FETI based algorithms for modelling of fibrous composite materials with debonding

Zdeněk Dostál\textsuperscript{a,b,\ast,\ast}, David Horák\textsuperscript{a,\ast}, Oldřich Vlach\textsuperscript{a,\ast}

\textsuperscript{a}FEI VŠB-Technical University of Ostrava, Ostrava, Czech Republic
\textsuperscript{b}Institute of Geonics of AS CR, Ostrava, Czech Republic

Abstract

We show how we can exploit our recently proposed algorithms for the solution of contact problem of elasticity to the 2D analysis of the interfacial debonding of samples that consist of several fibres embedded in a homogeneous matrix, aligned in the longitudinal direction. The performance of the algorithm is demonstrated on analysis of deformations of samples of the fibrous composite material.

Key words: fibrous composites, domain decomposition, contact problems

1 Introduction

The composite materials are increasingly important in many modern engineering designs. To exploit effectively the attractive properties of these new materials, it is necessary to understand properly their macroscopic response to tractions. However, it turns out that it is not easy to describe the macroscopic mechanical properties of the composite materials even under the assumption that the microstructure is perfectly bonded [9].

It seems that it was P. Wriggers who first presented the results based on numerical analysis that take into account the effect of the interface strength for multiple fibers [15]. He reduced his analysis to 2D plain strain problem observing that the aggregate longitudinal stiffness (parallel to the fibres) is usually not significantly affected, since the stiffness is essentially that of the fibres, but the aggregate transverse stiffness is essentially that of the fibers. The resulting special contact problem is still quite challenging due to the strong non-linearity related to the non-penetration conditions and the finite

\* This research was supported by the grant 101/05/0423 of the GA CR and by the project 1ET400300415 of the Ministry of Education of the Czech Republic.
\* Corresponding author.

\textit{Email addresses: zdenek.dostal@vsb.cz} (Zdeněk Dostál),
david.horak@vsb.cz (David Horák), oldrich.vlach2@vsb.cz (Oldřich Vlach).

\hspace{1cm}Preprint submitted to Elsevier 10 November 2006
interface strength that must be considered on relatively large, disconnected and a priori unknown debonding surfaces. To solve it, P. Wriggers used the node to segment implementation of the non-penetration condition [14] and the original nested contact algorithm scheme based on the active set strategy to effectively simulate multiple interacting unilateral constraints.

In this paper we suggest to use an alternative algorithm that is based on modification of the FETI (Finite Element Tearing and Interconnecting) methods proposed by Farhat and Roux [12] for parallel solution of linear problems. Its key ingredient is decomposition of the spatial domain into non-overlapping subdomains that are ”glued” by Lagrange multipliers, so that, after eliminating the primal variables, the original problem is reduced to a small, relatively well conditioned, typically equality constrained quadratic programming problem that is solved iteratively. Observing that the equality constraints may be used to define so called ”natural coarse grid”, Farhat, Mandel and Roux [11] modified the basic FETI algorithm so that they were able to prove its numerical scalability.

If the FETI procedure is applied to the problems with the boundary non-linearity, the resulting quadratic programming problem has not only the equality constraints, but also the bound constraints. However, it turned out that even such problems can be solved very efficiently provided the FETI methods are combined with a modification of the special augmented Lagrangian method [4] which generates the approximations of the Lagrange multipliers in the outer loop while the bound constrained quadratic programming problems are solved approximately by efficient algorithms [8] in the inner loop. The algorithms have been proved to enjoy a kind of optimal convergence and most recently, scalability has been proved for FETI with these algorithms [7,5]. Alternative application of domain decomposition based methods to modelling of microstructure was presented by Zohdi and Wriggers [16].

After describing the conditions of equilibrium of the sample of a composite material with enclosed fibres (zero interface strength), we briefly review the FETI methodology that turns the variational inequality into the well conditioned quadratic programming problem with bound and equality constraints, so that our efficient algorithms can be used. Finally we discuss modelling of the composites with given interface strength and give results of numerical experiments.

2 Composite with inclusions in plane strain

We shall first consider a sample of composite with enclosed fibres as in Figure 2.1 assuming the plain strain in the transversal plane. We shall model it as a system of homogeneous isotropic elastic bodies, each of which occupies, in a reference configuration, a domain \( \Omega_p \) in \( \mathbb{R}^2 \) with boundary \( \Gamma_p \). To prepare for effective application of our domain decomposition algorithm, we shall decompose the cross-section into the square cells, each of which contains exactly one fiber. Thus each cell comprises two bodies, the outer body being part of the matrix surrounding the enclosed fiber. Let us denote the overall number of bodies by \( s \). Suppose that each \( \Gamma_p, p = 1, \ldots, s \) consists of four disjoint parts \( \Gamma_p^U, \Gamma_p^F, \Gamma_p^G \) and \( \Gamma_p = \Gamma_p^U \cup \Gamma_p^F \cup \Gamma_p^G \cup \Gamma_p^C \), and that the displacements \( \mathbf{U}^p : \Gamma_p^U \to \mathbb{R}^d \) and forces \( \mathbf{F}^p : \Gamma_p^F \to \mathbb{R}^d \) are given. The part \( \Gamma_G \) denotes the
artificial interface between cells, and the part $\Gamma^p_C$ denotes the part of $\Gamma^p$ which is the interface between the matrix and the fiber. We assume the linearized nonpenetration condition on $\Gamma^p_C$ to be described later. We shall denote by $\Gamma^{pq}_C$ the part of the artificial interface $\Gamma^p$ which is "glued" to the corresponding part of $\Omega^q$, and by $\Gamma^{qp}_C$ the part of $\Gamma^p$ that can be, in the solution, in contact with the body $\Omega^q$. In our case, when fibre $\Omega^p$ is inserted into the matrix $\Omega^q$, then

$$\Gamma^p_C = \Gamma^{pq}_C = \Gamma^{qp}_C = \Gamma^q_C.$$  

The gluing conditions require continuity of displacements and of their normal derivatives across $\Gamma_C$.

Figure 2.1 Fiber composite

Let $c_{ijkl}^p : \Omega^p \to \mathbb{R}^d$ and $g^p : \Omega^p \to \mathbb{R}^d$ denote the entries of the elasticity tensor and a vector of body forces, respectively. For any sufficiently smooth displacement $u : \Omega^1 \times \ldots \times \Omega^s \to \mathbb{R}^d$, the total potential energy is defined by

$$J(u) = \sum_{p=1}^s \left\{ \frac{1}{2} \int_{\Omega^p} a(u^p, u^p) d\Omega - \int_{\Omega^p} (g^p)^T u^p d\Omega - \int_{\Gamma^p_F} (F^p)^T u^p d\Gamma \right\}$$  \hspace{1cm} (2.1)$$

where

$$a^p(u^p, v^p) = \frac{1}{2} \int_{\Omega^p} c_{ijkl}^p e_{ij}^p(u^p) e_{kl}^p(v^p) d\Gamma$$  \hspace{1cm} (2.2)$$

$$e_{kl}^p(u^p) = \frac{1}{2} \left( \frac{\partial u^p_k}{\partial x^p_\ell} + \frac{\partial u^p_\ell}{\partial x^p_k} \right).$$  \hspace{1cm} (2.3)$$

We suppose that the elasticity tensor satisfies natural physical restrictions so that

$$a^p(u^p, v^p) = a(v^p, u^p) \quad \text{and} \quad a(u^p, u^p) \geq 0.$$  \hspace{1cm} (2.4)$$

To describe the linearized non-interpenetration conditions, let us define for each $p < q$ a one-to-one continuous mapping $O^{pq}_C : \Gamma^p_C \to \Gamma^q_C$ that assigns to
each \( \mathbf{x} \in \Gamma_{pq}^p \) some point \( \mathbf{y} \in \Gamma_{pq}^q \) that is near to \( \mathbf{x} \). In our case, we take \( \mathbf{y} = \mathbf{x} \). The linearized non-interpenetration condition at \( \mathbf{x} \in \Gamma_{pq}^p \) then reads

\[
(u^p(\mathbf{x}) - u^q(\mathbf{O}^{pq}x))\mathbf{n}^p \leq (\mathbf{O}^{pq}(\mathbf{x}) - \mathbf{x})\mathbf{n}^p, \quad \mathbf{x} \in \Gamma_{pq}^p, \quad p < q. \tag{2.5}
\]

Now let us introduce the Sobolev space

\[
\mathcal{V} = H^1(\Omega_1)^d \times \cdots \times H^1(\Omega_s)^d, \tag{2.6}
\]

and let \( \mathbf{K} = \mathbf{K}^E \cap \mathbf{K}^I \) denote the set of all kinematically admissible displacements, where

\[
\mathbf{K}^E = \{ \mathbf{v} \in \mathcal{V} : \mathbf{v}^p = \mathbf{U} \text{ on } \Gamma_U^p \text{ and } \mathbf{v}^p(\mathbf{x}) = \mathbf{v}^q(\mathbf{x}), \mathbf{x} \in \Gamma_{pq}^G \} \tag{2.7}
\]

and

\[
\mathbf{K}^I = \{ \mathbf{v} \in \mathcal{V} : (\mathbf{v}^p(\mathbf{x}) - \mathbf{v}^q(\mathbf{O}^{pq}x))\mathbf{n}^p \leq (\mathbf{O}^{pq}(\mathbf{x}) - \mathbf{x})\mathbf{n}^p, \quad \mathbf{x} \in \Gamma_{pq}^p, p < q \}. \tag{2.8}
\]

The displacement \( \mathbf{u} \in \mathbf{K} \) of the system of bodies in equilibrium satisfies

\[
J(\mathbf{u}) \leq J(\mathbf{v}) \text{ for any } \mathbf{v} \in \mathbf{K}. \tag{2.9}
\]

Conditions that guarantee existence and uniqueness may be expressed in terms of coercivity of \( J \) and may be found, for example, in [10]. More general boundary conditions, such as prescribed normal displacements and zero forces in the tangential plane, may be used to enhance the algorithm without any conceptual difficulties.

### 3 Discretization and reduction to the interface

The finite element discretization of \( \Omega = \Omega_1 \cup \cdots \cup \Omega_s \) with suitable numbering of nodes results in the quadratic programming (QP) problem

\[
\frac{1}{2} \mathbf{u}^T \mathbf{K} \mathbf{u} - \mathbf{f}^T \mathbf{u} \rightarrow \min \quad \text{subject to } \mathbf{B}_I \mathbf{u} \leq \mathbf{c}, \tag{3.1}
\]

with a symmetric positive definite or positive semidefinite block-diagonal matrix \( \mathbf{K} = \text{diag}(K_1, \ldots, K_s) \) of order \( n \), an \( m \times n \) full rank matrix \( \mathbf{B}_I \), \( \mathbf{f} \in \mathbb{R}^n \), and \( \mathbf{c} \in \mathbb{R}^m \). For the sake of simplicity, we shall assume that the grid match across the contact ad the "gluing" interfaces. The matrix \( \mathbf{B}_I \) and the vector \( \mathbf{c} \) describe the linearized incremental non-interpenetration conditions. The rows \( b_i \) of \( \mathbf{B}_I \) are formed by zeros and appropriately placed coordinates of outer unit normals, so that the change of normal distance due to the displacement \( \mathbf{u} \) is
given by \( u^T b_i \), and the entry \( c_i \) of \( c \) describes the normal distance between the \( i \)-th couple of corresponding nodes on the contact interface in the reference configuration. In our case \( c = 0 \) as fibers are in the reference configuration in contact with the matrix, \( n \) is large and \( m \) is much smaller than \( n \). Some care should be taken to guarantee that \( B_I \) is a full rank matrix. The vector \( f \) describes the nodal forces arising from the volume forces and/or some other imposed tractions. The diagonal blocks \( K_p \) that correspond to subdomains \( \Omega^p \) are positive definite or semidefinite sparse matrices. Moreover, we shall assume that the nodes of the discretization are numbered in such a way that \( K_p \) are banded matrices that can be effectively decomposed, possibly after some regularization, by means of the Cholesky factorization.

The continuity of the displacements across auxiliary interfaces requires that \( u^T b_i = 0 \), where \( b_i \) are vectors of order \( n \) with zero entries except 1 and \(-1\) at appropriate positions. If \( B_E \) is the matrix with rows \( b_i \), then the discretization of problem (3.1) with the secondary decomposition results in the QP problem

\[
\frac{1}{2} u^T K u - f^T u \rightarrow \min \text{ subject to } B_I u \leq c \text{ and } B_E u = 0. \tag{3.2}
\]

Some care should be taken to describe the gluing conditions at the corner nodes in order to guarantee that \( B_E \) is a full rank matrix.

Even though (3.1) and (3.2) are standard convex quadratic programming problems, their formulation is not suitable for numerical solution. The reasons are that \( K \) is singular and that the feasible set is in general so complex that projections into it can hardly be effectively computed. These complications may be essentially reduced by applying the duality theory of convex programming.

The Lagrangian associated with problem (3.2) is

\[
L(u, \lambda_I, \lambda_E) = \frac{1}{2} u^T K u - f^T u + \lambda_I^T (B_I u - c) + \lambda_E^T B_E u, \tag{3.3}
\]

where \( \lambda_I \) and \( \lambda_E \) are the Lagrange multipliers associated with the inequality and equality constraints of (3.3), respectively. Introducing notation

\[
\lambda = \begin{bmatrix} \lambda_I \\ \lambda_E \end{bmatrix}, \quad B = \begin{bmatrix} B_I \\ B_E \end{bmatrix}, \quad \text{and} \quad \hat{c} = \begin{bmatrix} c \\ 0 \end{bmatrix},
\]

we can write the Lagrangian briefly as

\[
L(u, \lambda) = \frac{1}{2} u^T K u - f^T u + \lambda^T (B u - \hat{c}).
\]

It is well known [2] that (3.2) is equivalent to the saddle point problem

\[
\text{Find } (u, \lambda) \text{ s.t. } \quad L(u, \lambda) = \sup_{\lambda_I \geq 0} \ inf_{u} L(u, \lambda). \tag{3.4}
\]
For fixed \( \lambda \), the Lagrange function \( L(\cdot, \lambda) \) is convex in the first variable and the minimizer \( u \) of \( L(\cdot, \lambda) \) satisfies
\[
Ku - f + B^T \lambda = 0. \tag{3.5}
\]
Equation (3.5) has a solution iff
\[
f - B^T \lambda \in \text{Im}K, \tag{3.6}
\]
which can be expressed more conveniently by means of a matrix \( R \) whose columns span the null space of \( K \) as
\[
R^T (f - B^T \lambda) = 0. \tag{3.7}
\]
The matrix \( R \) may be formed directly using the known rigid body modes of each subdomains. If the fibres have circle cross-section, we shall omit their rotations so that \( R^T B^T \) is a full rank matrix.

Now assume that \( \lambda \) satisfies (3.6) and denote by \( K^\dagger \) any matrix that satisfies
\[
KK^\dagger K = K. \tag{3.8}
\]
It may be verified directly that if \( u \) solves (3.5), then there is a vector \( \alpha \) such that
\[
u = K^\dagger (f - B^T \lambda) + R \alpha. \tag{3.9}
\]
After substituting expression (3.9) into problem (3.4) and a change of signs, we shall get the minimization problem
\[
\begin{align*}
\min \Theta(\lambda) \quad & \text{s.t.} \quad \lambda_I \geq 0 \quad \text{and} \quad R^T (f - B^T \lambda) = 0, \\
\end{align*}
\tag{3.10}
\]
where
\[
\begin{align*}
\Theta(\lambda) = \frac{1}{2} \lambda^T BK^\dagger B^T \lambda - \lambda^T (BK^\dagger f - \hat{c}).
\end{align*}
\tag{3.11}
\]
Once the solution \( \lambda \) of (3.10) is obtained, the vector \( u \) that solves (3.4) can be evaluated provided the vector \( \alpha \) of (3.9) is known. The formula for \( \alpha \) reads
\[
\alpha = (R^T \tilde{B}^T \tilde{B} R)^{-1} R^T \tilde{B}^T (\tilde{c} - \tilde{B} K^\dagger (f - B^T \lambda)) \tag{3.12}
\]
where \([\tilde{B}_I, \tilde{c}]\) is the matrix formed by the rows of \( B_I \) and \( c \) that correspond to active constraints, the latter being characterized by \( \lambda_i = 0 \). The evaluated \( \alpha \) then can be substituted into (3.9) to get \( u \). If the fibres have circle cross-section, then some modifications described in [13] may be necessary to recover the displacements of the fibres.
4 Natural coarse grid projectors

Even though problem (3.10) is much more suitable for computations than (3.2) and was used for efficient solution of contact problems, further improvement may be achieved by adapting some simple observations and the results of Farhat, Mandel and Roux [11]. We shall formulate a problem that is equivalent to (3.10) but its augmented Lagrangian has such a spectral distribution that the rate of convergence of unconstrained minimization by the conjugate gradients depends neither on penalisation nor discretization parameters.

Let us denote
\[ F = BK^\dagger B^T, \quad \tilde{d} = BK^\dagger f, \]
\[ \tilde{G} = R^T B^T, \quad \tilde{e} = R^T f \]
and let \( T \) denote a regular matrix that defines the orthonormalization of the rows of \( \tilde{G} \) so that the matrix \( G = T\tilde{G} \) has orthogonal rows. After denoting \( e = T\tilde{e} \), problem (3.10) reads

\[
\min \frac{1}{2} \lambda^T F \lambda - \lambda^T \tilde{d} \quad \text{s.t.} \quad \lambda_I \geq 0 \quad \text{and} \quad G\lambda = e. \quad (4.1)
\]

Next we shall transform the problem of minimization on the subset of the affine space to that on the subset of the vector space by means of arbitrary \( \ell \) that satisfies \( G\ell = e \). To this purpose, we shall look for the solution of (4.1) in the form \( \lambda = \mu - \ell \). Since

\[
\frac{1}{2} \lambda^T F \lambda - \lambda^T \tilde{d} = \frac{1}{2} \mu^T F \mu - \mu^T (\tilde{d} + F \ell) + \frac{1}{2} \ell^T F \ell + \ell^T \tilde{d},
\]
problem (4.1) is, after returning to the old notation, equivalent to

\[
\min \frac{1}{2} \lambda^T F \lambda - d^T \lambda \quad \text{s.t.} \quad G\lambda = 0 \quad \text{and} \quad \lambda_I \geq \ell_I. \quad (4.2)
\]

with \( d = \tilde{d} - F\ell \).

Our final step is based on observation that the augmented Lagrangian for problem (4.2) may be decomposed by the orthogonal projectors

\[ Q = G^T G \quad \text{and} \quad P = I - Q \]
on the image space of \( G^T \) and on the kernel of \( G \), respectively. Indeed, problem (4.2) is equivalent to

\[
\min \frac{1}{2} \lambda^T PFP \lambda - \lambda^T Pd \quad \text{s.t.} \quad G\lambda = 0 \quad \text{and} \quad \lambda_I \geq \ell_I. \quad (4.3)
\]

The point is that the Hessian \( H = PFP + \rho Q \) of the augmented Lagrangian

\[
L(\lambda, \mu, \rho) = \frac{1}{2} \lambda^T (PFP + \rho Q) \lambda - \lambda^T Pd + \mu^T G\lambda \quad (4.4)
\]
is decomposed by the projectors $P$ and $Q$ whose image spaces are invariant subspaces of $H$, so that we can assume fast convergence even for large penalty parameters [3]. The problem 4.3 may then be solved efficiently by our SMALBE (Semimonotonic Augmented Lagrangians for Bound and Equality constrained problems) [4] with our MPRGP (Modified proportioning with Reduced Gradient Projections) [8] in inner loop.

5 Modelling of the interface strength

It is rather easy to modify the algorithm so that we can solve the problems with prescribed interface strength. To this end, we shall add to the matrix $B$ new lines for relative tangential displacements, and prescribe suitable non-zero lower bound corresponding to the tensile strength on multipliers for normal constraints and lower and upper bounds for the tangential ones. We shall get the problem of the same structure as above which we can solve by the algorithms of Section 5. When we get the solution, we set the bounds on the multipliers that reached their bounds to zero. The latter implements the non-penetration condition. Repeating the procedure, we shall reach the solution in a finite number of steps as the set of the debonded multipliers increases monotonically. The solution of auxiliary step may be interpreted as solution of problem of material which can sustain for a moment critical stress before the debonding takes place. Alternatively, some incremental procedure may be considered.

6 Numerical experiments

We have implemented the algorithm in MATLAB and tested it on solution of two model problems.

We first considered modelling of a square sample of fiber composite comprising $4 \times 4$ fibres inserted into the matrix without gluing. The Young modulus and the Poisson ratio of the fiber was 100000 MPa and 0.2, respectively, the Young modulus and the Poisson ratio of the matrix was 1000 MPa and 0.4, respectively. We assumed that the sample was fixed in the horizontal direction on the left and in the vertical direction on the bottom. The tensile distributed forces with the intensity -20 MPa acted on the upper boundary of the sample. The problem was discretized by 3104 nodal displacements and 926 Lagrange multipliers. The resulting displacements compared with that of the homogeneous sample are in Figure 7.1 To solve the problem required 794 conjugate gradient iterations.

To demonstrate the capability of the algorithm to model the interface strength, we considered the square sample of the same material properties as above and comprising $4 \times 4$ fibres fixed in the matrix by glue with normal tensile strength and tangential strength equal to 5 MPa. The problem was discretized by 6176 nodal displacements and 1374 Lagrange multipliers. To solve the problem required 3730 conjugate gradient iterations and 6 outer iterations. To compare the effect of gluing, we have solved the same problem also without gluing. The deformation of the samples is in Figure 7.2.
The numbers of iterations are still quite high and some improvements should be considered. Let us point out that our examples do not satisfy the assumptions on problems for which the optimality results are known [5], but the algorithms are still effective.

7 Comments and conclusions

We have presented an algorithm for numerical analysis of fiber composites that enables to take into account the effect of the interface strength for multiple fibers. The algorithm combines a variant of the FETI method with projectors to the natural coarse grid and new algorithms for the solution of special quadratic programming problems. A new feature of these algorithms is the adaptive control of precision of the solution of auxiliary problems with effective usage of the projections to the natural coarse grid. The algorithm may be
effectively implemented on parallel computers. It is supported by the theory which grants that the solution is always found. Numerical examples presented indicate that the algorithm is effective.

References