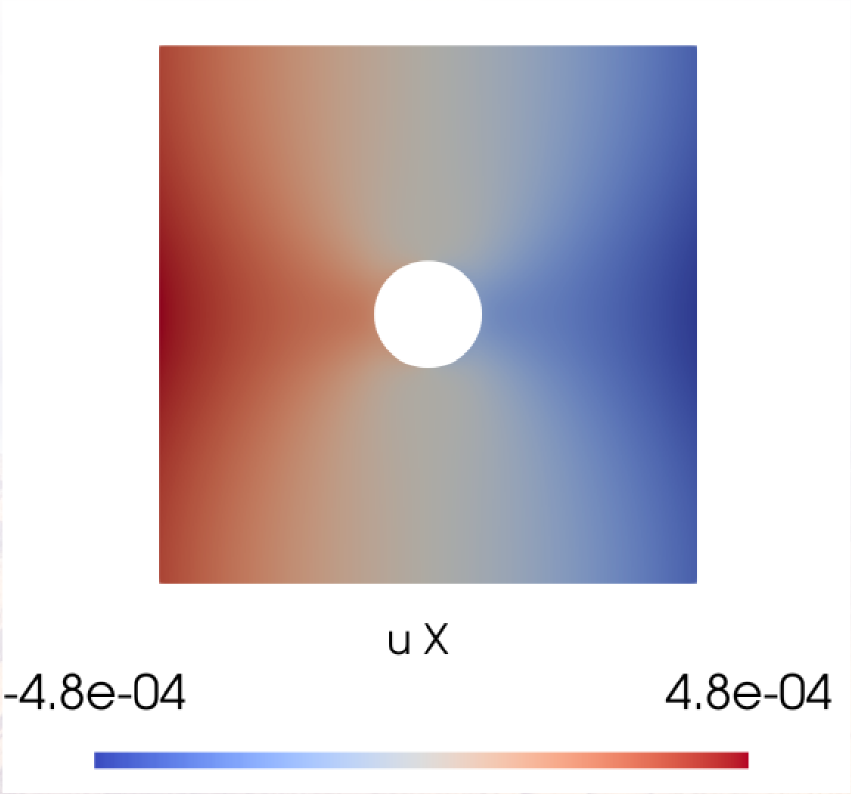
$$\left(\frac{\partial \boldsymbol{R}_n^m}{\partial \boldsymbol{\xi}_n^m}\right)^{T\prime} \boldsymbol{Z}_n^m + \left(\frac{\partial \boldsymbol{C}_n^m}{\partial \boldsymbol{\xi}_n^m}\right)^{T\prime} \phi_n^m = -\left(\frac{\partial \mathcal{Q}_n^m}{\partial \boldsymbol{\xi}_n^m}\right)' - \left(\frac{\partial \boldsymbol{C}_{n+1}^m}{\partial \boldsymbol{\xi}_n^m}\right)^{T\prime} \phi_{n+1}^m.$$

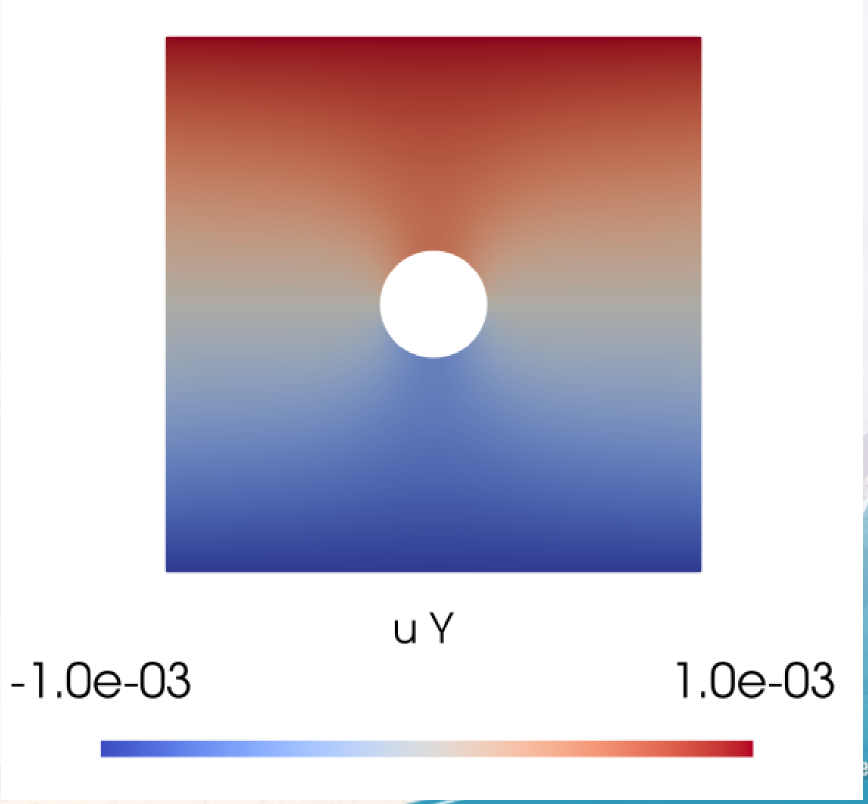
- Compute element-level error contributions η^e:

$$\eta^e = (\boldsymbol{Z}_n^e)^T \underbrace{(\boldsymbol{R}_n^e)'}_{=\boldsymbol{0}} + (\phi_n^e)^T (\boldsymbol{C}_n^e)'.$$

Proof-of-Concept Demonstration

- "Hello world!" for goal-oriented MFE estimation:
  - Two linear elastic models (plane strain, quarter symmetry):
    - Coarse model: E = 200 GPa , υ = 0.3 .
    - Fine model: E = 150 GPa , υ = 0.25 .
  - Local state variable: Cauchy stress.
  - QoI: Average of displacement components (in quarter).





Verification Check

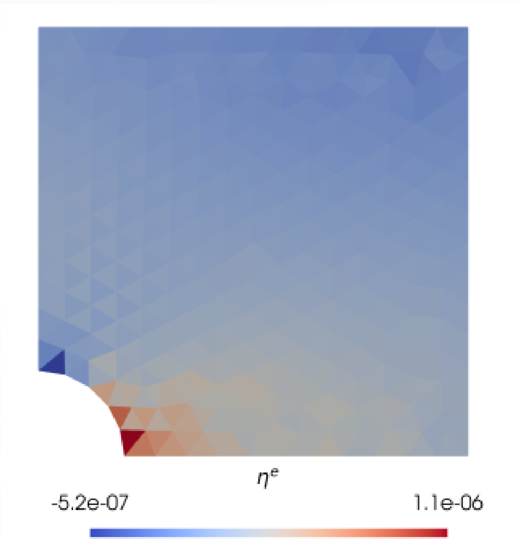
- Compute $Q^m - Q^M$ two ways:
  1. Solve the forward problem twice (E_exact).
  2. Compute the adjoint-based estimate (E_computed):
     1. Solve the forward problem with the "M" model.
     2. Solve the adjoint problem with the "m" model (always linear).
     3. Compute the element-level error estimates η^e and sum.

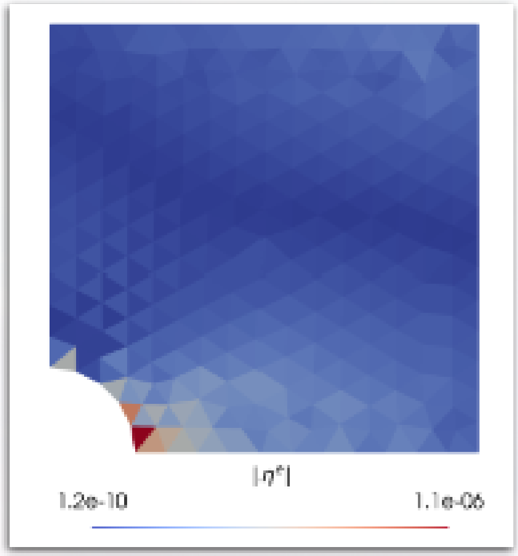
- Code output:

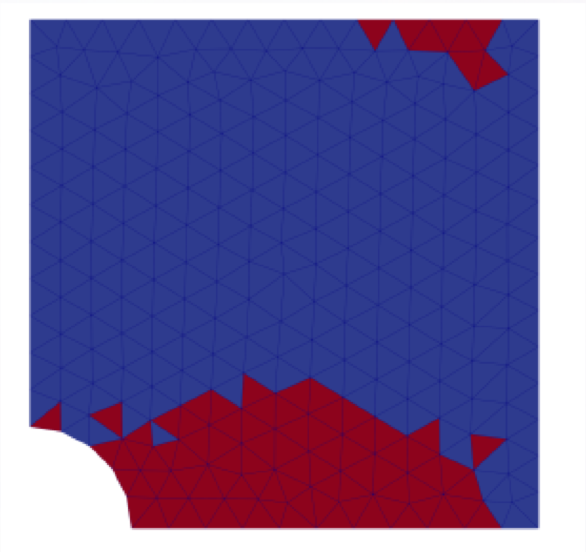
```
Q^M: 1.6118517806566819e-04
Q^m: 1.8159857938902549e-04

E_exact: 2.0413401323357300e-05
E_computed: 2.0413401323357283e-05

E_computed - E_exact: 2.3716922523120409e-20
E_computed / E_exact: 1.0000000000000011e+00
```

Error Localization and Adaptivity

- Estimate, localize, mark, and refine:





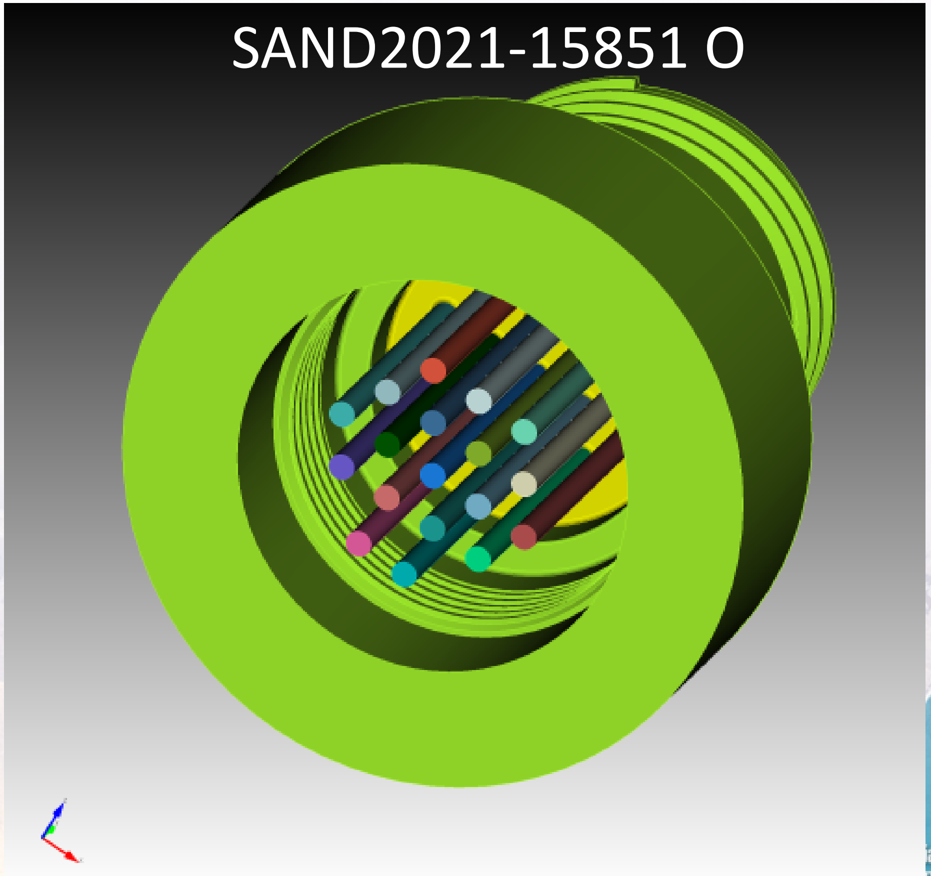


base model (M)
fine model (m)

```
Q^m: 1.8159857938902549e-04

First solve/estimate:

  Q^M: 1.6118517806566819e-04

  error estimate: 2.0413401323357283e-05
  error bound:  < 5.0339224699379316e-05

89 ELEMENTS MARKED FOR REFINEMENT

Second solve/estimate:

  Q^M: 1.8205643929058302e-04

  error estimate: -4.5785990155757729e-07
  error bound: < 2.3044739576808756e-05
```

Motivating Application: Glass to Metal Seals

The connector is uniformly cooled from 600 ℃ to room temperature, which causes stresses to build up due to differing coefficients of thermal expansion.



Adjoints required:

- Pins and shell: metal elastoplasticity — https://doi.org/10.1002/nme.6843 .
- Glass: thermoviscoelastic.

Thermoviscoelastic Materials I

- Time-varying, temperature-dependent material response.
- Important for modeling of aging components.
- Linear constitutive model:

$$\begin{aligned}\dot{\sigma}_{ij} &= K^{\infty}\left(\dot{\varepsilon}_{kk} - 3\alpha^{\infty}\dot{T}\right)\delta_{ij} + 2\mu^{\infty}\dot{\varepsilon}'_{ij} \\ &+\Delta K\,\dot{J}^{1}\delta_{ij} - 3\Delta\left(\alpha K\right)\dot{J}^{3}\delta_{ij} + 2\Delta\mu\dot{J}^{2}_{ij}.\end{aligned}$$

Lester and Long 2020, SAND2020-4973R .

- Hereditary integrals:

$$J^{1} = \sum_{n=1}^{n_v} w_k^v J^{1(k)}, \qquad J^{1(k)} = \int_0^t \exp\left(-\frac{t^* - s^*}{\tau_k^v}\right)\frac{\partial \varepsilon_{mm}}{\partial s} ds, \qquad t^* = \int_0^t \frac{ds}{a\left(s\right)}$$

Thermoviscoelastic Materials II

- Hereditary integral discrete evolution equation:

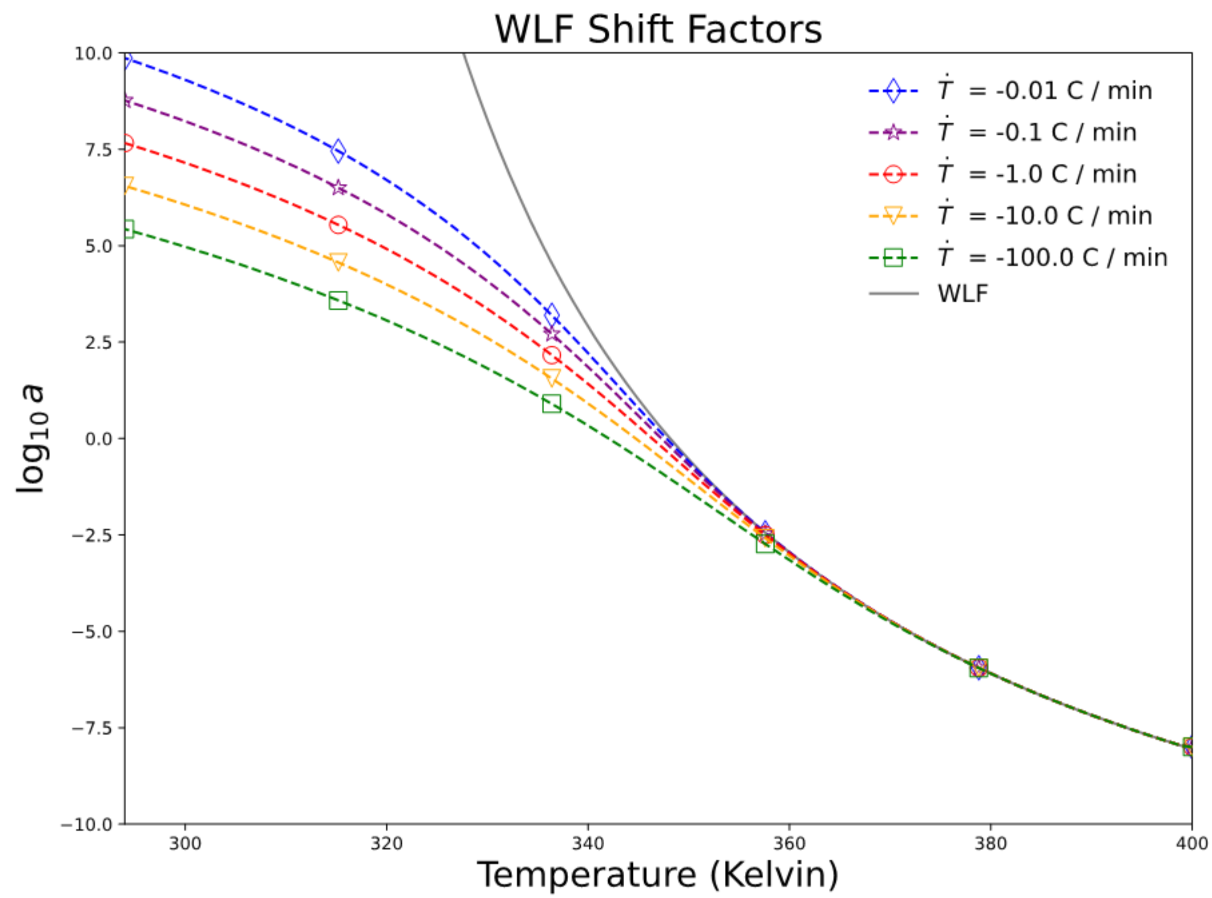
$$J_{n+1}^{1(k)} = \frac{a^{n+1}\tau_k^v}{a^{n+1}\tau_k^v + \Delta t}\left(J_n^{1(k)} + \Delta t \dot{\varepsilon}_{mm}^{n+1}\right).$$

- Shift factor:

$$\log_{10} a^{\mathrm{WLF\_Lag}} = \frac{-C_1\left(T - T_{\mathrm{ref}} - \int_0^t f_v\left(t^* - s^*\right)\frac{\partial T}{\partial s} ds\right)}{C_2 + \left(T - T_{\mathrm{ref}} - \int_0^t f_v\left(t^* - s^*\right)\frac{\partial T}{\partial s} ds\right)}.$$

Thermoviscoelastic Materials III

- Shift factor temperature dependence:



Thermoviscoelastic Materials IV

- Prony series:

Term	τ_k^v (s)	w_k^v (-)	τ_k^s (s)	w_k^s (-)
1	1.0×10^{-10}	1.06×10^{-2}	1.0×10^{-10}	4.96×10^{-3}
2	1.0×10^{-9}	1.14×10^{-2}	1.0×10^{-9}	6.85×10^{-3}
3	1.0×10^{-8}	1.64×10^{-2}	1.0×10^{-8}	1.14×10^{-2}
4	1.0×10^{-7}	2.27×10^{-2}	1.0×10^{-7}	1.97×10^{-2}
5	1.0×10^{-6}	2.63×10^{-2}	1.0×10^{-6}	2.64×10^{-2}
6	3.16×10^{-6}	8.85×10^{-3}	3.16×10^{-6}	1.13×10^{-2}
7	1.0×10^{-5}	2.52×10^{-2}	1.0×10^{-5}	2.98×10^{-2}
8	3.16×10^{-5}	1.94×10^{-2}	3.16×10^{-5}	2.75×10^{-2}
9	1.0×10^{-4}	2.80×10^{-2}	1.0×10^{-4}	4.02×10^{-2}
10	3.16×10^{-4}	2.83×10^{-2}	3.16×10^{-4}	4.58×10^{-2}
11	1.0×10^{-3}	3.41×10^{-2}	1.0×10^{-3}	5.76×10^{-2}
12	3.16×10^{-3}	3.70×10^{-2}	3.16×10^{-3}	6.74×10^{-2}
13	1.0×10^{-2}	4.19×10^{-2}	1.0×10^{-2}	7.90×10^{-2}
14	3.16×10^{-2}	4.58×10^{-2}	3.16×10^{-2}	8.85×10^{-2}
15	1.0×10^{-1}	5.02×10^{-2}	1.0×10^{-1}	9.56×10^{-2}
16	3.16×10^{-1}	5.39×10^{-2}	3.16×10^{-1}	9.72×10^{-2}
17	1.0×10^{-0}	5.71×10^{-2}	1.0×10^{-0}	9.17×10^{-2}
18	3.16×10^{-0}	5.93×10^{-2}	3.16×10^{-0}	7.79×10^{-2}
19	1.0×10^{1}	6.03×10^{-2}	1.0×10^{1}	5.75×10^{-2}
20	3.16×10^{1}	5.97×10^{-2}	3.16×10^{1}	3.49×10^{-2}
21	1.0×10^{2}	5.72×10^{-2}	1.0×10^{2}	1.63×10^{-2}
22	3.16×10^{2}	5.30×10^{-2}	3.16×10^{2}	5.26×10^{-3}
23	1.0×10^{3}	4.66×10^{-2}	1.0×10^{3}	1.05×10^{-3}
24	3.16×10^{3}	3.95×10^{-2}	3.16×10^{3}	8.72×10^{-5}
25	1.0×10^{4}	3.03×10^{-2}	1.0×10^{4}	1.29×10^{-5}
26	3.16×10^{4}	2.34×10^{-2}	1.0×10^{5}	2.67×10^{-6}
27	1.0×10^{5}	1.34×10^{-2}	1.0×10^{-6}	4.17×10^{-7}
28	3.16×10^{5}	1.12×10^{-2}	-	-
29	1.0×10^{6}	1.56×10^{-2}	-	-
30	3.16×10^{6}	4.84×10^{-3}	-	-

Table 2: Prony series fit of the volumetric and deviatoric spectra for verification parameters from fit in Kuether [27].

Thermoviscoelastic Materials V

- Constitutive model:

$$
\begin{aligned}
\sigma_{ij}^{n+1} &= \sigma_{ij}^{n} + \bar{K} d\varepsilon_{kk}\delta_{ij} + 2\bar{\mu} d\varepsilon'_{ij} - 3\left(\bar{\alpha K}\right) dT\delta_{ij} \\
&-\Delta K \Delta t \sum_{n=1}^{n_v} \frac{w_k^v}{a^{n+1}\tau_k^v + \Delta t}\left(J_n^{1(k)} + d\varepsilon_{kk}\right)\delta_{ij} + 3\Delta t \Delta\left(\alpha K\right) \sum_{n=1}^{n_v} \frac{w_k^v}{a^{n+1}\tau_k^v + \Delta t}\left(J_n^{3(k)} + dT\right)\delta_{ij} \\
&-2\Delta\mu\Delta t \sum_{k=1}^{n_s} \frac{w_k^s}{a^{n+1}\tau_k^s + \Delta t}\left(\left(J_{ij}^{2(k)}\right)_n + d\varepsilon'_{ij}\right),
\end{aligned}
$$

- Leads to ~ 200 local state variables… not tractable!

- We have a solution.

Thermoviscoelastic Coupled Formulation

- Original coupled approach:

$$\boldsymbol{R}^n\left(\boldsymbol{U}^n, \boldsymbol{\xi}^n\right) = \boldsymbol{0}, \quad n = 1, \ldots, N_L,$$
$$\boldsymbol{C}_e^n\left(\boldsymbol{U}_e^n, \boldsymbol{U}_e^{n-1}, \boldsymbol{\xi}_e^n, \boldsymbol{\xi}_e^{n-1}\right) = \boldsymbol{0}, \quad e = 1, \ldots, n_{el}, \; n = 1, \ldots, N_L.$$

- New coupled approach:

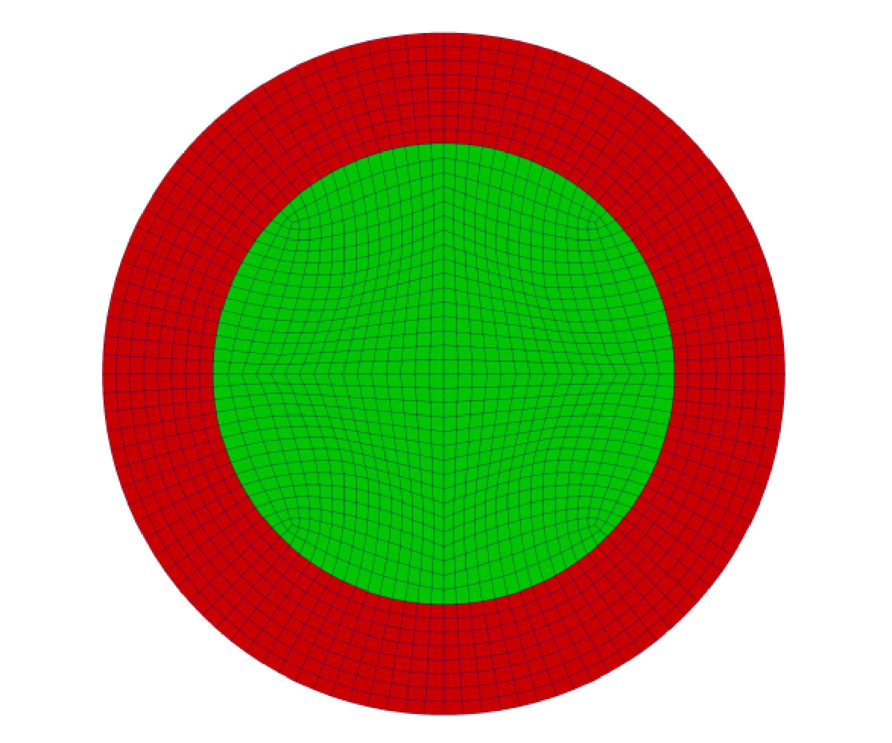
$$\boldsymbol{R}^n\left(\boldsymbol{U}^n, \boldsymbol{\xi}^n\right) = \boldsymbol{0}, \quad n = 1, \ldots, N_L,$$
$$\boldsymbol{C}_e^n\left(\boldsymbol{U}_e^n, \boldsymbol{U}_e^{n-1}, \boldsymbol{\xi}_e^n, \boldsymbol{\xi}_e^{n-1}, \boldsymbol{\chi}_e^{n-1}\right) = \boldsymbol{0}, \quad e = 1, \ldots, n_{el}, \; n = 1, \ldots, N_L,$$
$$\boldsymbol{D}_e^n\left(\boldsymbol{U}_e^n, \boldsymbol{U}_e^{n-1}, \boldsymbol{\chi}_e^n, \boldsymbol{\chi}_e^{n-1}\right) = \boldsymbol{0}, \quad e = 1, \ldots, n_{el}, \; n = 1, \ldots, N_L.$$

- Hereditary integral discrete evolution equation:

$$J_{n+1}^{1(k)} = \frac{a^{n+1}\tau_k^v}{a^{n+1}\tau_k^v + \Delta t}\left(J_n^{1(k)} + \Delta t \dot{\varepsilon}_{mm}^{n+1}\right).$$

Glass-to-Metal Seal Exemplar

- Two materials (low-fidelity / high-fidelity):
  - Glass: thermoelastic / thermoviscoelastic.
  - Metal shell: thermoelastic / thermoplastic.
  - QoI: Average of σ_{rr} or $\sigma_{\theta\theta}$ in the glass near the interface.



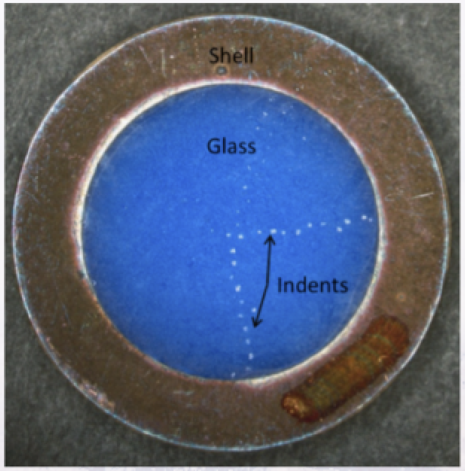


Figure 3. Photo of the Concentric Glass-to-Metal Seal Used for Validation Purposes.

SAND2017-10894

Glass-to-Metal Seal Exemplar

- Two materials (low-fidelity / high-fidelity):
  - Glass: thermoelastic / thermoviscoelastic.
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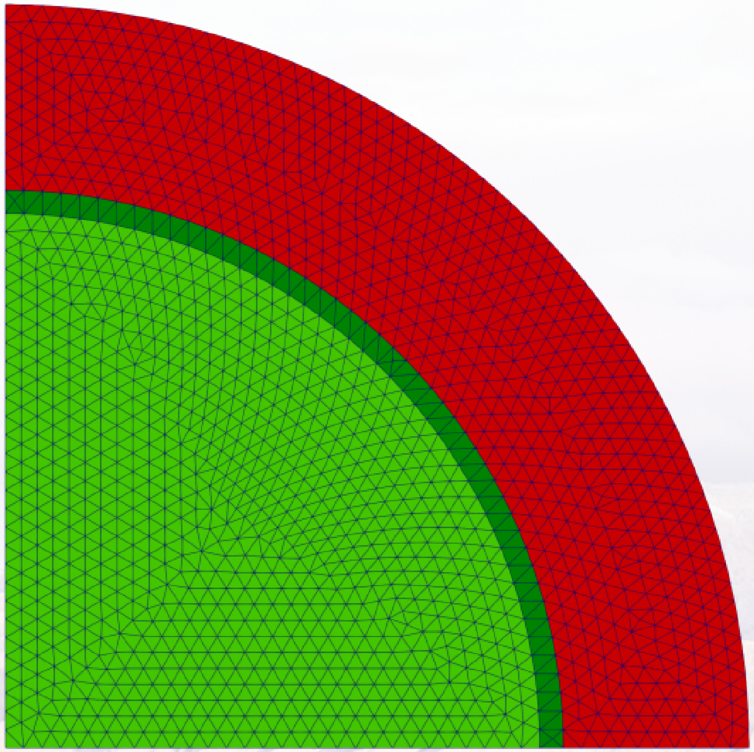
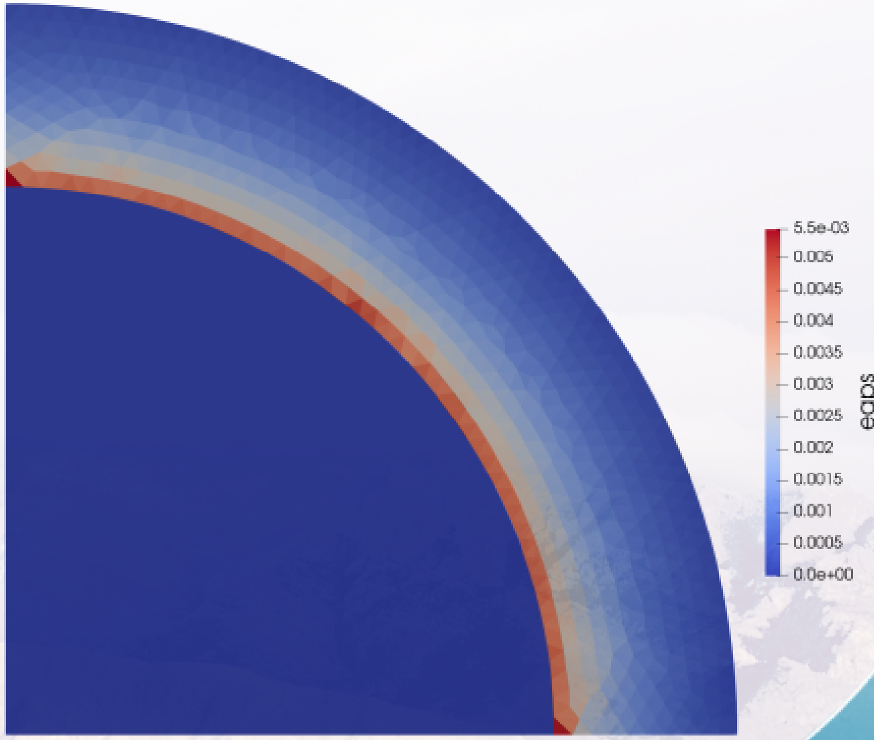


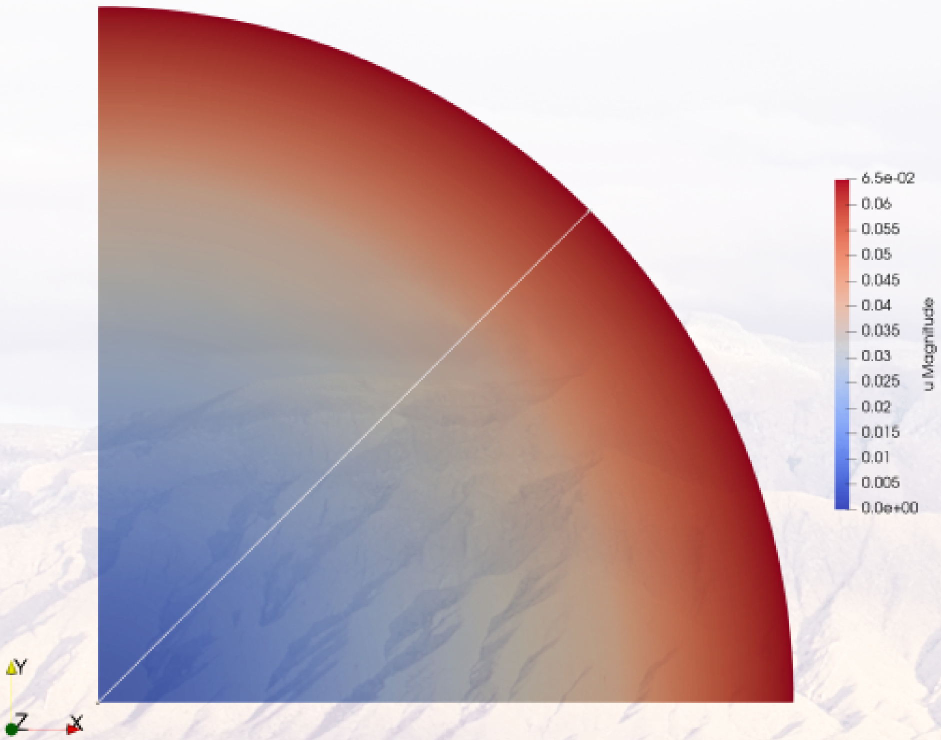
Element blocks

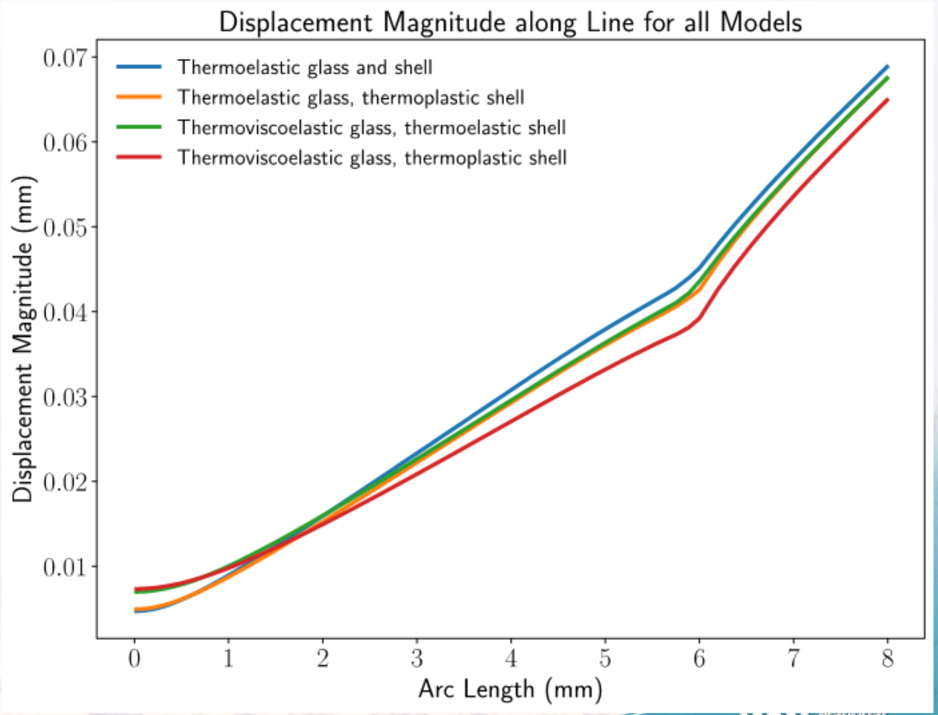


Compression from cooling (plastic)

Glass-to-Metal Seal Exemplar

- Two materials (low-fidelity / high-fidelity):
  - Glass: thermoelastic / thermoviscoelastic.
  - Metal shell: thermoelastic / thermoplastic.
  - QoI: Average of σ_{rr} or $\sigma_{\theta\theta}$ in the glass near the interface.





Glass-to-Metal Seal Exemplar I

- Two materials (low-fidelity / high-fidelity):
  - Glass: thermoelastic .
  - Metal shell: thermoelastic / thermoplastic.
  - **QoI: Average of σ_{rr} in the glass near the interface.**

- Forward solves: coarse + fine times ~ 5.5 min .
  - Q^M = -157 MPa .
  - Q^m = -123 MPa .
  - E_exact = $Q^m - Q^M$ = 34.04 MPa .

- Adjoint-based error estimate: 2.5 min!
  - E_estimated ~ 33.95 MPa .
  - Effectivity = 0.997 .
  - Close estimate at half the cost (46%).

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Glass-to-Metal Seal Exemplar I

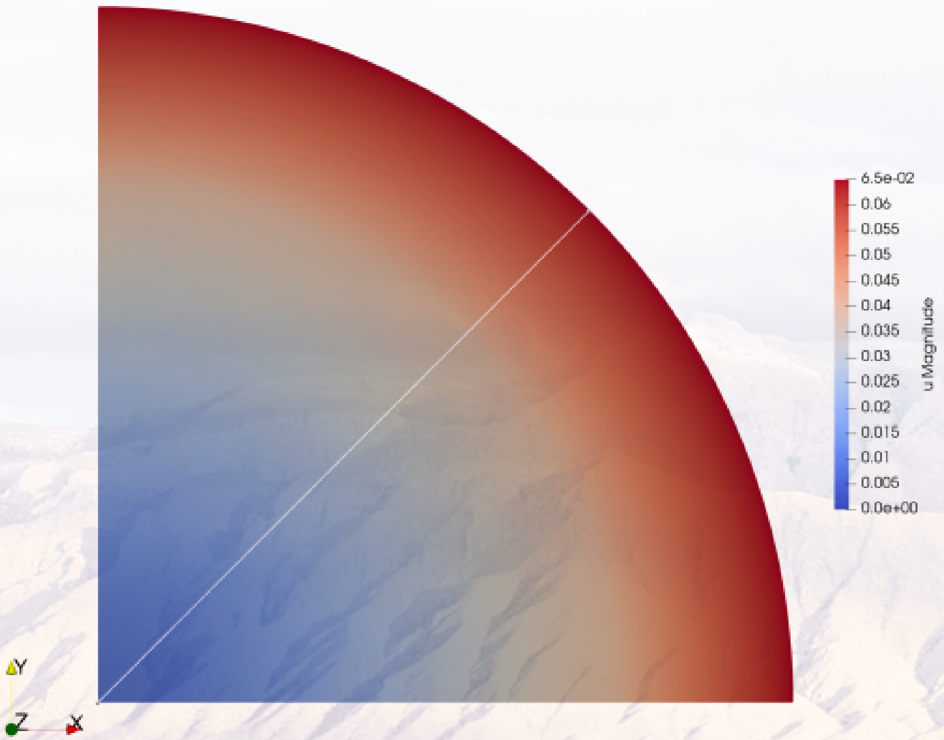
- Two materials (low-fidelity / high-fidelity):
  - Glass: thermoelastic .
  - Metal shell: thermoelastic / thermoplastic.
  - **QoI: Average of $\sigma_{\theta\theta}$ in the glass near the interface.**

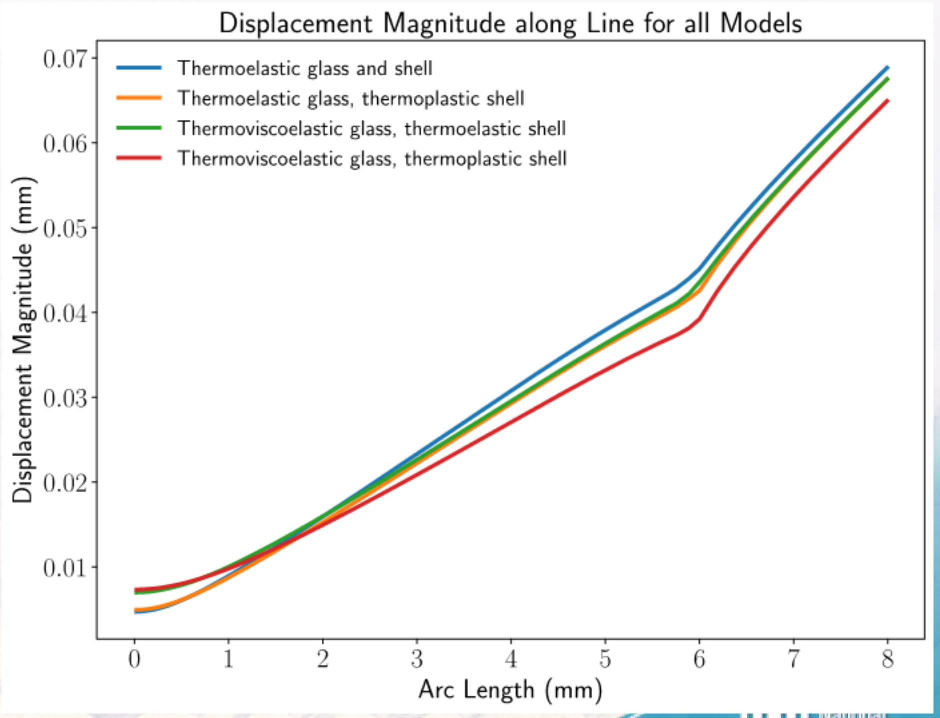
- Forward solves: coarse + fine times ~ 5.5 min .
  - Q^M = -204 MPa .
  - Q^m = -162 MPa .
  - E_exact = $Q^m - Q^M$ = 42.24 MPa .

- Adjoint-based error estimate: 2.5 min!
  - E_computed ~ 40.08 MPa .
  - Effectivity = 0.949 .
  - Close estimate at half the cost (46%).

Glass-to-Metal Seal Exemplar II

- Two materials (low-fidelity / high-fidelity):
  - Glass: thermoelastic / thermoviscoelastic.
  - Metal shell: thermoelastic / thermoplastic.
  - QoI: Average of σ_{rr} or $\sigma_{\theta\theta}$ in the glass near the interface.





Glass-to-Metal Seal Exemplar II

- Two materials (low-fidelity / high-fidelity):
  - Glass: thermoelastic / thermoviscoelastic.
  - Metal shell: thermoelastic / thermoplastic.
  - **QoI: Average of σ_{rr} in the glass near the interface.**

- Forward solves: coarse + fine times ~ 8.66 min .
  - Q^M = -157 MPa .
  - Q^m = -124 MPa .
  - E_exact = $Q^m - Q^M$ = 33.19 MPa .

- Adjoint-based error estimate: 4.33 min!
  - E_estimated ~ 34.10 MPa .
  - Effectivity = 1.03 .
  - Close estimate at half the cost (50%).

Glass-to-Metal Seal Exemplar II

- Two materials (low-fidelity / high-fidelity):
  - Glass: thermoelastic / thermoviscoelastic.
  - Metal shell: thermoelastic / thermoplastic.
  - **QoI: Average of $\sigma_{\theta\theta}$ in the glass near the interface.**

- Forward solves: coarse + fine times ~ 8.66 min .
  - Q^M = -204 MPa .
  - Q^m = -155 MPa .
  - E_exact = $Q^m - Q^M$ = 49.63 MPa .

- Adjoint-based error estimate: 4.33 min!
  - E_estimated ~ 61.88 MPa .
  - Effectivity = 1.25 .
  - Close-ish estimate at half the cost (50%).

Summary and Conclusions

- Goal-oriented constitutive model form error estimation:
  - Split equilibrium PDE and constitutive equations.
  - Solve coupled adjoint problem and use its solution in the error estimate.
  - Possibilities for constitutive model adaptivity.

- Adjoints for thermoviscoelasticity:
  - Hereditary integrals introduce many new local state variables.
  - Our formulation introduces new constraints to minimize storage costs.

- Application to nonlinear glass-to-metal seal problem:
  - Error estimate often close to exact error and costs less to obtain than the brute force approach.

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