Augmented Lagrangian Contact of Compressible Hyperelastic Cube

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1 Problem Definition

This document is based on the original FEniCS hyperelasticity demo, but uses a different formulation. In the original demo, the weak form is not written explicitly and instead the demo uses an energy minimization scheme.

1.1 Energy Density Function

The energy density function for compressible Neo-Hookean materials is:

$$W = \frac{\mu}{2}(I_1 - 3 - 2\ln J) + \frac{\lambda}{2}(\ln J)^2 \tag{1}$$

where μ and λ are Lamé Parameters and can be defined in terms of the Young's modulus, E, and Poisson's ratio ν

$$\mu = \frac{E}{2(1+\nu)} \quad \lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \tag{2}$$

The first and third invariant of the deformation:

$$I_1 = \mathrm{tr}(\mathbf{C}) \quad J = \det(\mathbf{F}) \tag{3}$$

1.2 Equilibrium equation

The nominal stress tensor is defined as:

$$P_{iJ} = \frac{\partial W}{\partial F_{iJ}} \tag{4}$$

Use the chain rule to find the expression for the nominal stress tensor using the energy density function:

$$\begin{aligned}
\frac{\partial W}{\partial F_{iJ}} &= \frac{\partial W}{\partial I_1}\frac{\partial I_1}{\partial F_{iJ}} + \frac{\partial W}{\partial I_3}\frac{\partial I_3}{\partial F_{iJ}} \quad \text{See Proof section} \\
\mathbf{P} &= \frac{\mu}{2}(2\mathbf{F}) + \left[\frac{\mu}{2}(-\frac{2}{I_3}) + \frac{\lambda}{2}2\frac{\ln J}{J}\right]J\mathbf{F}^{-T} \\
&= \mu\mathbf{F} - \left[\frac{\mu}{I_3} + \lambda\frac{\ln I_3}{I_3}\right]J\mathbf{F}^{-T} \\
&= \mu\mathbf{F} - \mu\mathbf{F}^{-T} + \lambda\ln J\mathbf{F}^{-T}
\end{aligned}$$

Rearranging we can obtain the nominal stress tensor, P:

$$\mathbf{P} = \mu(\mathbf{F} - \mathbf{F}^{-T}) + \lambda\ln J\mathbf{F}^{-T} \tag{5}$$

1.3 Proofs

Proof of the derivative $\frac{\partial I_1}{\partial \mathbf{F}}$ in indicial:

$$
\begin{aligned}
\frac{\partial \operatorname{tr}(\mathbf{F^T F})}{\partial \mathbf{F}} &= \frac{\partial F_{kI} F_{kI}}{\partial F_{pQ}} \quad \text{Product Rule} \\
&= \frac{\partial F_{kI}}{\partial F_{pQ}} F_{kI} + F_{kI} \frac{\partial F_{kI}}{\partial F_{pQ}} \\
&= \delta_{kp}\delta_{IQ} F_{kI} + F_{kI}\delta_{kp}\delta_{IQ} \\
&= F_{pQ} + F_{pQ} = 2F_{pQ}
\end{aligned}
$$

Therefore, we have the following relationship:

$$
\frac{\partial \operatorname{tr}(\mathbf{F^T F})}{\partial \mathbf{F}} = 2\mathbf{F} \tag{6}
$$

Relationship for $\frac{\partial I_3}{\partial \mathbf{F}}$

$$
\frac{\partial \det \mathbf{F}}{\partial \mathbf{F}} = \det \mathbf{F}\mathbf{F}^{-\mathbf{T}} = \mathbf{J}\mathbf{F}^{-\mathbf{T}}
$$

2 Strong and Weak Forms

$$
\frac{\partial P_{iJ}}{\partial X_J} + b_i = 0 \tag{7}
$$

Take Eq. 7 and multiply by a test function

$$
\begin{aligned}
\frac{\partial P_{iJ}}{\partial X_J} \mathbf{e_i} \cdot v_j \mathbf{e_j} &= -b_i \mathbf{e_i} \cdot v_j \mathbf{e_j} \\
\frac{\partial P_{iJ}}{\partial X_J} v_j \delta_{ij} &= -b_i v_j \delta_{ij} \\
\frac{\partial P_{iJ}}{\partial X_J} v_i &= -b_i v_i \quad \text{Integrate over domain} \\
\int_{\Omega_o} \frac{\partial P_{iJ}}{\partial X_J} v_i dV &= -\int_{\Omega_o} b_i v_i dV \quad \text{Use integration by parts } f'g = (fg)' - fg' \\
\int_{\Omega_o} (P_{iJ} v_i)_{,J} dV - \int_{\Omega_o} P_{iJ} v_{i,J} dV &= -\int_{\Omega_o} b_i v_i dV \quad \text{Use divergence theorem} \\
\int_{\partial\Omega_o} P_{iJ} N_J v_i dS - \int_{\Omega_o} P_{iJ} v_{i,J} dV &= -\int_{\Omega_o} b_i v_i dV \quad \text{Recognize traction } P_{iJ} N_J = T_i \\
\int_{\partial\Omega_o} T_i v_i dS - \int_{\Omega_o} P_{iJ} v_{i,J} dV &= -\int_{\Omega_o} b_i v_i dV \quad \text{rearrange} \\
\int_{\Omega_o} P_{iJ} v_{i,J} dV &= \int_{\Omega_o} b_i v_i dV + \int_{\partial\Omega_o} T_i v_i dS
\end{aligned}
$$

Rewrite in direct notation to obtain weak form:

$$
\int_{\Omega_o} P : \operatorname{Grad}(v) dV = \int_{\Omega_o} bv dV + \int_{\partial\Omega_o} Tv dS \tag{8}
$$

3 Contact

The rigid indenter with a spherical surface can be approximated by a parobolic equation instead of explicitly modeled and meshed. Consider the indenter radius, R, to be sufficiently large with respect to the contact region characteristic size (R >> a). This relationship, R >> a, allows the spherical surface to be approximated by a parabola.

$$\begin{aligned} h(x,z) &= -h_o + \frac{1}{2R}(x^2+z^2) \quad \text{about origin} \\ h(x,z) &= -h_o + \frac{1}{2R}\big[(x-0.5)^2+(z-0.5)^2\big] \quad \text{about point } (0.5,0.5) \end{aligned} \tag{9}$$

where the gap is defined as

$$g_N = u_N - h$$

Where there are several cases

$$\begin{aligned} g_N &\geq 0 \\ p_N &\leq 0 \quad \text{ on } \Gamma_c \\ p_N g_N &= 0 \end{aligned} \tag{10}$$

The definition of the MacKauley bracket:

$$\begin{aligned} <x> &= \frac{x+|x|}{2} \\ <x> &= \begin{cases} 0 \text{ for } x \leq 0, \\ x \text{ for } x > 0 \end{cases} \end{aligned} \tag{11}$$

3.1 Penalty Approach

Adding a penalty term to the energy, Π.

$$\Pi_N^P = \frac{1}{2}\int_{\Gamma_c} k_{pen}(g_N)^2 dA \quad \text{where } k_{pen} > 0 \tag{12}$$

Take the variation of Eq. 12, this holds for pure stick. This is the addition to the weak form:

$$\begin{aligned} C_N^P &= k_{pen}\int_{\Gamma_c} \big(g_N \delta g_N\big) dA \\ C_N^P &= k_{pen}\int_{\Gamma_c} \big(g_N \delta u_N\big) dA \end{aligned}$$

3.1.1 Incorporating into weak form

$$\begin{aligned} k_{pen}\int_{\partial\Omega_0} g_N \delta u_N \, dS + \int_{\Omega_0} \mathbf{P} : \mathrm{Grad}(\boldsymbol{\delta}\mathbf{u})\, dV - \int_{\Omega_0} \mathbf{B}\cdot\boldsymbol{\delta}\mathbf{u}\, dV - \int_{\partial\Omega_0} \mathbf{T}\cdot\boldsymbol{\delta}\mathbf{u}\, dS = 0 \\ \int_{\Omega_0} \left(C - C^t\right)\delta\mu dV - \int_{\Omega_0} \mathbf{J}\cdot\frac{\delta\mu}{\delta X}\Delta t dV - \int_{\partial\Omega_0} i\delta\mu\Delta t dS - \int_{\Omega_0} r\delta\mu\Delta t dV = 0 \end{aligned}$$

3.2 Lagrange Multiplier Method

Lagrange multiplier to add constraints:

$$\Pi_N^L = \int_{\Gamma_c} \lambda_N g_N dA$$

Take the variation

$$C_N^L = \int_{\Gamma_c} \big(\delta\lambda_N g_N + \lambda_N \delta g_N\big) dA$$
$$C_N^L = \int_{\Gamma_c} \big(g_N \delta\lambda_N + \lambda_N \delta u_N\big) dA$$

3.2.1 Incorporating into weak form

$$\begin{aligned}
\int_{\partial\Omega_0} \lambda_N \delta u_N \, dS + \int_{\Omega_0} \mathbf{P} : \mathrm{Grad}(\boldsymbol{\delta}\mathbf{u}) \, dV - \int_{\Omega_0} \mathbf{B} \cdot \boldsymbol{\delta}\mathbf{u} \, dV - \int_{\partial\Omega_0} \mathbf{T} \cdot \boldsymbol{\delta}\mathbf{u} \, dS = 0 \\
\int_{\Omega_0} \left(C - C^t\right) \delta\mu dV - \int_{\Omega_0} \mathbf{J} \cdot \frac{\delta\mu}{\delta X} \Delta t dV - \int_{\partial\Omega_0} i\delta\mu\Delta t dS - \int_{\Omega_0} r\delta\mu\Delta t dV = 0 \\
\int_{\partial\Omega_0} g_N \delta\lambda_N dS = 0
\end{aligned}$$

3.3 Augmented Lagrange Approach

3.3.1 Augmented Lagrange Methods: Wriggers

We introduce the following augmented lagrangian term.

$$\hat{\lambda}_N = \lambda_N + k_{pen} g_N$$

Possible contact cases

$$\begin{aligned}
\text{Contact: } & g_N = 0, \quad \lambda_N < 0, \quad \hat{\lambda}_N < 0 \\
\text{No Contact: } & g_N > 0, \quad \lambda_N = 0, \quad \hat{\lambda}_N > 0 \\
\text{Interpenetration: } & g_N < 0, \quad \lambda_N < 0, \quad \hat{\lambda}_N = 0
\end{aligned} \tag{13}$$

where the gap is defined as

$$g_N = u_N - h$$

The main idea of this method is combining the penalty method with Lagrange multiplier methods. The augmented Lagrange functional is introduced for normal contact:

$$\Pi_N^{AL} = \begin{cases} \int_{\Gamma_c} (\lambda_N g_N + \frac{1}{2}\epsilon_N g_N^2) d\Gamma & \text{for } \hat{\lambda}_N \le 0, \\ \int_{\Gamma_c} -\frac{1}{2\epsilon_N} |\lambda_N|^2 d\Gamma & \text{for } \hat{\lambda}_N > 0 \end{cases} \tag{14}$$

where $\hat{\lambda}_N \leq 0$ indicates that the gap is closed and $\hat{\lambda}_N > 0$ means the gap is open. Taking the variation of Eq. 14 gives the following, where we recognize the augmented lagrangian

$$C_N^{AL} = \begin{cases} \int_{\Gamma_c} (\delta\lambda_N g_N + \lambda_N \delta g_N + \epsilon_N g_N \delta g_N) d\Gamma & \text{for } \hat{\lambda}_N \leq 0, \\ \int_{\Gamma_c} -\frac{1}{\epsilon_N} \lambda_N \delta\lambda_N d\Gamma & \text{for } \hat{\lambda}_N > 0 \end{cases}$$

$$C_N^{AL} = \begin{cases} \int_{\Gamma_c} \Big(\delta\lambda_N g_N + (\lambda_N + \epsilon_N g_N) \delta g_N \Big) d\Gamma & \text{for } \hat{\lambda}_N \leq 0, \\ \int_{\Gamma_c} -\frac{1}{\epsilon_N} \lambda_N \delta\lambda_N d\Gamma & \text{for } \hat{\lambda}_N > 0 \end{cases}$$

Final equation for variation:

$$C_N^{AL} = \begin{cases} \int_{\Gamma_c} \Big(\delta\lambda_N g_N + \hat{\lambda}_N \delta g_N \Big) d\Gamma & \text{for } \hat{\lambda}_N \leq 0, \\ \int_{\Gamma_c} -\frac{1}{\epsilon_N} \lambda_N \delta\lambda_N d\Gamma & \text{for } \hat{\lambda}_N > 0 \end{cases} \tag{15}$$

3.3.2 Augmented Lagrange: Contact Methods in Finite Element Simulations

Defined with the Mackauley bracket where p $= \epsilon_N$

$$\Pi_N^{AL} = \frac{1}{2k_{pen}} < -(\lambda_N + k_{pen} g_N) >^2$$

If we take the variation of this equation:

$$C_N = \frac{2}{2k_{pen}} < -(\lambda_N + k_{pen} g_N) > \delta\lambda_N + \frac{2}{2k_{pen}} < -(\lambda_N + k_{pen} g_N) > k_{pen} \delta g_N$$
$$C_N = \frac{1}{k_{pen}} < -(\lambda_N + k_{pen} g_N) > \delta\lambda_N + < -(\lambda_N + k_{pen} g_N) > \delta g_N$$

3.3.3 Addition into weak form

The formulation that works is the source which utilizes the Mackauley bracket, with a removal of the Mackauley bracket of the first term. Note that this is the same as placing the Mackauley bracket around $\hat{\lambda}_N$ in the Wriggers formulation:

$$C_N = \frac{1}{k_{pen}} \big[-(\lambda_N + k_{pen} g_N) \big] \delta\lambda_N + < -(\lambda_N + k_{pen} g_N) > \delta g_N$$
$$C_N = -\frac{1}{k_{pen}} \lambda_N \delta\lambda_N + g_N \delta\lambda_N + < -(\lambda_N + k_{pen} g_N) > \delta g_N \quad \text{define } g_N = u - h(x,z)$$
$$C_N = -\frac{1}{k_{pen}} \lambda_N \delta\lambda_N + g_N \delta\lambda_N + < -\hat{\lambda} > \delta u_N$$

The addition of the lagrange multiplier augments the solution space and increases the number of equations in the weak form by 1 equation.

$$\begin{aligned}
\int_{\partial\Omega_0} < -\hat{\lambda}_N > \delta u_N \, dS + \int_{\Omega_0} \mathbf{P} : \mathrm{Grad}(\boldsymbol{\delta}\mathbf{u}) \, dV - \int_{\Omega_0} \mathbf{B} \cdot \boldsymbol{\delta}\mathbf{u} \, dV - \int_{\partial\Omega_0} \mathbf{T} \cdot \boldsymbol{\delta}\mathbf{u} \, dS = 0 \\
\int_{\Omega_0} \left(C - C^t\right) \delta\mu dV - \int_{\Omega_0} \mathbf{J} \cdot \frac{\delta\mu}{\delta X} \Delta t dV - \int_{\partial\Omega_0} i\delta\mu\Delta t dS - \int_{\Omega_0} r\delta\mu\Delta t dV = 0 \\
-\frac{1}{k_{pen}} \int_{\partial\Omega_o} \lambda_N \delta\lambda_N \, dS + \int_{\partial\Omega_o} g_N \delta\lambda_N \, dS = 0
\end{aligned}$$

Without fluid diffusion

$$\begin{aligned}
\int_{\partial\Omega_o} < -\hat{\lambda} > \boldsymbol{\delta}\mathbf{u} \, dS + \int_{\Omega_o} \mathbf{P} : \mathrm{Grad}(\boldsymbol{\delta}\mathbf{u}) \, dV - \int_{\Omega_o} \mathbf{B} \cdot \boldsymbol{\delta}\mathbf{u} \, dV - \int_{\partial\Omega_o} \mathbf{T} \cdot \boldsymbol{\delta}\mathbf{u} \, dS = 0 \\
-\frac{1}{k_{pen}} \int_{\partial\Omega_o} \lambda\delta\lambda \, dS + \int_{\partial\Omega_o} g_N \delta\lambda \, dS = 0
\end{aligned}$$

3.3.4 Question

Without

$$\begin{aligned}
\int_{\Omega_0} \mathbf{P} : \boldsymbol{\nabla}_X \boldsymbol{\delta}\mathbf{u} \, dV - \int_{\Omega_0} \mathbf{B} \cdot \boldsymbol{\delta}\mathbf{u} \, dV - \int_{\partial\Omega_0} \mathbf{T} \cdot \boldsymbol{\delta}\mathbf{u} \, dS = 0 \\
\int_{\Omega_0} \left(C - C^t\right) \delta\mu \, dV - \int_{\Omega_0} \mathbf{J} \cdot \nabla_X \, \delta\mu \, \Delta t \, dV - \int_{\partial\Omega_0} i \, \delta\mu \, \Delta t \, dS - \int_{\Omega_0} r \, \delta\mu \, \Delta t \, dV = 0
\end{aligned}$$

We introduce the following augmented lagrangian term.

$$\begin{aligned}
\hat{\lambda}_N &= \lambda_N + k_{pen} g_N \\
g_N &= h - u_N
\end{aligned}$$

First

$$\begin{aligned}
\int_{\partial\Omega_0} < \hat{\lambda}_N > \delta u_N \, dS - \int_{\partial\Omega_0} \hat{\lambda}_N \delta u_N \, dS + \int_{\Omega_0} \mathbf{P} : \boldsymbol{\nabla}_X \boldsymbol{\delta}\mathbf{u} \, dV - \int_{\Omega_0} \mathbf{B} \cdot \boldsymbol{\delta}\mathbf{u} \, dV - \int_{\partial\Omega_0} \mathbf{T} \cdot \boldsymbol{\delta}\mathbf{u} \, dS = 0 \\
\int_{\Omega_0} \left(C - C^t\right) \delta\mu \, dV - \int_{\Omega_0} \mathbf{J} \cdot \nabla_X \, \delta\mu \, \Delta t \, dV - \int_{\partial\Omega_0} i \, \delta\mu \, \Delta t \, dS - \int_{\Omega_0} r \, \delta\mu \, \Delta t \, dV = 0 \\
-\frac{1}{k_{pen}} \int_{\partial\Omega_o} \lambda_N \delta\lambda \, dS + \int_{\partial\Omega_o} g_N \delta\lambda \, dS = 0
\end{aligned}$$

Note that this is the full expression

$$\begin{aligned}
\int_{\partial\Omega_0} < \hat{\lambda}_N > \delta u_N \, dS - \int_{\partial\Omega_0} \hat{\lambda}_N \delta u_N \, dS + \int_{\Omega_0} \mathbf{P} : \boldsymbol{\nabla}_X \boldsymbol{\delta}\mathbf{u} \, dV - \int_{\Omega_0} \mathbf{B} \cdot \boldsymbol{\delta}\mathbf{u} \, dV - \int_{\partial\Omega_0} \mathbf{T} \cdot \boldsymbol{\delta} \\
-k_{s1} \int_{\Omega_0} \big(\nabla_X(\mu - \mu^t) \cdot \nabla_X \, \delta\mu\big) dV + \int_{\Omega_0} \left(C - C^t\right) \delta\mu \, dV - \int_{\Omega_0} \mathbf{J} \cdot \nabla_X \, \delta\mu \, \Delta t \, dV - \int_{\partial\Omega_0} i \, \delta\mu \, \Delta t \, dS - \int_{\Omega_0} r \, \delta\mu \, \Delta \\
-k_{s2} \int_{\Omega_0} \big(\nabla_X(\lambda_N - \lambda_N^t) \cdot \nabla_X \delta\lambda\big) dV - \frac{1}{k_{pen}} \int_{\partial\Omega_o} \lambda_N \delta\lambda \, dS + \int_{\partial\Omega_o} g_N \delta
\end{aligned}$$