An overview of the Moertel package for non-conformal mesh tying or simple contact problems

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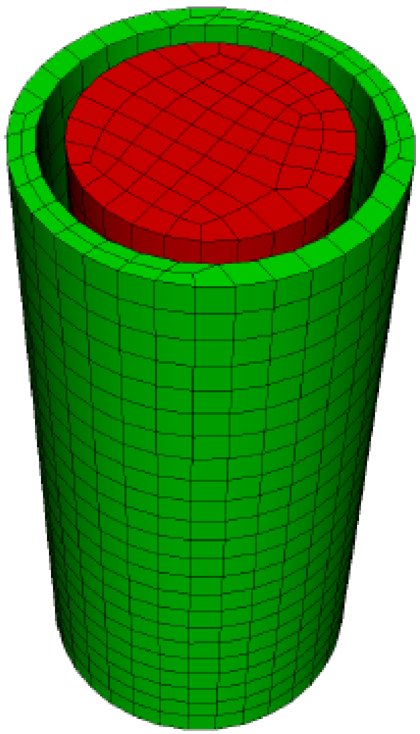
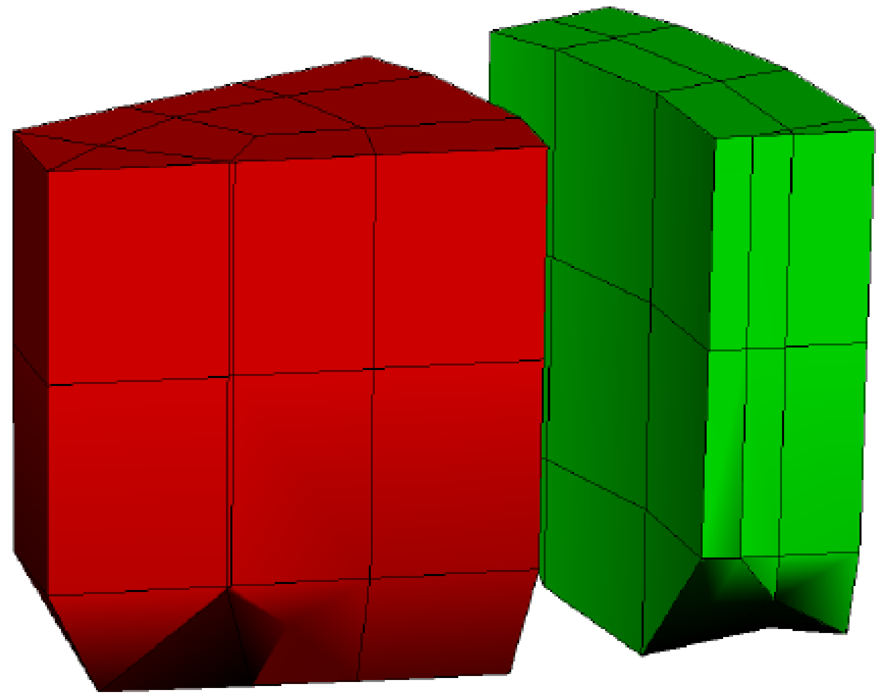
MOERTEL

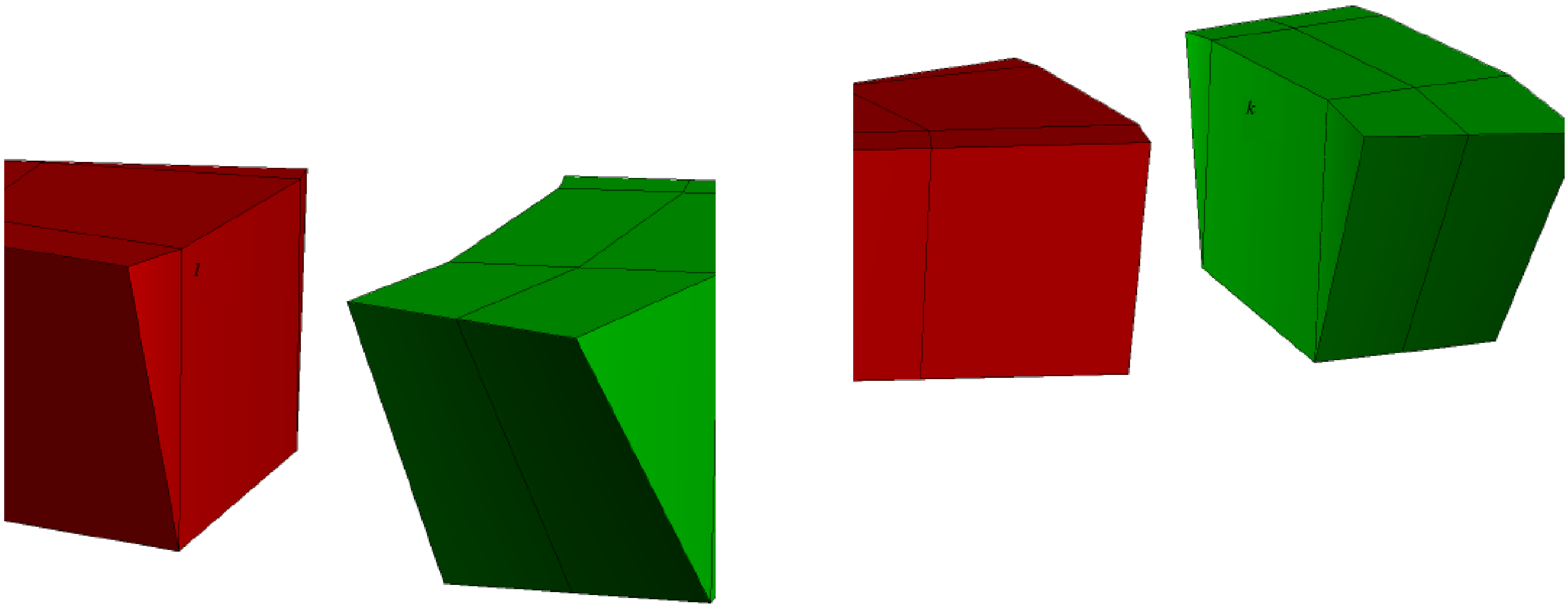
- Moertel is a Trilinos package that supplies capabilities for nonconformal mesh tying and contact formulations in 2 and 3D.
- Mortar methods are a form of Lagrange multiplier constraint useful for contact formulations, mesh tying, and domain decomposition techniques.
- Moertel uses the meshes on the tentatively-contacting interfaces to build the M and D coupling matrices needed to couple nonconformal interfaces in a mortar FE formulation.
- Moertel is German for "mortar," pronounced "mor-del." The package was developed by Michael Gee, now at TUM.

Mortar method basics





Mortar integration space



(a) Pellet view, element face l

(b) Cladding view, element face k

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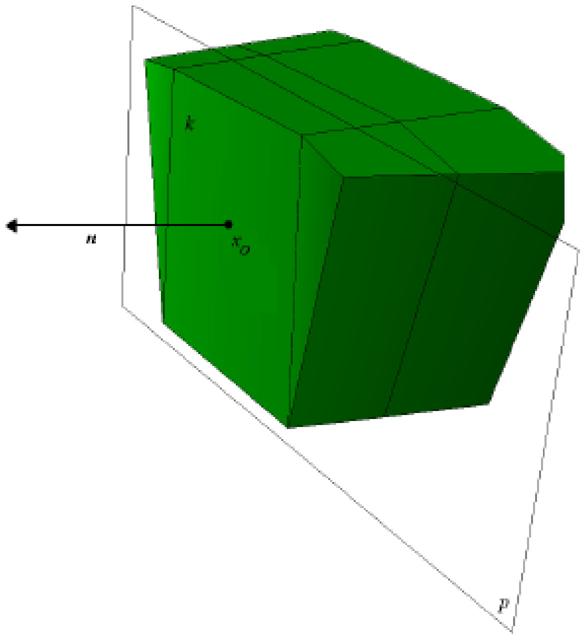
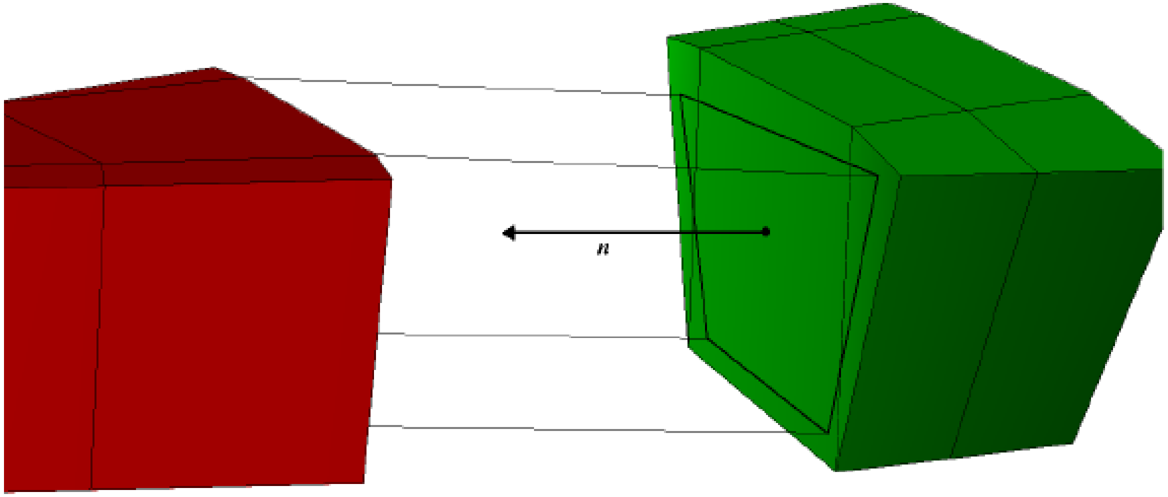
Mortar integration space

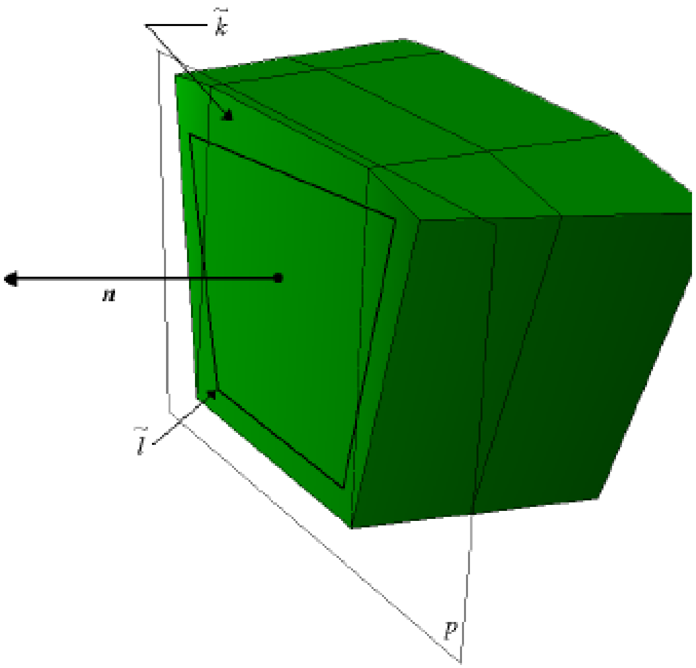


(a) Outward normal of plane p through x_o

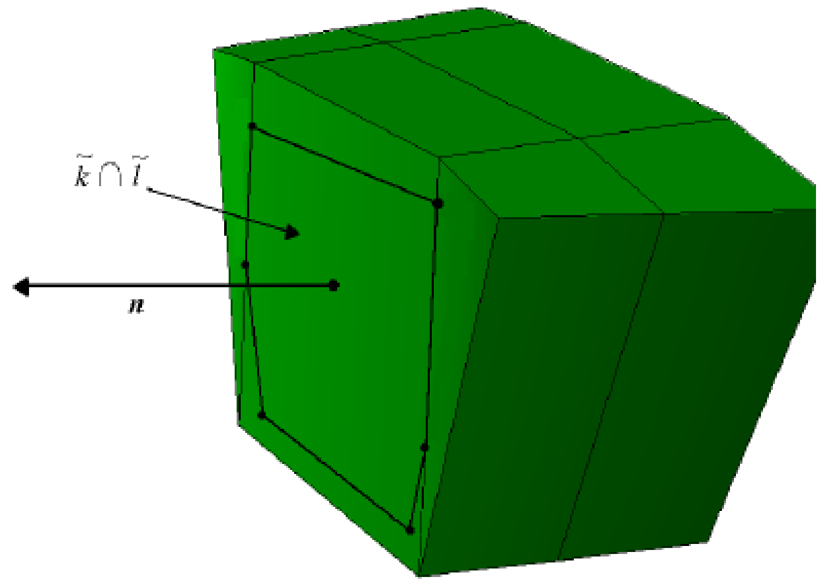


(b) Back-projection of nodes of l along n

Mortar integration space

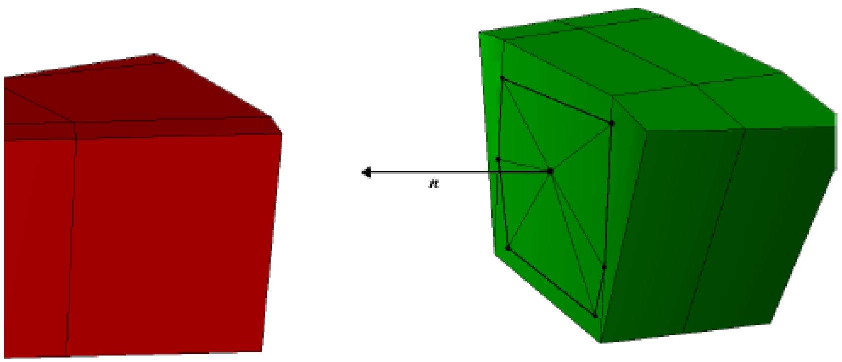


(a) New facets $\tilde{k}$ and $\tilde{l}$ on p

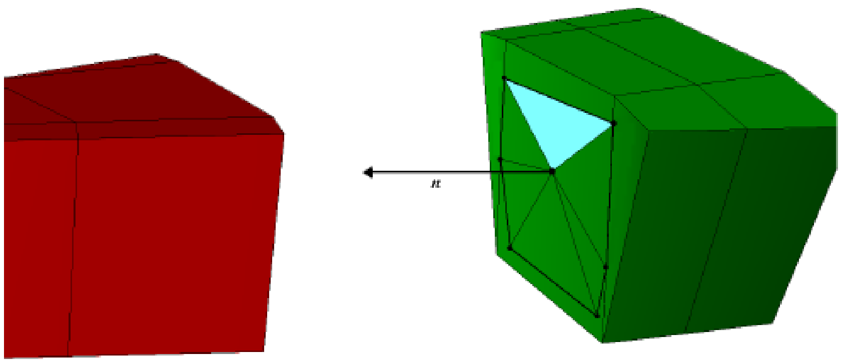


(b) New polygonal facet $\tilde{k} \cap \tilde{l}$

Mortar integration space



(a) Center x_o allows triangulation of the polygon



(b) Triangular common integration face

- **Ultimately, M and D matrices are formed that couple the mortar and non-mortar (l and k) surfaces to the Lagrange multipliers**

$$M = \int_{\Gamma^C} \mathbf{N}_m^T \mathbf{N}_\lambda d\Gamma^C \quad D = -\int_{\Gamma^C} \mathbf{N}_s^T \mathbf{N}_\lambda d\Gamma^C$$

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Two motivating applications

- **Mesh tying – solution of the heat equation across a nonconformal interface**
- **Coupled thermomechanical contact involving a cylinder within an annulus filled with a conductive gas (He)**

Heat equation

- **Weak form of heat equation**

$$(\rho C_p T_t - Q, v) + (k\nabla T, \nabla v) - \langle q(T), v\rangle_{\Gamma_F} = 0$$

- **Let**

$$a_T(T, v) = (k\nabla T, \nabla v)$$

- **and**

$$F_T(T, v) = (\rho C_p T_t - Q, v)$$

- **then**

$$a_T(T, v) + F_T(T, v) = 0.$$

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Thermal constraints

- **Kuhn-Tucker conditions describe the thermal constraints**

$$\Delta T = T^s - T^m \geq 0$$

$$\mathbf{q} \geq 0$$

- **The heat flux across the non-conformal interface is expressed as**

$$q = U(T^s - T^m) = U\Delta T$$

- **Which results in the Lagrange multiplier constraint equation**

$$c_T(T, \lambda_T) = \int_{\Gamma^c} \lambda_T (T^s - T^m) d\Gamma^c$$

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Thermal problem

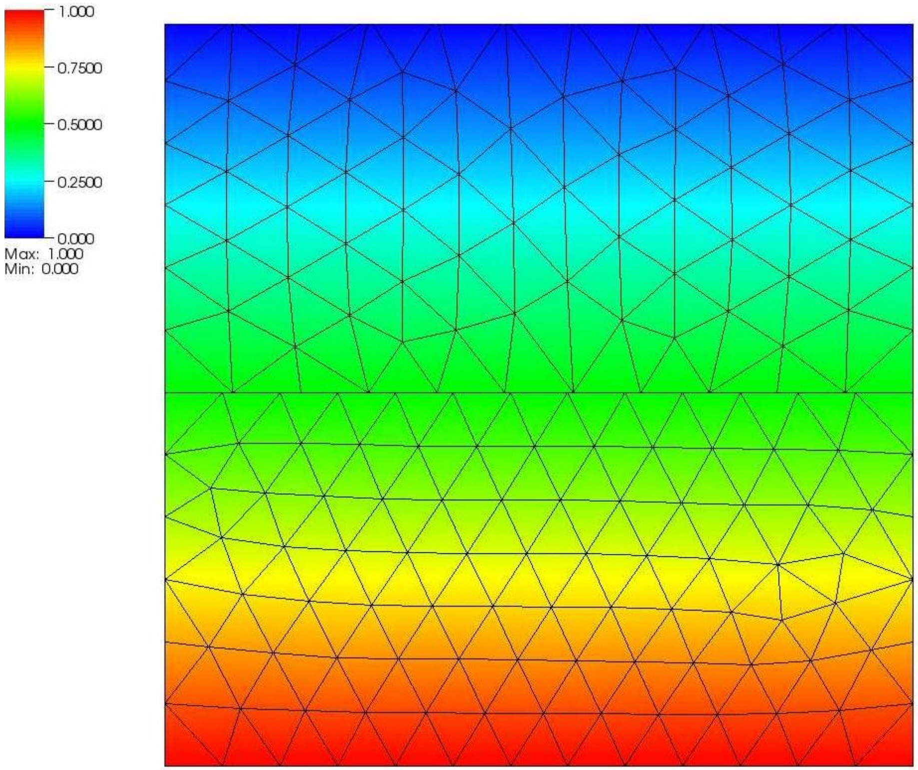
- **We seek solutions to the aggregate constrained problem**

$$\begin{aligned} a_T^h(T,v) + c_T^h(v,\lambda_T) &= -F_T^h(T,v) & \forall\, v^h \in V^h \\ c_T^h(T,\mu_T) &= 0 & \forall\, \mu_T^h \in \mathcal{M}^h \end{aligned}$$

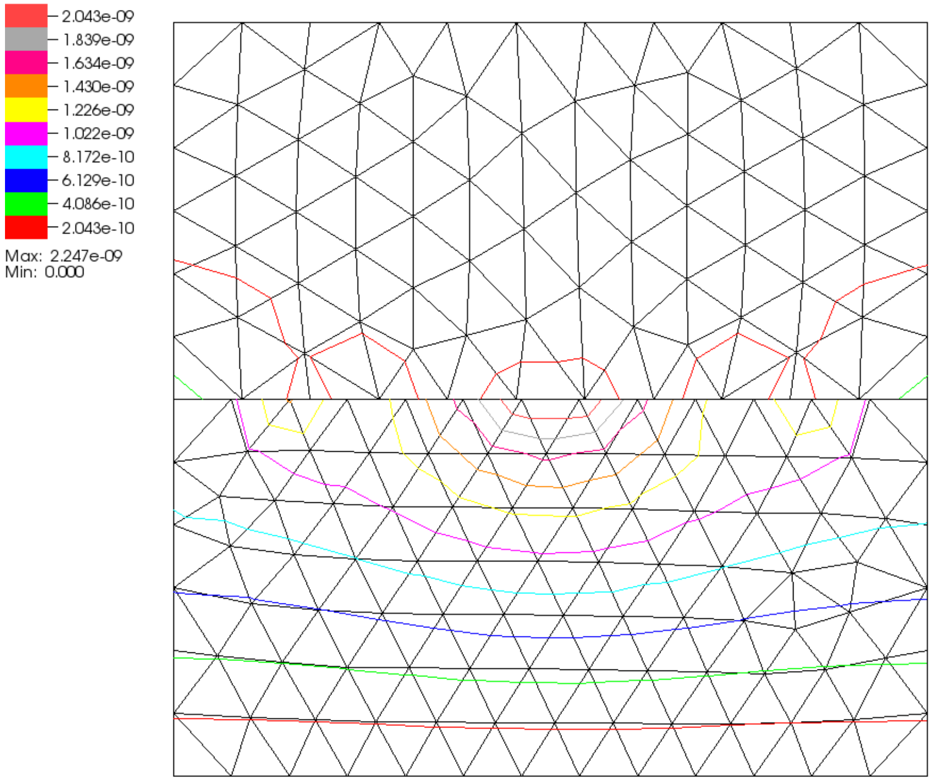
- **Resulting in the thermal problem in matrix form**

$$a_T^h(T,v) + c_T^h(v,\lambda_T) + c_T^h(T,\mu_T) = \left(\mathbf{T}_i^T\ \mathbf{T}_m^T\ \mathbf{T}_s^T\ {\lambda_T}^T\right) \begin{pmatrix} A_{ii} & A_{im} & A_{is} & 0 \\ A_{mi} & A_{mm} & 0 & M \\ A_{si} & 0 & A_{ss} & D \\ 0 & M^T & D^T & 0 \end{pmatrix} \begin{pmatrix} \mathbf{v}_i \\ \mathbf{v}_m \\ \mathbf{v}_s \\ \mu_T \end{pmatrix}$$

Performance of thermal model



Linear hear conduction in rectangle



Error contours

Thermomechanical problem

- **Transient, nonlinear heat conduction**

$$\rho C_p T_t - \nabla \cdot k \nabla T - q = 0$$

- **Linear elastic model, nonlinear material properties**

$$\begin{aligned}(u_{tt}, \phi) &+ \mu S(u, \phi) + \lambda(\nabla \cdot u, \nabla \cdot \phi) \\ &- (f, \phi) - \langle g, \phi \rangle - (\alpha T, \nabla \phi) = 0\end{aligned}$$

$$S(u, \phi) = \sum_{i,j=1}^{3} (\partial_j u_i + \partial_i u_j)(\partial_j \phi_i + \partial_i \phi_j)$$

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Thermal problem

- **Weak form of heat equation**

$$(\rho C_p T_t - Q, v) + (k\nabla T, \nabla v) - \langle q(T), v\rangle_{\Gamma_F} = 0$$

- **Let**

$$a_T(T, v) = (k\nabla T, \nabla v)$$

- **and**

$$F_T(T, v) = (\rho C_p T_t - Q, v)$$

- **then**

$$a_T(T, v) + F_T(T, v) = 0.$$

Thermal constraints

- **Kuhn-Tucker conditions describe the thermal constraints**

$$\Delta T = T^s - T^m \geq 0$$

$$\mathbf{q} \geq 0$$

- **The heat flux across the gap is expressed as**

$$q = U(T^s - T^m) = U\Delta T$$

- **where***

$$U = U(g) = \frac{k_g}{d_g + 1.5(R_f + R_c) + g_f + g_c}$$

*Ross and Stoute

- **This is simplified to**

$$U(g) = \frac{k_g}{d_g}$$

Thermal problem

- **Results in the Lagrange multiplier constraint equation**

$$c_T(T, \lambda_T) = \int_{\Gamma^C} \lambda_T (T^s - T^m - \frac{\lambda_T}{U}) d\Gamma^C$$

- **We seek solutions to the aggregate constrained problem**

$$\begin{array}{lcll} a_T^h(T, v) + c_T^h(v, \lambda_T) & = & -F_T^h(T, v) & \forall\, v^h \in V^h \\ c_T^h(T, \mu_T) & = & 0 & \forall\, \mu_T^h \in \mathcal{M}^h \end{array}$$

- **Resulting in the thermal contribution to the global solution**

$$a_T^h(T, v) + c_T^h(v, \lambda_T) + c_T^h(T, \mu_T) = \left(\mathbf{T}_i^T \; \mathbf{T}_m^T \; \mathbf{T}_s^T \; {\lambda_T}^T \right) \begin{pmatrix} A_{ii} & A_{im} & A_{is} & 0 \\ A_{mi} & A_{mm} & 0 & M \\ A_{si} & 0 & A_{ss} & D \\ 0 & M^T & D^T & \frac{2}{\mathbf{U}} \end{pmatrix} \begin{pmatrix} \mathbf{v}_i \\ \mathbf{v}_m \\ \mathbf{v}_s \\ \mu_T \end{pmatrix}$$

Mechanical problem

- **Weak form**

$$\left(\mathbf{u}_{tt}, \mathbf{w}\right) + \mu S\left(\mathbf{u}, \mathbf{w}\right) + \lambda\left(\nabla \cdot \mathbf{u}, \nabla \cdot \mathbf{w}\right)$$

$$- \left((T - T_{\text{ref}})\mathbf{a}, \mathbf{w}\right) = 0,$$

$$S\left(\mathbf{u}, \mathbf{w}\right) = \sum_{i,j=1}^{3} \left(\partial_j u_i + \partial_i u_j\right)\left(\partial_j w_i + \partial_i w_j\right),$$

- **The system gap vector at the LMs can be written as**

$$\mathbf{G} = D\mathbf{x}^s - M\mathbf{x}^m$$

- **Where**

$$\mathbf{x}^s = \mathbf{X}^s + \mathbf{u}^s$$

$$\mathbf{x}^m = \mathbf{X}^m + \mathbf{u}^m$$

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Mechanical constraints

- **Kuhn-Tucker conditions describe the mechanical constraints**

$$\mathbf{g} = \mathbf{x}^s - \mathbf{x}^m \geq 0$$

$$\mathbf{t} \geq 0$$

- **The pressure of the gases (He initially) in the gap changes over time**
  - Compute aggregate plenum volume by integrating the gap over the segment areas
  - Equation of state gives transient plenum pressure
- **Must also regularize Newton's method**
- **The overall pressure in the gap is expressed as**

$$P_c = A_{seg} P_o e^{\left[S_{NE}(\xi - g_n)^2\right]}$$

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Mechanical problem

- **Results in the Lagrange multiplier constraint equation**

$$\Pi_{\mathbf{u}} = \int_{\Gamma^C} t_n(g_n - \frac{t_n}{P_c})d\Gamma^C$$

- **We seek solutions to the aggregate constrained problem**

$$\begin{aligned} a^h_{\mathbf{u}}(\mathbf{u},\mathbf{w}) + c^h_{\mathbf{u}}(\mathbf{w},\lambda_{\mathbf{u}}) &= -F^h_{\mathbf{u}}(T,\mathbf{u},\mathbf{w}) && \forall\ \mathbf{w}^h \in W^h \\ c^h_{\mathbf{u}}(\mathbf{u},\mu_{\mathbf{u}}) &= 0 && \forall\ {\mu_{\mathbf{u}}}^h \in \mathcal{M}^h \end{aligned}.$$

- **Resulting in the mechanical contribution to the global solution**

$$a^h_{\mathbf{u}}(\mathbf{u},\mathbf{w}) + c^h_{\mathbf{u}}(\mathbf{w},\lambda_{\mathbf{u}}) + c^h_{\mathbf{u}}(\mathbf{u},\mu_{\mathbf{u}})$$

$$= \begin{pmatrix} \mathbf{u}_i^T\ \mathbf{u}_m^T\ \mathbf{u}_s^T\ {\lambda_u}^T \end{pmatrix} \begin{pmatrix} A_{ii} & A_{im} & A_{is} & 0 \\ A_{mi} & A_{mm} & 0 & M \\ A_{si} & 0 & A_{ss} & D \\ 0 & M^T & D^T & \frac{2}{P_c} \end{pmatrix} \begin{pmatrix} \mathbf{w}_i \\ \mathbf{w}_m \\ \mathbf{w}_s \\ \mu_u \end{pmatrix}$$

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JFNK implemented using Trilinos

NOX

1. $n = 0, ... \quad Do$
2. set $U_0 = U^n$
3. For $k = 0, ...$ till converge Do
4. solve $J^k(\mathbf{U}^k)\delta\mathbf{U}^k = -F(\mathbf{U^k})$
5. $\mathbf{U}^{k+1} = \mathbf{U}^k + \delta\mathbf{U}^k$
6. EndDo
7. $t_{n+1} = t_n + \Delta t$
8. Enddo

Stratimikos / Belos

1. Compute $r_0 = -F(\mathbf{U}^n), \beta = ||r_0||_2$, and $v_1 = r_0/\beta$
2. For $j = 1, ...m Do:$
3. Compute $w := JM^{-1}v_j$
4. For $i = 1, ...j, Do:$
5. $h_{i,j} := (w, v_i)$
6. $w := w - h_{i,j}v_i$
7. EndDo
8. Compute $h_{j+1,j} = ||w||_2$ and $v_{j+1} = w/h_{j+1,j}$
9. Define $V_m := [v_1, ..., v_m], H_m = h_{ij}{}_{1\leq i\leq j+1; 1\leq j\leq m}$
10. EndDo
11. Compute $y_m = argmin_y||\beta e_1 - \hat{H}_m y||_2$ and $\delta\mathbf{U}_m = \delta\mathbf{U}_0 + M^{-1}V_m y_m$

NOX::Epetra::MatrixFree

$$JM^{-1}\mathbf{v} \approx \frac{F(\mathbf{U} + \varepsilon M^{-1}\mathbf{v}) - F(\mathbf{U})}{\varepsilon}$$

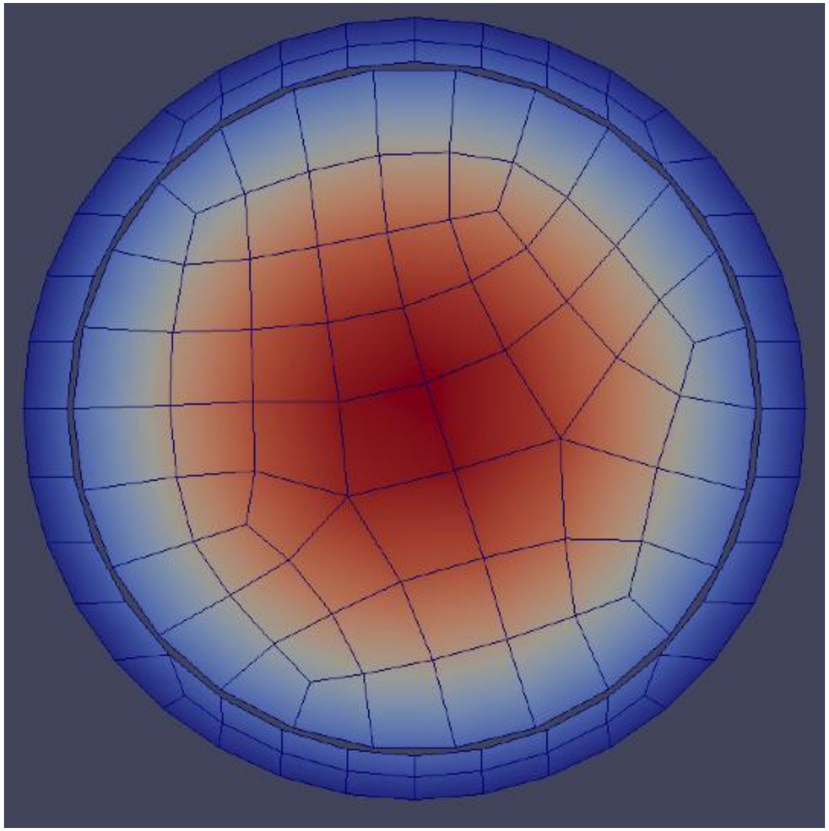
IFPACK

1. $z = M^{-1}v$
2. $JM^{-1}v = Jz \approx \dfrac{F(\mathbf{U} + \varepsilon z) - F(\mathbf{U})}{\varepsilon}$

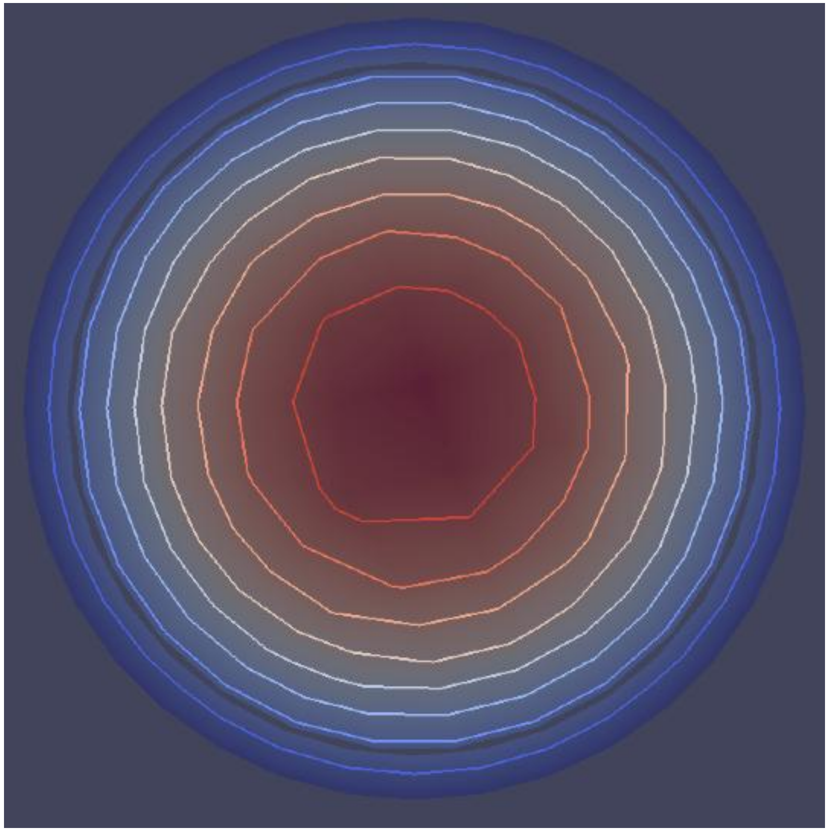
Trilinos packages in use:

- Moertel – mortar methods package
- Teuchos, Epetra, Seacas
- Ifpack for preconditioning

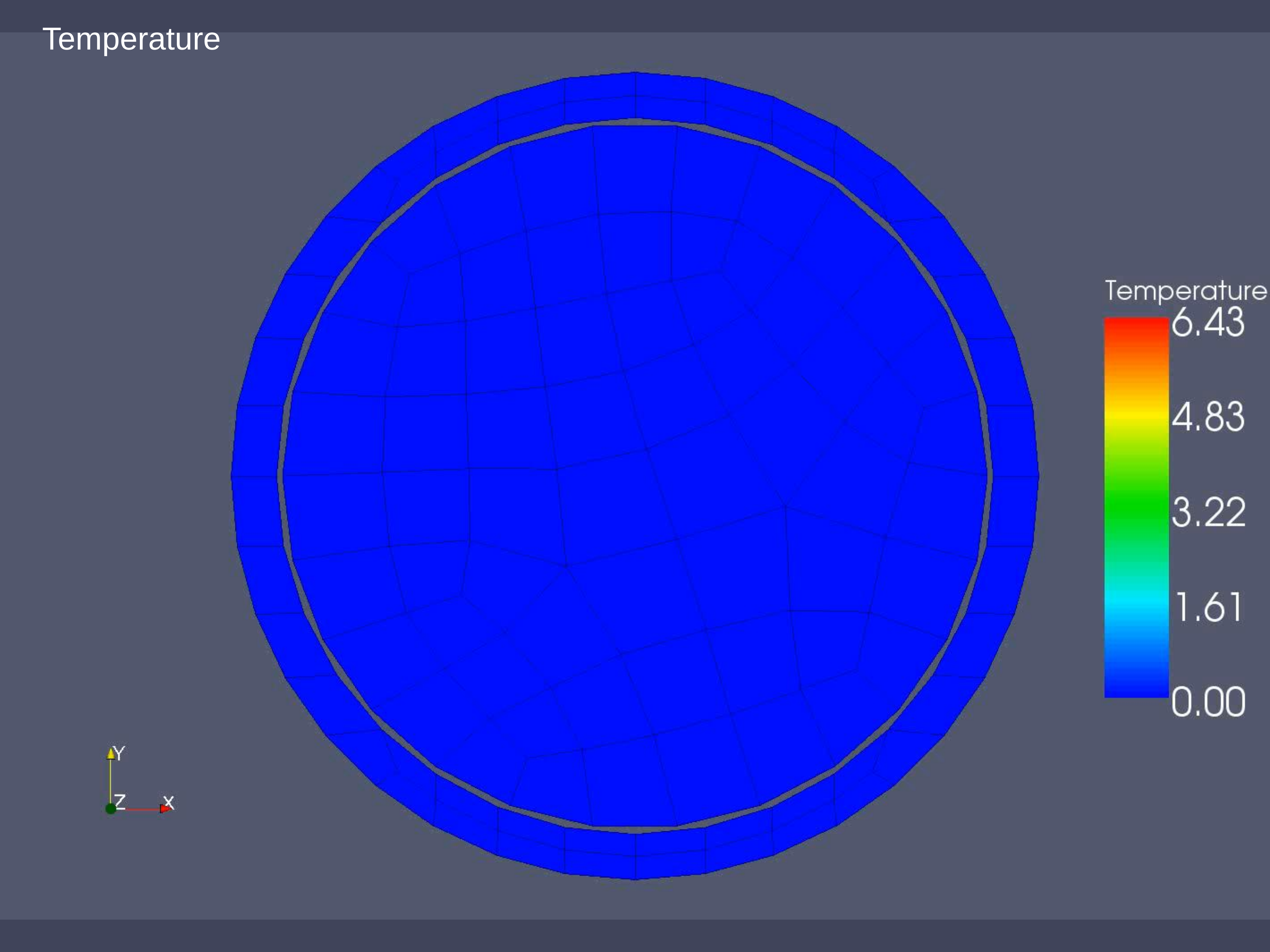
Thermal result



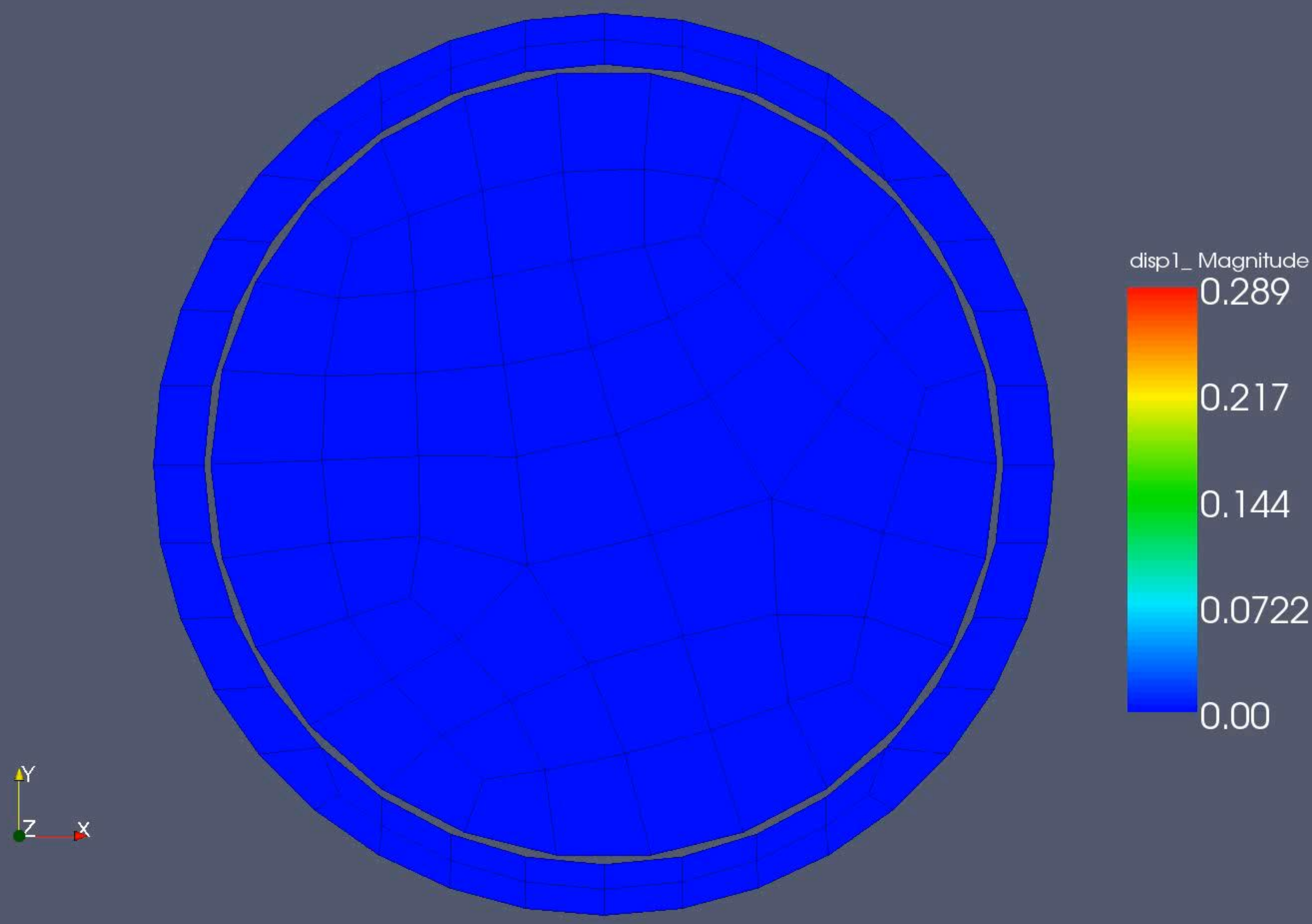
Nonlinear heat conduction from pellet



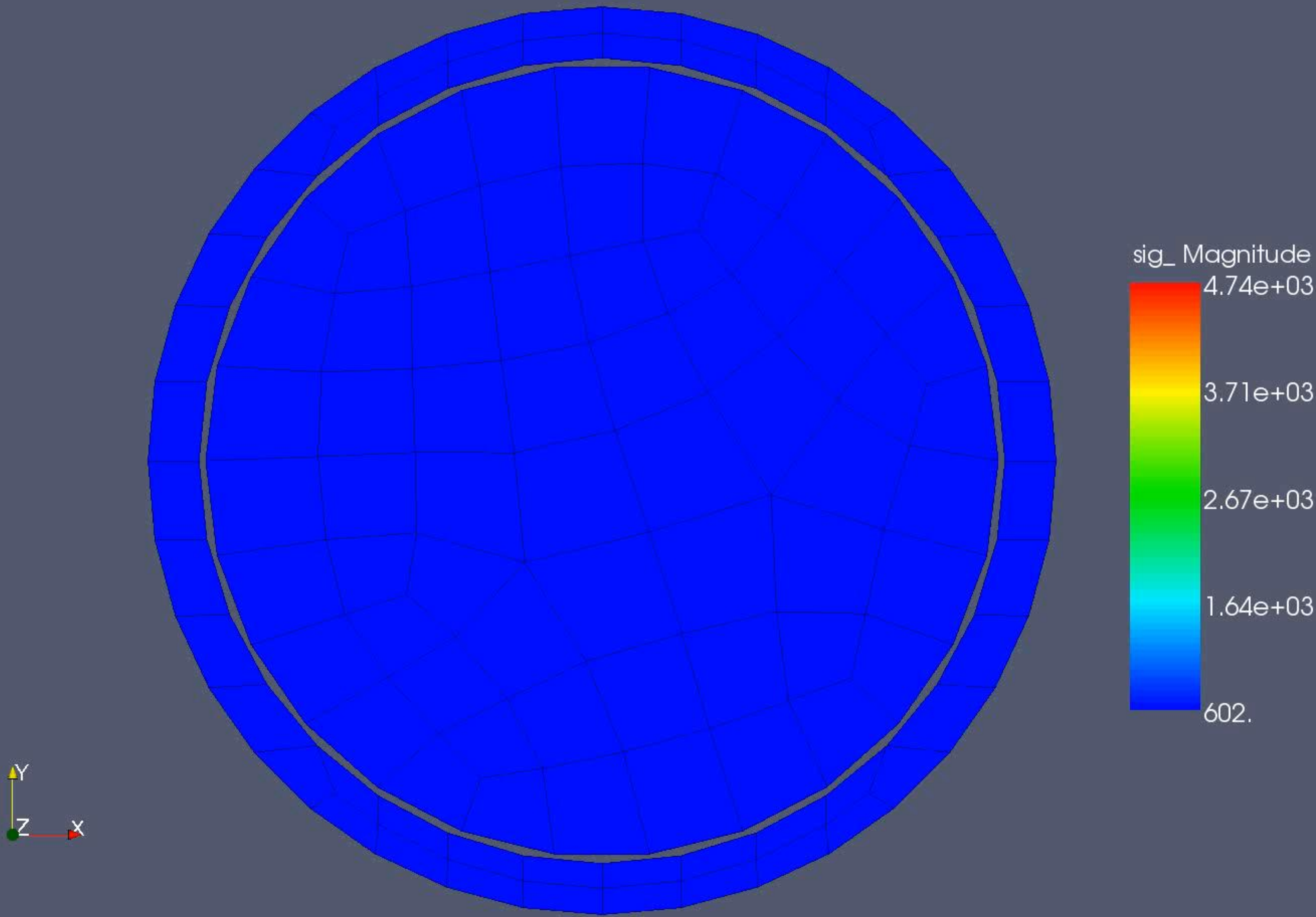
Temperature contours


Temperature
Temperature
6.43
4.83
3.22
1.61
0.00
Y
Z
X

Displacement



Stress



In closing

- **Please email if you're interested in Moertel, encounter issues, or have questions:**

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