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PARALLEL MULTI-SCALE FINITE ELEMENT PROCEDURE FOR PIEZOELECTRIC MATERIAL

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ABSTRACT

This paper presents a parallel computing procedure for the multi-scale piezoelectric analysis based on the crystallographic homogenization method. In the finite element (FE) equation for the conventional piezoelectric analysis, coefficient matrix is not positive definite and ill-condition because of the electromechanical coupling problem [1], [2]. A parallel computing technique for piezoelectric FE analysis is newly developed based on the iterative partitioned coupling method with the parallel conjugate gradient (CG) solver.

We assume that the piezoelectric material may have averaged properties in a macro continuum body. The characteristic function vectors $\boldsymbol{\chi}^{mn}$, $\boldsymbol{\varphi}^{mn}$, $\boldsymbol{\Phi}^{p}$ and $\boldsymbol{R}^{p}$ are obtained by solving the microscopic FE equations for a representative volume element (RVE),

$$\begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{u\phi} \\ \mathbf{K}_{\phi u} & -\mathbf{K}_{\phi\phi} \end{bmatrix} \begin{Bmatrix} \boldsymbol{\chi}^{mn} \\ \boldsymbol{\varphi}^{mn} \end{Bmatrix} = \begin{Bmatrix} \mathbf{t}^{mn} \\ \mathbf{q}^{mn} \end{Bmatrix}, \quad \begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{u\phi} \\ \mathbf{K}_{\phi u} & -\mathbf{K}_{\phi\phi} \end{bmatrix} \begin{Bmatrix} \boldsymbol{\Phi}^{p} \\ \boldsymbol{R}^{p} \end{Bmatrix} = \begin{Bmatrix} \mathbf{t}^{p} \\ \mathbf{q}^{p} \end{Bmatrix}, \tag{1}$$

where the characteristic functions have nine components $(m,n)=(1,1), (2,2), (3,3), (2,3), (3,1), (1,2)$, $p=1,2,3$. Since the diagonal terms in sub-matrix $-\mathbf{K}_{\phi\phi}$ are negative, the coefficient matrix of the liner equations (1) are not positive definite. The iterative solver such as the CG method is inapplicable to the equations.

The system equations are rewritten to partition forms as follows:

$$\begin{cases} [\mathbf{K}_{uu}]\{\boldsymbol{\chi}^{mn}\} = \{\mathbf{t}^{mn}\} - [\mathbf{K}_{u\phi}]\{\boldsymbol{\varphi}^{mn}\} \\ [\mathbf{K}_{\phi\phi}]\{\boldsymbol{\varphi}^{mn}\} = -\{\mathbf{q}^{mn}\} + [\mathbf{K}_{u\phi}]^{T}\{\boldsymbol{\chi}^{mn}\} \end{cases}, \quad \begin{cases} [\mathbf{K}_{uu}]\{\boldsymbol{\Phi}^{p}\} = \{\mathbf{t}^{p}\} - [\mathbf{K}_{u\phi}]\{\boldsymbol{R}^{p}\} \\ [\mathbf{K}_{\phi\phi}]\{\boldsymbol{R}^{p}\} = -\{\mathbf{q}^{p}\} + [\mathbf{K}_{u\phi}]^{T}\{\boldsymbol{\Phi}^{p}\} \end{cases}, \tag{2}$$

in order to maintain positive definite of coefficient matrices. The parallel CG solver is applied respectively to partitioned equations until unknown vectors $\boldsymbol{\chi}^{mn}$ and $\boldsymbol{\varphi}^{mn}$ are converged with substituting the coupling terms based on the block Gauss-Seidel method. In the parallel analysis code, two types of parallel methods using PC cluster are implemented and compared on parallel performance. A hierarchical process distribution for parallel computing is introduced to reduce amount of data for communication.

Figure 1 and 2 show convergence history of CG solver for solving $\boldsymbol{\chi}^{11}$ component and

iterative partitioned coupling method for microscopic analysis of a lead titanate $PbTiO_3$, respectively. The result shows safe convergence of both the iterative coupling method and the CG solver without applying preconditioning by using the partitioning procedure into structural and electrical fields. Number of iterations for iterative coupling method depends on problems such as crystal orientation distribution. Figure 3 shows relation between normalized remanent polarization and number of iterations for coupling analysis. The number of iterations is increased by coupling effect which corresponds to the piezoelectric constant d_{33}^H.

Parallel performance is evaluated by using PC cluster (AMD Opteron 244 1.8GHz CPU, 2GB RAM, SuSE Linux OS, Giga-bit Ethernet network) based on estimation of parallel computing time. The estimated parallel computing time agrees very well to real execution time as shown in Fig. 4. The parallel performance of hierarchical parallel method is higher than horizontal one.

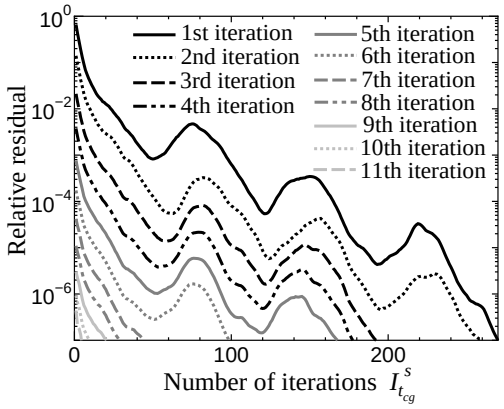

Fig. 1 Convergence history of χ^{11} in CG solver

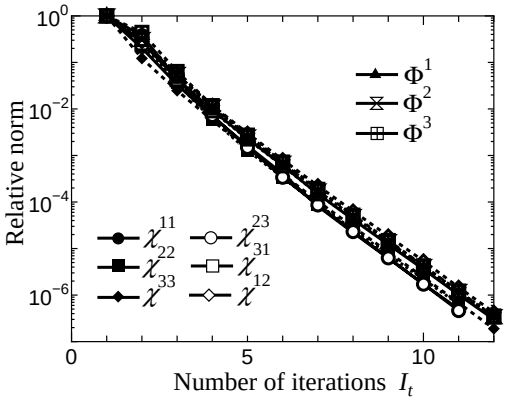

Fig. 2 Convergence history of iterative coupling method

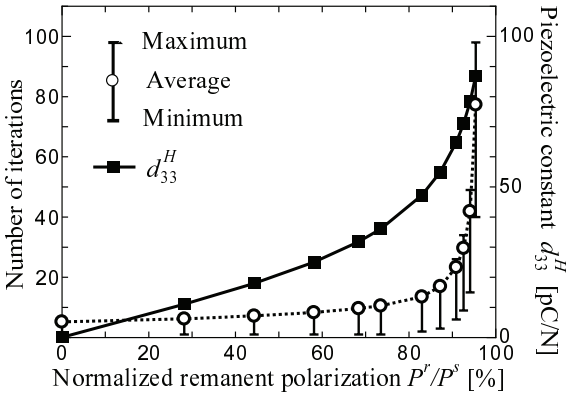

Fig. 3 Relation between number of iterations and normalized remanent polarization

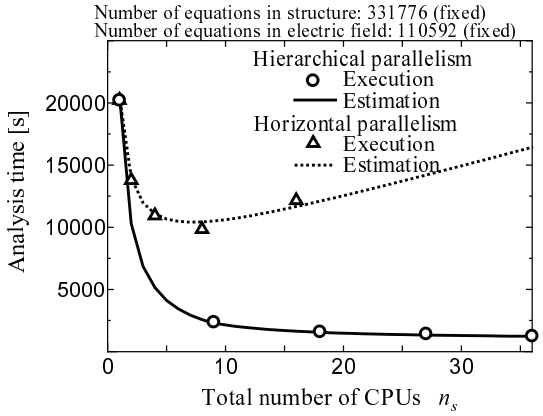

Fig. 4 Relation between parallel analysis time and total number of CPUs

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