Optimizing contact-based assemblies, supplementary material

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1 Contact

Consider the region on the boundary, Γ_C, representing the contact region of the main object with a rigid body. The PDE could be then summarized as following:

$$
\begin{aligned}
-\nabla \cdot \sigma = 0 & \text{ (external force)} \\
& \text{such that:} \\
& u = \hat{u} \quad \text{on } \Gamma_D \\
& \sigma n = g \quad \text{on } \Gamma_N \\
& u \cdot n \leqslant 0 \quad \text{on } \Gamma_C \\
& \sigma n \cdot n \leqslant 0 \quad \text{on } \Gamma_C \\
& (\sigma n \cdot n)(u \cdot n) = 0 \quad \text{on } \Gamma_C
\end{aligned}
$$

First equation on Γ_C says that displacement should be (if existent) on opposite direction of the normal. The second equation says that the normal force on this boundary should be 0 or on the opposite direction of the normal. And finally, the last one guarantees that there is nonzero force if and only if the bodies are touching (considering the displacement).

This problem has the following weak form:

$$\int_\Omega \varepsilon(u) : C : \varepsilon(w) dV \geqslant \int_\Omega f \cdot w dV + \int_{\Gamma_N} g \cdot w dS \quad \text{for any } w \in K(\Omega)$$

where $K(\Omega) = \{v \in (H^1(\Omega))^d, v = 0 \text{ on } \Gamma_D \text{ and } v \cdot n \leqslant 0 \text{ on } \Gamma_C\}$ and $u \in K(\Omega)$. Also, g here is the traction (force per area) on the boundary and f represents the forcing function (which we consider non existing, for this work). The problem can also be thought as an optimization problem with the following energy:

$$\underset{v \in K(\Omega)}{\operatorname{argmin}} \frac{1}{2} \int_\Omega \varepsilon(v) : C : \varepsilon(v) dV - \int_\Omega f \cdot v dV - \int_{\Gamma_N} g \cdot v dS$$

The work from Maury et al. [2] shows that the solution u admits at most a conical derivative and argues that it is difficult to use the concept in numerical practice, since it requires a subgradient optimization method. The idea then is to remove u from its convex set $K(\Omega)$ by penalizing the inequality $u \cdot n \leqslant 0$. We end up with the following formula approximating the normal contact effect:

$$\underset{v}{\operatorname{argmin}} \frac{1}{2} \int_\Omega \varepsilon(v) : C : \varepsilon(v) dV - \int_\Omega f \cdot v dV - \int_{\Gamma_N} g \cdot v dS + \frac{1}{\epsilon} j_N(v) \tag{1}$$

where $j_N(v)$ penalizes penetration. This problem can then be rewritten in the weak form as:

$$\int_\Omega \varepsilon(w) : C : \varepsilon(u)\, dV + j'_{N,\alpha}(u, w) = \int_\Omega w \cdot f + \int_{\Gamma_N} w \cdot g\, dS$$

where

$$j'_{N,\alpha}(u, w) = \frac{1}{\alpha} \int_{\Gamma_C} h_\eta(u \cdot n)\ w \cdot n\, dS$$

and

$$h_\eta(y) = \begin{cases} 0 & y \leqslant -\eta \\ \frac{1}{4\eta}y^2 + \frac{1}{2}y + \frac{\eta}{4} & -\eta \leqslant y \leqslant \eta \\ y & y \geqslant \eta \end{cases}$$

1.1 Deformable-deformable (DD) contact

Another case of contact is considered when dealing with other non-rigid objects, like an object with same material. The constraints are very similar to the one presented before, with the main difference that displacements and stress measurements on both sides of the contact region are considered. Region Γ_S defines the region of contact between two objects Ω^- and Ω^+. We refer to Γ_S on Ω^- (Ω^+) side as Γ_{S-} (Γ_{S+}).

The term $J'_{S,\alpha}(u,w)$ in this case is defined as:

$$j'_{S,\alpha}(u,w) = \frac{1}{\alpha}\int_{\Gamma_S} h_\eta([u]\cdot n^-)\ [w]\cdot n^-\,dS$$

where

$$[\theta] = \theta^- - \theta^+$$

We can rewrite this using two separate terms, one for each side of the contact region.

$$\begin{aligned} j'_{S,\alpha}(u,w) = \frac{1}{\alpha}\int_{\Gamma_{S-}} h_\eta([u]\cdot n^-)\ w\cdot n\,dS \quad + \\ +\frac{1}{\alpha}\int_{\Gamma_{S+}} h_\eta([u]\cdot n^-)\ w\cdot n\,dS \end{aligned}$$

where we assume that ϕ and n correspond to the side being integrated. Notice that the argument for h_η is always the same and contains n^-. We could rewrite the argument as:

$$\begin{aligned} [u]\cdot n^- &= u^-\cdot n^- - u^+\cdot n^- \\ &= u^-\cdot n^- + u^+\cdot n^+ \end{aligned}$$

1.2 FEM formulation

With the consideration of contact and neglecting the forcing function we obtain the equation:

$$\underbrace{\int_\Omega \varepsilon(w) : C : \varepsilon(u)\,dV}_{T_E} + \underbrace{j'_{N,\alpha}(u,w)}_{T_C} + \underbrace{j'_{S,\alpha}(u,w)}_{T_S} = \underbrace{\int_{\Gamma_N} w\cdot g\,dS}_{T_N} \tag{2}$$

When constructing the finite dimensional approximation, the first term T_E becomes:

$$T_E = \sum_e \sum_{A,B} \sum_{i,j} w_i^A \left(\int_{\Omega^e} \varepsilon(\varphi^A I_i) : C : \varepsilon(\varphi^B I_j)\,dV\right) u_j^B = \sum_e \sum_{A,B} \sum_{i,j} w_i^A K_{i,j}^{A,B} u_j^B$$

where i, j are representing the coordinates of each vector variable, A, B represents the local nodes in each element e of Ω. Also, I_j corresponds to the j column of a identity matrix of size equal to the number of dimensions we are working with.

In matrix vector form, we have

$$T_E = \sum_e \sum_{A,B} (w^A)^T K^{A,B} u^B = \sum_e w_e^T K_e u_e$$

where both w^A and u^B are vectors of size equal to N. Also, $K^{A,B} \in GL(2)$. On the final per element form, all vectors and matrices have size $N * n_{nel}$. The global form can be rewritten as follows:

$$T_E = \bar{w}^T K \bar{u}$$

Let's now talk about T_N that also appears in the linear elasticity formulation. Using the piecewise finite dimensional approximation:

$$\begin{aligned}
T_N &= \sum_{e \in E_n} \sum_{A,i} w_i^A \left(\int_{\Gamma_N^e} \varphi^A g_i \, dS \right) \\
&= \sum_{e \in E_N} \sum_{A,i} w_i^A (F_N)_i^A \\
&= \sum_{e \in E_N} \sum_{A} (w^A)^T (F_N)^A \\
&= \sum_{e \in E_N} (w_e)^T F_{Ne} \\
&= w^T F_N
\end{aligned}$$

RD Term.

Similar to the T_N term, T_C can be obtained:

$$\begin{aligned}
T_C &= \sum_{e \in E_C} \sum_{A,i} w_i^A \left(\frac{1}{\alpha} \int_{\Gamma_C^e} \varphi^A n_i \;\; h_\eta(u^h \cdot n) \, dS \right) \\
&= \sum_{e \in E_C} \sum_{A,i} w_i^A (N_{Ce})_i^A (\bar{u}) \\
&= \sum_{e \in E_C} \sum_{A} (w^A)^T (N_{Ce})^A (\bar{u}) \\
&= \sum_{e \in E_C} w_e^T N_{Ce}(\bar{u}) \\
&= \bar{w}^T N_C(\bar{u})
\end{aligned}$$

DD Term. Finally, we can look at the DD term T_S:

$$\begin{aligned}
T_S &= \sum_{e \in E_S} \frac{1}{\alpha} \int_{\Gamma_S} h_\eta([u] \cdot n^-) \; (w^- - w^+) \cdot n^- \, dS \\
&= \sum_{e^- \in E_{S-}} \frac{1}{\alpha} \int_{\Gamma_S} h_\eta([u] \cdot n^-) \; w^- \cdot n^- \, dS \\
&- \sum_{e^+ \in E_{S+}} \frac{1}{\alpha} \int_{\Gamma_S} h_\eta([u] \cdot n^-) \; w^+ \cdot n^- dS \\
&= \sum_{e^- \in E_{S-}} \sum_{A^-,i} w_i^{A^-} \left(\frac{1}{\alpha} \int_{\Gamma_S^{e^-}} \varphi^{A^-} n_i^- \, h_\eta([u] \cdot n^-) \; dS \right) \\
&- \sum_{e^+ \in E_{S+}} \sum_{A^+,i} w_i^{A^+} \left(\frac{1}{\alpha} \int_{\Gamma_S^{e^+}} \varphi^{A^+} n_i^- \, h_\eta([u] \cdot n^-) \; dS \right)
\end{aligned}$$

Because $n^- = -n^+$, we can rewrite T_S as:

$$\begin{aligned}
T_S = & \sum_{e^-\in E_{S-}} \sum_{A^-,i} w_i^{A^-} \left(\frac{1}{\alpha} \int_{\Gamma_S^{e^-}} \varphi^{A^-} n_i^- \, h_\eta([u]\cdot n^-) \; dS \right) \\
+ & \sum_{e^+\in E_{S+}} \sum_{A^+,i} w_i^{A^+} \left(\frac{1}{\alpha} \int_{\Gamma_S^{e^+}} \varphi^{A^+} n_i^+ \, h_\eta([u]\cdot n^-) \; dS \right) \\
= & \sum_{e^-\in E_{S-}} \sum_{A^-,i} w_i^{A^-} (N_{Se^-})_i^{A^-} + \sum_{e^+\in E_{S+}} \sum_{A^+,i} w^{A^+} (N_{Se^+})_i^{A^+} \\
= & \sum_{e^-\in E_{S-}} \sum_{A^-} (w^{A^-})^T N_{Se^-}^{A^-}(\bar{u}) + \sum_{e^+\in E_{S+}} \sum_{A^+} (w^{A^+})^T N_{Se^+}^{A^+}(\bar{u}) \\
= & \sum_{e^-\in E_{S-}} (w_{e^-})^T N_{Se^-}(\bar{u}) + \sum_{e^+\in E_{S+}} (w_{e^+})^T N_{Se^+}(\bar{u}) \\
= & \, \bar{w}^T N_{S-}(\bar{u}) + \bar{w}^T N_{S+}(\bar{u}) \\
= & \, \bar{w}^T (N_{S-}(\bar{u}) + N_{S+}(\bar{u})) \\
= & \, \bar{w}^T (N_S(\bar{u}))
\end{aligned}$$

1.3 Complete discretization

Putting all terms together from section 1.2 together:

$$\begin{aligned}
T_E + T_C + T_S &= T_N \\
\bar{w}^T K\bar{u} + \bar{w}^T N_C(\bar{u}) + \bar{w}^T (N_{S-}(\bar{u}) + N_{S+}(\bar{u})) &= \bar{w}^T F_N \\
\bar{w}^T (K\bar{u} - F_N + N_C(\bar{u}) + N_{S-}(\bar{u}) + N_{S+}(\bar{u})) &= 0 \\
F(\bar{u}) = \underbrace{K\bar{u} - F_N}_{\text{linear elasticity}} + N_C(\bar{u}) + N_{S-}(\bar{u}) + N_{S+}(\bar{u}) &= 0
\end{aligned}$$

Notice that $F(\bar{u})$ is nonlinear, because term $N_C(\bar{u})$ and DD terms are not linear in u. To solve $F(\bar{u}) = 0$, we can use methods for solving nonlinear equations, such as Newton Method:

$$\bar{u}_{it+1} = \bar{u}_{it} + DF(\bar{u}_{it})^{-1}(F(\bar{u}_{it+1}) - F(\bar{u}_{it}))$$

where $DF(\bar{u})$ is the Jacobian of $F(\bar{u})$ and index it refers to the iteration number.

But we want $F(\bar{u}_{it+1})$ to be zero! So,

$$\begin{aligned}
\Delta\bar{u}_{it} &= DF(\bar{u}_{it})^{-1}(-F(\bar{u}_{it})) \\
DF(\bar{u}_i)\Delta\bar{u}_{it} &= -F(\bar{u}_{it})
\end{aligned}$$

$F(\bar{u})$ is known. Now we compute the Jacobian $DF(\bar{u})$.

$$DF(\bar{u}) = K + DN_C(\bar{u}) + DN_{S-}(\bar{u}) + DN_{S+}(\bar{u})$$

Jacobian of contact term. We can compute each element $[DN_C(\bar{u})]_{i,j}$ individually. Notice that i and j corresponds each to a coordinate of a node. So, we can write

$$[DN_C(\bar{u})]_{i,j} = [DN_C(\bar{u})]_{k,l}^{A,B} = \frac{\partial (N_C)_k^A}{\partial u_l^B}$$

where A, B are global node indices and $k, l = 1, 2$ ($, 3$ in 3D) are the coordinate indices.

Then,

$$\frac{\partial (N_C)_k^A}{\partial u_l^B} = \sum_{e\in E_{AB}} \frac{\partial (N_{Ce})_k^{\bar{A}}}{\partial u_l^{\bar{B}}}$$

where E_{AB} contains all elements with nodes A and B. Moreover, $\bar{A}$ and $\bar{B}$ correspond to the local indices of global nodes A and B in element e.

$$\begin{aligned}
\frac{\partial (N_{Ce})_k^{\bar{A}}}{\partial u_l^{\bar{B}}} &= \frac{\partial}{\partial u_l^{\bar{B}}} \left(\frac{1}{\alpha} \int_{\Gamma_C^e} \varphi^A n_i \;\; h_\eta (u^h \cdot n) \, dS \right) \\
&= \frac{1}{\alpha} \int_{\Gamma_C^e} \varphi^A n_i \;\; \frac{\partial}{\partial u_l^{\bar{B}}} \big(h_\eta (u^h \cdot n) \big) \, dS \\
&= \frac{1}{\alpha} \int_{\Gamma_C^e} \varphi^A n_i \;\; \frac{\partial}{\partial u_l^{\bar{B}}} \left(h_\eta \left(\underbrace{\sum_{C,j} \varphi^C u_j^C n_j}_{y} \right) \right) dS
\end{aligned}$$

Using chain rule:

$$\frac{\partial h_\eta}{\partial u_l^{\bar{B}}} = \frac{\partial h_\eta}{\partial y} \frac{\partial y}{\partial u_l^{\bar{B}}}$$

Where we know

$$\frac{\partial h_\eta}{\partial y} = \begin{cases} 0 & y \leqslant -\eta \\ \frac{y}{2\eta} + \frac{1}{2} & -\eta \leqslant y \leqslant \eta \\ 1 & y \geqslant \eta \end{cases}$$

And

$$\frac{\partial y}{\partial u_l^{\bar{B}}} = \varphi^{\bar{B}} n_l$$

Finally,

$$\frac{\partial (N_{Ce})_k^{\bar{A}}}{\partial u_l^{\bar{B}}} = \frac{1}{\alpha} \int_{\Gamma_C^e} \varphi^{\bar{A}} n_k \;\; \frac{\partial h_\eta}{\partial y} (u^h \cdot n) \varphi^{\bar{B}} n_l \, dS \tag{3}$$

Notice that φ^P, n and u^h depend on x, so they cannot leave the integral.

Jacobian of DD terms. When computing the jacobian of the DD terms, we notice many similarities with the normal contact term. One difference is on the derivative of $h_\eta([u^h] \cdot n^-)$, which appears on both positive and negative terms.

$$h_\eta([u^h] \cdot n^-) = h_\eta(\underbrace{(u^- - u^+) \cdot n^-}_{y*})$$

$$\frac{\partial h_\eta(y*)}{\partial u_l^{\bar{B}}} = \frac{\partial h_\eta(y*)}{\partial y*} \frac{\partial y*}{\partial u_l^{\bar{B}}}$$

We already know $\frac{\partial h_\eta(y*)}{\partial y*}$, so:

$$\begin{aligned}
\frac{\partial y*}{\partial u_l^{\bar{B}}} &= \frac{\partial}{\partial u_l^{\bar{B}}} \left(\sum_j n_j^- \left(\sum_{C^-} \varphi^{C^-} u_j^{C^-} - \sum_{C^+} \varphi^{C^+} u_j^{C^+} \right) \right) \\
&= \begin{cases} \varphi^{\bar{B}} n_l^- & \text{if } \bar{B} \text{ on } S- \\ -\varphi^{\bar{B}} n_l^- & \text{if } \bar{B} \text{ on } S+ \end{cases} \\
&= \begin{cases} \varphi^{\bar{B}} n_l^- & \text{if } \bar{B} \text{ on } S- \\ \varphi^{\bar{B}} n_l^+ & \text{if } \bar{B} \text{ on } S+ \end{cases}
\end{aligned}$$

Using this information, we can build the full formula for the individual terms for $\frac{\partial (N_{Se^-})_k^{\bar{A}}}{\partial u_l^{\bar{B}}}$ and $\frac{\partial (N_{Se^+})_k^{\bar{A}}}{\partial u_l^{\bar{B}}}$.

$$\frac{\partial (N_{Se^-})_k^{\bar{A}}}{\partial u_l^{\bar{B}}} = \frac{1}{\alpha} \int_{\Gamma_S^{e-}} \varphi^{\bar{A}} n_k \ \frac{\partial h_\eta}{\partial y}([u^h] \cdot n^-) \varphi^{\bar{B}} n_l \, dS \tag{4}$$

$$\frac{\partial (N_{Se^+})_k^{\bar{A}}}{\partial u_l^{\bar{B}}} = \frac{1}{\alpha} \int_{\Gamma_S^{e+}} \varphi^{\bar{A}} n_k \ \frac{\partial h_\eta}{\partial y}([u^h] \cdot n^-) \varphi^{\bar{B}} n_l \, dS \tag{5}$$

Notice that the normal direction is implied (where possible) from the element we are integrating. By looking closely to the previous equations, we can conclude that formulas for both N_{Se^-} and N_{Se^+} are exactly the same, noting that the argument of h_η is always n^-. The same also happens with the Jacobian individual terms.

Linear system. In the original linear elasticity formulation, an SPSD (symmetric positive semi-definite) solver is used, since K is SPSD. The matrix is symmetric by exchanging nodes and indices given formula 5. Also, since the energy minimization problem in Equation 1 is convex, we can conclude that our jacobian is also SPSD. Note that this is only true if we don't consider friction forces, which is presented in the following sections.

2 Shape Optimization With Contact

The process of obtaining the shape derivative when dealing with linear elasticity is well explained in literature. We used here a similar approach to Panetta et al. work [3]. The details on how to compute the derivative can be found in [3] and its supplemental material.

The formula for the discrete shape derivative of a function $J(\bar{u}) = \int_\Omega e(\bar{u}, x)dx$, considering only linear elasticity, is shown below:

$$S_m^e[u, \rho] = \left(\int_\Omega [e - \varepsilon(\rho) : \sigma] \nabla \lambda_m + [\nabla \lambda_m \cdot (\sigma p_n + (\epsilon(\rho) : C - \tau) u_n)] dV \right) + \\ \left(-\frac{1}{|\Gamma_N|} \left(\int_{\Gamma_N} \rho \cdot g \, d\Gamma_N \right) \left(\int_{\Gamma_N} \nabla \lambda_m \, d\Gamma_N \right) + \left(\int_{\Gamma_N} (\rho \cdot g) \, \nabla \lambda_m \, d\Gamma_N \right) \right) \tag{6}$$

We focus here on how to obtain the shape derivative related to the new contact terms, since adding new terms to the elasticity problem leads to a change in the shape optimization.

2.1 Derivative of contact term in PDE

We need to add the following to the weak form:

$$\begin{aligned} T_C' &= \frac{d}{dt}\Big|_{t=0} (j_{N,\alpha}'(u, w)) \\ &= \frac{d}{dt}\Big|_{t=0} \left(\frac{1}{\alpha} \int_{\Gamma_C} h_\eta(u \cdot n) \ w \cdot n \, dS \right) \end{aligned}$$

By assuming the contact shape does not change during optimization, we can pass the derivative inside integral:

$$\begin{aligned} T_C' &= \frac{1}{\alpha} \int_{\Gamma_C} \frac{d}{dt}\Big|_{t=0} (h_\eta(u \cdot n) \ w \cdot n) \, dS \\ &= \frac{1}{\alpha} \int_{\Gamma_C} \frac{d}{dt}\Big|_{t=0} (h_\eta(u \cdot n)) \ w \cdot n \ + h_\eta(u \cdot n) \ \frac{d}{dt}\Big|_{t=0} (w \cdot n) \, dS \end{aligned}$$

But because $D[w]=0$ in our discretization (and shape of Γ_C does not change), we can keep only the first term. We need to compute the following:

$$\begin{aligned}\frac{d}{dt}\Big|_{t=0}(h_\eta(u\cdot n)) &= \frac{dh_\eta}{dy}\frac{dy}{dt}\\ &= \frac{\partial h_\eta}{\partial y}\frac{d(u\cdot n)}{dt}\\ &= h'_\eta(u\cdot n)\,(D[u]\cdot n)\end{aligned}$$

So, T'_C term corresponds to:

$$T'_C = \frac{1}{\alpha}\int_{\Gamma_C}\left(h'_\eta(u\cdot n)\,(D[u]\cdot n)\right)\; w\cdot n\, dS$$

Complete derivative (contact shape may not be fixed). If we consider the more interesting case where shape on contact region is allowed to be perturbed during optimization, we have the following.

Consider the mapping $f_t(X) = X + tv(X)$ that represents the perturbation with velocity v of a point X in the original shape to its new position x in the perturbed shape. (The inverse of f_t is then $f_t^{-1}(x) = x - tv$). The jacobian of the map is then ∇f_t and equals $F_t = I + t\nabla v$. (As we know, the jacobian of f_t^{-1} corresponds to F_t^{-1}).

Then,

$$\begin{aligned}T'^{*}_C &= \frac{d}{dt}\Big|_{t=0}\left(j'_{N,\alpha}(u,w)\right)\\ &= \frac{d}{dt}\Big|_{t=0}\left(\frac{1}{\alpha}\int_{\Gamma_C^t} h_\eta(u\cdot n)\; w\cdot n\, dS\right)\\ &= \frac{d}{dt}\Big|_{t=0}\left(\frac{1}{\alpha}\int_{\Gamma_C^0} h_\eta(u\cdot n)\; w\cdot n\;\det(F_t)\, dS\right)\\ &= \frac{1}{\alpha}\int_{\Gamma_C^0}\frac{d}{dt}\Big|_{t=0}(h_\eta(u\cdot n)\; w\cdot n\;\det(F_t))\, dS\\ &= \frac{1}{\alpha}\int_{\Gamma_C}\frac{d}{dt}\Big|_{t=0}(h_\eta(u\cdot n))\; w\cdot n\;\det(F_0) + h_\eta(u\cdot n)\;\frac{d}{dt}\Big|_{t=0}(w\cdot n)\det(F_0) + h_\eta(u\cdot n)\; w\cdot n\;\frac{d}{dt}\Big|_{t=0}(\det(F_t))\, dS\end{aligned}$$

Note that F_0 is the identity and that $D[w]=0$. We arrive at the following equation:

$$\begin{aligned}T'^{*}_C &= \frac{1}{\alpha}\left[\int_{\Gamma_C} h'_\eta(u\cdot n)(n\cdot D[u] + u\cdot D[n])w\cdot n dS + \int_{\Gamma_C} h_\eta(u\cdot n)(w\cdot D[n])dS + \int_{\Gamma_C} h_\eta(u\cdot n)(w\cdot n)\nabla\cdot v dS\right]\\ &= T'_C - H'_C\end{aligned}$$

where

$$H'_C = -\frac{1}{\alpha}\left[\int_{\Gamma_C} h'_\eta(u\cdot n)(u\cdot D[n])w\cdot n dS + \int_{\Gamma_C} h_\eta(u\cdot n)(w\cdot D[n])dS + \int_{\Gamma_C} h_\eta(u\cdot n)(w\cdot n)\nabla\cdot v\, dS\right]$$

2.2 Derivative of the DD term in PDE

In a similar way, we can also compute the derivative of the DD term T_S in Equation (2) with respect to time. Without considering the shape moving on the DD boundary, we obtain:

$$T'_S = \frac{1}{\alpha}\int_{\Gamma_S}\left(h'_\eta([u]\cdot n^-)\,(D[[u]]\cdot n^-)\right)\; w\cdot n\, dS$$

where $\Gamma_S = \Gamma_{S+}\cup\Gamma_{S-}$.

Complete derivative (DD regions may not be fixed). If we decide to consider the DD region moving, we have:

$$\begin{aligned}T'^{*}_S = \frac{1}{\alpha}\Bigg[&\int_{\Gamma_S}\left(h'_\eta([u]\cdot n^-)\,(D[[u]]\cdot n^- + [u]\cdot D[n^-])\right)\;(w\cdot n)\, dS\\ &+ \int_{\Gamma_S} h_\eta([u]\cdot n^-)(w\cdot D[n])\, dS + \int_{\Gamma_S} h_\eta([u]\cdot n^-)(w\cdot n)\nabla\cdot v\, dS\Bigg]\\ = T'_S - H'_S\end{aligned}$$

where

$$H_S^{'} = -\frac{1}{\alpha}\Bigg[\int_{\Gamma_S} h_\eta'([u]\cdot n^-)\,([u]\cdot D[n^-])\;(w\cdot n)\,dS +$$
$$+\int_{\Gamma_S} h_\eta([u]\cdot n^-)(w\cdot D[n])\,dS + \int_{\Gamma_S} h_\eta([u]\cdot n^-)(w\cdot n)\nabla\cdot v\,dS$$

2.3 Final derivative including RD and DD terms

The complete derivative of the PDE is then:

$$\boxed{\int_\Omega \varepsilon(w):C:\varepsilon(D[u])dV + \boldsymbol{T_C'} + \boldsymbol{T_S'} = \boldsymbol{H_C'} + \boldsymbol{H_S'} + \int_\Omega (\nabla w\nabla v):\sigma + \epsilon(w):C:(\nabla u\nabla v) - (\epsilon(w):\sigma)(\nabla\cdot v)dX-}$$
$$\boxed{-\left(\int_{\Gamma_N}(\nabla\cdot v)\,d\Gamma_N\right)\left(\int_{\Gamma_N} w\cdot g\,d\Gamma_N\right) + \left(\int_{\Gamma_N}(w\cdot g)\,(\nabla\cdot v)\,d\Gamma_N\right)} \quad (7)$$

2.4 The adjoint PDE

Without contact, we have equation below define the adjoint equation.

$$\int_\Omega \tau:\varepsilon(\psi)\,dV = \int_\Omega \varepsilon(\rho):C:\varepsilon(\psi)\,dV \quad (8)$$

where $\tau = 2e'\sigma : C$.

For the new weak form derivative we need to add in the T_C' term. As derived in [2], the T_C' term should be in form of:

$$\int_{\Gamma_C} \frac{\partial j}{\partial u}(u,\rho,n)\cdot\psi\,dS$$

where, in our case, j corresponds to the integrand of $j_{N,\alpha}'$ which equals $\frac{1}{\alpha}h_\eta(u\cdot n)\;w\cdot n$.

In fact, we can modify and reorder our derivative in the previous subsection in the following way:

$$T_C' = \int_{\Gamma_C} \underbrace{\frac{1}{\alpha}h_\eta'(u\cdot n)\;(\rho\cdot n)\,n}_{\text{integrand of } \frac{\partial j_{N,\alpha}'}{\partial u}}\;\cdot\, D[u]\;dS$$

Thus, we can write the new adjoint problem as the following:

$$\int_\Omega \epsilon(\rho):C:\epsilon(\psi)\,dV + \underbrace{\int_{\Gamma_C}\frac{1}{\alpha}h_\eta'(u\cdot n)\,(\rho\cdot n)\;n\cdot\psi\,dS}_{AT_C} = \int_\Omega \tau:\epsilon(\psi)\,dS$$

Notice that, in our FEM discretization, in each element we have $\sum_A \psi^A\varphi^A(x)$ and $\sum_B \rho^B\varphi^B(x)$. Then, discretizing the new term AT_C:

$$\begin{aligned}
AT_C &= \sum_{e\in E_C}\int_{\Gamma_C^e}\frac{1}{\alpha}h_\eta'(u^h\cdot n)\left(\sum_B \rho^B\varphi^B\cdot n\right)\;\left(n\cdot\sum_A \psi^A\varphi^A\right)dS\\
&= \sum_{e\in E_C}\int_{\Gamma_C^e}\frac{1}{\alpha}h_\eta'(u^h\cdot n)\left(\sum_B \rho_j^B\varphi^B n_j\right)\;\left(n_i\sum_A \psi_i^A\varphi^A\right)dS\\
&= \sum_{e\in E_C}\sum_{A,B}\sum_{i,j}\psi_i^A\left[\int_{\Gamma_C^e}\frac{1}{\alpha}h_\eta'(u^h\cdot n)\varphi^A\varphi^B n_i\,n_j\,dS\right]\rho_j^B\\
&= \psi^T\,[AN_C]\,\rho
\end{aligned}$$

where $[AN_C]$ is a matrix with same size as K. Note that this corresponds exactly to the Jacobian formulation, which means that the matrix we should use in the adjoint PDE resolution is the same as the result of the last iteration Newton's method for the original PDE.

This means we still have a linear equation to solve as adjoint problem. However, the stiffness matrix K is not the only term on the left hand side. Instead, we have:

$$\psi^T K\rho + \psi^T [AN_C]\rho = \psi^T D$$

where D is a vector corresponding to the "forcing function" $-\nabla \cdot \tau$ (or $\int_\Omega \tau : \epsilon(\psi)\, dS$ in the weak form). Rewriting the equation above we have:

$$\psi^T (K + [AN_C])\, \rho - D) = 0$$

This is the same as solving a linear system:

$$(K + [AN_C])\, \rho = D$$

Notice that we do **not** need to consider fixed terms due to Dirichlet values being all zeros for the adjoint problem. So, directly eliminating rows and columns suffices. Similar terms are added to the system for DD contact and both friction types (to be presented in Section 3).

2.5 Final Discrete Shape Derivative

If we assume that the area of contact is not optimized, meaning it is fixed from the beginning, we can compute the shape derivative the same way we did before, by just replacing ρ with the one obtained with the new adjoint system.

On the other hand, if the contact area is not fixed, we need to add terms related to H'_C (as well as H'_S) to the formula in Equation 6. To produce the final version, we use the following:

$$D[n](v) = -\nabla_t (v \cdot n) \text{ on } \partial\Omega$$
$$\text{where } \nabla_t \theta = \nabla\theta - (\nabla\theta \cdot n)n$$

So,

$$D[n](v) = -\nabla(v \cdot n) + (\nabla(v \cdot n) \cdot n)n$$

By discretizing $v(x) = \sum_m \lambda_m(x)\, \delta q_m$, we can obtain:

$$D[n](v) = \sum_m -\nabla\lambda_m\, (n \cdot \delta q_m) + n\, (\nabla\lambda_m \cdot n)\, (n \cdot \delta q_m)$$

With this, we can compute $(\theta \cdot D[n])$ (needed on H'_C formula), for any vector θ:

$$\theta \cdot D[n](v) = \sum_m [-(\theta \cdot \nabla\lambda_m)n + (\theta \cdot n)(\nabla\lambda_m \cdot n)n] \cdot \delta q_m$$

Then, adding this to the discretized terms in H'_C and H'_S, we obtain:

$$\begin{aligned} H'_{Cd}[v] = \sum_m -\frac{1}{\alpha}\Bigg[& \int_{\Gamma_C} h'_\eta(u \cdot n)\ (w \cdot n)\ (-(u \cdot \nabla\lambda_m) + (u \cdot n)(\nabla\lambda_m \cdot n))\ dS\ n + \\ & + \int_{\Gamma_C} h_\eta(u \cdot n)\ (-(w \cdot \nabla\lambda_m) + (w \cdot n)(\nabla\lambda_m \cdot n))\ dS\ n + \\ & + \int_{\Gamma_C} h_\eta(u \cdot n)\ (w \cdot n)\, dS\ \nabla\lambda_m \Bigg] \cdot \delta q_m \end{aligned}$$

$$\begin{aligned} H'_{Sd}[v] = \sum_m -\frac{1}{\alpha}\Bigg[& \int_{\Gamma_S} h'_\eta([u] \cdot n^-)\ (w \cdot n)\ \Big[-([u] \cdot \nabla\lambda_m) + ([u] \cdot n^-)(\nabla\lambda_m \cdot n^-)\Big]\ dS\ n^- + \\ & + \int_{\Gamma_S} h_\eta([u] \cdot n^-)\ (-(w \cdot \nabla\lambda_m) + (w \cdot n)(\nabla\lambda_m \cdot n))\ dS\ n + \\ & + \int_{\Gamma_S} h_\eta([u] \cdot n^-)\ (w \cdot n)\, dS\ \nabla\lambda_m \Bigg] \cdot \delta q_m \end{aligned}$$

By switching w to ρ, after solving the adjoint PDE, we reach the formulations presented in the appendix of the paper, described as S_C (from H'_{Cd}) and S_S (from H'_{Sd}).

3 Adding Friction to Contact

Although we include normal contact force in previous sections, we still need to add friction, which is an important force to keep objects in place or to reduce their movement in the presence of significantly small forces. In the case of contact with a rigid surface, we add the following constraints:

$$\begin{aligned}
&\|(\sigma n)_t\| \leqslant \mu|(\sigma n)_n| \text{ on } \Gamma_C \\
&\|(\sigma n)_t\| < \mu|(\sigma n)_n| \implies u_t = 0 \text{ on } \Gamma_C \\
&\|(\sigma n)_t\| = \mu|(\sigma n)_n| \implies u_t = -\lambda(\sigma n)_t
\end{aligned}$$

where $\lambda > 0$.

The first inequality says that the tangent force should be always less than or equal to the normal force multiplied by friction coefficient μ. The second equation represents the case where, if the force is lower than the normal force term (multiplied by μ), the object does not move in the tangential direction of the surface. Consider the example of a box on a rigid surface. A minimum force is required to move box to counteract the static friction. The last equation describes scenarios after this minimum force is applied. The box starts to move in the opposite direction of the friction force. Notice that the force is constant after the object starts moving in the tangential direction.

Adding these constraints to the elasticity problem makes the problem much more difficult since friction is dissipative and the physical problem cannot be represented as a minimization of potential energy anymore. We have to work directly with the variational inequality form (since there is also no corresponding variational equality):

$$\int_\Omega \varepsilon(u) : C : \varepsilon(w) dV + \underbrace{\int_{\Gamma_C} \mu|(\sigma n)_n| \, \|w_t\| dS - \int_{\Gamma_C} \mu|(\sigma n)_n| \, \|u_t\| dS}_{\text{new friction terms}} \geqslant \int_\Omega f \cdot w dV + \int_{\Gamma_N} g \cdot w dS$$

for any $\phi \in K(\Omega)$. Here, θ_t corresponds to the tangential component of a vector $\theta_t = \theta - (\theta \cdot n)n$.

Approximating the norm function by a smooth function $N_\eta(v)$ and using the previous penalization on penetration, we arrive at a variational equality, as shown in [1]. The final variational equality (which also includes the case of DD contact) is shown below:

$$\underbrace{\int_\Omega \varepsilon(w) : C : \epsilon(u) \, dV}_{T_E} + \underbrace{j'_{N,\alpha}(u,w)}_{T_C} + \underbrace{j'_{S,\alpha}(u,w)}_{T_S} + \underbrace{j'_{CF,\alpha}(u,w)}_{T_{CF}\text{: RD friction}} + \underbrace{j'_{SF,\alpha}(u,w)}_{T_{SF}\text{: DD friction}} = \underbrace{\int_{\Gamma_N} w \cdot g \, dS}_{T_N} \tag{9}$$

And here are the formulas for both the DD and the RD terms:

$$j'_{CF,\alpha}(u,w) = \int_{\Gamma_C} \frac{\mu}{\alpha} h_\eta(u \cdot n) \; N'_\eta(u_t) \cdot w_t \; dS \tag{10}$$

$$j'_{SF,\alpha}(u,w) = \int_{\Gamma_S} \frac{\mu}{\alpha} h_\eta([u] \cdot n^-) \; N'_\eta([u]_t) \cdot [w]_t \; dS \tag{11}$$

where $N_\eta(x)$ is an approximation of the $L2$ norm function:

$$N_\eta(y) = \begin{cases} \|y\| & \|y\| \geqslant \eta \\ -\frac{1}{8\eta^3}\|y\|^4 + \frac{3}{4\eta}\|y\|^2 + \frac{3}{8}\eta & \|y\| \leqslant \eta \end{cases} \tag{12}$$

and, therefore,

$$N'_\eta(y) = \begin{cases} \frac{1}{\|y\|} y & \|y\| \geqslant \eta \\ -\frac{\|y\|^2}{2\eta^3} y + \frac{3}{2\eta} y & \|y\| \leqslant \eta \end{cases} \tag{13}$$

Now, we can work on discretizing the new friction terms (T_{CF} and T_{SF}) for FEM.

3.1 FEM Formulation

First, consider the RD term:

$$
\begin{aligned}
T_{CF} &= \sum_{e\in E_C}\sum_{A,i} w_i^A \left(\frac{\mu}{\alpha}\int_{\Gamma_C^e} \varphi^A \;\; h_\eta(u\cdot n)\,[N'_\eta(u_t)]_i\,dS\right) - \sum_{B,j} w_j^B \left(\frac{\mu}{\alpha}\int_{\Gamma_C^e}\varphi^B \;\; h_\eta(u\cdot n)\;(N'_\eta(u_t)\cdot n)\,n_j\,dS\right)\\
&= \sum_{e\in E_C}\sum_{A,i} w_i^A \left(\underbrace{\left(\frac{\mu}{\alpha}\int_{\Gamma_C^e}\varphi^A \;\; h_\eta(u\cdot n)\,[N'_\eta(u_t)]_i\,dS\right)}_{F_C} - \underbrace{\left(\frac{\mu}{\alpha}\int_{\Gamma_C^e}\varphi^A \;\; h_\eta(u\cdot n)\;(N'_\eta(u_t)\cdot n)\,n_i\,dS\right)}_{F_C^2}\right)
\end{aligned}
$$

But notice that the second term F_C^2 contains a multiplication with $N'_\eta(u_t)\cdot n$. As shown in N'_η formula, it keeps the direction of its argument. Thus, $N'_\eta(u_t) = \lambda u_t$ and, consequently, $N'_\eta(u_t)\cdot n = \lambda(u_t\cdot n) = 0$. So

$$
\begin{aligned}
T_{CF} &= \sum_{e\in E_C}\sum_{A,i} w_i^A \left(\frac{\mu}{\alpha}\int_{\Gamma_C^e}\varphi^A \;\; h_\eta(u\cdot n)\,[N'_\eta(u_t)]_i\,dS\right)\\
&= \sum_{e\in E_C}\sum_{A,i} w_i^A (F_{Ce})_i^A(\bar{u})\\
&= \sum_{e\in E_C}\sum_{A} (w^A)^T (F_{Ce})^A(\bar{u})\\
&= \sum_{e\in E_C} w_e^T F_{Ce}(\bar{u})\\
&= \bar{w}^T F_C(\bar{u})
\end{aligned}
$$

Then, we can apply similar operations to find the FEM formulation term for the DD friction term:

$$
\begin{aligned}
T_{SF} = &\sum_{e\in E_{S-}}\sum_{A-,i} w_i^{A-}\left(\frac{\mu}{\alpha}\int_{\Gamma_{S-}^e}\varphi^{A-}\;\; h_\eta([u]\cdot n^-)\,[N'_\eta([u]_t)]_i\,dS\right) +\\
&- \sum_{e\in E_{S+}}\sum_{A+,i} w_i^{A+}\left(\frac{\mu}{\alpha}\int_{\Gamma_{S+}^e}\varphi^{A+}\;\; h_\eta([u]\cdot n^-)\,[N'_\eta([u]_t)]_i\,dS\right) +\\
&- \sum_{e\in E_{S-}}\sum_{B-,j} w_j^{B-}\left(\frac{\mu}{\alpha}\int_{\Gamma_{S-}^e}\varphi^{B-}\;\; h_\eta([u]\cdot n^-)\;(N'_\eta([u]_t)\cdot n)\,n_j\,dS\right) +\\
&+ \sum_{e\in E_{S+}}\sum_{B+,j} w_j^{B+}\left(\frac{\mu}{\alpha}\int_{\Gamma_{S+}^e}\varphi^{B+}\;\; h_\eta([u]\cdot n^-)\;(N'_\eta([u]_t)\cdot n)\,n_j\,dS\right)
\end{aligned}
$$

But notice that $N'_\eta([u]_t) = N'_\eta(u_t^- - u_t^+) = -N'_\eta(u_t^+ - u_t^-) = -N'_\eta(-[u]_t)$. This makes it possible to reduce to only two sums, like the RD term.

$$
\begin{aligned}
T_{SF} = &\sum_{e\in E_S}\sum_{A,i} w_i^A\left(\frac{\mu}{\alpha}\int_{\Gamma_S^e}\varphi^A\;\; h_\eta([u]\cdot n^-)\,[N'_\eta(u_t - u_t^o)]_i\,dS\right) +\\
&- \sum_{e\in E_S}\sum_{B,j} w_j^B\left(\frac{\mu}{\alpha}\int_{\Gamma_S^e}\varphi^B\;\; h_\eta([u]\cdot n^-)\;(N'_\eta(u_t - u_t^o)\cdot n)\,n_j\,dS\right)\\
= &\sum_{e\in E_S}\sum_{A,i} w_i^A\left(\frac{\mu}{\alpha}\int_{\Gamma_S^e}\varphi^A\;\; h_\eta([u]\cdot n^-)\,[N'_\eta(u_t - u_t^o)]_i\,dS\right) +\\
&\qquad - w_i^A\left(\frac{\mu}{\alpha}\int_{\Gamma_S^e}\varphi^A\;\; h_\eta([u]\cdot n^-)\;(N'_\eta(u_t - u_t^o)\cdot n)\,n_i\,dS\right)
\end{aligned}
$$

Again, the second term can be eliminated due to $(N'_\eta(u_t - u^o_t) \cdot n) = 0$

$$\begin{aligned} T_{SF} &= \sum_{e\in E_S} \sum_{A,i} w_i^A \left(\frac{\mu}{\alpha} \int_{\Gamma_S^e} \varphi^A \;\; h_\eta([u]\cdot n^-) \, [N'_\eta(u_t - u^o_t)]_i \, dS \right) \\ &= \sum_{e\in E_C} \sum_{A,i} w_i^A (F_{Se})_i^A(\bar{u}) \\ &= \sum_{e\in E_C} \sum_{A} (w^A)^T (F_{Se})^A(\bar{u}) \\ &= \sum_{e\in E_C} w_e^T F_{Se}(\bar{u}) \\ &= \bar{w}^T F_S(\bar{u}) \end{aligned}$$

where u^o is the displacement on the opposite edge of each e (boundary element).

3.2 Jacobian of RD term

We can compute each $[DF_C(\bar{u})]_{i,j}$ individually. Notice that i and j corresponds to a different coordinate of a node respectively. So, we can write

$$[DF_C(\bar{u})]_{i,j} = [DF_C(\bar{u})]_{k,l}^{A,B} = \frac{\partial (F_C)_k^A}{\partial u_l^B}$$

where A, B are global node indices and $k, l = 1, 2$ $(, 3$ in 3D) are the coordinate indices.

Then,

$$\frac{\partial (F_C)_k^A}{\partial u_l^B} = \sum_{e\in E_{AB}} \frac{\partial (F_{Ce})_k^{\bar{A}}}{\partial u_l^{\bar{B}}}$$

where E_{AB} contains all elements with nodes A and B. Moreover, $\bar{A}$ and $\bar{B}$ correspond to the local indices of global nodes A and B in element e.

We can develop it:

$$\begin{aligned} \frac{\partial (F_{Ce})_k^{\bar{A}}}{\partial u_l^{\bar{B}}} &= \frac{\partial}{\partial u_l^{\bar{B}}} \left(\frac{\mu}{\alpha} \int_{\Gamma_C^e} \varphi^{\bar{A}} \;\; h_\eta(u\cdot n) \, [N'_\eta(u_t)]_k \, dS \right) \\ &= \frac{\mu}{\alpha} \int_{\Gamma_C^e} \varphi^{\bar{A}} \;\; \left(\frac{\partial}{\partial u_l^{\bar{B}}} (h_\eta(u\cdot n)) \, [N'_\eta(u_t)]_k + h_\eta(u\cdot n) \, \frac{\partial}{\partial u_l^{\bar{B}}} ([N'_\eta(u_t)]_k) \right) dS \end{aligned}$$

We know from the normal contact force that

$$\frac{\partial}{\partial u_l^{\bar{B}}} (h_\eta(\overbrace{u\cdot n}^{y})) = \frac{\partial h_\eta}{\partial y} \frac{\partial y}{\partial u_l^{\bar{B}}}$$

Where we know

$$\frac{\partial h_\eta}{\partial y} = \begin{cases} 0 & y \leqslant -\eta \\ \frac{y}{2\eta} + \frac{1}{2} & -\eta \leqslant y \leqslant \eta \\ 1 & y \geqslant \eta \end{cases}$$

And

$$\frac{\partial y}{\partial u_l^{\bar{B}}} = \varphi^{\bar{B}} n_l$$

We also need to compute $\frac{\partial}{\partial u_l^{\bar{B}}}([N'_\eta(u_t)]_k)$:

$$\frac{\partial}{\partial u_l^{\bar{B}}} ([N'_\eta(\overbrace{u_t}^{w})]_k) = \frac{\partial [N'_\eta]_k}{\partial w} \frac{\partial w}{\partial u_l^{\bar{B}}}$$

We can compute the term $\frac{\partial}{\partial w}([N'_\eta(w)]_k)$ from symmetric matrix $\frac{\partial}{\partial w}([N'_\eta(w)])$.

$$\frac{\partial}{\partial w}([N'_\eta(w)]) = \begin{cases} \frac{1}{\|w\|} I - \frac{1}{\|w\|^3} ww^T \\ -\frac{ww^T}{\eta^3} - \frac{\|w\|^2}{2\eta^3} I + \frac{3}{2\eta} I \end{cases}$$

And

$$\frac{\partial w}{\partial u_l^{\bar{B}}} = \frac{\partial}{\partial u_l^{\bar{B}}}(u - (u \cdot n)n) = \varphi^B (I_l - n_l n)$$

Finally,

$$\frac{\partial (F_{Ce})_k^{\bar{A}}}{\partial u_l^{\bar{B}}} = \frac{\mu}{\alpha} \int_{\Gamma_C^e} \varphi^{\bar{A}} \varphi^{\bar{B}} \left(\frac{\partial h_\eta}{\partial y}(u \cdot n) \, [N'_\eta(u_t)]_k n_l + h_\eta(u \cdot n) \left[\frac{\partial N'_\eta}{\partial w}(u_t) \right]_k^T (I_l - n_l n) \right) dS \tag{14}$$

Using Equation 14 we can build the full Jacobian related to friction $DF_C(\bar{u})$.

3.3 Jacobian of the DD term

Now, let's do the same for the DD term of friction.

$$[DF_S(\bar{u})]_{i,j} = [DF_S(\bar{u})]_{k,l}^{A,B} = \frac{\partial (F_S)_k^A}{\partial u_l^B}$$

where A, B are global node indices and $k, l = 1, 2$ (, 3 in 3D) are the coordinate indices.

Then,

$$\frac{\partial (F_S)_k^A}{\partial u_l^B} = \sum_{e \in E_{AB}} \frac{\partial (F_{Se})_k^{\bar{A}}}{\partial u_l^{\bar{B}}}$$

where E_{AB} contains all elements with nodes A and B. Moreover, $\bar{A}$ and $\bar{B}$ correspond to the local indices of global nodes A and B in element e.

For the first part we have:

$$\begin{aligned} \frac{\partial (F_{Se})_k^{\bar{A}}}{\partial u_l^{\bar{B}}} &= \frac{\partial}{\partial u_l^{\bar{B}}} \left(\frac{\mu}{\alpha} \int_{\Gamma_S^e} \varphi^{\bar{A}} \;\; h_\eta([u] \cdot n^-) \, [N'_\eta(u_t - u_t^o)]_k \, dS \right) \\ &= \frac{\mu}{\alpha} \int_{\Gamma_S^e} \varphi^{\bar{A}} \;\; \left(\frac{\partial}{\partial u_l^{\bar{B}}} (h_\eta([u] \cdot n^-)) \, [N'_\eta(u_t - u_t^o)]_k + h_\eta([u] \cdot n^-) \, \frac{\partial}{\partial u_l^{\bar{B}}} ([N'_\eta(u_t - u_t^o)]_k) \right) dS \end{aligned}$$

To compute this, we need the answer to

$$\frac{\partial}{\partial u_l^{\bar{B}}} (N'_\eta(\overbrace{u_t - u_t^o}^{w})) = \frac{\partial N'_\eta}{\partial w} \frac{\partial w}{\partial u_l^{\bar{B}}}$$

where

$$\frac{\partial (u_t - u_t^o)}{\partial u_l^{\bar{B}}} = \begin{cases} \;\;\varphi^{\bar{B}} (I_l - n_l n) & \text{if } \bar{B} \text{ is on } e \text{ (current edge) side} \\ -\varphi^{\bar{B}} (I_l - n_l n) & \text{if } \bar{B} \text{ is on side opposite to } e \end{cases}$$

Also,

$$h_\eta([u] \cdot n^-) = h_\eta(\underbrace{u \cdot n - u^o \cdot n}_{y})$$

$$\frac{\partial}{\partial u_l^{\bar{B}}} h_\eta([u] \cdot n^-) = \frac{\partial h_\eta}{\partial y} \frac{\partial y}{\partial u_l^{\bar{B}}}$$

$$\frac{\partial([u]\cdot n^-)}{\partial u_l^{\bar{B}}} = \frac{\partial u\cdot n}{\partial y} - \frac{\partial u^o\cdot n}{\partial y} = \begin{cases} \varphi^{\bar{B}} n_l & \text{if } \bar{B} \text{ is on } e \text{ (current edge) side} \\ -\varphi^{\bar{B}} n_l & \text{if } \bar{B} \text{ is on side opposite to } e \end{cases}$$

So, summarizing

$$\frac{\partial(F_{Se})_k^{\bar{A}}}{\partial u_l^{\bar{B}}} = op(e,\bar{B})\ \frac{\mu}{\alpha}\int_{\Gamma_S^e} \varphi^{\bar{A}}\,\varphi^{\bar{B}}\left(\frac{\partial h_\eta}{\partial y}([u]\cdot n^-)\ n_l\,[N'_\eta(u_t-u_t^o)]_k + h_\eta([u]\cdot n^-)\left[\frac{\partial N'_\eta}{\partial w}(u_t-u_t^o)\right]_k^T (I_l - n_l n)\right)dS$$

where

$$op(e,A) = \begin{cases} 1 & \text{if node } A \text{ is } \textbf{on } e \text{ (current edge) side} \\ -1 & \text{if node } A \text{ is on } \textbf{opposite} \text{ side of } e \end{cases}$$

Note that the Jacobian with respect to friction is not SPSD anymore, and not even symmetric.

4 Shape Optimization With Friction

The addition of friction terms to our elasticity problem with contact adds complexity to the shape optimization.

4.1 Derivative of contact term in PDE

First, consider the case of contact with a rigid body, represented by the term T_{CF}.

$$\begin{aligned} T'^{*}_{CF} &= \frac{d}{dt}\Big|_{t=0}\big(j'_{CF,\alpha}(u,w)\big) \\ &= \frac{d}{dt}\Big|_{t=0}\left(\int_{\Gamma_C}\frac{\mu}{\alpha}\,h_\eta(u\cdot n)\ N'_\eta(u_t)\cdot w_t\ dS\right) \end{aligned}$$

Passing the derivative inside the integral:

$$\begin{aligned} T'^{*}_{CF} &= \frac{\mu}{\alpha}\int_{\Gamma_C}\frac{d}{dt}\Big|_{t=0}\big(h_\eta(u\cdot n)\ N'_\eta(u_t)\cdot w_t\ \det(F_t)\big)\ dS \\ &= \frac{\mu}{\alpha}\int_{\Gamma_C}\frac{d}{dt}\Big|_{t=0}(h_\eta(u\cdot n))\ N'_\eta(u_t)\cdot w_t\ \det(F_t) + h_\eta(u\cdot n)\ \frac{d}{dt}\Big|_{t=0}\big(N'_\eta(u_t)\cdot w_t\big)\ \det(F_t) + \\ &\quad + h_\eta(u\cdot n)\,N'_\eta(u_t)\cdot w_t\ \frac{d}{dt}\Big|_{t=0}(\det(F_t)) \quad dS \\ &= \frac{\mu}{\alpha}\int_{\Gamma_C}\left(\frac{d}{du}(h_\eta(u\cdot n))\cdot D[u] + \frac{d}{dn}(h_\eta(u\cdot n))\cdot D[n]\right)\ N'_\eta(u_t)\cdot w + \\ &\quad + h_\eta(u\cdot n)\left(\frac{d}{du_t}\big(N'_\eta(u_t)\big)\,(D[u]-((D[u]\cdot n + u\cdot D[n])n - (u\cdot n)D[n]))\cdot w_t + N'_\eta(u_t)\cdot D[w]\right) + \\ &\quad + h_\eta(u\cdot n)\ N'_\eta(u_t)\cdot w_t\ \nabla\cdot v \quad dS \end{aligned}$$

Let's work on some individual terms of our derivative:

$$\begin{aligned} \frac{d}{du}(h_\eta(u\cdot n)) &= h'_\eta(u\cdot n)\,\frac{d(u\cdot n)}{du} = h'_\eta(u\cdot n)\,n \\ \frac{d}{dn}(h_\eta(u\cdot n)) &= h'_\eta(u\cdot n)\,\frac{d(u\cdot n)}{dn} = h'_\eta(u\cdot n)\,u \end{aligned}$$

And

$$\begin{aligned} &\frac{dN'_\eta(u_t)}{du_t}(D[u]-((D[u]\cdot n + u\cdot D[n])n + (u\cdot n)D[n])) = \\ &= N''_\eta(u_t)\Big(\big(I - nn^T\big)D[u] - (u\cdot D[n])n - (u\cdot n)D[n]\Big) \\ &= N''_\eta(u_t)\,(I-nn^T)D[u] - N''_\eta(u_t)((u\cdot D[n])n + (u\cdot n)D[n]) \end{aligned}$$

So, going back to our derivative:

$$
\begin{aligned}
T_{CF}^{'*} = \frac{\mu}{\alpha} \int_{\Gamma_C} & h_\eta'(u \cdot n)(n \cdot D[u] + u \cdot D[n]) \; N_\eta'(u_t) \cdot w + \\
& + h_\eta(u \cdot n) \, N_\eta''(u_t) \Big(I - nn^T \Big) \, D[u] \cdot w + \\
& - h_\eta(u \cdot n) \, N_\eta''(u_t)((u \cdot D[n])n + (u \cdot n) D[n]) \cdot w + \\
& + h_\eta(u \cdot n) \; N_\eta'(u_t) \cdot w_t \; \nabla \cdot v \quad dS
\end{aligned}
$$

We can split it in two parts:

$$
T_{CF}^{'*} = T_{CF}' - H_{CF}'
$$

where

$$
\begin{aligned}
T_{CF}' = \frac{\mu}{\alpha} \int_{\Gamma_C} & h_\eta'(u \cdot n)(n \cdot D[u]) \; N_\eta'(u_t) \cdot w + \\
& + h_\eta(u \cdot n) \, N_\eta''(u_t) \Big(I - nn^T \Big) \, D[u] \cdot w \quad dS
\end{aligned}
$$

$$
\begin{aligned}
H_{CF}' = -\frac{\mu}{\alpha} \int_{\Gamma_C} & h_\eta'(u \cdot n)(u \cdot D[n]) \; N_\eta'(u_t) \cdot w + \\
& - h_\eta(u \cdot n) \, N_\eta''(u_t)((u \cdot D[n])n + (u \cdot n) D[n]) \cdot w + \\
& + h_\eta(u \cdot n) \; \Big(N_\eta'(u_t) \cdot w \Big) \; \nabla \cdot v \quad dS
\end{aligned}
$$

If we do the same with the term related to soft body contact, we have:

$$
\begin{aligned}
T_{SF}^{'*} &= \frac{d}{dt}\Big|_{t=0} \big(j_{SF,\alpha}'(u, w) \big) \\
&= \frac{d}{dt}\Big|_{t=0} \left(\int_{\Gamma_S} \frac{\mu}{\alpha} \, h_\eta([u] \cdot n^-) \; N_\eta'([u]_t) \cdot [w]_t \; dS \right) \\
&= \frac{d}{dt}\Big|_{t=0} \left(\int_{\Gamma_{S-}} \frac{\mu}{\alpha} \, h_\eta([u] \cdot n^-) \; N_\eta'((u^- - u^+)_t) \cdot w^- \; dS \right) - \\
&\quad - \frac{d}{dt}\Big|_{t=0} \left(\int_{\Gamma_{S+}} \frac{\mu}{\alpha} \, h_\eta([u] \cdot n^-) \; N_\eta'((u^- - u^+)_t) \cdot w^+ \; dS \right) \\
&= \frac{d}{dt}\Big|_{t=0} \left(\int_{\Gamma_{S-} \, \cup \, \Gamma_{S+}} \frac{\mu}{\alpha} \, h_\eta([u] \cdot n^-) \; N_\eta'((u - u^o)_t) \cdot w \; dS \right)
\end{aligned}
$$

Passing the derivative inside the integral:

$$
\begin{aligned}
T_{SF}^{'*} &= \frac{\mu}{\alpha} \int_{\Gamma_{S-} \, \cup \, \Gamma_{S+}} \frac{d}{dt}\Big|_{t=0} \Big(h_\eta([u] \cdot n^-) \; \Big(N_\eta'((u - u^o)_t) \cdot w \Big) \; \det(F_t) \Big) \; dS \\
&= \frac{\mu}{\alpha} \int_{\Gamma_{S-} \, \cup \, \Gamma_{S+}} \frac{d}{dt}\Big|_{t=0} \Big(h_\eta([u] \cdot n^-) \Big) \; \Big(N_\eta'((u - u^o)_t) \cdot w \Big) \; \det(F_t) + \\
&\quad + h_\eta([u] \cdot n^-) \, \frac{d}{dt}\Big|_{t=0} \Big(N_\eta'((u - u^o)_t) \cdot w \Big) \; \det(F_t) + \\
&\quad + h_\eta([u] \cdot n^-) \; \Big(N_\eta'((u - u^o)_t) \cdot w \Big) \; \frac{d}{dt}\Big|_{t=0} (\det(F_t)) \quad dS \\
&= \frac{\mu}{\alpha} \int_{\Gamma_{S-} \, \cup \, \Gamma_{S+}} \left(\frac{d}{d[u]} \Big(h_\eta([u] \cdot n^-) \Big) \cdot D[[u]] + \frac{d}{dn^-} \Big(h_\eta([u] \cdot n^-) \Big) \cdot D[n^-] \right) \; \Big(N_\eta'((u - u^o)_t) \cdot w \Big) + \\
&\quad + h_\eta([u] \cdot n^-) \left(\frac{d}{dw} \Big(N_\eta'((u - u^o)_t) \Big) D[(u - u^o)_t] \cdot w + N_\eta'((u - u^o)_t) \cdot D[w] \right) + \\
&\quad + h_\eta([u] \cdot n^-) \; \Big(N_\eta'((u - u^o)_t) \cdot w \Big) \, \nabla \cdot v \quad dS \\
&= \frac{\mu}{\alpha} \int_{\Gamma_{S-} \, \cup \, \Gamma_{S+}} \Big(h_\eta'([u] \cdot n^-) \, n \cdot D[u - u^o] + h_\eta'([u] \cdot n^-)(u - u^o) \cdot D[n] \Big) \; \Big(N_\eta'((u - u^o)_t) \cdot w \Big) + \\
&\quad + h_\eta([u] \cdot n^-) \Big(N_\eta''((u - u^o)_t) \, (I - nn^T) D[u - u^o] \cdot w \Big) + \\
&\quad + h_\eta([u] \cdot n^-) \; \Big(N_\eta'((u - u^o)_t) \cdot w \Big) \, \nabla \cdot v \quad dS
\end{aligned}
$$

We can split it in two parts:

$$T'^{*}_{SF} = T'_{SF} - H'_{SF}$$

where

$$T'_{SF} = \frac{\mu}{\alpha} \int_{\Gamma_{S-} \bigcup \Gamma_{S+}} \left(h'_\eta([u]\cdot n^-)\, n \cdot D[u-u^o]\right) \left(N'_\eta((u-u^o)_t)\cdot w\right)$$
$$+ h_\eta([u]\cdot n^-)\, N''_\eta((u-u^o)_t)\Big(I - nn^T\Big)\, D[u-u^o]\cdot w \quad dS$$

$$H'_{SF} = -\frac{\mu}{\alpha} \int_{\Gamma_{S-} \bigcup \Gamma_{S+}} \left(h'_\eta([u]\cdot n^-)(u-u^o)\cdot D[n]\right) \left(N'_\eta((u-u^o)_t)\cdot w\right) +$$
$$- h_\eta([u]\cdot n^-)\, N''_\eta((u-u^o)_t)(((u-u^o)\cdot D[n])n + ((u-u^o)\cdot n)D[n])\cdot w +$$
$$+ h_\eta([u]\cdot n^-)\, \left(N'_\eta((u-u^o)_t)\cdot w\right) \nabla\cdot v \quad dS$$

4.2 Final derivative including RD and DD contact

The complete derivative of the PDE is then:

$$\boxed{\int_\Omega \varepsilon(w) : C : \varepsilon(D[u])dV + \boldsymbol{T'_C} + \boldsymbol{T'_S} + \boldsymbol{T'_{CF}} + \boldsymbol{T'_{SF}} = \boldsymbol{H'_C} + \boldsymbol{H'_S} + \boldsymbol{H'_{CF}} + \boldsymbol{H'_{SF}} +}$$
$$\boxed{+ \int_\Omega (\nabla w \nabla v) : \sigma + \varepsilon(w) : C : (\nabla u \nabla v) - (\varepsilon(w):\sigma)(\nabla\cdot v) dX -}$$
$$\boxed{-\frac{1}{|\Gamma_N|}\left(\int_{\Gamma_N} (\nabla\cdot v)\, d\Gamma_N\right)\left(\int_{\Gamma_N} w\cdot T\, d\Gamma_N\right) + \left(\int_{\Gamma_N} (w\cdot T)\,(\nabla\cdot v)\, d\Gamma_N\right)} \quad (15)$$

After computing the PDE derivative with our new friction terms, we can again use the left side (T'_{CF}, T'_{SF}) to compute the adjoint PDE solution and the right side terms (H'_{CF}, H'_{SF}) to compute the discrete shape derivatives, presented in Appendix of the paper as S_{CF} and S_{SF}.

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