Shape optimization for contact problems based on isogeometric analysis

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Abstract. We consider the shape optimization for mechanical connectors. To avoid the gap between the representation in CAD systems and the finite element simulation used by mathematical optimization, we choose an isogeometric approach for the solution of the contact problem within the optimization method. This leads to a shape optimization problem governed by an elastic contact problem. We handle the contact conditions using the mortar method and solve the resulting contact problem with a semismooth Newton method. The optimization problem is nonconvex and nonsmooth due to the contact conditions. To reduce the number of simulations, we use a derivative based optimization method. With the adjoint approach the design derivatives can be calculated efficiently. The resulting optimization problem is solved with a modified Bundle Trust Region algorithm.

Introduction
There are different works on shape optimization for contact problems with standard finite elements e.g. [1] or shape optimization based on isogeometric analysis without contact e.g. [2]. In this work we present a optimization scheme for mechanical connectors based on isogeometric analysis. In the first part we describe the underlying system of partial differential equations, which represents the physical model. After that we give a short introduction in isogeometric analysis. The third part deals with the presentation of the shape optimization problem and the used optimization algorithm. Followed by an exemplary numerical result. Finally we give a short outlook on future research.

1. Physical Model
We describe the structural mechanic behavior of the connection through a system of partial differential equations (PDE). For simplicity reasons we assume that only one part of the connection is elastic. The other part is assumed to be rigid. Further we consider frictionless contact. This setting is called Signorini problem. The elastic body $\Omega$ is fixed on $\Gamma_D$ and a surface load $f^S$ acts on $\Gamma_N$ and a volume load $f^V$ on the whole body. The potential contact zone $\Gamma_C$ includes the a-priori unknown contact zone, where $\partial\Omega = \Gamma_N \cup \Gamma_D \cup \Gamma_C$. The gap between $\Omega$ and the obstacle is denoted by $g$. One can formulate the Signorini Problem as a constrained convex quadratic optimization problem. It can be shown that for Problem 1 exists a unique solution. For further details we refer to [3, 4].
Problem 1 (Weak Formulation of the frictionless Signorini Problem)

Find \( y \in K := \{ v \in H^1_D(\Omega) : Bv - g \leq 0 \text{ on } \Gamma_C \} \) such that

\[
J_{pe}(y) = \min_{v \in K} J_{pe}(v) := \frac{1}{2} \int_\Omega \varepsilon(v) : C \varepsilon(v) \, dx - \int_\Omega f^v \cdot v \, dx + \int_{\Gamma_N} f^s \cdot v \, dS(x),
\]

where \( B \) denotes the normal trace operator and \( H^1_D(\Omega) := \{ v \in H^1(\Omega) : v = 0 \text{ on } \Gamma_D \} \). The objective function \( J_{pe} \) denotes the potential energy.

For the following we denote the saddle point formulation of Problem 1 by

\[
C(y, \lambda, u) := \left( A(u)y - F(u) + B^*(u)\lambda \right) = 0,
\]

where \( u \) denotes the design of \( \Omega \), \( y \) represents the displacement and \( \lambda \in H^2(\Gamma_C) \) constitutes the Lagrange multipliers of the contact conditions, since we apply a mortar method [5, 6, 7]. The state equation is solved by a semismooth Newton method. To allow for a convergence theory of the semismooth Newton method in function space, we introduce a regularization parameter \( \alpha \), see [8]. The state equation (2) is the nonsmooth reformulation of the optimality system of Problem 1. For a more detailed derivation of the nonsmooth reformulation we refer to [8]. To discretize the state equation we use the approach of isogeometric analysis.

2. Isogeometric Analysis

The approach of isogeometric analysis follows an isoparametric idea. The characteristic is that we use the basis functions of the geometry description as basis functions for the solution space not like it is common in isoparametric settings the other way around. This gives us the advantage of a direct link from the CAD geometry to the finite element simulation and additionally that we can directly perform the simulation on the correct geometry, without the need to approximate it. In particular for contact mechanics the smooth boundaries lead to better results compared to standard finite elements [9]. Since in isogeometric analysis NURBS are used both as geometry description and ansatz function, we shortly summarize the basic concept of NURBS.

Definition 1 (NURBS curve) For a degree \( p \), a set of \( d \)-dimensional control points \( \{P_1, \ldots, P_n\} \), \( d \geq 1 \), \( n \geq p + 1 \), a set of real valued weights \( \{w_1, \ldots, w_n\} \), with \( w_i \geq 0 \) and an open knot vector \( \Xi := \{\xi_1, \ldots, \xi_{n+p+1}\} \), with \( \xi_i \in [0, 1] \) and \( \xi_1 = \cdots = \xi_p = 0 \) and \( \xi_{n+1} = \cdots = \xi_{n+p+1} = 1 \), the resulting NURBS curve is defined as

\[
G(\xi) = \sum_{i=1}^n R^p_i(\xi)P_i, \quad \text{with } R^p_i(\xi) := \frac{w_i N^p_i(\xi)}{\sum_{j=1}^n w_j N^p_j(\xi)},
\]

where the basis functions \( N^p_i : [0, 1] \to \mathbb{R} \) are defined through the recurrence formula due to Cox, deBoor and Mansfield [10].

Through the knot vector \( \Xi \) one can not only control the geometry of the curve but also the differentiability. With the concept of multiple knots, e.g. \( \xi_1 = \cdots = \xi_{s+k-1} \), one reduces the smoothness at \( \xi_i \) from \( C^{p-1} \) to \( C^{p-k} \), where the case of \( C^{-1} \) denotes a point of discontinuity of the considered curve. In this work we assume an open knot vector. As a result the NURBS curve is interpolatory at both ends. A detailed introduction in NURBS theory is given in [10].
Definition 2 (NURBS solid) A d-dimensional NURBS solid \( V(\xi, \eta, \zeta) \), with \((\xi, \eta, \zeta) \in [0, 1]^3\) of degree \((p, q, r) \in \mathbb{N}_0^3\) is defined as the tensor product of three NURBS curves defined as in Definition 1,

\[
V(\xi, \eta, \zeta) = \sum_{i=1}^{n} \sum_{j=1}^{m} \sum_{k=1}^{l} R_{i,j,k}^{p,q,r}(\xi, \eta, \zeta) P_{i,j,k},
\]

with \( R_{i,j,k}^{p,q,r}(\xi, \eta, \zeta) := \frac{w_{i,j,k} N_i^p(\xi) M_j^q(\eta) L_k^r(\zeta)}{\sum_{a=1}^{n} \sum_{b=1}^{m} \sum_{c=1}^{l} w_{a,b,c} N_a^p(\xi) M_b^q(\eta) L_c^r(\zeta)} \), \( P_{i,j,k} \in \mathbb{R}^d \).

3. Optimization problem

The aim of our optimization scheme is to find a shape \( \Omega \) for a connector such that the stiffness is maximized under different constraints. One way to do this is to minimize the compliance of the considered connection. The compliance can be defined as

\[
J_c(y, u) = \int_{\Omega(u)} f \cdot y \, dx + \int_{\Gamma_N(u)} q \cdot y \, dS(x), \quad (3)
\]

To determine subgradients with respect to the shape parameters, we use an adjoint approach. Since we know that Problem 1 has a unique solution for a given domain \( \Omega \), we can define a nonsmooth solution operator \( S : U \rightarrow (K \times H^2(\Gamma_C))^* \) that maps each shape \( u \in U \) of \( \Omega \) to the corresponding unique solution of (2). Thereby we can define the reduced form of (3) by

\[
j_c(u) := J_c(u, S(u)).
\]

It can be checked that in points of strict complementarity, i.e., if the contact forces do not vanish in all contact nodes, the shape gradient can be obtained by

\[
j'_c(u) = \frac{\partial}{\partial u} J_c(S(u), u) + p^\top \frac{\partial}{\partial u} C(S(u), u), \quad (4)
\]

where the adjoint \( p \) is defined through the adjoint equation

\[
\frac{\partial}{\partial (y, \lambda)} C(\lambda, y, u)^\top p = -\frac{\partial}{\partial (y, \lambda)} J_c(y, \lambda, u).
\]

If strict complementarity is violated, a perturbation argument justifies to compute an approximate subgradient by (4). The shape optimization problem has the following form:

\[
\min_{u \in U_{ad}} j_c(u), \quad (5)
\]

with the set of admissible designs \( U_{ad} := \{ u \in U : h(u) = 0, g(u) \leq 0, u \leq \pi \} \). The differentiable functions \( h(\cdot) \) and \( g(\cdot) \) can describe different constraints like volume, distance or curvature restrictions. The resulting optimization problem (5) is nonsmooth and nonconvex. We therefore apply a nonconvex Bundle Trust Region (BTR) method, as shown in [11]. In general the BTR method generates a cutting plane model to approximate the objective function from below. For this purpose one calculates a subgradient in the current point and adds the plane defined through this subgradient to the bundle of planes already generated. Then the optimization problem is solved over the cutting plane model. If the step satisfy a sufficient descend condition the step is called essential step and will be performed. If not it is called null step. A null step is an indicator for a bad approximation of the real objective function by the cutting plane model and so it has to be improved by adding an additional cutting plane and start the optimization again. In [11] a BTR method for the unconstrained case is proposed. We have modified the inner loop of the algorithm such that the calculated steps are always within the feasible set.
4. Numerical Results

Now we give a short application of the algorithm. We assume the following scenario. The bar has the size of $12 \text{mm} \times 3 \text{mm} \times 1.5 \text{mm}$. From the top there is a homogeneous down acting force applied, see upper detached plane in Fig. 1. We additionally assume gravity. The bar is in contact with a rigid obstacle at the outer $2 \text{mm}$, see the lower two gray planes in Fig. 1. For an improved visibility the Neumann boundary is plotted with a constant offset towards the bar. The colour in Fig. 1 represents the von Mises stress. The displacement is scaled by a factor of 100. As objective function we choose the compliance (3). The tri-cubic reference mesh consisting of two elements and 80 control points. The mesh has been refined through knot insertion up to 1200 elements and 4362 control points. The degrees of freedom in this example have been the 20 control points of the upper surface in the reference mesh. There was no change in the $x$ and $y$ direction allowed. Under the constraint of constant volume, a minimal height of $0.5 \text{mm}$ and a maximal height of $10 \text{mm}$ we could reduce the compliance about $30.57\%$ within 13 iterations.

Outlook and Acknowledgment

The next steps of our work are to consider multibody contact and an extension of the current physical model due to nonlinear elasticity and large deformations. This work was supported by the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) Research Grant CRC 666 Subproject A2.

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