Application of Boundary Conditions via Facet Elements in the `imitor` Finite Element Code

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Acquiring necessary data on a facet element

For three-dimensional conventional finite elements, the element residual and tangent stiffness equations for facets involve area integrals in $\mathbb{R}^3$. The quantities necessary to calculate these integrals are: shape function values N_a, ratio of differential areas between reference configuration and parent space J, reference configuration normal $\mathbf{N}$, and in-plane shape function gradients $\mathbf{g}_a$. Shape function values can be easily evaluated at integration points. The process by which to determine the other three quantities is described below.

Assume a parametrization $\mathbf{X} \in \Omega^m$ for a particular element m is available in the reference configuration of the physical space. For conventional finite element methods, the parametrization is provided by shape functions defined in the parent space: $X_i = \sum\limits_a X_{ia} N_a(\xi_i)$.

Define parametrization variables ξ_j, regardless of whether or not they are defined on a parent space. Consider a three-dimensional problem, in which facets are defined on 2D subsets of $\mathbb{R}^3$. The cross product of $\frac{\partial \mathbf{X}}{\partial \xi_1}$ and $\frac{\partial \mathbf{X}}{\partial \xi_2}$ defines a vector that points normal to the facet in the reference configuration, with magnitude equal to the differential area spanned by $\frac{\partial \mathbf{X}}{\partial \xi_1}$ and $\frac{\partial \mathbf{X}}{\partial \xi_2}$. This magnitude and direction are indeed the J and $\mathbf{N}$ we desire, respectively.

In order to calculate the in-plane shape function gradients, first define two orthonormal in-plane directions $\mathbf{M}_1$ and $\mathbf{M}_2$. Calculation of the material line segment $\mathbf{M}_1$ is performed by first choosing the basis vector $\mathbf{e}_p$ that is closest to lying in the plane defined by $\mathbf{N}$. It is then projected onto that plane and scaled to be unit magnitude. The second direction $\mathbf{M}_2$ is calculated simply by $\mathbf{N} \times \mathbf{M}_1$.

Define in-plane shape function gradients in the reference configuration as $\mathbf{g}_a = h_{1a}\mathbf{M}_1 + h_{2a}\mathbf{M}_2$. If we define $\mathbf{M}$ as the 3×2 matrix whose columns are $\mathbf{M}_1$ and $\mathbf{M}_2$, and if $\mathbf{h}_a$ is a column vector with components h1a and h2a, we may write $\mathbf{g}_a = \mathbf{M}\mathbf{h}_a$. We may then define shape function gradients with respect to the parametrization variables as $\frac{\partial N_a}{\partial \xi_i} = \mathbf{g}_a \cdot \frac{\partial \mathbf{X}}{\partial \xi_i}$. Using the definition for $\mathbf{g}_a$ above, this can be written as $\frac{\partial N_a}{\partial \boldsymbol{\xi}} = \mathbf{g}_a \cdot \frac{\partial \mathbf{X}}{\partial \boldsymbol{\xi}} = \mathbf{M}\mathbf{h}_a \cdot \frac{\partial \mathbf{X}}{\partial \boldsymbol{\xi}} = (\frac{\partial \mathbf{X}}{\partial \boldsymbol{\xi}}^T \mathbf{M})\mathbf{h}_a = \mathbf{H}\mathbf{h}_a$. The matrix $\mathbf{H}$ maps in-plane shape function gradients h_{ia} acting in directions $\mathbf{M}_i$ into shape function gradients in directions of parameterized variables ξ_i. The components h_{ia} are found from $\mathbf{h}_a = \mathbf{H}^{-1}\frac{\partial N_a}{\partial \boldsymbol{\xi}}$. Finally $\mathbf{g}_a$ is formed using the relation $\mathbf{g}_a = h_{1a}\mathbf{M}_1 + h_{2a}\mathbf{M}_2$.

In order to use the same approach for a 1D facet in 2D space, assign $\frac{\partial \mathbf{X}}{\partial \xi_2} = \mathbf{e}_3$. The cross product $\frac{\partial \mathbf{X}}{\partial \xi_1} \times \mathbf{e}_3$ gives $\mathbf{dA} = J\mathbf{N} = |\frac{\partial \mathbf{X}}{\partial \xi_1}|\mathbf{N}$. This produces the appropriate values for J and $\mathbf{N}$ for the lower dimensional case. Calculations for shape function gradients simplify to scalar operations rather than matrix operations, and $\mathbf{g}_a = h_{1a}\mathbf{M}_1$ only.

Algorithm (In elems_nodes_m.f):
For each integration point of a particular 2D facet element in 3D space:

$$\frac{\partial X_i}{\partial \xi_j} = \sum_a X_i \frac{\partial N_a}{\partial \xi_j}, \quad i = 1, \mathrm{NC}, \quad j = 1, \mathrm{NCF} \tag{1}$$

$$\mathbf{dA} = \frac{\partial \mathbf{X}}{\partial \xi_1} \times \frac{\partial \mathbf{X}}{\partial \xi_2} \tag{2}$$

$$J = |\mathbf{dA}| \tag{3}$$

$$\mathrm{IP\_WTS} \leftarrow \mathrm{IP\_WTS} * J \tag{4}$$

$$\mathrm{NRML} \leftarrow \mathbf{N} = \mathbf{dA}/J \tag{5}$$

$$N_p = \min_i |N_i| \tag{6}$$

$$\mathbf{M}_1 = \frac{(\mathbf{I} - \mathbf{N} \otimes \mathbf{N})\mathbf{e}_p}{|(\mathbf{I} - \mathbf{N} \otimes \mathbf{N})\mathbf{e}_p|} \tag{7}$$

$$\mathbf{M}_2 = \mathbf{N} \times \mathbf{M}_1 \tag{8}$$

$$H_{ij} = \frac{\partial \mathbf{X}}{\partial \xi_i} \cdot \mathbf{M}_j, \quad i = 1, \mathrm{NCF}, \quad j = 1, \mathrm{NCF} \tag{9}$$

$$\mathbf{h}_a = \mathbf{H}^{-1} \frac{\partial N_a}{\partial \boldsymbol{\xi}} \tag{10}$$

$$\mathrm{SF\_GRADS} \leftarrow \mathbf{g}_a = h_{1a}\mathbf{M}_1 + h_{2a}\mathbf{M}_2 \tag{11}$$

For 1D facet elements in 2D space, the same algorithm applies, with the addition $\frac{\partial \mathbf{X}}{\partial \xi_2} = \mathbf{e}_3$ and the modification $\mathbf{g}_a = h_{1a}\mathbf{M}_1$.

Applying particular BCs

Six types of boundary conditions are allowed: Cauchy tractions, Piola tractions, Cauchy pressures, Piola pressures, Cauchy follower loads, and Piola follower loads. Cauchy boundary conditions are distinguished from Piola in that they are scaled by the ratio of areas in the current configuration and reference configuration α. Cauchy and Piola BCs always act in the same direction. Follower loads are a specific type of traction, described momentarily.

All calculations are based on the formation of $\mathbf{da} = \alpha\mathbf{n}$. The quantity $\alpha\mathbf{n}$ is found by crossing orthonormal in-plane deformed material line directions in the current configuration: $\alpha\mathbf{n} = \mathbf{F}\mathbf{M}_1 \times \mathbf{F}\mathbf{M}_2$. The vectors $\mathbf{M}_1$ and $\mathbf{M}_2$ are chosen to be defined in the same manner as the previous section, although they need not be. All other quantities, and their derivatives, can be formed from this definition.

The algorithm laid out in the following section may equally well be used for 1D facets belonging to 2D space, provide that one prescribes $\mathbf{M}_2 = \mathbf{e}_3$ and $\mathbf{M}_1 = \mathbf{M}_2 \times \mathbf{N}$. The deformation gradient $\mathbf{F}$ is formed using the in-plane shape function gradients $\mathbf{g}_a$, and by construction $\mathbf{g}_a \cdot \mathbf{e}_3 = 0$. Thus, $\alpha\mathbf{n} = \mathbf{F}\mathbf{M}_1 \times \mathbf{F}\mathbf{e}_3 = \mathbf{F}\mathbf{M}_1 \times \mathbf{e}_3 = |\mathbf{F}\mathbf{M}_1|\mathbf{n}$ as desired. Also, for the purposes of computing $\frac{\partial(\alpha\mathbf{n})}{\partial\hat{\mathbf{u}}}$, the quantity $\frac{\partial\mathbf{F}}{\partial\hat{\mathbf{u}}}\mathbf{M}_2$ is needed. It can be shown that when $\mathbf{M}_2 = \mathbf{e}_3$, $\frac{\partial\mathbf{F}}{\partial\hat{\mathbf{u}}}\mathbf{M}_2 = 0$, as desired. So indeed, this algorithm can be used exactly the same for 1D facets belonging to 2D space, as long as $\mathbf{M}_2 = \mathbf{e}_3$ is prescribed. $\mathbf{M}_1$ is formed in this manner as opposed to that done in 3D so that the counterclockwise orientation convention may be obeyed.

Follower loads

Define a traction $\mathbf{L}(t) = -p(t)\mathbf{N} + \tau(t)\mathbf{S}$, where $\mathbf{L}$ acts on a facet in the reference configuration. It is decomposed into normal and in-plane components, where $p(t)$ is the pressure, $\tau(t)$ is the shear force magnitude, $\mathbf{N}$ is the facet normal in the reference configuration, and $\mathbf{S}$ is the shear force direction. The components $L_i(t)$ shall be provided by the user, with no knowledge *a priori* of normal and in-plane considerations.

Now define a *follower load* as a particular type of traction defined by $\boldsymbol{\ell}(t) = -p(t)\mathbf{n}(t) + \tau(t)\mathbf{s}(t)$. These loads "follow" the local orientation of the facet in the current configuration. Define $\mathbf{n}$ as the current configuration normal. Also, consider a material fiber direction defined by $\mathbf{S}$ that lies in the plane of the facet in the reference configuration. Define $\mathbf{s}$ as the direction of the deformed fiber in the current configuration, acting in the direction of $\mathbf{F}\mathbf{S}$. Thus, in the same manner that a pure pressure "follows" the normal, a follower follows both the normal direction and a particular in-plane direction.

The current normal $\mathbf{n}$ is calculated in the same way as before, and the current shear direction is simply $\mathbf{s} = \mathbf{F}\mathbf{S}/|\mathbf{F}\mathbf{S}|$. Special care is taken for cases where $\tau = 0$. Again, a follower load is distinguished as Cauchy if the magnitude of pressure and shear are scaled by the area ratio α. Otherwise, it is deemed of Piola type. It is worth reiterating that the follower load itself is not prescribed by the user, but rather the load that acts on the reference configuration.

Algorithm (In lcl_elem_fct_m.f):
For each integration point of the particular facet element (either 1D facet in 2D space or 2D facet in 3D space):

$$F_{ij} = \delta_{ij} + \sum_a u_{ia} g_{ja}, \qquad \text{or} \qquad \mathbf{F} = \mathbf{I} + \sum_a \mathbf{u}_a \otimes \mathbf{g}_a \tag{12}$$

$$\frac{\partial F_{ij}}{\partial \hat{u}_{kb}} = \delta_{ik} g_{jb} \tag{13}$$

Reference configuration normal $\mathbf{N}$ is given from the previous algorithm. If NCF = 1, set $\mathbf{M}_2 = \mathbf{e}_3$ and $\mathbf{M}_1 = \mathbf{M}_2 \times \mathbf{N}$. Otherwise, recompute $\mathbf{M}_1$ and $\mathbf{M}_2$ in the same manner as before. Check to see which boundary condition is imposed:

1. If Cauchy pressure prescribed: $\overline{\mathbf{p}} = -p\alpha\mathbf{n}$ and $\frac{\partial \overline{\mathbf{p}}}{\partial \hat{\mathbf{u}}} = -p\frac{\partial(\alpha\mathbf{n})}{\partial \hat{\mathbf{u}}}$.

$$\alpha\mathbf{n} = \mathbf{F}\mathbf{M}_1 \times \mathbf{F}\mathbf{M}_2 \tag{14}$$

$$\frac{\partial(\alpha\mathbf{n})}{\partial \hat{\mathbf{u}}} = (\frac{\partial \mathbf{F}}{\partial \hat{\mathbf{u}}}\mathbf{M}_1 \times \mathbf{F}\mathbf{M}_2) + (\mathbf{F}\mathbf{M}_1 \times \frac{\partial \mathbf{F}}{\partial \hat{\mathbf{u}}}\mathbf{M}_2) \tag{15}$$

2. If Cauchy traction prescribed: $\overline{\mathbf{p}} = \alpha\mathbf{t}$ and $\frac{\partial \overline{\mathbf{p}}}{\partial \hat{\mathbf{u}}} = \frac{\partial \alpha}{\partial \hat{\mathbf{u}}}\mathbf{t}$.

$$\text{compute } \alpha\mathbf{n}, \ \frac{\partial(\alpha\mathbf{n})}{\partial \hat{\mathbf{u}}} \text{ as before} \tag{16}$$

$$\alpha^2 = \alpha\mathbf{n} \cdot \alpha\mathbf{n} \tag{17}$$

$$\alpha = \sqrt{\alpha^2} \tag{18}$$

$$\frac{\partial(\alpha^2)}{\partial \hat{\mathbf{u}}} = 2\frac{\partial(\alpha\mathbf{n})}{\partial \hat{\mathbf{u}}} \cdot \alpha\mathbf{n} \tag{19}$$

$$\frac{\partial \alpha}{\partial \hat{\mathbf{u}}} = \frac{1}{2\alpha}\frac{\partial(\alpha^2)}{\partial \hat{\mathbf{u}}} \tag{20}$$

3. If Piola pressure prescribed: $\overline{\mathbf{p}} = -p\mathbf{n}$ and $\frac{\partial \overline{\mathbf{p}}}{\partial \hat{\mathbf{u}}} = -p\frac{\partial \mathbf{n}}{\partial \hat{\mathbf{u}}}$.

$$\text{compute } \alpha\mathbf{n}, \ \frac{\partial(\alpha\mathbf{n})}{\partial \hat{\mathbf{u}}}, \ \alpha, \ \frac{\partial \alpha}{\partial \hat{\mathbf{u}}} \text{ as before} \tag{21}$$

$$\mathbf{n} = \frac{1}{\alpha}(\alpha\mathbf{n}) = \frac{1}{\alpha}(\mathbf{F}\mathbf{M}_1 \times \mathbf{F}\mathbf{M}_2) \tag{22}$$

$$\frac{\partial \mathbf{n}}{\partial \hat{\mathbf{u}}} = -\frac{1}{\alpha^2}\frac{\partial \alpha}{\partial \hat{\mathbf{u}}}(\alpha\mathbf{n}) + \frac{1}{\alpha}\frac{\partial(\alpha\mathbf{n})}{\partial \hat{\mathbf{u}}} \tag{23}$$

4. If Piola traction prescribed: $\overline{\mathbf{p}}$ is explicitly defined and $\frac{\partial \overline{\mathbf{p}}}{\partial \hat{\mathbf{u}}} = \mathbf{0}$.

5. If Cauchy follower traction prescribed: $\overline{\mathbf{p}} = \alpha\boldsymbol{\ell}$ and $\frac{\partial\overline{\mathbf{p}}}{\partial\hat{\mathbf{u}}} = \frac{\partial(\alpha\boldsymbol{\ell})}{\partial\hat{\mathbf{u}}}$, where $\alpha\boldsymbol{\ell} = -p(\alpha\mathbf{n}) + \tau(\alpha\mathbf{s})$, $\frac{\partial(\alpha\boldsymbol{\ell})}{\partial\hat{\mathbf{u}}} = -p\frac{\partial(\alpha\mathbf{n})}{\partial\hat{\mathbf{u}}} + \tau\frac{\partial(\alpha\mathbf{s})}{\partial\hat{\mathbf{u}}}$, and $\mathbf{L}(t) = -p(t)\mathbf{N} + \tau(t)\mathbf{S}$.

$$\text{compute } \alpha\mathbf{n},\ \frac{\partial(\alpha\mathbf{n})}{\partial\hat{\mathbf{u}}},\ \alpha,\ \frac{\partial\alpha}{\partial\hat{\mathbf{u}}} \text{ as before} \tag{24}$$

$$p = -(\mathbf{L}\cdot\mathbf{N}) \tag{25}$$

$$\tau\mathbf{S} = \mathbf{L} + p\mathbf{N} \tag{26}$$

$$\tau = |\mathbf{L} + p\mathbf{N}| \tag{27}$$

$$\mathbf{S} = \frac{\tau\mathbf{S}}{\tau} \tag{28}$$

$$\beta\mathbf{s} = \mathbf{F}\mathbf{S} \tag{29}$$

$$\beta^2 = \mathbf{F}\mathbf{S}\cdot\mathbf{F}\mathbf{S} \tag{30}$$

$$\beta = \sqrt{\beta^2} \tag{31}$$

$$\alpha\mathbf{s} = \alpha\frac{\mathbf{F}\mathbf{S}}{\beta} \tag{32}$$

$$\frac{\partial\beta^2}{\partial\hat{\mathbf{u}}} = 2\frac{\partial\mathbf{F}}{\partial\hat{\mathbf{u}}}\mathbf{S}\cdot\mathbf{F}\mathbf{S} \tag{33}$$

$$\frac{\partial\beta}{\partial\hat{\mathbf{u}}} = \frac{1}{2\beta}\frac{\partial\beta^2}{\partial\hat{\mathbf{u}}} \tag{34}$$

$$\frac{\partial(\alpha\mathbf{s})}{\partial\hat{\mathbf{u}}} = \frac{\partial\alpha}{\partial\hat{\mathbf{u}}}\frac{1}{\beta}\mathbf{F}\mathbf{S} - \alpha\frac{1}{\beta^2}\frac{\partial\beta}{\partial\hat{\mathbf{u}}}\mathbf{F}\mathbf{S} + \alpha\frac{1}{\beta}\frac{\partial\mathbf{F}}{\partial\hat{\mathbf{u}}}\mathbf{S} \tag{35}$$

$$\alpha\boldsymbol{\ell} = -p(\alpha\mathbf{n}) + \tau(\alpha\mathbf{s}) \tag{36}$$

$$\frac{\partial(\alpha\boldsymbol{\ell})}{\partial\hat{\mathbf{u}}} = -p\frac{\partial(\alpha\mathbf{n})}{\partial\hat{\mathbf{u}}} + \tau\frac{\partial(\alpha\mathbf{s})}{\partial\hat{\mathbf{u}}} \tag{37}$$

6. If Piola follower traction prescribed: $\overline{\mathbf{p}} = \boldsymbol{\ell}$ and $\frac{\partial \overline{\mathbf{p}}}{\partial \hat{\mathbf{u}}} = \frac{\partial \boldsymbol{\ell}}{\partial \hat{\mathbf{u}}}$, where $\boldsymbol{\ell} = -p\mathbf{n} + \tau\mathbf{s}$, $\frac{\partial \boldsymbol{\ell}}{\partial \hat{\mathbf{u}}} = -p\frac{\partial \mathbf{n}}{\partial \hat{\mathbf{u}}} + \tau\frac{\partial \mathbf{s}}{\partial \hat{\mathbf{u}}}$, and $\mathbf{L}(t) = -p(t)\mathbf{N} + \tau(t)\mathbf{S}$.

$$\text{compute } \alpha\mathbf{n},\ \frac{\partial(\alpha\mathbf{n})}{\partial \hat{\mathbf{u}}},\ \alpha,\ \frac{\partial \alpha}{\partial \hat{\mathbf{u}}} \text{ as before} \tag{38}$$

$$p = -(\mathbf{L} \cdot \mathbf{N}) \tag{39}$$

$$\tau\mathbf{S} = \mathbf{L} + p\mathbf{N} \tag{40}$$

$$\tau = |\mathbf{L} + p\mathbf{N}| \tag{41}$$

$$\mathbf{S} = \frac{\tau\mathbf{S}}{\tau} \tag{42}$$

$$\beta\mathbf{s} = \mathbf{F}\mathbf{S} \tag{43}$$

$$\beta^2 = \mathbf{F}\mathbf{S} \cdot \mathbf{F}\mathbf{S} \tag{44}$$

$$\beta = \sqrt{\beta^2} \tag{45}$$

$$\mathbf{s} = \frac{\mathbf{F}\mathbf{S}}{\beta} \tag{46}$$

$$\frac{\partial \beta^2}{\partial \hat{\mathbf{u}}} = 2\frac{\partial \mathbf{F}}{\partial \hat{\mathbf{u}}}\mathbf{S} \cdot \mathbf{F}\mathbf{S} \tag{47}$$

$$\frac{\partial \beta}{\partial \hat{\mathbf{u}}} = \frac{1}{2\beta}\frac{\partial \beta^2}{\partial \hat{\mathbf{u}}} \tag{48}$$

$$\frac{\partial \mathbf{s}}{\partial \hat{\mathbf{u}}} = -\frac{1}{\beta^2}\frac{\partial \beta}{\partial \hat{\mathbf{u}}}\mathbf{F}\mathbf{S} + \frac{1}{\beta}\frac{\partial \mathbf{F}}{\partial \hat{\mathbf{u}}}\mathbf{S} \tag{49}$$

$$\boldsymbol{\ell} = -p\mathbf{n} + \tau\mathbf{s} \tag{50}$$

$$\frac{\partial \boldsymbol{\ell}}{\partial \hat{\mathbf{u}}} = -p\frac{\partial \mathbf{n}}{\partial \hat{\mathbf{u}}} + \tau\frac{\partial \mathbf{s}}{\partial \hat{\mathbf{u}}} \tag{51}$$