Predictor-corrector interior point method for contact analysis models with multi-point constraints

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Abstract
Recently, interior point methods are focused as an efficient strategy for large scale contact problems. In this paper, we present a method based on a predictor-corrector method for contact problems with multi-point constraints. Furthermore, we implement our algorithm into FrontISTR, which is an open-source and large scale finite element structural analysis software, and investigate the performance.

Keywords contact problems, interior point method, predictor-corrector method, finite element method

Research Activity Group Scientific Computation and Numerical Analysis

1. Introduction

Structural analysis based on a finite element method is widely used in a design process of industrial products in order to ensure the structural reliability and to reduce the cost of experimental productions. It becomes common for structural analysis to consider multiple parts and interactions such as contact constraints and tied constraints to evaluate the stiffness of the whole body. Elastic analysis with frictionless contacts and tied constraints is formulated by a constrained optimization problem which includes non penetration constraints and multi-point constraints. Therefore, we can apply solution methods for constrained optimization problems.

Major algorithms to solve contact problems are introduced by Wriggers [1]. An active set method is well known as a simple and widely used method for contact problems. In order to determine which non penetration constraints are active, the set of active constraints is updated iteratively based on the result of trial analysis until it converges. However, the number of iterations rapidly increases as the number of contact constraints becomes large and it leads to the increase of calculation time. Structural analysis of portable electronic devices such as laptop PCs and smartphones is one of the cases which encounter this kind of problem in the industrial field. These devices consist of covers, circuit boards, CPUs and many other thin and small parts and they are densely placed inside the body. Thus, the potential contact area tends to be wide and the number of contact constraints becomes large.

Recently, interior point methods are focused as an efficient strategy for this kind of problem. A primal-dual interior point method is applied to contact analysis [2] and the efficiency for large scale problems is confirmed by numerical experiments [3]. In addition, the combination of active set method and primal interior point method is proposed [4].

In this paper, we introduce Mehrotra’s predictor-corrector method [5] to elastic analysis with frictionless contacts and tied constraints. Although theoretical bound of complexity is not given for this method, it is widely used because of its actual performance. We implement our algorithm into FrontISTR [6], which is an open-source and large scale finite element structural analysis software, and investigate the performance.

2. Formulation of contact analysis with multipoint constraints

We consider a three-dimensional, small deformation and frictionless contact problem of elastic bodies that are discretized by finite element method. Let n and nC denote the number of nodes and the number of contact constraints, and \( u \in \mathbb{R}^{3n} \), \( f \in \mathbb{R}^{3n} \) and \( K \in \mathbb{R}^{3n \times 3n} \) denote the nodal displacement vector, the external load vector and the stiffness matrix, respectively. The contact problem with multi-point constraints is given by

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} u^T Ku - f^T u, \\
\text{subject to} & \quad T_i^T u + h_i \geq 0 \quad (i = 1, 2, \ldots, n_C), \\
& \quad B_i^T u = 0 \quad (i = 1, 2, \ldots, n_M),
\end{align*}
\]

where \( T_i \in \mathbb{R}^{3n} \) is the vector that projects the displacement of concerned nodes to the contact direction. For the node-to-segment contact shown in Fig. 1, the components of \( T_i \) is calculated from the normal vector and the shape function at the projection point of the slave node to the master segment. \( h_i \) is the initial gap of \( i \)-th contact constraint, then the gap at current configuration can be represented by \( T_i^T u + h_i \). \( n_M \) is the number of multi-point constraints and \( B_i \) is the coefficient vector of \( i \)-th multi-point constraint.
We note that the equilibrium equations under contact constraints and multi-point constraints are the Karush Kuhn Tucker (KKT) condition of the contact problem with multi-point constraints, and they are given as follows:

\[ Ku = f + \sum_{i=1}^{n_C} T_i r_i, \]  
\[ r_i(T_i^T u + h_i) = 0 \quad (i = 1, 2, \ldots, n_C), \]  
\[ r_i \geq 0 \quad (i = 1, 2, \ldots, n_C), \]  
\[ T_i^T u + h_i \geq 0 \quad (i = 1, 2, \ldots, n_C), \]  
\[ B_i^T u = 0 \quad (i = 1, 2, \ldots, n_M), \]  

where \( r_i \) is the contact force for \( i \)-th contact constraint. A contact candidate node is said to be free when the gap is positive and the contact force is zero, and is said to be in contact when its gap is zero and contact force is positive. Eqs. (2), (3) and (4) mean that a contact state is either free or in contact.

3. Primal-dual interior point method for contact problems

In this section, we describe the primal-dual interior point method for contact problems introduced by Tanoh [3]. We remove multi-point constraints by a quadratic penalty method, then the minimization problem to be solved becomes as follows:

\[
\text{minimize } I(u) \equiv \frac{1}{2} u^T Ku - f^T u + \frac{1}{2} \rho \sum_{i=1}^{n_M} u^T B_i B_i^T u,
\]

subject to \( T_i^T u + h_i \geq 0 \quad (i = 1, 2, \ldots, n_C), \) 

where \( \rho \) is a sufficiently large positive real number.

The main idea of an interior point method is to remove inequality constraints by using a logarithmic barrier function:

\[ I_\mu(u) \equiv I(u) - \mu \sum_{i=1}^{n_C} \log (T_i^T u + h_i). \]

\( \mu \) is a positive real parameter and is called the barrier parameter. The optimal point of \( I_\mu(u) \) converges to that of the minimization problem (6) if \( \mu \) tends to zero under certain assumptions. Based on this property, an interior point method repeats the following two procedures until \( u \) converges; to take a step to reduce \( I_\mu(u) \) by the Newton method and to reduce \( \mu \) according to a certain criteria.

The procedure to obtain the step is as follows. The first order optimal condition of \( I_\mu(u) \):

\[ Ku + \rho \sum_{i=1}^{n_M} B_i B_i^T u - f - \sum_{i=1}^{n_C} T_i r_i = 0, \]  
\[ r_i(T_i^T u + h_i) = \mu \quad (i = 1, 2, \ldots, n_C), \]  
\[ r_i > 0 \quad (i = 1, 2, \ldots, n_C), \]  
\[ T_i^T u + h_i > 0 \quad (i = 1, 2, \ldots, n_C). \]

Here, we define \( r_i \equiv \mu/(T_i^T u + h_i) \). For a primal-dual interior point method, a dual variable \( r_i \) is treated as an independent variable. From (8) and (9), we can obtain the newton direction \( \Delta u \) for \( I_\mu(u) \) by solving following linear equations:

\[
\begin{aligned}
(K + \rho \sum_{i=1}^{n_M} B_i B_i^T) \Delta u &= -\sum_{i=1}^{n_C} T_i \Delta r_i \\
&= - \left( Ku + \rho \sum_{i=1}^{n_M} B_i B_i^T u - f - \sum_{i=1}^{n_C} T_i r_i \right), \\
&= \mu - r_i(T_i^T u + h_i) \quad (i = 1, 2, \ldots, n_C).
\end{aligned}
\]

This step size is decreased not to get out of the interior of (10) and (11).

Then, \( \mu \) is decreased and the Newton direction for updated \( \mu \) is calculated repeatedly until the residual of (8) and (9):

\[ \phi(u, r, \mu) = \left[ \left\| Ku - f - \sum_{i=1}^{n_C} T_i r_i \right\|^2 - \sum_{i=1}^{n_C} r_i(T_i^T u + h_i) - \mu \right]^{\frac{1}{2}}, \]

where \( r = (r_1, r_2, \ldots, r_{n_C}) \), converges. We show the procedure of a primal-dual interior point method for contact problems as follows:

**primal-dual interior point method**

1. Set \( \mu > 0, \varepsilon_1 > 0, \varepsilon_2 > 0, 0 < \eta < 1 \) and \( k = 0 \). Choose initial \( u = u_0 \) and \( r = r_0 \).
2. Get \( \Delta u \) and \( \Delta r \) from (8) and (9).
3. Let \( \sigma_{\text{max}1} \) and \( \sigma_{\text{max}2} \) denote the maximum value of \( \sigma_1 \) and \( \sigma_2 \) that satisfy

\[
T_i^T (u_k + \sigma_{\text{max}1} \Delta u) + h_i \geq 0 \quad (i = 1, 2, \ldots, n_C),
\]

\[
r_{i,k} + \sigma_{\text{max}2} \Delta r_i \geq 0 \quad (i = 1, 2, \ldots, n_C).
\]

Then, set \( \sigma_i = \min(0.99\sigma_{\text{max}}, 1), (i = 1, 2) \).
4. Update \( u \) and \( r \):

\[
u_{k+1} = u_k + \sigma_1 \Delta u, r_{k+1} = r_k + \sigma_2 \Delta r
\]
5. Decrease \( \mu : \mu = [\sigma_1 + (1 - \sigma)\mu] \), where \( \sigma = (\sigma_1 + \sigma_2)/2 \)
6. If \( \phi(u_{k+1}, r_{k+1}, \mu) < \varepsilon_1 \) and \( \mu < \varepsilon_2 \), the algorithm stops. Otherwise, set \( k = k + 1 \) and go to step 2.
4. Predictor-corrector method for contact problems

In this section, we introduce a predictor-corrector method [5] to primal-dual interior point method described in the previous section. A predictor-corrector method consists of two steps: the prediction step and the correction step. In the prediction step, the affine scaling direction \((\Delta \bar{u}, \Delta \bar{r})\) is calculated from (8) and (9) with \(\mu = 0\). In the correction step, the barrier parameter \(\mu\) is updated at first. Let us define a duality gap \(g(u, r)\) as

\[
g(u, r) = \sum_{i=1}^{nC} r_i (T_i^T u + h_i) \tag{14}
\]

and define \(\sigma_{max1}\) and \(\sigma_{max2}\) in the same way as \(\sigma_{max1}\) and \(\sigma_{max2}\) in the previous section. Then, the update criteria of \(\mu\) is given by

\[
\mu_{new} = \left[ \frac{g(u + \sigma_{max1} \Delta u, r + \sigma_{max2} \Delta r)}{g(u, r)} \right] ^\gamma \mu_{old}. \tag{15}
\]

Since Mehrotra [5] proposed to set \(\gamma = 2\) or 3, we use \(\gamma = 3\) here. Second, the corrector \((\Delta \bar{u}, \Delta \bar{r})\) is given as follows in order to move prediction point \((u + \Delta u, r + \Delta r)\) towards the optimal point of \(I_{new}\). By substituting \((u + \Delta \bar{u} + \Delta \tilde{u}, r + \Delta \bar{r} + \Delta \tilde{r})\) to (8) and (9), we obtain

\[
K(u + \Delta \bar{u} + \Delta \tilde{u}) + \rho \sum_{i=1}^{nC} B_i B_i^T (u + \Delta \bar{u} + \Delta \tilde{u})
\]

\[
- f - \sum_{i=1}^{nC} T_i (r + \Delta \bar{r} + \Delta \tilde{r}) = 0, \tag{16}
\]

\[
(r + \Delta \bar{r} + \Delta \tilde{r}) [T_i^T (u + \Delta \bar{u} + \Delta \tilde{u}) + h_i] = \mu_{new} \quad (i = 1, 2, \ldots, nC). \tag{17}
\]

From the definition of \((\Delta \bar{u}, \Delta \bar{r})\), it holds

\[
\left( K + \rho \sum_{i=1}^{nC} B_i B_i^T \right) \Delta \bar{u} - \sum_{i=1}^{nC} T_i \Delta \bar{r}_i = 0 \tag{18}
\]

\[
r_i T_i^T \Delta \bar{u} + (T_i^T u + h_i) \Delta \bar{r}_i
\]

\[
= \mu_{new} - \tilde{r}_i T_i^T \Delta \bar{u} - \tilde{r}_i T_i^T \Delta \tilde{u} - \tilde{r}_i T_i^T \Delta u
\]

\[
- \tilde{r}_i T_i^T \Delta \tilde{u} \quad (i = 1, 2, \ldots, nC). \tag{19}
\]

Ignoring the terms that include \(\Delta \tilde{u}\) and \(\Delta \tilde{r}\) from the RHS of (19), we obtain the linear equation of \((\Delta \bar{u}, \Delta \bar{r})\) as follows:

\[
r_i T_i^T \Delta \bar{u} + (T_i^T u + h_i) \Delta \bar{r}_i
\]

\[
= \mu_{new} - \tilde{r}_i T_i^T \Delta \bar{u} \quad (i = 1, 2, \ldots, nC). \tag{20}
\]

Thus, the corrector \((\Delta \bar{u}, \Delta \bar{r})\) is given from (18) and (20). In a predictor-corrector method, we have to solve linear equations twice per iteration to obtain \((\Delta \bar{u}, \Delta \bar{r})\) and \((\Delta \bar{u}, \Delta \bar{r})\). However, since the coefficient matrix to obtain \((\Delta \bar{u}, \Delta \bar{r})\) is the same as the coefficient matrix to obtain \((\Delta \bar{u}, \Delta \bar{r})\), the matrix solver time for second time can be reduced considerably by keeping the LU factorization of the first time.

The total step direction is given by \((\Delta \bar{u} + \Delta \tilde{u}, \Delta \bar{r} + \Delta \tilde{r})\). This step size is decreased not to get out of the interior of (10) and (11) in the same way as the previous section. The procedure of a predictor-corrector method for contact problems is summarized as follows:

**predictor-corrector method**

1. Set \(\mu > 0, \varepsilon_1 > 0, \varepsilon_2 > 0\) and \(k = 0\). Choose initial \(u = u_0\) and \(r = r_0\).

2. **prediction step**

   2. Set \(\mu = 0\) and get \(\Delta \bar{u}\) and \(\Delta \bar{r}\) from (8) and (9).

   3. Let \(\sigma_{max1}\) and \(\sigma_{max2}\) denote the maximum value of \(\sigma_1\) and \(\sigma_2\) that satisfy

   \[
   T_i^T (u_k + \sigma_{max1} \Delta u) + h_i \geq 0 \quad (i = 1, 2, \ldots, nC),
   \]

   \[
   r_{i,k} + \sigma_{max2} \Delta r_i \geq 0 \quad (i = 1, 2, \ldots, nC).
   \]

   Then, set \(\sigma_i = \min(0.99 \sigma_{max}, 1)\), \(i = 1, 2\).

4. **correction step**

   4. Update \(\mu = \mu_{new}\) by (15).

   5. Get \(\Delta \bar{u}\) and \(\Delta \bar{r}\) from (18) and (20).

   \[
   \Delta u = \Delta \bar{u} + \Delta \tilde{u} + \Delta \bar{r} + \Delta \tilde{r}.
   \]

   6. Let \(\sigma_{max1}\) and \(\sigma_{max2}\) denote the maximum value of \(\sigma_1\) and \(\sigma_2\) that satisfy

   \[
   T_i^T (u_k + \sigma_{max1} \Delta u) + h_i \geq 0 \quad (i = 1, 2, \ldots, nC),
   \]

   \[
   r_{i,k} + \sigma_{max2} \Delta r_i \geq 0 \quad (i = 1, 2, \ldots, nC).
   \]

   Then, set \(\sigma_i = \min(0.99 \sigma_{max}, 1)\), \(i = 1, 2\).

   7. Update \(u\) and \(r\):

   \[
   u_{k+1} = u_k + \sigma_1 \Delta u, \quad r_{k+1} = r_k + \sigma_2 \Delta r
   \]

   8. If \(\phi(u_{k+1}, r_{k+1}, \mu) < \varepsilon_1\) and \(\mu < \varepsilon_2\), the algorithm stops. Otherwise, set \(k = k + 1\) and go to step 2.

5. Numerical experiments

In this section, we present the results of numerical experiments. We implemented an active set method (ASM), a primal-dual interior point method (PDPIM) and a predictor corrector method (PCM) for contact problems into FrontISTR [6]. Since FrontISTR supports contact analysis function by an active set method and an augmented Lagrange method, we could easily implement our algorithm by using its data structure in the contact analysis module.

Fig. 2 and Table 1 shows models which we use for numerical experiments. The model 1 is a simple two-beams which gets into contact when a pressure is applied to the pushing jig. The model 2 is a two-plates model that has a larger number of DOFs than the model 1. The model 3 is a smartphone case model. The model 4 is a laptop PC model in order to evaluate stress at the liquid crystal display when the rear cover is pressed by an external force. The model 5 is the CPU side of a laptop PC model and has a larger number of DOFs than model 4.

The numerical experiments were performed on a machine with Intel(R) Xeon(R) CPU X5675 @ 3.07GHz,12core and 72GB RAM. We also used a sparse direct solver Pardiso in the Intel Math Kernel Library 11.2.

We compared the number of iterations of the main loop and the nodal displacements between the three
methods. We note that a sparse matrix solver routine is executed once per iteration in ASM and PDIPM, and is executed twice per iteration in PCM. Therefore, we also compared calculation time of the three methods for model 5 that has the largest number of DOFs.

We set the initial value of the barrier parameter $\mu$ to 0.5. We also set the convergence threshold $\epsilon_1 = \epsilon_2 = 10^{-10}$ for the model 2 and $10^{-6}$ for other models because $10^{-10}$ was necessary for model 2 in order to obtain the same result as ASM. Since the number of iterations strongly depends on $\eta$ for PDIPM, we used 0.01, 0.1, 0.3, 0.5 and 0.7 for $\eta$. As for the contact conditions of which initial gap is to be zero, we set $h_i$ to $10^{-8}$ so that the initial solution $u = 0$ is an interior point. The penalty value $\rho$ was set to $10^6$ for three methods.

To confirm that the same solution is obtained by ASM, PDIPM and PCM briefly, we show the maximum nodal displacement of five test models in Table 2. As for the model 5, we also show the nodal displacement contour in Fig. 3. For each model, the values of maximum displacement are the same for the three methods.

Table 3 shows the number of iterations of the main loop. As the number of DOFs and that of constraints increase, PDIPM become faster than ASM. PCM spends 50% or less number of iterations of PDIPM. Computational time of the model 5 is shown in Table 4. Computational time per iteration of PCM increases at most by 20% compared to other methods and it makes total time of PCM the smallest.

### 6. Conclusion

We proposed a method for contact problems with multi-point constraints and investigated the performance of this algorithm. By the numerical experiments, it is confirmed that the proposed method converges faster than conventional methods for electronic models that have a large number of DOFs and constraints. As for theoretical upper bound of complexity, it is given for some variant of the predictor-corrector method [7]. Comparison with the theoretical upper bound using these methods is necessary.

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