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The Schur Complement Algorithm for the Solution of Contact Problems

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ABSTRACT. We present a modification of the Schur complement algorithm for the solution of the systems of linear equations in order to solve quadratic programming problems with inequality constraints. We give elementary proof that the algorithm is correct and discuss possible improvements.

1. Introduction

The problem to find an equilibrium of bodies in contact is of natural interest for the domain decomposition methods. This statement is based on two observations. First, the physical domain of such problems often consists of several subdomains, so that no additional data describing the decomposition of the domain are necessary. Second, the numerical solution of such problems is usually reduced to numerical solution of the sequence of related linear problems, so that there is a good chance that some more expensive preliminary computations may pay off.

In this paper, we present the basic nonoverlapping domain decomposition algorithm which combines the well known conjugate gradient algorithm for the solution of quadratic programming problems and the basic Schur complement precondtitioning. The minimization of the energy functional on each subspace generated by the active set strategy is carried out in two steps. First the functional is minimized on interiors of subdomains using the Schur complement in some conjugate projector, which amounts to the solution of Dirichlet problems for all subregions. Then the same projector is used to the preconditioning of auxiliary linear problem.

The algorithm has already been described in Reference 4, however, here we give different reasoning to show that the algorithm is correct under relaxed assumptions. We restrict our attention to the numerical solution of discretized contact problem without friction formulated in terms of quadratic programming as described in References 1,2 and 6.

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2. Notations and preliminaries

Let K denote the stiffness matrix of the order n resulting from the finite element discretization of a system of elastic bodies which occupy regions $\Omega_1, \cdots, \Omega_p$. For simplicity, we suppose that bilateral boundary conditions are enhanced in K. With suitable numbering of nodes, we can achieve that $K = \text{diag}(K_1, \cdots, K_p)$, where K_i is banded stiffness matrix of the body which occupies the region Ω_i. The matrices K_i are known to be possitive semidefinite.

The linearized incremental contact conditions are supposed to be defined by the matrix B and the vector c,

$$B = (b_{\cdot 1}, \ldots, b_{\cdot k}) = \begin{pmatrix} b_{1\cdot}^T \\ \vdots \\ b_{n\cdot}^T \end{pmatrix}, \qquad c = \begin{pmatrix} \gamma_1 \\ \vdots \\ \gamma_k \end{pmatrix}.$$

The columns $b_{\cdot i}$ of B are vectors which enable us to evaluate the change of the distance $\gamma_i \geq 0$ between two potential contact surfices in a reference configuration in a given pair of nodes; the formula for the displacement u is $b_{\cdot i}^T u$. The matrix B is sparse as nonzero entries of $b_{\cdot i}$ may be only in positions of nodal variables which correspond to the nodes involved in some constraint.

Let U_i denote the matrix which we obtain from the identity matrix of the order n by crossing out the columns which do not correspond to the displacements of nodes in the interior of Ω_i. Thus U_i is the 0–1 matrix that maps the local displacements of interior points of Ω_i into the global displacements and $B^T U_i = O$.

For any subset J of $\{1, \ldots, k\}$, denote by B^J and c^J the parts of B and c consisting of the columns $b_{\cdot i}, i \in J$ and γ_i, respectively.

Our problem is to minimize the energy functional

$$j(u, f) = \frac{1}{2} u^T K u - f^T u \tag{1}$$

on the set

$$\mathscr{B} = \{u : B^T u \leq c\}.$$

3. CG on the range of symmetric matrix

Let us recall here few observations which are useful for minimization of the energy functional on the range $\mathscr{C}$ of a symmetric positive semidefinite matrix C by the CG method. For any $M \in R^{nn}$ and $b \in R^n$, let $\mathscr{K}_i(b, M)$ denote the subspace which is spanned by $b, Mb, \ldots, M^{i-1}b$, and put $\mathscr{K}_i = \mathscr{K}_i(b, KC)$.

If $x_i \in \mathscr{K}_i$ minimizes $j(u,b)$ for $u \in C\mathscr{K}_i$, then $r_i = b - Kx_i$ is orthogonal to $C\mathscr{K}_i$, so that Cr_i is orthogonal to $\mathscr{K}_i$. Moreover, $r_i \in \mathscr{K}_{i+1}$ and $Cr_i = o$ implies $j(x_i, b) = \min\{j(u,b) : u \in \mathscr{C}\}$.

As $KC\mathscr{K}_{i-1} \subset \mathscr{K}_i$ and Cr_i is orthogonal to $\mathscr{K}_i$, it follows that Cr_i is orthogonal to $KC\mathscr{K}_{i-1}$, so that Cr_i is K-conjugate to $C\mathscr{K}_{i-1}$.

Now suppose that $p_0, \ldots, p_{j-1}$ form the K-conjugate basis of $C\mathscr{K}_j$, $j = 1, \ldots, i$. Then, if $Cr_i \neq o$ and $Kp_{i-1} \neq o$, we can extend $p_0, \ldots, p_{i-1}$ to the basis of $C\mathscr{K}_{i+1}$ by taking

$$p_i = Cr_i - \beta_{i-1}p_{i-1}, \qquad \beta_{i-1} = r_i^T CKp_{i-1}/p_{i-1}^T Kp_{i-1}. \tag{2}$$

Thus we can get K-conjugate basis of $C\mathscr{K}_i$ by the reccurrence (2) starting from $p_0 = Cb$. Computation of x_i is then reduced to the standard one dimensional searches

$$x_i = x_{i-1} + \alpha_{i-1}p_{i-1}; \quad \alpha_{i-1} = r_{i-1}^T p_{i-1}/p_{i-1}^T Kp_{i-1} \tag{3}$$

starting from $x_0 = o$. If $Cr_i \neq o$ and $Kp_{i-1} = o$, then, using recurrences for p_i and r_i and orthogonality relations, it may be shown that

$$j(x_{i-1} + \alpha p_{i-1}, b) = j(x_{i-1}, b) - \alpha r_{i-1}^T Cr_{i-1}$$

so that no minimum of $j(u,b)$ exists and p_{i-1} is the decrease direction.

4. Projector preconditioning on subspace

We shall exploit the observations of the Section 3 to shape the algorithm which first looks for the minimum on a subspace $\mathscr{U} \subset \mathscr{C}$ and then continues by iterations. The subspace $\mathscr{U}$ will be defined as the range of a full rank matrix U. We suppose that $U^T KU$ is invertible.

Using the gradient argument, we observe that $\min j(u,b)$ for $u \in \mathscr{U}$ is attained at

$$x_0 = U(U^T KU)^{-1}U^T b. \tag{4}$$

Now let us introduce the conjugate projector $Q = I - U(U^T KU)^{-1}U^T K$ with the range $\mathscr{V} = (K\mathscr{U})^{\perp}$ and notice that

$$Q\mathscr{C} \subset \mathscr{C}, \quad Q^T r_o = r_o \quad \text{and} \quad KQ = Q^T KQ = Q^T K. \tag{5}$$

Let us show that $\mathscr{V} \cap \mathscr{C}$ is the range of QCQ^T.

LEMMA 1 *If C is positive semidefinite, then the range of QCQ^T is $\mathscr{V} \cap \mathscr{C}$.*

PROOF: Suppose that $x \in \mathscr{C} \cap \mathscr{V}$, so that there are $y \in \mathscr{C}$ and $z \in \mathscr{V}$ such that $x = Cy = Qz$. As $Q^2 = Q$, it follows that x belongs to the range of QC. On the other hand, if $x = QCy$, then $x \in \mathscr{V} \cap \mathscr{C}$ by (5).

As C is positive semidefinite, it follows that there is positive semidefinite $C^{1/2}$ with the same range $\mathscr{C}$, so that $\mathscr{V} \cap \mathscr{C}$ is equal to the range of $QC^{1/2}$. To finish the proof, it is enough to observe that the range of $QC^{1/2}$ is the orthogonal complement of the kernel of $C^{1/2}Q^T$ and that the kernel of $C^{1/2}Q^T$ is that of QCQ^T. □

Now we can look for x_c which minimizes $j(x_o + u, b)$ or $j(u, b - Kx_o)$ for $u \in \mathscr{V} \cap \mathscr{C}$ using the formulae (2) and (3) with C replaced by QCQ^T.

If $\mathscr{C} = R^n$ and K is invertible, the algorithm reduces to the projector preconditioning algorithm whose preconditioning effect has been studied in Reference 5.

5. Algorithm

The proposed algorithm reads as follows:

A. Initialization

(i) Define $U = (U_1, \ldots, U_p)$. It follows that $B^T U = O$, or, in other words, that the range $\mathscr{U}$ of U satisfies $\mathscr{U} \subset \mathscr{B}$. Moreover, $u \in \mathscr{B}$ implies $u + \mathscr{U} \subset \mathscr{B}$. We shall suppose that $U^T KU$ is invertible.

(ii) Find the factorization $LL^T = U^T KU = \mathrm{diag}(U_1^T K_1 U_1, \ldots, U_p^T K_p U_p)$.

(iii) $u = o, r = f$.

B. Update of the set of active contraints

(iv) Put $J = \{i : b_{\cdot i}^T u = \gamma_i\}$.

(v) Extend U to the full rank $n \times m$ matrix $V = (U, V_0)$ whose range form the basis of the kernel $\mathscr{B}^J$ of B^{JT} and whose blocks satisfy $U^T V_0 = O$. Details may be found in Reference 4.

C. Reducing the residuum on $\mathscr{U}$.

(vi) $u = u + UL^{-T}L^{-1}U^T r$.

(vii) $r = f - Ku, \quad p = VV^T r$.

D. Test of the residuum and of the contact conditions.

(viii) $r0 = V^T r$.

(ix) If $| r0 | \neq 0$ go to (xiii).

(x) Evaluate the Lagrange multipliers λ_i by solving $B^T \lambda = r$.

(xi) If all λ_i are greater or equal to zero go to (xx).

(xii) Remove from J indices of negative λ_i and go to (v).

E. Conjugate gradient iterations on $(K\mathscr{U})^{\perp} \cap \mathscr{B}^J$

(xiii) $q = (I - UL^{-T}L^{-1}U^TK)p$.

(xiv) If $Kq \neq o$, then put $\alpha = r^Tq/q^TKq$ and

$$\alpha 1 = \min\left\{\frac{\gamma_i - b_{\cdot i}^T u}{b_{\cdot i}^T q} : b_{\cdot i}^T q > 0\right\}.$$

If $Kq = o$ and α_1 is not defined (minimum over empty set), signal no solution and stop.
If $Kq = o$ and α_1 is defined, put $\alpha = \alpha 1$.

(xv) $u = u + \min(\alpha, \alpha 1)q$.

(xvi) $r = r - \min(\alpha, \alpha 1)Kq$.

(xvii) $\beta = r^TVV^TKq/q^TKq$.

(xviii) $p = VV^Tr - \beta p$.

(xix) If $\alpha < \alpha 1$ go to (viii), else to go (iv).

(xx) Return u as the desplacement of the solution. Nodal contact forces may be extracted from λ.

Apart from the observations of Section 4 applied to $C = VV^T$, we have used the identity $Q^Tr = r$, which is a consequence of (5) and (xvi). The algorithm differs from the standard active set algorithm in two steps minimization (parts C and E of the algorithm), so that it preserves its finite termination property.

6. Comments

The algorithm is the domain decomposition algorithm due to the special choice of U which implies that U^TKU is block diagonal, each diagonal block being the stiffnes matrix of the body Ω_i with enhanced Dirichlet conditions. Thus the decomposition of (ii) reduces to the decomposition of blocks which may be done in parallel. The same holds for the implementation of the most expensive steps (vi) and (xiii), which involve solution of the Dirichlet problem for each domain.

If the matrix V^TKV is regular, the preconditioning effect which results from reduction of the problem to the boundary and contact zone may be observed. The point is that this reduction is performed by means of the projector which does not change with the change of the active sets. The algorithm has been implemented for the solution 2D contact problems and it has been shown that even in serial implementation there are problems for which the performance of the algorithm is considerably better than that of the standard active set algorithm. Details may be found in Reference 4.

We belive that some improvement may be achieved with additional preconditioning and with improved strategy of the update of the active set. For example the preconditioner of the References 3, 7 and 9 may be useful as it is efficient and its update to the current contact surface may be not expensive. The inspiration for modification of the update of the active set may be found in Reference 8.

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