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To cite this version:

A. Barka, F.X. Roux. Validation of FETI-2LM formulation for EBG material prediction and optimal strategy for multiple RHS.. ISAP 2013, Oct 2013, NANJING, China. hal-01057692

HAL Id: hal-01057692

https://onera.hal.science/hal-01057692v1

Submitted on 25 Aug 2014

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Validation of FETI-2LM formulation for EBG material prediction and optimal strategy for multiple RHS

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Abstract This paper presents the validation of finite element tearing and interconnecting (FETI) methods for solving electromagnetic frequency domain problems encountered in the design of electromagnetic band gap (EBG) materials. Validation results presented at the EM-ISAE 2012 workshop are discussed.

I. Introduction

The Finite Element Method (FEM) is one of the most successful frequency domain computational methods for electromagnetic simulations . It combines, very efficiently, a geometrical adaptability and ability to handle arbitrary materials for modelling complex geometries and materials of arbitrary composition, including meta-materials that have recently become popular. Finite element approximation of Maxwell's equations leads to a sparse linear system, usually solved by using direct or iterative solvers. However, modern engineering applications dealing with antennas, scatterers or microwave circuits, style require the solution of problems with hundred millions of unknowns.

Domain Decomposition Methods have demonstrated efficiency and accuracy for the solution of Maxwell equations in the frequency domain for both RCS applications and antenna structures interactions [2]. In the domain of finite element methods (FEM), and for the solution of acoustic Helmoltz equations, efficient sub-domain connecting techniques have been applied and called dual-primal finite element tearing and interconnecting [3][4]. These techniques are known under the acronym FETI-DP and have been adapted to electromagnetics (FETI-DPEM) for the calculation of antenna arrays and metamaterial periodic structures [5][6].

This paper presents some recent developments on the Finite Element Tearing and Interconnecting with two lagrange multipliers (FETI-2LM) techniques, for solving large scale FEM problems encountered in electromagnetic applications. Validation results presented at the EM-ISAE 2012 workshop are discussed including cross comparison of the FETI-2LM techniques with FDTD, MLFMM, and Time Domain Discontinuous Galekin methods (TDDG).

II. FETI-2LM Formulation

A. Weak formulation

The general principle of the FETI methods for Maxwell equations is to decompose the global computational domain in non overlapping sub-domains in which local solution fields are calculated by solving the finite element system with a direct method. We then impose the tangent field continuity on the interfaces by using Lagrange multiplier. It results in a reduced problem on interfaces and can be solved by an iterative method. The solution of the interface problem is used as a boundary condition for evaluating the field in each sub-domain. We denote $\Omega = \Omega_1 \cup \Omega_2 .... \Omega_N$ a partition of the initial computation domain. In each sub-domain Ω_i (Fig. 1), we are calculating the scattered fields $\vec{E}^i$ verifying on Ω_i:

$$\nabla\times(\mu_{r,i}^{-1}\nabla\times\vec{E}^i)-k_0^2\varepsilon_{r,i}\vec{E}^i = k_0^{\,2}(\varepsilon_{r,i}-\mu_{r,i}^{-1})\vec{E}_{incident} \quad (1)$$

$$\vec{n}_{ext}\times\nabla\times\vec{E}^i + jk_0\vec{n}_{ext}\times(\vec{n}_{ext}\times\vec{E}^i) = 0 \quad (2)$$

The vector $\vec{E}_{incident}$ is representing the electric incident field in the volume Ω_i. Γ_{ABC} represents the boundary of the volume Ω_i, where the field is verifying absorbing boundary conditions (ABC).

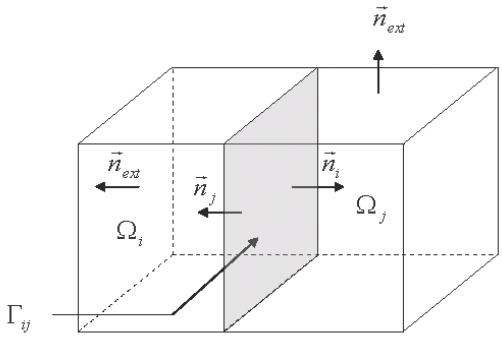

Fig. 1. Interface problem.

In the following, we will denote with $\vec{E}_j^i$ the electric field on the interface of the sub domain Ω_i adjacent to the sub domain Ω_j . On the interfaces Γ_{ij}^{robin} separating two sub-

domains Ω_i and Ω_j, we impose Robin type boundary conditions by using Lagrange multipliers $\vec{\Lambda}^i_j$ and $\vec{\Lambda}^j_i$ which will be the new unknowns:

$$\vec{n}_i \times (\mu_{r,i}^{-1} \nabla \times \vec{E}^i_j) + jk_0 \vec{n}_i \times (\vec{n}_i \times \vec{E}^i_j) = \vec{\Lambda}^i_j \quad (3)$$

$$\vec{n}_j \times (\mu_{r,j}^{-1} \nabla \times \vec{E}^j_i) + jk_0 \vec{n}_j \times (\vec{n}_j \times \vec{E}^j_i) = \vec{\Lambda}^j_i \quad (4)$$

The tangential electric and magnetic field continuity on the interfaces Γ_{ij}^{robin} separating the two sub domains Ω_i and Ω_j leads to the following relations that should be verified by the two Lagrange multipliers $\vec{\Lambda}^i_j$ and $\vec{\Lambda}^j_i$ on Γ_{ij}^{robin}:

$$\begin{aligned} \Lambda^i_j + \Lambda^j_i - 2jk_0 \vec{n}_i \times (\vec{n}_i \times \vec{E}^i_j) = 0 \\ \Lambda^i_j + \Lambda^j_i - 2jk_0 \vec{n}_j \times (\vec{n}_j \times \vec{E}^j_i) = 0 \end{aligned} \quad (5)$$

The weak formulation used for the computation of the scattered fields $\vec{E}^i$ belonging to the space $H(Rot^0, \Omega_i)$ in each volume Ω_i is:

$$\begin{aligned} &\int_{\Omega_i} \left[\mu_{r,i}^{-1} (\nabla \times \vec{E}^i).(\nabla \times \vec{W}) - k_0^2 \varepsilon_{r,i} \vec{E}^i.\vec{W} \right] d\Omega \\ &+ jk_0 \int_{\Gamma_{ext}} (\vec{n} \times \vec{E}^i).(n \times \vec{W}) d\Gamma \\ &+ jk_0 \int_{\Gamma_{ij}^{robin}} (\vec{n} \times \vec{E}^i_j).(n \times \vec{W}) d\Gamma \\ &= k_0^2 \int_{\Omega_i} (\varepsilon_{r,i} - \mu_{r,i}^{-1}) \vec{E}^i.\vec{W} d\Omega \end{aligned} \quad (6)$$

The iterative resolution of the interface problem (5) is based on a Krylov sub-space method. We write equivalently:

$$\lambda^i_j + \lambda^j_i - (M^i_j + M^j_i) E^i_j = 0 \quad \forall \quad i = 1,..,N \quad (7)$$

where j is neighbouring i and

$$M^i_j = jk_0 \int_{\Gamma_{ij}} (\vec{n}_i \times \vec{W}_i).(\vec{n}_i \times \vec{W}_i) d\Gamma \quad (8)$$

The iterative method consists of four steps:

1. Calculation of local solutions in each sub domain with the use of Robin type conditions by solving the problem (5).
2. Exchange fields $\vec{E}$ and Lagrange multipliers $\vec{\Lambda}$ on each interface.
3. $g^i_j = \lambda^i_j + \lambda^j_i - (M^i_j + M^j_i) E^i_j$ computation on each interface.
4. Implementation of ORTHODIR iterations with a stop criterion $\|g\| < \varepsilon$.

B. Optimal strategy for multiple Right Hand Sides

Iteration algorithms, for all FETI methods, are based on Krylov space methods with full orthogonalizations, such as those found in the CG, ORTHODIR or GMRES algorithms. In the event that the same problem must be solved with several right hand sides, one drawback with iterative methods is that they generally need to restart from scratch for each new right hand side. The cost of storing and orthogonalizing a set of interface vectors is small compared to the cost of computing one matrix-vector product for the condensed interface operator.

Let us consider equation $Ax = b$. Once the problem has been solved for the first right hand side, a set of search direction vectors has been built. If the Krylov space method is the conjugate gradient method, these n_c vectors, $(v_j), 1 \le j \le n_c$, as well as their products by the FETI operator, $(Av_j), 1 \le j \le n_c$ have been computed and can be stored in memory. They provide a natural set of vectors to be used to implement a preconditioner based on projection for the next right hand side. Furthermore the $V^t AV$ matrix associated with this set of vectors is diagonal, and it has also been computed during the iterations. Thus, the computation of the projection associated with V is easy.

The new search direction vectors to be computed for the next series of iterations using the preconditioner based on projection would be automatically A-orthogonal to V, and would also be A-orthogonal to one another, thanks to the properties of the conjugate gradient algorithm. So the initial set of vectors can be augmented, for each new right hand side, with the set of newly computed search direction vectors. With this technique, the number of actual new iterations required for each new right hand side tends to decrease dramatically [7].

Of course this method requires us to store all the successive search direction vectors, and to perform a full orthogonalization procedure when computing the projection. But the associated overhead is not so large in the context of the FETI method. Furthermore, the number of stored vectors can be arbitrary limited on demand, for instance according to some memory limits. In practice, the full orthogonalization procedure may also be used for the search direction vectors of the current iterations. It makes the conjugate gradient method even more robust, because it prevents loss of orthogonality due to accumulated round-off errors.

For the case of a non-spd FETI method, if the ORTHODIR algorithm is used, all the search direction vectors as well as their product by the FETI operator have to be stored anyway. They are $A^* A$-orthogonal. They can be straightforwardly used to implement the optimal projection operator with a matrix $V^* A^* AV$ that has already been computed during the ORTHODIR iterations, and is

diagonal. The set of vectors can be augmented with the new search direction vectors built for any new right hand side.

The same methodology can be implemented with GMRES, but it is a little bit more technical since the basis built by GMRES is not A^*A-orthogonal, but simply orthogonal. Nevertheless, the advantage of GMRES over ORTHODIR is not so evident, in the context of FETI methods, since the storage of extra interface vectors is not so expensive. Furthermore, GMRES does not compute the value of the approximate solution of the condensed interface problem at each iteration. It is necessary to derive the approximate solution to compute the associated approximate solution of the global problem if the convergence is to be monitored according to the residual of the global problem.

III. EBG MATERIAL

C. EM-ISAE-2012 WORKSHOP

We consider the test of the EBG material designed by ONERA for the EM-ISAE 2012 Workshop.

This test is concerned with the simulation of the fields diffracted by an 8x20 EBG array comprising of alumina dielectric rods (Fig. 2) and centred at the origin (0,0,0). All the dimensions are given in millimetre (mm) in the Table I.

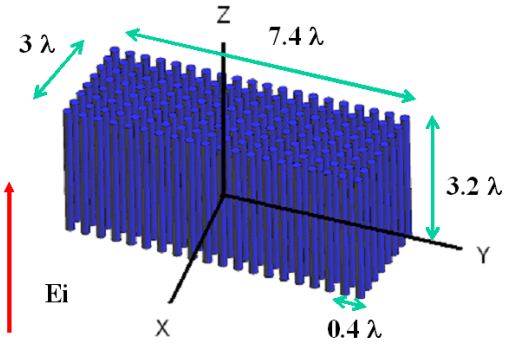

Fig. 2. 8x20 EBG array

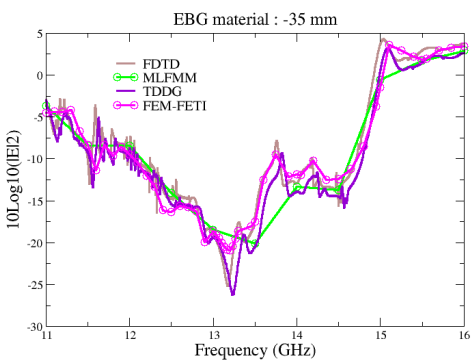

Fig. 3. Near field at point (-35,0,0) mm.

Table I
Geometry of EBG rods.

Rods diameter (mm)	4
Rod length (mm)	60
Array step (mm)	7
Alumina permittivity	$\varepsilon_r = 9.4$

The array is excited by a uniform and unitary plane wave (|Ei|=1), whose electric field is polarized parallel to the axis OZ of the rods and whose incidence direction is collinear to the OX axis (ɵ=90, φ=0). The parameters to be simulated are the total electric field transmitted behind the array at point (-35 mm,0,0).

The results are obtained with the Finite Element module of the FACTOPO frequency domain code [2] calling the FETI-2LM [1] library. Four empty unit cells are introduced around the 8x20 array to keep the ABC surface sufficiently far away from the scatterer. The size of the simulated array is then 16x28 corresponding to 448 sub-domains. Each domain contains one rod and is meshed with 139,547 edges. The total number of unknowns is 62.52 millions, and the computation parameters are presented in the Table II. The zero-order Whitney edge elements (6 degree of freedom in each tetrahedral) are considered. The local linear system resolution in each sub-domain is performed with the Intel MKL PARDISO solver. The sub domains are connected together iteratively with the ORTHODIR and the simulation results are plotted in pink on Fig. 3. They are in good agreement with the Finite Difference Time Domain simulations (FDTD [2], brown curve), Time Domain Discontinuous Galerkin simulations [1] (TDDG [3], magenta curve) and Multi Leval Fast Multipole Methods simulations (MLFMM [4], green curve). The FEM-FETI results need to be improved for the lowest levels by implementing the PML layers instead of the ABC. The calculation of the electric field in the EBG structure also shows a strong attenuation of the field (Fig. 4) in the band gap around 12 GHz.

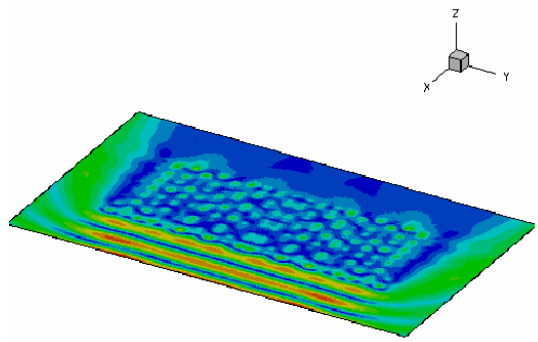

Fig. 4. E field at 12 GHz.

Table II
EBG: computation parameters.

[1] FEM-FETI results provided by the FACTOPO code of ONERA, France
[2] FDTD results provided by the SOPHIE code of CEA, France
[3] TDDG results provided by the SEMBA code of CASSIDIAN/UGR, Spain
[4] MLFMM results provided by the HP-TEST code of CASSIDIAN, Spain

Unknowns	62.52 millions
Longest edge	λ/13
Elapse time per frequency	1,372 s
Computer	448 cores X5560, 2.8 GHz
Memory used per core	1.8 Gb
Iterations par frequency	500
Residual (stop criteria)	1e-3

D. Analysis of scalability

The convergence of the FETI-2LM method is analysed by considering arrays with progressively increasing size (2x3, 4x7, 8x14, 16x28). The unit cell was done, as previously with 139,547 edges, for all of the arrays. The elapse time and the evolution of the number of iterations required for a convergence lower than 10^{-3} is indicated in Table. III. It is observed a linear increase of the number of iterations required for convergence as the array size is increased. This is due mainly to the global distribution of the diffracted field induced by the plane wave in the EBG material, which leads to strong interactions between the cells of the array.

Table III
EBG: statistics versus array size.

Array size	2x3	4x7	8x14	16x28
Cores (X5560 2.8 GHz)	6	28	112	448
Unknowns (millions)	0.837	3.9	15.6	62.52
Elapse time (s)	113	232	785	1,372
Iterations (stop criteria 10^{-3})	70	123	201	500

E. Assessment of the multiple Right Hand Side strategy

Radar Cross Section (RCS) analysis is requiring the computation of the diffracted fields for the vertical and horizontal polarisation of the incident field and a large number of incidence directions. Similarly, in the context of antenna array applications, there is an interest in evaluating the coupling levels between the array elements. This information is usually obtained by calculating the scattering matrix of the array. The procedure consists of sequentially exciting all of the elements of the array and computing the behaviour of the electromagnetic fields at all the feeding ports. The number of right hand sides is potentially prohibitive and one drawback with iterative methods is that they need to restart from scratch for each new right hand side. The optimal strategy developed in subsection II.B is assessed for the EBG material test. We consider a uniform plane wave exciting the arrays 2x3 and 8x14 for 10 incidences angles varying from (ϴ=90, φ=0) to (ϴ=90$, φ=10) with an angular step of 1 degree. We observe from Fig. 5 that the number of iterations required for convergence is significantly reduced by a factor of 8 and 5.6 respectively for the 2x3 and 8x14 arrays. The maximum number of direction vectors stored (subsection II.B) is 150 for the 2x3 array, while it is 656 for the 8x14 array.

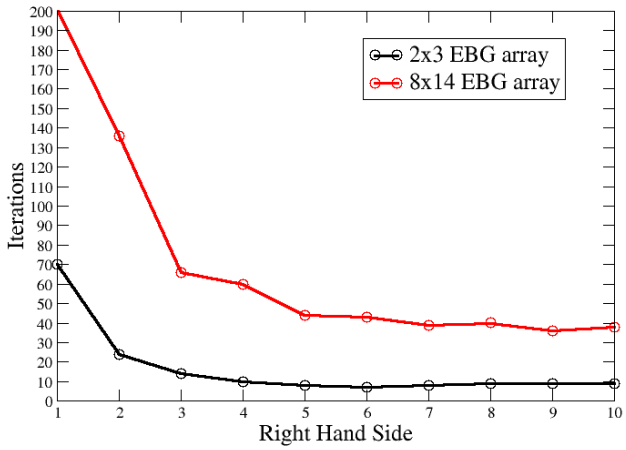

Fig. 5. EBG: iterations versus right hand side

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