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

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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 $k$
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

$$M = \int_{\Gamma_C} N_m^T N_\lambda d\Gamma^C \quad D = - \int_{\Gamma_C} N_s^T N_\lambda d\Gamma^C$$
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)
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

\[ \Delta T = T^s - T^m \geq 0 \]
\[ q \geq 0 \]

- 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

\[ c_T(T, \lambda_T) = \int_{\Gamma^c} \lambda_T(T^s - T^m) d\Gamma^c \]
Thermal problem

- We seek solutions to the aggregate constrained problem

\[ a^h_T(T, v) + c^h_T(v, \lambda_T) = -F^h_T(T, v) \quad \forall \: v^h \in V^h \]
\[ c^h_T(T, \mu_T) = 0 \quad \forall \: \mu^h_T \in M^h \]

- Resulting in the thermal problem in matrix form

\[ a^h_T(T, v) + c^h_T(v, \lambda_T) + c^h_T(T, \mu_T) = \begin{pmatrix} T_i^T & T_m^T & T_s^T & \lambda_T^T \end{pmatrix} \begin{pmatrix} A_{ii} & A_{im} & A_{is} & 0 \\ A_{mi} & A_{mm} & 0 & M \\ A_{si} & 0 & A_{ss} & D \\ 0 & M^T & D^T & 0 \end{pmatrix} \begin{pmatrix} v_i \\ v_m \\ v_s \\ \mu_T \end{pmatrix} \]
Performance of thermal model

Linear heat 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
  \[
  (u_{tt}, \phi) + \mu S(u, \phi) + \lambda (\nabla \cdot u, \nabla \cdot \phi) \\
  - (f, \phi) - \langle g, \phi \rangle - (\alpha T, \nabla \phi) = 0
  \]
  \[
  S(u, \phi) = \sum_{i,j=1}^{3} (\partial_j u_i + \partial_i u_j)(\partial_j \phi_i + \partial_i \phi_j)
  \]
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

\[ \Delta T = T^s - T^m \geq 0 \]
\[ q \geq 0 \]

- The heat flux across the gap is expressed as

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

- where*

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

- This is simplified to

\[
U(g) = \frac{k_g}{d_g}
\]

*Ross and Stoute
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

$$a_T^T(T, \nu) + c_T^h(\nu, \lambda_T) = -F_T^h(T, \nu) \quad \forall \nu^h \in V^h$$

$$c_T^h(T, \mu_T) = 0 \quad \forall \mu_T^h \in M^h$$

- Resulting in the thermal contribution to the global solution

$$a_T^T(T, \nu) + c_T^h(\nu, \lambda_T) + c_T^h(T, \mu_T) = \begin{pmatrix} T_i^T & T_m^T & T_s^T & \lambda_T^T \end{pmatrix} \begin{pmatrix} A_{ii} & A_{im} & A_{is} & 0 \\ A_{mi} & A_{mm} & 0 & M \\ A_{si} & 0 & A_{ss} & D \\ 0 & M^T & D^T & \frac{2}{U} \end{pmatrix} \begin{pmatrix} \nu_i \\ \nu_m \\ \nu_s \\ \mu_T \end{pmatrix}$$
Mechanical problem

- Weak form

$$(u_{tt}, w) + \mu S(u, w) + \lambda (\nabla \cdot u, \nabla \cdot w) - ((T - T_{\text{ref}}) a, w) = 0,$$

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

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

$$G = Dx^s - Mx^m$$

- Where

$$x^s = X^s + u^s$$

$$x^m = X^m + u^m$$
Mechanical constraints

- Kuhn-Tucker conditions describe the mechanical constraints
  \[ g = x^s - x^m \geq 0 \]
  \[ t \geq 0 \]

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

- Results in the Lagrange multiplier constraint equation
  \[ \Pi_u = \int_{\Gamma C} t_n (g_n - \frac{t_n}{P_c}) d\Gamma^C \]

- We seek solutions to the aggregate constrained problem
  \[ a^h_u(u, w) + c^h_u(w, \lambda_u) = -F^h_u(T, u, w) \quad \forall \ w^h \in W^h \]
  \[ c^h_u(u, \mu_u) = 0 \quad \forall \ \mu_u^h \in M^h . \]

- Resulting in the mechanical contribution to the global solution
  \[ a^h_u(u, w) + c^h_u(w, \lambda_u) + c^h_u(u, \mu_u) \]
  \[ = \begin{pmatrix} u_i^T & u_m^T & u_s^T & \lambda_u^T \end{pmatrix} \begin{pmatrix} A_{ii} & A_{im} & A_{is} & 0 \\ A_{mi} & A_{mm} & 0 & M \\ A_{si} & 0 & A_{ss} & D \\ 0 & M^T & D^T & \frac{2}{P_c} \end{pmatrix} \begin{pmatrix} w_i \\ w_m \\ w_s \\ \mu_u \end{pmatrix} \]
JFNK implemented using Trilinos

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

Trilinos packages in use:
- Moertel – mortar methods package
- Teuchos, Epetra, Seacas
- Ifpack for preconditioning
Thermal result

Nonlinear heat conduction from pellet

Temperature contours
Temperature
In closing

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

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