CSMA 2026
17ème Colloque National en Calcul des Structures
18-22 Mai 2026, Presqu'île de Giens (Var)

FETI-DP method with interface reduction for numerical simulations of periodic structures under thermal loading

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Abstract — This paper investigates the static analysis of plate-like periodic structures under thermal loading. Notably, this analysis targets the deformation of industrial wafers, where complex periodic patterns are usually involved. To alleviate the computational burden and memory storage issues associated with a direct finite element analysis, the FETI-DP domain decomposition method is considered in this paper. Subsequent speedups can be obtained by reducing the number of Lagrange multipliers at the substructure interfaces. Numerical experiments are carried out on a silicon plate with 400 substructures.
Keywords — FETI-DP method, periodic structures, Lagrange multipliers, model reduction.

1 Introduction

This study focuses on silicon wafers with periodic patterns, which are common devices found in many electronic components. Those wafers represent thin layers of various materials and micro-metric thicknesses piled on a thicker substrate, and are subjected to severe thermal loading and critical strains during the manufacturing process [1, 2].

In this work, an efficient numerical strategy able to compute the mechanical deformation of wafers under thermal loading is proposed. To address the numerical issues involved in finite element (FE) simulations of wafers with many "periodic" substructures, the FETI-DP (FE Tearing and Interconnecting - Dual-Primal) domain decomposition method is used [3]. Indeed, preliminary works conducted on a wafer with 225 substructures have highlighted the relevance of this numerical method in terms of accuracy and computational speedups. Here, a model reduction strategy is proposed to further improve the computational efficiency of the FETI-DP method. This relies on approximating the Lagrange multipliers at the substructure interfaces via interpolation functions and a reduced number of interpolation points, and using parallel computing. This model reduction strategy appears to be suitable for structures built up from many substructures (periodic pattern) like those involved in industrial applications, and for which the computational times involved in standard FETI simulations would become significant (even though this method enables strong decrease of the computational times compared to the direct FE method).

The rest of the paper is organized as follows. In Sec. 2, the principles of the FETI-DP method are recalled together with the related algorithm procedure (preconditioned conjugate gradient method). In Sec. 3, the interface reduction strategy is detailed. In Sec. 4, numerical experiments are conducted on a silicon wafer with a large number of substructures.

2 FETI-DP method

A whole periodic structure, built from identical elastic substructures (see Fig. 1), may be described through the following FE-based static equation:

$$\mathbf{K}\mathbf{u} = \mathbf{f} \tag{1}$$

with $\mathbf{K}$ the stiffness matrix, and $\mathbf{u}$ the displacement vector; also, $\mathbf{f}$ is the force vector that results from thermal loading ΔT and related prescribed strains ε_{th} [6]:

$$\varepsilon_{th} = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{yy} & \varepsilon_{zz} & 2\varepsilon_{yz} & 2\varepsilon_{zx} & 2\varepsilon_{xy} \end{bmatrix}_{th}^{T} = \alpha \Delta T \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \end{bmatrix}^{T} \tag{2}$$

with α a thermal expansion coefficient.

To avoid computing the stiffness matrix $\mathbf{K}$ of the periodic structure, and computing the static equation (1) explicitly, domain decomposition techniques can be used. In this case, a whole periodic structure is partitioned into N_s several substructures with local stiffness matrices $\mathbf{K}^s$, subjected to coupling forces (Lagrange multipliers) $\boldsymbol{\lambda}^s$ as shown in Fig. 2. Notably, the FETI-DP method involves considering several local substructure problems, and determining the Lagrange multipliers $\boldsymbol{\lambda}^s$ at the substructure interface using an iterative solver [3].

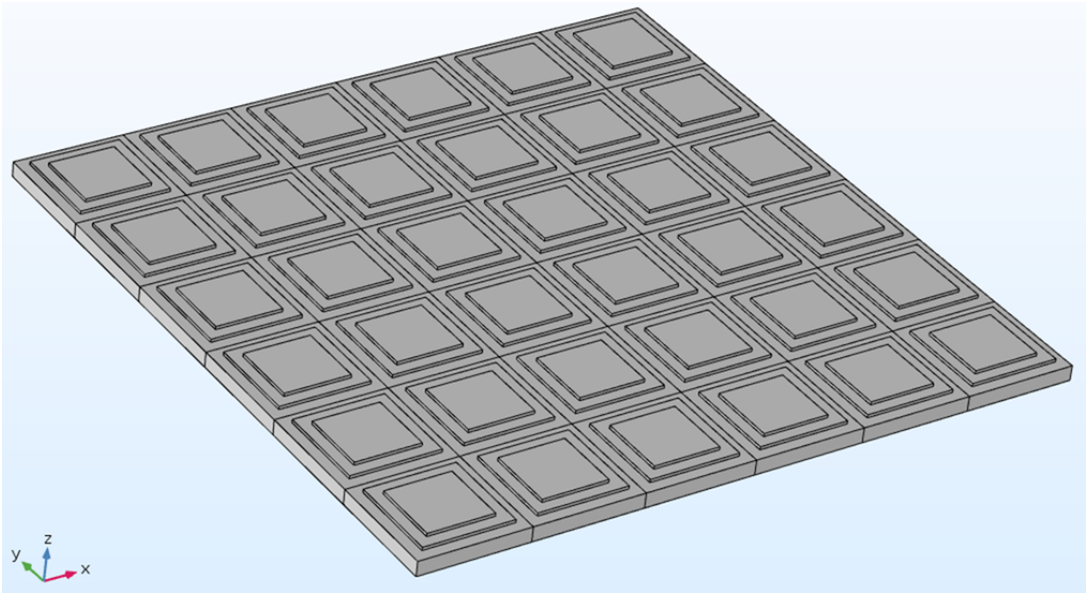

Figure 1: Schematic of a plate-like periodic structure.

Within the framework of the FETI-DP method, the substructure interface DOFs are described in terms of primal variables $\mathbf{u}_c^s$ at the substructure corners, and dual variables $\boldsymbol{\lambda}^s$ at the remaining interface DOFs (see Fig. 2). Then, coupling conditions between substructures can be enforced through strong compatibility conditions at the corner "primal" DOFs (i.e., ensuring that the displacements are equal at these DOFs), and weak compatibility conditions for the remaining DOFs. In this case, Lagrange multipliers (dual variables) are introduced into the substructure equation in order to verify the following compatibility constraint for the remaining DOFs $\mathbf{u}_r^s$:

$$\sum_{s=1}^{N_s} \mathbf{B}_r^s \mathbf{u}_r^s = \mathbf{0}. \tag{3}$$

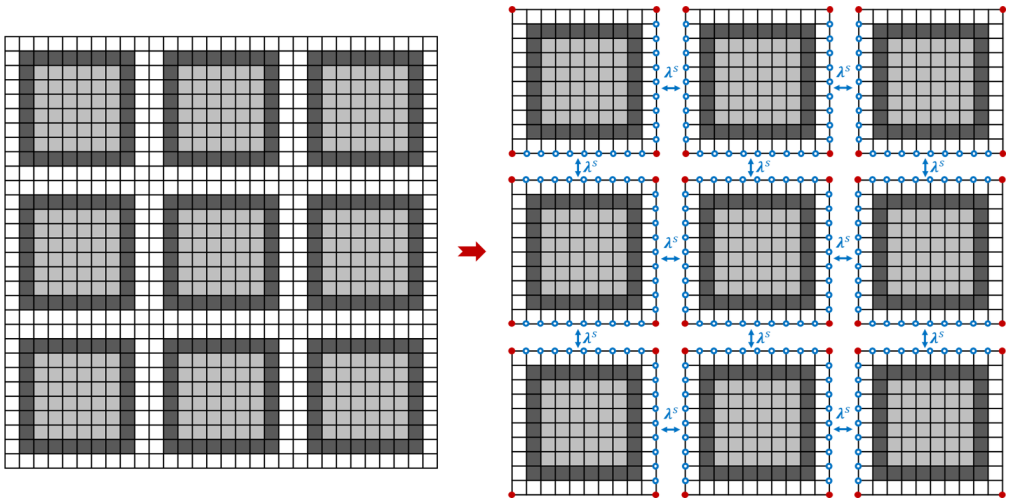

Figure 2: Schematic of a periodic structure and related decomposition into N_s substructures ($N_s = 9$ here). Red dots highlight corner DOFs; blue dots highlight other interface DOFs.

where $\mathbf{B}_r^s$ denotes signed Boolean matrices. In this case, the static equation of a substructure s ($s = 1,\ldots,N_s$) would be written as:

$$\begin{bmatrix} \mathbf{K}_{rr}^s & \mathbf{K}_{rc}^s \\ (\mathbf{K}_{rc}^s)^T & \mathbf{K}_{cc}^s \end{bmatrix} \begin{bmatrix} \mathbf{u}_r^s \\ \mathbf{u}_c^s \end{bmatrix} = \begin{bmatrix} \mathbf{f}_r^s \\ \mathbf{f}_c^s \end{bmatrix} + \begin{bmatrix} \boldsymbol{\lambda}^s \\ \mathbf{0} \end{bmatrix}. \tag{4}$$

The first block row of (4) yields:

$$\mathbf{u}_r^s = (\mathbf{K}_{rr}^s)^{-1}(-\mathbf{K}_{rc}^s\,\mathbf{u}_c^s + \mathbf{f}_r^s - (\mathbf{B}_r^s)^T\,\boldsymbol{\lambda}), \tag{5}$$

with $\boldsymbol{\lambda}$ the global vector of dual variables. Let us denote the global vector primal variables as $\mathbf{u}_c$. Then, introducing (5) into (3) and the second block row of (4) yields, after standard FE assembly procedure of the local substructure equations:

$$\begin{bmatrix} \mathbf{F}_{rr} & \mathbf{F}_{rc} \\ (\mathbf{F}_{rc})^T & -\mathbf{K}_{cc}^\star \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \mathbf{u}_c \end{bmatrix} = \begin{bmatrix} \mathbf{d}_r \\ -\mathbf{f}_c^\star \end{bmatrix}. \tag{6}$$

Here:

$$\begin{array}{rcl} \mathbf{F}_{rr} & = & \sum_{s=1}^{N_s} \mathbf{B}_r^s\,(\mathbf{K}_{rr}^s)^{-1}\,(\mathbf{B}_r^s)^T, \\ \mathbf{F}_{rc} & = & \sum_{s=1}^{N_s} \mathbf{B}_r^s\,(\mathbf{K}_{rr}^s)^{-1}\,\mathbf{K}_{rc}^s\,\mathbf{B}_c^s, \\ \mathbf{K}_{cc}^\star & = & \sum_{s=1}^{N_s} (\mathbf{B}_c^s)^T\,(\mathbf{K}_{cc}^s\,\mathbf{B}_c^s - (\mathbf{K}_{rc}^s)^T\,(\mathbf{K}_{rr}^s)^{-1}\,\mathbf{K}_{rc}^s, \\ \mathbf{d}_r & = & \sum_{s=1}^{N_s} \mathbf{B}_r^s\,(\mathbf{K}_{rr}^s)^{-1}\,(\mathbf{B}_r^s)^T\,\mathbf{f}_r^s, \\ \mathbf{f}_c^\star & = & \sum_{s=1}^{N_s} (\mathbf{B}_c^s)^T\,\mathbf{f}_c^s - \sum_{s=1}^{N_s} (\mathbf{B}_c^s)^T\,(\mathbf{K}_{rc}^s)^T\,(\mathbf{K}_{rr}^s)^{-1}\,\mathbf{f}_r^s, \end{array} \tag{7}$$

with $\mathbf{B}_c^s$ a Boolean localization matrix defined as $\mathbf{u}_c^s = \mathbf{B}_c^s\,\mathbf{u}_c$. Eventually, condensing the primal DOFs $\mathbf{u}_c$ onto the dual ones $\boldsymbol{\lambda}$ gives the following equation (for $\boldsymbol{\lambda}$):

$$\mathbf{F}\,\boldsymbol{\lambda} = \mathbf{d}, \tag{8}$$

where:

$$\mathbf{F} = \mathbf{F}_{rr} + \mathbf{F}_{rc}\,(\mathbf{K}_{cc}^\star)^{-1}\,\mathbf{F}_{rc}^T, \tag{9}$$

and

$$\mathbf{d} = \mathbf{d}_r - \mathbf{F}_{rc}\,(\mathbf{K}_{cc}^\star)^{-1}\,\mathbf{f}_c^\star. \tag{10}$$

The resolution of (8) can be done in a standard way using the conjugate gradient method (PCG) with a Dirichlet preconditioner $(\bar{\mathbf{F}}_I)^{-1}$ [3] (see Algorithm 1). The algorithm works iteratively by minimizing, at each new iteration n, a residual $\mathbf{r}_n = \mathbf{d} - \mathbf{F}\boldsymbol{\lambda}_n$ in the direction "$\mathbf{p}_n$" perpendicular to it. Finally note that, to speed up the computational times, the numerical steps $S2-1$, $S2-2$ and $S2-3$ involved in the algorithm procedure can be parallelized [5]. Also, the periodicity properties of the structure can be advantageously considered to strongly reduce the number of matrix products at the substructure level (in the sense most of these matrix terms are similar between the substructures).

3 Interface reduction

A strategy is proposed to reduce the number of Lagrange multipliers at the substructure interfaces, which allows the computational times to be further reduced. The proposed strategy focuses on square 3D substructures with rectangular sides Γ^s, where the idea is to express the Lagrange multipliers at a reduced number of points (see Fig. 3). For instance, for a side associated with a central coordinate system (O,x,y) ($x_{min} \le x \le x_{max}$, $y_{min} \le y \le y_{max}$), those points may represent Gauss points (x_i^G, y_i^G) with coordinates:

$$x_i^G = \frac{x_{max}+x_{min}}{2} + \frac{x_{max}-x_{min}}{2}\,\xi_i^G \quad ; \quad y_i^G = \frac{y_{max}+y_{min}}{2} + \frac{y_{max}-y_{min}}{2}\,\eta_i^G \tag{11}$$

with (ξ_i^G, η_i^G) the Gauss point positions expressed in natural coordinates, e.g., $\xi_i^G, \eta_i^G \in \{-1/\sqrt{3}, 1/\sqrt{3}\}$ for 2×2 points. Then, the Lagrange multiplier at a given node (x_j, y_j) may be obtained from the Lagrange multipliers at the Gauss points as follows:

$$\lambda_j \approx \sum_{i=1}^{n^G} N_i(x_j,y_j)\lambda_i^G, \tag{12}$$

Algorithm 1 Preconditioned conjugate gradient method (PCG)

Initialize:

$\boldsymbol{\lambda}_0 \leftarrow \mathbf{0}$; $\mathbf{r}_0 \leftarrow \mathbf{d}$; $\mathbf{w}_0 \leftarrow (\bar{\mathbf{F}}_I)^{-1}\mathbf{r}_0$; $\mathbf{p}_0 = \mathbf{w}_0$

for $n = 0$ to n_{max} **do**

S1: $\boldsymbol{\delta}_n = \mathbf{F}_{rr}\mathbf{p}_n$

S2-1: $\mathbf{y}_n = (\mathbf{F}_{rc})^T\mathbf{p}_n$

S2-2: $\mathbf{x}_n = (\mathbf{K}^*_{cc})^{-1}\mathbf{y}_n$

S2-3: $\mathbf{z}_n = \mathbf{F}_{rc}\mathbf{x}_n$

$\mathbf{F}\mathbf{p}_n = \boldsymbol{\delta}_n + \mathbf{z}_n$; $\alpha_n = \frac{\mathbf{r}_n^T\mathbf{w}_n}{\mathbf{p}_n^T\mathbf{F}\mathbf{p}_n}$

$\boldsymbol{\lambda}_{n+1} = \boldsymbol{\lambda}_n + \alpha_n\mathbf{p}_n$; $\mathbf{r}_{n+1} = \mathbf{r}_n - \alpha_n\mathbf{F}\mathbf{p}_n$; $\mathbf{w}_{n+1} = (\bar{\mathbf{F}}_I)^{-1}\mathbf{r}_{n+1}$

if $\frac{\|\mathbf{r}_{n+1}\|}{\|\mathbf{d}\|} < \varepsilon = 10^{-6}$ **then**

break

end if

$\mathbf{p}_{n+1} = \mathbf{w}_{n+1} + \frac{\mathbf{r}_{n+1}^T\mathbf{w}_{n+1}}{\mathbf{r}_n^T\mathbf{w}_n}\mathbf{p}_n$

end for

where $N_i(x_j, y_j)$ represent standard interpolation functions of the form:

$$N_i(x_j, y_j) = \left(\prod_{k\neq i}\frac{x_j - x_k^G}{x_i^G - x_k^G}\right)\left(\prod_{k\neq i}\frac{y_j - y_k^G}{y_i^G - y_k^G}\right). \tag{13}$$

An interface reduction for each side of a substructure is obtained by considering a small number of Lagrange multipliers at the Gauss points. A a result, the interface DOFs of a whole substructure may be described as:

$$\boldsymbol{\lambda}^s \approx \mathbf{N}^s\tilde{\boldsymbol{\lambda}}^s, \tag{14}$$

with $\tilde{\boldsymbol{\lambda}}^s$ the vector of Lagrange multipliers at Gauss points (four sides), and $\mathbf{N}^s$ the related matrix of interpolation functions. Then, the interface reduction at the structure level may be described as:

$$\boldsymbol{\lambda} \approx \mathbf{N}\tilde{\boldsymbol{\lambda}}. \tag{15}$$

Following the FETI framework and the Galerkin projection technique, a reduced equation for the Lagrange multipliers $\tilde{\boldsymbol{\lambda}}$ may therefore be proposed as follows:

$$\tilde{\mathbf{F}}\tilde{\boldsymbol{\lambda}} = \tilde{\mathbf{d}}, \tag{16}$$

where

$$\tilde{\mathbf{F}} = \mathbf{N}^T\mathbf{F}\mathbf{N}, \tag{17}$$

and

$$\tilde{\mathbf{d}} = \mathbf{N}^T\mathbf{d}. \tag{18}$$

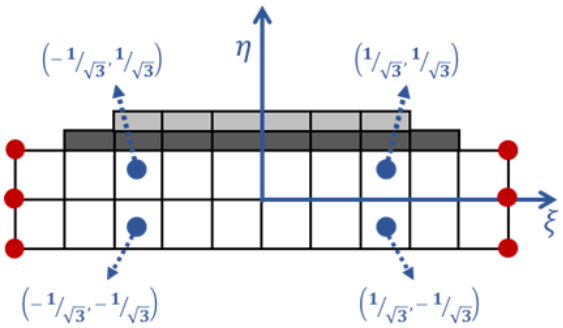

Figure 3: Example of a interface with $n^G = 2 \times 2$ Gauss points.

4 Numerical results

The FETI-DP method is used to assess the deformation of a square silicon plate (size 150×150 mm^2) with a periodic pattern of thin layers of different materials. The plate is supposed to be clamped at the central position of its bottom side and free elsewhere, the final geometry being therefore reduced to a plate quarter of size 75×75 mm^2. Here, $N_s = 20 \times 20 = 400$ substructures like those described in Fig. 2 are considered, where each substructure consists of a lower square silicon base, and two upper thin films of different dimensions and material properties (see Tab. 1).

Table 1: Properties of the substructures.

Layer	Thickness	Square basis dimensions	Young's modulus	Poisson's ratio	Thermal coefficient
Silicon base	500 µm	3.7×3.7 mm^2	130 GPa	0.27	$2.8\,10^{-6}$ K^{-1}
Intermediary layer	1 µm	3.0×3.0 mm^2	69 GPa	0.33	$24\,10^{-6}$ K^{-1}
Upper layer	1 µm	2.2×2.2 mm^2	58 GPa	0.30	$30\,10^{-6}$ K^{-1}

The right and top sides of the whole structure quarter are free, while symmetry boundary conditions are applied to the left and bottom sides. In addition, the left-bottom corner of the structure is fixed at the lower surface (see Fig. 4). In this case, each substructure is meshed using 300 twenty-node hexahedrons (three DOFs per node), leading to $1,915,215$ DOFs for the whole structure.

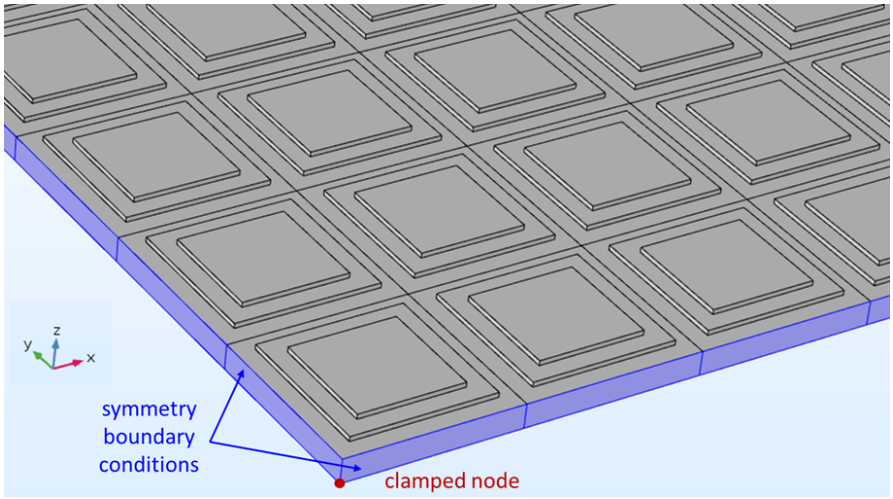

Figure 4: Boundary conditions applied to the quarter of the structure: symmetry (left and bottom sides), clamped (lowest node, left-bottom corner); other boundaries are free.

The mechanical deformation of the structure resulting from a temperature rise of $\Delta T = 200°C$ (thermal loading) is investigated. For this purpose, the following modeling strategies are considered: (i) reference FE approach, where Eq. (1) is solved directly ($1,915,215$ DOFs); (ii) standard FETI-DP method, where $171,000$ Lagrange multipliers are considered; (iii) FETI-DP method with interface reduction, where $9,120$ Lagrange multipliers (as obtained using four interpolation points on each substructure side) are considered. Numerical simulations are carried out with Matlab for the three methods. Regarding the FETI-DP method, 26 iterations are required to reach convergence of the solution with the standard strategy, while it takes 113 iterations with the model reduction strategy. Notably, the transverse displacement field of the structure that results from the two FETI-DP strategies appear to be in good agreement as shown in Fig. 5.

An overview of the numerical results is presented in Tab. 2. Here, the error between the FETI-DP solutions and the reference solutions are computed as:

$$\text{Error} = \frac{\|\mathbf{u}_{\text{direct}} - \mathbf{u}_{\text{FETI}}\|}{\|\mathbf{u}_{\text{direct}}\|} \tag{19}$$

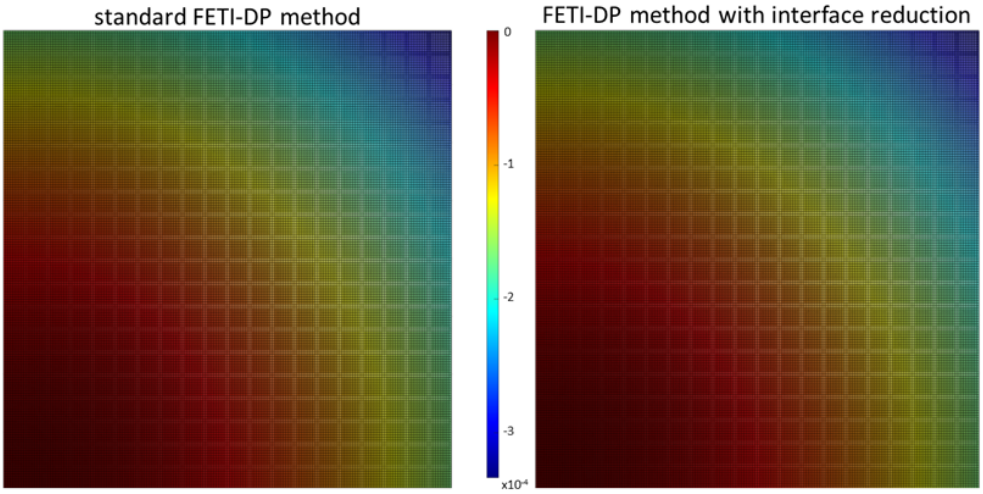

Figure 5: Transverse displacement field of the periodic plate (20×20 substructures). (left) standard FETI-DP method; (right) FETI-DP method with interface reduction.

with $\mathbf{u}_{\text{direct}}$ and $\mathbf{u}_{\text{FETI}}$ the full displacement vector of the periodic structure computed with the direct and FETI-DP methods. Overall, the two FETI-DP strategies yield accurate solutions (i.e., less than 1% for the two methods), as well as they allow strong reduction of the computational times compared to the direct approach (regarding the FETI strategies, it is worth noting that the offline steps (e.g., matrix assemblies) and the online steps (PCG) steps are accounted for in the computational times).

Importantly, the FETI-DP method with interface reduction is 57.78 % faster than the standard technique (even though the number of iterations involved in the PCG is larger with the model reduction strategy). The numerical performance of the model reduction strategy over the standard method is even better for larger number of DOFs, as this can be checked for a periodic structure with 50×50 substructures. In this case, the FETI-DP method with interface reduction ($58,800$ Lagrange multipliers) only requires 344 s to compute the structure deformation, compared to 991 s with the standard FETI-DP method. This represents a reduction of about 65 % of the computational time.

Table 2: Overview of the numerical results.

Method	Number of DOFs	Time	Reduction	Error
Direct (reference)	$1,915,212$	$2,055.0$ s	-	-
Standard FETI-DP	$171,000$	88.1 s	95.71 %	0.01 %
FETI-DP with interface reduction	$9,120$	37.2 s	98.19 %	0.61 %

5 Conclusion

In this paper, a FETI-DP approach combined with an interface reduction strategy has been proposed to predict the deformation of periodic structures under thermal loading. The proposed strategy enables strong reduction of the computational times, and alleviates the memory storage burden involved in standard (direct) FE analyses. Numerical results have been proposed concerning a silicon plate with periodic patterns built from thin layers of different materials (400 substructures). Those results have confirmed the relevance of the proposed strategy to drastically reduce the computational times and provide accurate displacement results. Importantly, one of the findings of this research is that the FETI-DP method with interface enables additional time reduction compared to the standard FETI-DP method (about 60%). Notably, it is expected that the proposed strategy can provide better time reduction for periodic structures with more substructures, making it suitable for being used in an industrial context where wafers owning numerous substructures of more complex geometries are of concern.

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