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MATERIAL INTERFACE PROBLEMS SOLVED BY DOMAIN DECOMPOSITION METHODS

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Summary: *This contribution deals with description of various effects on material interface based on domain decomposition method. Especially perfect and imperfect interaction of fibre with composite matrix and discontinuous behaviour of some parameters in heat and mass transfer are studied. The domain solved is split into subdomains which are identical with material regions and the subdomain interfaces are identical with material interfaces. Conditions on material interfaces are simply implemented to numerical analysis as conditions on the subdomain interfaces.*

1. Introduction

Description of various effects on material interfaces based on the finite element method usually leads to difficulties. There are some variables which are discontinuous across the material interface. As an example can serve moisture content in the moisture transfer or displacement field of fibre and composite matrix in the case of imperfect bond Kruis and Bittnar (2007). The classical finite element method is derived for continuous problems and there are not enough nodal degrees of freedom at nodes for description of the discontinuity.

There are several strategies how to avoid the mentioned difficulties. In the case of moisture transfer, the discontinuous moisture content is replaced by the relative humidity which is continuous. Unfortunately, there are tasks where the moisture content is required and the previous trick cannot be used. In the case of fibre-matrix interaction, contact elements are used but suitable stiffness of such elements has to be defined. The main problems occur if the perfect bond has to be modelled during some part of analysis. Very large stiffness is needed and it deteriorates the properties of the system of algebraic equations. The condition number of such matrix is very large and therefore iterative methods require very large number of iterations. Even the direct methods suffer from cancellation errors in this case.

On the other hand, domain decomposition methods are very suitable for such problems. The main advantage is that the methods prescribe some interface conditions between subdomains which can be used for description of various effects on the material interface. Therefore, the decomposition of the original domain has to take into account the material regions (domains or parts of structure with the same material). It means that each material region is covered by one subdomain. In such case, the material interface coincides with the subdomain interface. The main advantage from the implementation point of view is that the nodes on the interface

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are doubled in the domain decomposition methods and therefore two different values from both sides of the interface can be simply stored.

It should be noted that the position of the material interface is assumed fixed and known in advance. If this assumption is not satisfied, methods like X-FEM have to be used. As was mentioned before, there is a class of problems where the material interface is fixed and the proposed strategy can be used. The description of effects on the material interface based on domain decomposition methods can work on a single processor computer as well as on a parallel computer. In the case of parallel computing, each material region can be further decomposed into smaller subdomains and the classical domain decomposition method can be used Kruis (2006).

The paper is organized as follows. Section 2 briefly summarizes the FETI method because many ideas of this method are used in this paper. Section 3 describes the heat and mass transfer. Section 4 deals with the interaction between fibre and composite matrix.

2. Brief overview of the FETI Method

The FETI is an abbreviation of Finite Element Tearing and Interconnecting method which was introduced by Farhat and Roux in 1991 in reference Farhat and Roux (1991). It is a non-overlapping domain decomposition method which enforces the continuity among subdomains by Lagrange multipliers. The FETI method or its variants have been applied to broad class of two and three dimensional problems of second and fourth order. More details can be found e.g. in Toselli and Widlund (2005), Farhat and Roux (1994) and Kruis (2006).

Let the original domain be decomposed to m subdomains. Unknown displacements defined on the j-th subdomain are located in the vector $\boldsymbol{u}^j$. All unknown displacements are located in the vector

$$\boldsymbol{u}^T = \left((\boldsymbol{u}^1)^T, (\boldsymbol{u}^2)^T, \ldots, (\boldsymbol{u}^m)^T\right) \tag{1}$$

The stiffness matrix of the j-th subdomain is denoted $\boldsymbol{K}^j$ and the stiffness matrix of the whole problem has the form

$$\boldsymbol{K} = \begin{pmatrix} \boldsymbol{K}^1 & & & \\ & \boldsymbol{K}^2 & & \\ & & \ddots & \\ & & & \boldsymbol{K}^m \end{pmatrix} \tag{2}$$

The nodal loads of the j-th subdomain are located in the vector $\boldsymbol{f}^j$ and the load vector of the problem has the form

$$\boldsymbol{f}^T = \left((\boldsymbol{f}^1)^T, (\boldsymbol{f}^2)^T, \ldots, (\boldsymbol{f}^m)^T\right) \tag{3}$$

Continuity among subdomains has the form

$$\boldsymbol{B}\boldsymbol{u} = \boldsymbol{0} \tag{4}$$

where the Boolean matrix $\boldsymbol{B}$ has the form

$$\boldsymbol{B} = \left(\boldsymbol{B}^1, \boldsymbol{B}^2, \ldots, \boldsymbol{B}^m\right) \tag{5}$$

The matrices $\boldsymbol{B}^j$ contain only entries equal to $1, -1, 0$. With the previously defined notation, the energy functional has the form

$$\Pi(\boldsymbol{u}, \boldsymbol{\lambda}) = \frac{1}{2}\boldsymbol{u}^T\boldsymbol{K}\boldsymbol{u} - \boldsymbol{u}^T\boldsymbol{f} + \boldsymbol{\lambda}^T\boldsymbol{B}\boldsymbol{u} \tag{6}$$

where the vector $\boldsymbol{\lambda}$ contains Lagrange multipliers. Stationary conditions of the energy functional have the form

$$\frac{\partial \Pi}{\partial \boldsymbol{u}} = \boldsymbol{K}\boldsymbol{u} - \boldsymbol{f} + \boldsymbol{B}^T\boldsymbol{\lambda} = \boldsymbol{0} \tag{7}$$

$$\frac{\partial \Pi}{\partial \boldsymbol{\lambda}} = \boldsymbol{B}\boldsymbol{u} = \boldsymbol{0} \tag{8}$$

The known feature of the FETI method is application of a pseudoinverse matrix in relationship for unknown displacements

$$\boldsymbol{u} = \boldsymbol{K}^+\left(\boldsymbol{f} - \boldsymbol{B}^T\boldsymbol{\lambda}\right) + \boldsymbol{R}\boldsymbol{\alpha} \tag{9}$$

which stems from floating subdomains. The stiffness matrix of a floating subdomain is singular. The matrix $\boldsymbol{R}$ contains the rigid body modes of particular subdomains and the vector $\boldsymbol{\alpha}$ contains amplitudes that specifies the contribution of the rigid body motions to the displacements. Except of utilization of the pseudoinverse matrix, a solvability condition in the form

$$\boldsymbol{R}^T\left(\boldsymbol{f} - \boldsymbol{B}^T\boldsymbol{\lambda}\right) = \boldsymbol{0} \tag{10}$$

has to be taken into account. Substitution of the unknown displacements to the continuity condition (4) leads to the form

$$\boldsymbol{B}\boldsymbol{K}^+\boldsymbol{B}^T\boldsymbol{\lambda} = \boldsymbol{B}\boldsymbol{K}^+\boldsymbol{f} + \boldsymbol{B}\boldsymbol{R}\boldsymbol{\alpha} \tag{11}$$

Usual notation in the FETI method is the following

$$\boldsymbol{F} = \boldsymbol{B}\boldsymbol{K}^+\boldsymbol{B}^T \tag{12}$$

$$\boldsymbol{G} = -\boldsymbol{B}\boldsymbol{R} \tag{13}$$

$$\boldsymbol{d} = \boldsymbol{B}\boldsymbol{K}^+\boldsymbol{f} \tag{14}$$

$$\boldsymbol{e} = -\boldsymbol{R}^T\boldsymbol{f} \tag{15}$$

The continuity and solvability conditions can be rewritten with the defined notation in the form

$$\begin{pmatrix} \boldsymbol{F} & \boldsymbol{G} \\ \boldsymbol{G}^T & \boldsymbol{0} \end{pmatrix}\begin{pmatrix} \boldsymbol{\lambda} \\ \boldsymbol{\alpha} \end{pmatrix} = \begin{pmatrix} \boldsymbol{d} \\ \boldsymbol{e} \end{pmatrix} \tag{16}$$

The system of equations (16) is called the coarse or interface problem. It is solved by the modified conjugate gradient method because the matrix $\boldsymbol{F}$ is not assembled. More details about the modified conjugate gradient method and its preconditioning can be found in references Kruis (2006), Farhat and Roux (1994), Rixen and Farhat (1999) and Rixen (2002).

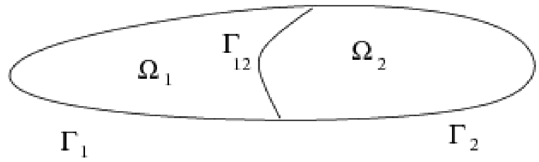

Figure 1: Domain containing two materials

3. Transport processes

For simplicity, let domain containing only two different materials be assumed and let the materials be separated by one material interface. The heat and mass transfer is assumed. The temperature is continuous while the volumetric moisture is discontinuous across the interface. The domain Ω is decomposed into two subdomains Ω_1 and Ω_2 with common edge Γ_{12}. The subdomains Ω_1 and Ω_2 correspond with material regions. The original boundary is split into parts Γ_1 and Γ_2. The situation is depicted in Figure 1. The finite element method is used for solution. The domains Ω_1 and Ω_2 are covered by two meshes which are conforming. The conformity is assumed also on the interface Γ_{12}. The system of ordinary differential equations after space discretization by the FEM has the form

$$\boldsymbol{C}\dot{\boldsymbol{r}} + \boldsymbol{K}\boldsymbol{r} + \boldsymbol{G}\boldsymbol{\lambda} = \boldsymbol{f} \tag{17}$$

$$\boldsymbol{G}^T\boldsymbol{r} = \boldsymbol{d} \tag{18}$$

where $\boldsymbol{C}$ denotes the capacity matrix, $\boldsymbol{K}$ denotes the conductivity matrix, $\boldsymbol{f}$ denotes the vector of prescribed nodal fluxes, $\boldsymbol{r}$ denotes the vector of nodal unknowns (temperature and volumetric moisture), $\dot{\boldsymbol{r}}$ denotes the time derivative of the nodal unknowns, $\boldsymbol{\lambda}$ denotes the vector of Lagrange multipliers, $\boldsymbol{G}$ denotes the Boolean matrix (similar to the matrices used in the FETI method Kruis (2006)) and $\boldsymbol{d}$ denotes the vector of jumps. Equation (17) is the balance equations while (18) describes the discontinuity across the material interface. The magnitude of discontinuity can be evaluated as follows

$$d = w_2 - f_2(g_1(w_1)) = f_1(g_2(w_2)) - w_1 \tag{19}$$

where w_1 and w_2 are moisture contents on subdomains Ω_1 and Ω_2, g and f denote the sorption isotherms. The magnitudes d are located in the vector $\boldsymbol{d}$.

Time discretization of the system (17) is done by the generalized trapezoidal method which can be found e.g. in reference Hughes (1987) and has the form

$$\tilde{\boldsymbol{r}}_{n+1} = \boldsymbol{r}_n + \Delta t(1-\alpha)\dot{\boldsymbol{r}}_n \tag{20}$$

$$\boldsymbol{r}_{n+1} = \tilde{\boldsymbol{r}}_{n+1} + \alpha\Delta t\dot{\boldsymbol{r}}_{n+1} \tag{21}$$

where $\tilde{\boldsymbol{r}}_{n+1}$ denotes the predictor, $\dot{\boldsymbol{r}}_n$ denotes the vector of time derivatives of the nodal values, α denotes a control parameter which defines whether the method is explicit or implicit and Δt denotes the time step. The system of algebraic equations has the form

$$\begin{pmatrix} \boldsymbol{C} + \alpha\Delta t\boldsymbol{K} & \alpha\Delta t\boldsymbol{G} \\ \alpha\Delta t\boldsymbol{G}^T & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{r}_{n+1} \\ \boldsymbol{\lambda}_{n+1} \end{pmatrix} = \begin{pmatrix} \alpha\Delta t\boldsymbol{f}_{n+1} + \boldsymbol{C}\tilde{\boldsymbol{r}}_{n+1} \\ \alpha\Delta t\boldsymbol{d} \end{pmatrix} \tag{22}$$

where the subscripts denote the iteration number.

First vector equation in the system (22) has the form

$$(\boldsymbol{C} + \alpha\Delta t\boldsymbol{K})\,\boldsymbol{r}_{n+1} + \alpha\Delta t\boldsymbol{G}\boldsymbol{\lambda}_{n+1} = \alpha\Delta t\boldsymbol{f}_{n+1} + \boldsymbol{C}\tilde{\boldsymbol{r}}_{n+1} \tag{23}$$

which resembles the vector equation (7) of the FETI method. But there is significant difference connected with the matrix $\boldsymbol{C}+\alpha\Delta t\boldsymbol{K}$ which corresponds to the matrix $\boldsymbol{K}$ in the FETI method. While the matrix $\boldsymbol{K}$ in the FETI method can be singular for subdomains without Dirichlet boundary conditions, the matrix $\boldsymbol{C}+\alpha\Delta t\boldsymbol{K}$ is always nonsingular because the capacity matrix $\boldsymbol{C}$ is always nonsingular (even for subdomains without Dirichlet boundary conditions). If all subdomain matrices are nonsingular, no rigid body modes can be computed and the coarse problem in the FETI method cannot be assembled. Similar problem was studied in connection with dynamic problems in the reference Farhat et al. (1995).

Because the matrix $\boldsymbol{C} + \alpha\Delta t\boldsymbol{K}$ is nonsingular, the unknown vector $\boldsymbol{r}_{n+1}$ can be expressed as

$$\boldsymbol{r}_{n+1} = (\boldsymbol{C} + \alpha\Delta t\boldsymbol{K})^{-1}\left(\alpha\Delta t\boldsymbol{f}_{n+1} + \boldsymbol{C}\tilde{\boldsymbol{r}}_{n+1} - \alpha\Delta t\boldsymbol{G}\boldsymbol{\lambda}_{n+1}\right) \tag{24}$$

Substitution of (24) to the second equation of (22) leads to the form

$$\alpha\Delta t\boldsymbol{G}^T(\boldsymbol{C} + \alpha\Delta t\boldsymbol{K})^{-1}\boldsymbol{G}\boldsymbol{\lambda}_{n+1} = \boldsymbol{G}^T(\boldsymbol{C} + \alpha\Delta t\boldsymbol{K})^{-1}\left(\alpha\Delta t\boldsymbol{f}_{n+1} + \boldsymbol{C}\tilde{\boldsymbol{r}}_{n+1}\right) - \boldsymbol{d} \tag{25}$$

Algebraic Babuška-Brezzi conditions Hughes (1987) for this problem have the form

- for all vectors $\boldsymbol{v}$ which satisfy the equation $\boldsymbol{G}^T\boldsymbol{v} = \boldsymbol{0}$ must hold $\boldsymbol{v}^T(\boldsymbol{C} + \alpha\Delta t\boldsymbol{K})\,\boldsymbol{v} > 0$,
- matrix $\boldsymbol{G}^T$ has linearly independent rows.

Both conditions are satisfied because the matrix $\boldsymbol{C}$ is positive definite and the matrix $\boldsymbol{K}$ is positive semidefinite. Therefore the matrix $\boldsymbol{C} + \alpha\Delta t\boldsymbol{K}$ is positive definite. The matrix $\boldsymbol{G}^T$ has linearly independent rows because it contains zero matrix entries everywhere except of two nonzero entries connected with two adjacent degrees of freedom across the interface in each row.

4. Fibre-matrix interaction

The classical FETI method uses the continuity condition (4) which enforces the same displacements at the boundary nodes. If there is a reason for different displacements between two neighbour subdomains, the continuity condition transforms itself to a slip condition. The slip condition can be written in the form

$$\boldsymbol{B}\boldsymbol{u} = \boldsymbol{s} \tag{26}$$

The vector $\boldsymbol{s}$ stores slips between boundary nodes. For this moment, the slip is assumed to be prescribed and constant.

Let the boundary unknowns be split to two disjunct parts. The boundary unknowns which satisfy the continuity condition are located in the vector $\boldsymbol{u}_c$, while the boundary unknowns which satisfy the slip condition are located in the vector $\boldsymbol{u}_s$. Similarly to the continuity condition in the FETI method, the vectors $\boldsymbol{u}_c$ and $\boldsymbol{u}_s$ can be written in the form

$$\boldsymbol{u}_c = \boldsymbol{B}_c\boldsymbol{u} \tag{27}$$

$$\boldsymbol{u}_s = \boldsymbol{B}_s\boldsymbol{u} \tag{28}$$

where $\boldsymbol{B}_c$ and $\boldsymbol{B}_s$ are the Boolean matrices. Now, the continuity condition has the form

$$\boldsymbol{B}_c\boldsymbol{u} = \boldsymbol{0} \tag{29}$$

and the slip condition has the form

$$\boldsymbol{B}_s\boldsymbol{u} = \boldsymbol{s} \tag{30}$$

The conditions (29) and (30) can be amalgamated to a new interface condition

$$\boldsymbol{B}\boldsymbol{u} = \begin{pmatrix} \boldsymbol{B}_c \\ \boldsymbol{B}_s \end{pmatrix} \boldsymbol{u} = \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{s} \end{pmatrix} = \boldsymbol{c} \tag{31}$$

The energy functional can be rewritten to the form

$$\Pi = \frac{1}{2}\boldsymbol{u}^T\boldsymbol{K}\boldsymbol{u} - \boldsymbol{u}^T\boldsymbol{f} + \boldsymbol{\lambda}^T(\boldsymbol{B}\boldsymbol{u} - \boldsymbol{c}) \tag{32}$$

The stationary conditions have the form

$$\boldsymbol{K}\boldsymbol{u} - \boldsymbol{f} + \boldsymbol{B}^T\boldsymbol{\lambda} = \boldsymbol{0} \tag{33}$$

$$\boldsymbol{B}\boldsymbol{u} = \boldsymbol{c} \tag{34}$$

As was mentioned before, the system of two stationary conditions is accompanied by the solvability condition (10). The expression of the vector $\boldsymbol{u}$ given in (9) remains the same and the interface conditions has the form

$$\boldsymbol{B}\boldsymbol{K}^+\boldsymbol{B}^T\boldsymbol{\lambda} = \boldsymbol{B}\boldsymbol{K}^+\boldsymbol{f} + \boldsymbol{B}\boldsymbol{R}\boldsymbol{\alpha} - \boldsymbol{c} \tag{35}$$

and the solvability condition has the form

$$\boldsymbol{R}^T\left(\boldsymbol{f} - \boldsymbol{B}^T\boldsymbol{\lambda}\right) = \boldsymbol{0} \tag{36}$$

The coarse problem can be written with the help of notation (12) - (15) in the form

$$\begin{pmatrix} \boldsymbol{F} & \boldsymbol{G} \\ \boldsymbol{G}^T & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda} \\ \boldsymbol{\alpha} \end{pmatrix} = \begin{pmatrix} \boldsymbol{d} - \boldsymbol{c} \\ \boldsymbol{e} \end{pmatrix} \tag{37}$$

The modified coarse problem (37) differs from the original coarse problem (16) by the vector of prescribed slips $\boldsymbol{c}$ on the right hand side.

The prescribed slip between two subdomains is not a common case. On the other hand, the slip often depends on shear stress. Discretized form of equations used in the coarse problem requires a discretized law between slip as a difference of two neighbour displacements and nodal forces as integrals of stresses along element edges. One of the simplest law is the linear relationship

$$\boldsymbol{c} = \boldsymbol{H}\boldsymbol{\lambda} \tag{38}$$

where $\boldsymbol{H}$ denotes the compliance matrix. Substitution of (38) to the coarse problem (37) leads to the form

$$\begin{pmatrix} \boldsymbol{F} + \boldsymbol{H} & \boldsymbol{G} \\ \boldsymbol{G}^T & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda} \\ \boldsymbol{\alpha} \end{pmatrix} = \begin{pmatrix} \boldsymbol{d} \\ \boldsymbol{e} \end{pmatrix} \tag{39}$$

It should be noted that the coarse system of equations (39) is usually solved by the modified conjugate gradient method. Details can be found in Farhat and Roux (1994) and Kruis (2006). The only difference with respect to the system (16) is the compliance matrix $\boldsymbol{H}$. Only one step, the matrix-vector multiplication, of the modified conjugate gradient method should be changed. The compliance matrix may be a diagonal or nearly diagonal matrix. More details about this modification can be found in reference Kruis and Bittnar (2007).

5. Conclusions

Two different problems connected with the material interface were studied. The transport processes lead sometimes to discontinuous response which means that some variables are not continuous. The second problem was connected with analysis of composite materials where perfect of imperfect bond between fibre and composite matrix has to be taken into account. The classical approach based on contact elements with some artificial stiffness works only for very simple examples. Both problems were formulated in the terms of domain decomposition methods, especially of the FETI method. Special conditions on the material interfaces are formulated as the interface conditions used in the domain decomposition methods. It is useful also from the implementation point of view. The nodes on subdomain interfaces are doubled and there are two times more components in arrays for storage of all necessary data which is not the case of the classical finite element method. It is known that the domain decomposition methods can be easily parallelized.

6. Acknowledgment

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