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Element-Independent Implementation for Method of Lagrange Multipliers

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***Abstract*—**Treatment for the non-matching interface is an important computational issue. To handle this problem, the method of Lagrange multipliers including classical and localized versions are the most popular technique. It essentially imposes the interface compatibility conditions by introducing Lagrange multipliers. However, the numerical system becomes unstable and inefficient due to the Lagrange multipliers. The interface element-independent formulation that does not include the Lagrange multipliers can be obtained by modifying the independent variables mathematically. Through this modification, more efficient and stable system can be achieved while involving equivalent accuracy comparing with the conventional method. A numerical example is conducted to verify the validity of the presented method.

***Keywords*—**Element-independent formulation, non-matching interface, interface coupling, methods of Lagrange multipliers.

I. Introduction

IN various engineering fields, the problems are becoming complex and enormous. To solve these problems efficiently, a total system should be divided into several subsystems to describe each other independently. In this case, the interface boundaries are naturally created between the subsystems and non-matching meshes are occurred on them. Also, when the multi-material and multi-physics, as well as contact problems, are considered, the non-matching meshes arise naturally on the interface boundaries due to the different behaviors of each system. Therefore, demand for developing approaches to connect non-matching meshes is gradually increased.

The method of Lagrange multipliers is the most popular way to satisfy the interface compatibility conditions on the non-matching meshes. This method imposes interface compatibility conditions by introducing Lagrange multipliers acting as contact forces in a variational sense. Depending on how to define interface conditions, it is divided into two methods [1]–[6]. One is the method of Classical Lagrange multipliers (CLM, widely named mortar method) [1]–[3], the other is the method of Localized Lagrange Multipliers (LLM) [5]–[7]. A distinctive feature compared with the method of CLM is a creation of independent frame domain between the interface boundaries to impose a unique set of constraint conditions [7].

From the computational point of view, the method of Lagrange multipliers is composed of two kinds of linear system. One is a system with Lagrange multipliers; the other is a system without Lagrange multipliers [8]-[10]. Due to the characteristics of a total system equation, the latter is preferred to improve numerical efficiency and stability. However, these are complicated to understand and implement easily to the practical engineering problems. Moreover, the studies have not been extended to the method of LLM. To overcome these drawbacks, straightforward and efficient method is proposed by modifying the method of Lagrange multipliers. The key idea of this study is the elimination of unnecessary variables that cause numerical instability. This means to construct a compact type of system mathematically by removing variables that do not cause problems even if they are removed from the analysis. Through this modification, we intend to derive a more efficient and stable system with the same accuracy compared with the conventional method.

The remainder of this paper is organized as follows. Section II introduces the conventional method of Lagrange multipliers including classical and localized versions with schematic and mathematical descriptions. Based on the formulations from Section II, the Modified Method of Lagrange Multipliers (MMLM) is proposed mathematically in Section III. To verify the effectiveness and exactness of the proposed method, a simple contact patch test is performed in Section IV. The characteristics of presented method are investigated compared with conventional method. Finally, purposes and comments are summarized in Section V.

II. Conventional Method of Lagrange Multipliers

This section introduces a basic concept for the conventional method of CLM and LLM to connect the non-matching meshes. A simple interface patch test problem consisting of two elastic bodies is used to demonstrate the features of each method as depicted in Fig. 1.

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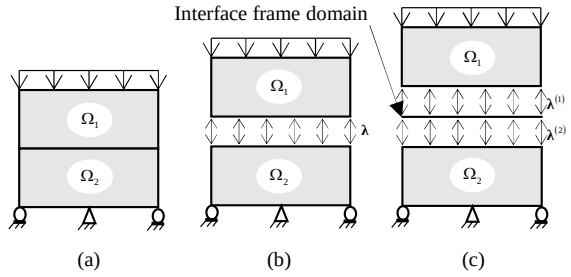

Fig. 1 Simple interface example; (a) a structure decomposed of two parts. Each part is connected by the method of (b) CLM, (c) LLM

To obtain finite element formulation for imposing interface compatibility conditions, the hybrid form of total energy functional has to be defined as

$$\Pi_{\text{TPE}} = \sum_{\Omega=1}^{N} \Pi_{\text{PE}}^{\Omega} - \Pi_c \tag{1}$$

where Π_{TPE} is the total energy functional, Π_c is the interface potential energy, N is a number of subdomains (In Fig. 1, N=2), and Π_{PE} is the potential energy for each subdomain in which it is given as

$$\begin{aligned} \Pi_{\text{PE}}^{\Omega} &= \int_{\Omega} \left[{}^{3}(u) - u_i f_i \right] d\Omega - \int_{\partial\Omega} u_i t_i d\Gamma \\ {}^{3}(\mathbf{u}) &= \frac{1}{2} D_{ijkl} \pounds_{ij} \pounds_{kl}, \quad \pounds_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) \end{aligned} \tag{2}$$

In (2), the potential energy is composed of the internal energy expressed in strain energy and the external energy induced from the body force f and surface traction t, where $\mathbf{u}$ is a displacement field at a subdomain Ω, D_{ijkl} is the 4th order elastic Young's modulus, conventional summation rule is in effect, and comma represents partial derivatives.

A. Method of Classical Lagrange Multipliers (CLM)

To obtain interface potential energy Π_c for the method of CLM, the Lagrange multipliers between subdomains have to be defined as shown in Fig. 1 (b). Then, interface potential energy is defined as

$$\Pi_c = \int_{\Gamma_I} \boldsymbol{\lambda}^T \left(\mathbf{u}^{(1)} - \mathbf{u}^{(2)} \right) d\Gamma \tag{3}$$

where Γ_I represents interface boundary, $\boldsymbol{\lambda}$ is the Lagrange multipliers, $\mathbf{u}^{(1)}$ and $\mathbf{u}^{(2)}$ are the displacement fields for each subdomain.

Substituting (3) into the total energy functional and taking the first variation to minimize the energy functional, a matrix form of total system equation can be obtained as

$$\begin{bmatrix} \mathbf{K}^{(1)} & 0 & \mathbf{B}_1\mathbf{Q}_1 \\ 0 & \mathbf{K}^{(2)} & -\mathbf{B}_2\mathbf{Q}_2 \\ \mathbf{Q}_1^T\mathbf{B}_1^T & -\mathbf{Q}_2^T\mathbf{B}_2^T & 0 \end{bmatrix} \begin{Bmatrix} \mathbf{u}^{(1)} \\ \mathbf{u}^{(2)} \\ \boldsymbol{\lambda} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}^{(1)} \\ \mathbf{f}^{(2)} \\ 0 \end{Bmatrix} \tag{4}$$
$$\mathbf{Q}_1 = \int_{\Gamma_I} \mathbf{N}_{u_{\Gamma 1}}^T \mathbf{N}_{\text{a}} d\Gamma, \quad \mathbf{Q}_2 = \int_{\Gamma_I} \mathbf{N}_{u_{\Gamma 2}}^T \mathbf{N}_{\text{a}} d\Gamma$$

where $\mathbf{B}_1$ and $\mathbf{B}_2$ are the Boolean matrices for filtering interface boundary components, $\mathbf{Q}_1$ and $\mathbf{Q}_2$ are the projection matrices to impose interface compatibility conditions, $\mathbf{N}$ is the shape function.

B. Method of LLM

The basic concept for the method of LLM is similar to the CLM. However, the fictitious frame domain is introduced to connect each subdomain as depicted in Fig. 1 (c). Therefore, the interface potential energy is scaled by the corresponding Lagrange multipliers with the interface constraints between each substructure and the frame.

$$\Pi_c = \int_{\Gamma_I} \left\{ \boldsymbol{\lambda}_1^T \left(\mathbf{u}^{(1)} - \mathbf{u}^{(f)} \right) + \boldsymbol{\lambda}_2^T \left(\mathbf{u}^{(2)} - \mathbf{u}^{(f)} \right) \right\} d\Gamma \tag{5}$$

where the Lagrange multipliers are depicted in Fig. 1 (c).

Comparing to the CLM, the number of independent variables is much larger, but the interface conditions can be defined uniquely and efficiently with no redundancy in the constraint equations [7].

To formulate the total potential energy, (5) has to be substituted in (1). Then, taking the first variation of the energy functional and setting it to zero, the matrix form of a total system equation is derived as

$$\begin{bmatrix} \mathbf{K}^{(1)} & 0 & \mathbf{B}_1\mathbf{Q}_1 & 0 & 0 \\ 0 & \mathbf{K}^{(2)} & 0 & \mathbf{B}_2\mathbf{Q}_2 & 0 \\ \mathbf{Q}_1^T\mathbf{B}_1^T & 0 & 0 & 0 & -\mathbf{W}_1 \\ 0 & \mathbf{Q}_2^T\mathbf{B}_2^T & 0 & 0 & -\mathbf{W}_2 \\ 0 & 0 & -\mathbf{W}_1^T & -\mathbf{W}_2^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}^{(1)} \\ \mathbf{u}^{(2)} \\ \boldsymbol{\lambda}^{(1)} \\ \boldsymbol{\lambda}^{(2)} \\ \mathbf{u}^{(f)} \end{bmatrix} = \begin{bmatrix} \mathbf{f}^{(1)} \\ \mathbf{f}^{(2)} \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
$$\mathbf{Q}_1 = \int_{\Gamma_I} \mathbf{N}_{u_{\Gamma 1}}^T \mathbf{N}_{\text{a}1} d\Gamma, \quad \mathbf{Q}_2 = \int_{\Gamma_I} \mathbf{N}_{u_{\Gamma 2}}^T \mathbf{N}_{\text{a}2} d\Gamma, \tag{6}$$
$$\mathbf{W}_1 = \int_{\Gamma_I} \mathbf{N}_{\text{a}1}^T \mathbf{N}_{uf} d\Gamma, \quad \mathbf{W}_2 = \int_{\Gamma_I} \mathbf{N}_{\text{a}2}^T \mathbf{N}_{uf} d\Gamma$$

where $\mathbf{Q}_1$, $\mathbf{Q}_2$, $\mathbf{W}_1$, and $\mathbf{W}_2$ are the projection matrices that represent the interface condition between interface boundary and the fictitious frame displacements.

III. Modified Method of Lagrange Multipliers

In this section, the proposed method is illustrated based on the conventional method discussed in section II. When the conventional method is solved numerically, a total system equation is ill-conditioned due to the Lagrange multipliers. To improve the numerical properties, many types of research are suggested to eliminate the Lagrange multipliers [8], [9]. In a

similar approach, the proposed method derives an efficient system by replacing unnecessary variables into essential parts mathematically on the variational form. In this method, the unnecessary variables indicate the Lagrange multipliers and interface boundary displacements that are overlapped. Therefore, a total system of the proposed method only contains the essential variables. Through the modification, more straightforward and efficient method while involving comparable accuracy should be obtained. Because the modification of the independent variables is the key idea of the proposed method, we have named MMLM.

A. Modification of the Method of CLM

In this section, the procedures for the CLM are presented. To eliminate unnecessary variables, a total displacement $\mathbf{u}$ has to be divided into internal $\mathbf{u}_i$ and interface boundary $\mathbf{u}_b$ for each subdomain as shown in Fig. 2. Then, the equilibrium equations can be expanded as:

$$\begin{aligned}
&\mathbf{K}_{ii}^{(1)}\mathbf{u}_i^{(1)}+\mathbf{K}_{ib}^{(1)}\mathbf{u}_b^{(1)}=\mathbf{f}_i^{(1)}\\
&\mathbf{K}_{bi}^{(1)}\mathbf{u}_i^{(1)}+\mathbf{K}_{bb}^{(1)}\mathbf{u}_b^{(1)}+\mathbf{Q}_1\boldsymbol{\lambda}=\mathbf{f}_b^{(1)}\\
&\mathbf{K}_{ii}^{(2)}\mathbf{u}_i^{(2)}+\mathbf{K}_{ib}^{(2)}\mathbf{u}_b^{(2)}=\mathbf{f}_i^{(2)}\\
&\mathbf{K}_{bi}^{(2)}\mathbf{u}_i^{(2)}+\mathbf{K}_{bb}^{(2)}\mathbf{u}_b^{(2)}-\mathbf{Q}_2\boldsymbol{\lambda}=\mathbf{f}_b^{(2)}\\
&\mathbf{Q}_1^T\mathbf{u}_b^{(1)}-\mathbf{Q}_2^T\mathbf{u}_b^{(2)}=0
\end{aligned} \tag{7}$$

To derive a modified total system equation, two steps should be performed by using (7). First, the relation between interface boundary displacements should be defined as

$$\begin{aligned}
&\mathbf{Q}_1^T\mathbf{u}_b^{(1)}-\mathbf{Q}_2^T\mathbf{u}_b^{(2)}=0\rightarrow\mathbf{u}_b^{(2)}=\mathbf{Q}_2^{-1}\mathbf{Q}_1^T\mathbf{u}_b^{(1)}\\
&\therefore\mathbf{u}_b^{(2)}=\mathbf{C}_{21}\mathbf{u}_b^{(1)}
\end{aligned} \tag{8}$$

Second, the Lagrange multipliers should be converted to the essential variables as

$$\begin{aligned}
&\mathbf{K}_{bi}^{(2)}\mathbf{u}_i^{(2)}+\mathbf{K}_{bb}^{(2)}\mathbf{u}_b^{(2)}-\mathbf{Q}_2\boldsymbol{\lambda}=\mathbf{f}_b^{(2)}\\
&\therefore\boldsymbol{\lambda}=\mathbf{Q}_2^{-1}\left(\mathbf{K}_{bi}^{(2)}\mathbf{u}_i^{(2)}+\mathbf{K}_{bb}^{(2)}\mathbf{C}_{21}\mathbf{u}_b^{(1)}-\mathbf{f}_b^{(2)}\right).
\end{aligned} \tag{9}$$

Therefore, the matrix form of a modified system equation for the method of CLM can be derived as

$$\begin{bmatrix}\mathbf{K}_{ii}^{(1)} & 0 & \mathbf{K}_{ib}^{(1)}\\ 0 & \mathbf{K}_{ii}^{(2)} & \mathbf{K}_{ib}^{(2)}\mathbf{C}_{21}\\ \mathbf{K}_{bi}^{(1)} & \mathbf{C}_{21}^T\mathbf{K}_{bi}^{(2)} & \mathbf{K}_{bb}^{(1)}+\mathbf{C}_{21}^T\mathbf{K}_{bb}^{(2)}\mathbf{C}_{21}\end{bmatrix}\begin{Bmatrix}\mathbf{u}_i^{(1)}\\ \mathbf{u}_i^{(2)}\\ \mathbf{u}_b^{(1)}\end{Bmatrix}=\begin{Bmatrix}\mathbf{f}_i^{(1)}\\ \mathbf{f}_i^{(2)}\\ \mathbf{f}_b^{(1)}+\mathbf{C}_{21}^T\mathbf{f}_b^{(2)}\end{Bmatrix} \tag{10}$$

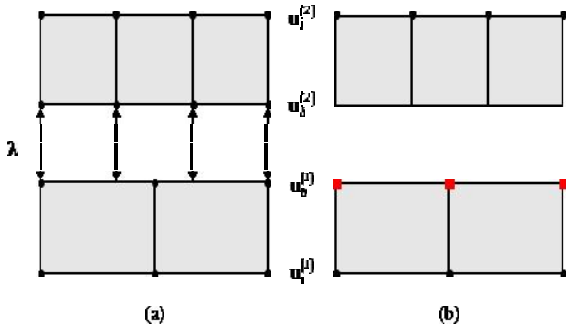

Fig. 2 Schematic descriptions of the MMLM for CLM; (a) conventional method, (b) modified method

B. Modification of the Method of LLM

To obtain a modified system of the LLM, (6) should be expanded by dividing internal and interface boundary displacements as shown in the previous section. Then, the unnecessary variables are converted to the union of essential variables. To eliminate overlapped displacements, the interface boundary displacements should be represented by the frame displacements as:

$$\begin{aligned}
&\mathbf{Q}_1^T\mathbf{u}_b^{(1)}-\mathbf{W}_1\mathbf{u}^{(f)}=0\\
&\therefore\mathbf{u}_b^{(1)}=\mathbf{Q}_1^{-1}\mathbf{W}_1\mathbf{u}^{(f)}=\mathbf{C}_{1f}\mathbf{u}^{(f)}\\
&\mathbf{Q}_2^T\mathbf{u}_b^{(2)}-\mathbf{W}_2\mathbf{u}^{(f)}=0\\
&\therefore\mathbf{u}_b^{(2)}=\mathbf{Q}_2^{-1}\mathbf{W}_2\mathbf{u}^{(f)}=\mathbf{C}_{2f}\mathbf{u}^{(f)}
\end{aligned} \tag{11}$$

Using (11), the Lagrange multipliers are defined as:

$$\begin{aligned}
&\mathbf{K}_{bi}^{(1)}\mathbf{u}_i^{(1)}+\mathbf{K}_{bb}^{(1)}\mathbf{u}_b^{(1)}+\mathbf{Q}_1\boldsymbol{\lambda}^{(1)}=\mathbf{f}_b^{(1)}\\
&\therefore\boldsymbol{\lambda}^{(1)}=\mathbf{Q}_1^{-1}\left(\mathbf{f}_b^{(1)}-\mathbf{K}_{bi}^{(1)}\mathbf{u}_i^{(1)}-\mathbf{K}_{bb}^{(1)}\mathbf{u}_b^{(1)}\right)\\
&\mathbf{K}_{bi}^{(2)}\mathbf{u}_i^{(2)}+\mathbf{K}_{bb}^{(2)}\mathbf{u}_b^{(2)}+\mathbf{Q}_2\boldsymbol{\lambda}^{(2)}=\mathbf{f}_b^{(2)}\\
&\therefore\boldsymbol{\lambda}^{(2)}=\mathbf{Q}_2^{-1}\left(\mathbf{f}_b^{(2)}-\mathbf{K}_{bi}^{(2)}\mathbf{u}_i^{(2)}-\mathbf{K}_{bb}^{(2)}\mathbf{C}_{21}\mathbf{u}_b^{(1)}\right)
\end{aligned} \tag{12}$$

Finally, a modified total system for the method of LLM can be derived as

$$\begin{bmatrix}\mathbf{K}_{ii}^{(1)} & 0 & \mathbf{K}_{ib}^{(1)}\mathbf{C}_{1f}\\ 0 & \mathbf{K}_{ii}^{(2)} & \mathbf{K}_{ib}^{(2)}\mathbf{C}_{2f}\\ \mathbf{C}_{1f}^T\mathbf{K}_{bi}^{(1)} & \mathbf{C}_{2f}^T\mathbf{K}_{bi}^{(2)} & \mathbf{C}_{1f}^T\mathbf{K}_{bb}^{(1)}\mathbf{C}_{1f}+\mathbf{C}_{2f}^T\mathbf{K}_{bb}^{(2)}\mathbf{C}_{2f}\end{bmatrix}\begin{Bmatrix}\mathbf{u}_i^{(1)}\\ \mathbf{u}_i^{(2)}\\ \mathbf{u}^{(f)}\end{Bmatrix}=\begin{Bmatrix}\mathbf{f}_i^{(1)}\\ \mathbf{f}_i^{(2)}\\ \mathbf{C}_{1f}^T\mathbf{f}_b^{(1)}+\mathbf{C}_{2f}^T\mathbf{f}_b^{(2)}\end{Bmatrix} \tag{13}$$

By solving (10) and (13), the essential variables are obtained directly, and others can be calculated using the relations between them.

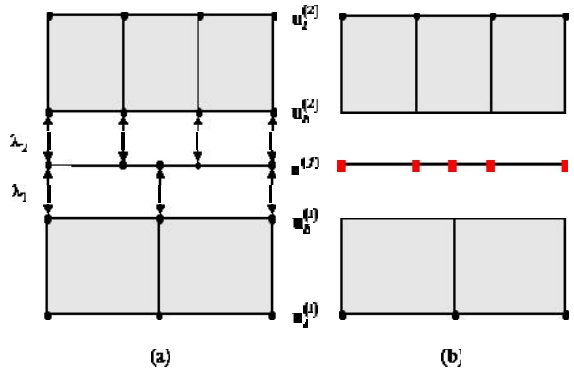

Fig. 3 Schematic descriptions of the MMLM for LLM; (a) conventional method, (b) modified method

IV. Simple Interface Patch Test Problem

A. Problem Definition

To verify effectiveness and exactness of the proposed method, a simple contact patch test containing non-matching meshes is considered [11]. The problem definition and boundary conditions are depicted in Fig. 4 (a). Each domain is discretized independently as shown in Fig. 4 (b). This example is in perfect contact with the interface. The material properties such as Young's modulus and Poisson's ratio are chosen as 20000000 and 0.3, respectively.

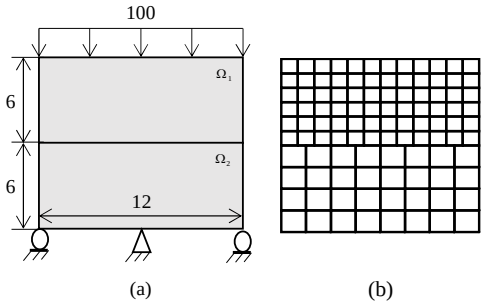

Fig. 4 Simple contact patch test; (a) problem definition, (b) discretization model

B. Result

To ensure efficiency and accuracy comparing with the conventional method, two parameters are checked. One is the condition number of a total system equation to investigate the efficiency and stability. Another is the norm of the stress error to confirm the accuracy.

Through the results of the norm of stress error for each method, the accuracy is confirmed that all methods are passed the contact patch test as shown in Fig. 5 (a). Also, the condition numbers of the proposed method are lower than conventional method about 10^1 as shown in Fig. 5 (a). From the simple contact patch test, the proposed method is proved that it derives more efficient and stable system while containing the accurate solution. Through these results, the validity of the proposed method can be verified by simple contact patch test.

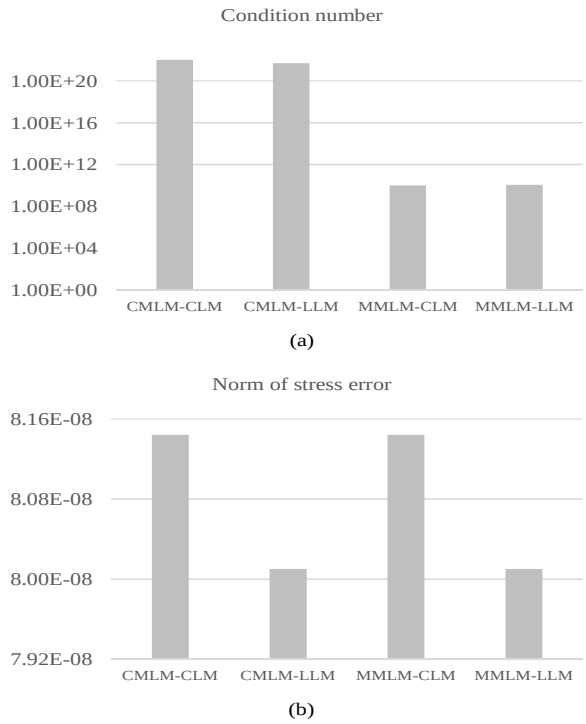

Fig. 5 Results of the simple contact patch test; (a) condition number, (b) norm of stress error

V. Conclusion

In this study, the method of Lagrange multiplier including classical (CLM) and localized (LLM) versions are considered to deal with problems modeled with non-matching meshes. To make more stable and efficient numerical system, the method to eliminate unnecessary variables is proposed. Using the proposed method, the modification of the method of CLM and LLM is conducted mathematically using a few formulas. The numerical characteristics of the proposed method are confirmed by the simple patch test problem.

Using the characteristics of the present method, we will apply the proposed method to the problems that inevitably create the non-matching meshes such as the multi-material and multi-physics as well as contact problems.

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