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Numerical model for contact with adhesion based on Kalker's variational principle.

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Micro Abstract
Kalker variational principle allows to solve consistently unilateral contact problems in terms of the normal traction as the prime unknown variable. It is particularly useful for the development of boundary elements for Boussinesq problem in half-space approximation. This principle is extended to account for adhesion between solids. The contact pressure may take negative values governed by an adhesive work potential and surface separation energy. The latter is evaluated via level-set.

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Introduction

One of the main problems of contact modeling is to determine the part of their interface where they touch each other. Typically the contact domain is iteratively adjusted to meet contact conditions by increments of finite size (let's say of a contact or a boundary element). Meanwhile more exact evaluation of the contact area is required by certain applications such as adhesive contact. Incorporation of the surface energy variation to the computational model urges for a formulation where the contact domain can change continuously. An example of such approach can be found in [1] with regard to the unilateral contact of a membrane and an obstacle.

We propose a method for modeling contact of elastic bodies with continuously changing contact domain. It is derived from the surface mechanical form of Kalker's variational principle. It treats the contact pressures as the unknown variables that are determined through minimization of the complementary energy functional. In order to include adhesion to the problem the conditions of contact pressure positiveness are abandoned. Instead the contact area is determined through a gap function that is positive outside of the contact domain. The compliance between gap and current guess contact area is enforced via a specially constructed penalty function and Lagrange multipliers. The stationarity of the derived weak functional which includes the adhesive surface energy defines the solution to the problem. In conclusion a discrete element approximation is shown for the case of axisymmetric contact.

1 Kalker's variational principle

This variational principle [4] formulates conditions that determine uniquely the solution to the unilateral contact problem with forces and not displacements as primal variable . It states that the true contact area and surface tractions are those which minimize the complementary energy functional

$$\Phi[p] = \frac{1}{2}\int\limits_S p \cdot u dS + \int\limits_S p \cdot (h-\delta) dS \to \min \tag{1}$$

subject to the constraint that the contact pressure S is nonnegative everywhere on the contact interface S. The functional is computed for given initial gap between the bodies h and rela-

tive approach δ and the total elastic normal displacement u corresponding to the tractions p acting on the interface. This problem statement provides an alternative to collocation methods when solving contact problems with boundary element methods. When discretizing (1) one gets symmetric influence coefficients matrix even for an irregular mesh or in the axisymmetric setting. The active set strategy while handling inequality constraint follows directly from basic mathematical programming with no apparent issues.

The optimality conditions for the original principle read as follows

$$\begin{cases} u + (h - \delta) = 0 & \text{where } p \geq 0 \\ u + (h - \delta) \geq 0 & \text{where } p = 0 \end{cases} \tag{2}$$

in terms of the gap $g = u + (h - \delta)$. Apparently the part of the surface C where contact pressure is positive is the contact area, where surfaces touch each other, while outside of this domain $S \backslash C$ no force is transmitted and the deformed bodies remain separated.

The optimality conditions for the original principle can be derived from the stationarity of the corresponding Lagrangian

$$\mathscr{L}[p, g] = \frac{1}{2} \int_S p \cdot u dS + \int_S p \cdot (h - \delta) dS - \int_S p \cdot g dS \to \text{stat} \tag{3}$$

with the introduced above gap serving as Lagrange multiplier. The Karush-Kuhn-Tucker conditions as expected are $p \geq 0$, $g \geq 0$, $g \cdot p = 0$. It should be noted that value of both the complementary energy (1) and the Lagrangian (3) for the solution of the problem equals to the opposite to the stored elastic energy $-\Pi_{\text{el}}$.

2 Adhesive interactions

If we discard the constraint on the positiveness of p and introduce the interaction energy Π_{surf} related to the gap one can compose the following functional to which a max/min principle applies

$$\max_g \min_p \left[\frac{1}{2} \int_S p \cdot u dS + \int_S p \cdot (h - \delta) dS - \int_S p \cdot g dS - \int_S \sigma(g) dS \right] \tag{4}$$

Its stationarity gives the following set of equations

$$\begin{cases} u + (h - \delta) = g \\ p = -\dfrac{\partial \sigma}{\partial g} \end{cases} \tag{5}$$

that are usually solved when the adhesive contact is analysed for the known regular interaction potential $\sigma(g)$, for instance the Lennard-Jones potential [2].

We look at the situation when the adhesion is determined by the surface energy γ that is released instantly when the bodies get separated and the free surface is created. The gain in energy is balanced by the additional elastic deformation required to bring bodies into contact over the larger area [3]. The surface energy is determined as in [5] up to an additive constant as the functional of the contact domain

$$\Pi_{\text{surf}}[C] = -\int_C \gamma dS \tag{6}$$

The gap g is now indirectly related to the contact set by the conditions $g = 0$ in C, $g \geq 0$ in $S\backslash C$. We can discard the zero values of g inside the contact zone and extend it by the arbitrary negative values. Then we can postulate that the boundary of C is determined by the zero level-set of g. If we introduce a penalty function

$$\zeta_C(g) = \begin{cases} H(g) & \text{in } C \\ H(-g) & \text{in } S\backslash C \end{cases} \tag{7}$$

defined in the entire domain S through the Heaviside function H we can enforce the conditions $g \leq 0$ in C and $g \geq 0$ in $S\backslash C$ demanding that $\zeta_C(g) \equiv 0$. This allows to constitute the following functional

$$\mathscr{L}_C\left[p, g, C, \mu\right] = \frac{1}{2}\int\limits_S p \cdot u dS + \int\limits_S p \cdot (h - \delta) dS - \int\limits_{S\backslash C} p \cdot g dS + \int\limits_C \gamma dS + \int\limits_S \mu \zeta_C(g) \tag{8}$$

The advantages of this functional is that it enables unconstrained variation of the unknown pressure p and gap g that are defined on the entire interface S rather than its corresponding parts C and $S\backslash C$. This means that these unknown fields can be discretized on a fixed mesh that will not vary with the change of the contact domain guess.

3 Approximate solution in the axisymmetric case

Let's demonstrate the application of the proposed variational functional to the derivation of an approximate solution in the axisymmetric case. We choose to approximate the unknown pressure p as piecewise constant and the extended gap function g as piecewise linear

$$p^c(r) = \sum_a p_a \phi_a(r) \qquad\qquad g^c = \sum_j g_j \psi_j(r) \tag{9}$$

on a regular mesh on the radial axis with the nodes $r_j = jc$, $j = 0, 1, \ldots N$ for the gap values and midpoints $r_a = ac$, $a = 1/2, 3/2, \ldots (N - 1/2)$ for the pressure values. The initial separation h uses same piecewise linear approximation as the gap g.

The Lagrange multipliers μ can only be properly determined where the constraint (7) is violated, since $\partial\zeta_C(g)/\partial g = 0$ wherever $\zeta_C(g) = 0$. This domain will be narrowed to the vicinity of the boundary ∂C of the contact area. Correspondingly the piecewise linear approximation of μ will only extend to the nodes j for which the support of the basis functions ψ_j intersects this boundary. For simplicity consider the case when the contact area is simply connected and is a circular domain C of radius ρ inside of the circular interface S of radius R.

The approximate Lagrangian with this choice of the discretization is computed as

$$\mathscr{L}_C^c\left[p_a, g_j, C, \mu_j\right] = \frac{1}{2}\, p_a C_{ab} p_b + p_a W_{aj}(h_j - \delta) - p_a \tilde{W}_{aj} g_j + \gamma|C| + \mu_j Z_j \tag{10}$$

where

$$C_{ab} = \int\limits_0^R \phi_a \cdot u[\phi_b]\ \pi r dr \qquad\qquad W_{aj} = \int\limits_0^R \phi_a \cdot \psi_j\ \pi r dr$$

$$W_{aj} = \int\limits_\rho^R \phi_a \cdot \psi_j\ \pi r dr \qquad\qquad Z_j = \int\limits_0^R \zeta_C \cdot \psi_j\ \pi r dr$$

Note that the way the penalty (7) was chosen and the suggested approximation (9) of the fields the function Z_j is continuous and differentiable with respect to the nodal values of the gap and the contact radius.

The stationarity conditions of (10) produce the following set of equations

$$C_{ab}p_b + W_{aj}(h_j - \delta) - \tilde{W}_{aj}g_j = 0 \tag{11}$$

$$-p_a\tilde{W}_{ak} + \mu_j\frac{\partial Z_j}{\partial g_k} = 0 \tag{12}$$

$$-p_a\frac{\partial\tilde{W}_{aj}}{\partial\rho}g_j + \gamma\frac{\partial|C|}{\partial\rho} + \mu_j\frac{\partial Z_j}{\partial\rho} = 0 \tag{13}$$

$$Z_j = 0 \tag{14}$$

that can be solved by Newton iterations. It should be noted that the values of the gap function can not be defined for the nodes that belong to the elements that are entirely located inside of the contact zone C where it is artificially extended. Similarly, the Lagrange multipliers μ_j are only determined for those elements where the penalty Z_j is not identically zero, which is across the boundary ∂C of the contact domain.

Conclusions

The proposed approach to modeling adhesive contact is distinguished by continuous variation of the contact area. This is achieved by writing the contact conditions in the weak surface mechanical form in terms of the unknown contact pressure and gap. The discretization of the problem is performed on a fixed mesh without the need of adjustment for the changing contact domain as shown for the axisymmetric case.

References

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