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Electromagnetic modelling/Modélisation électromagnétique

A numerical strategy for a high frequency electromagnetic scattering problem in a mixed formulation

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Abstract

We consider the electromagnetic scattering problem of an inhomogeneous obstacle. The methodology applied combines a volume finite element method with a boundary integral method. Both are numerically solved in an efficient way and coupled with a domain decomposition method. The main ingredients are: domain decomposition method with Després's transmission conditions and concentric subdomains, Després's integral equations, fast multipole method, and a parallel sparse direct solver. Numerical results on different inhomogeneity and complex geometries are presented. ***To cite this article: K. Mer-Nkonga et al., C. R. Physique 7 (2006).***

Résumé

Une stratégie de résolution d'un problème de diffraction électromagnétique à haute fréquence en formulation mixte. Notre but est de résoudre le problème de la diffraction électromagnétique par un obstacle hétérogène. La méthode que nous proposons couple une formulation volumique discrétisée par éléments finis avec une méthode intégrale surfacique. Ces deux formulations sont résolues numériquement par des méthodes efficaces et sont couplées à l'aide d'une méthode de décomposition de domaines. Les ingrédients principaux utilisés sont : la décomposition de domaines avec conditions de transmission de Després et des sous-domaines concentriques, les équations intégrales de Després, la méthode multipôle rapide, et enfin un solveur direct creux parallèle. Nous présentons des résultats obtenus pour différentes hétérogénéités sur des géométries complexes. ***Pour citer cet article : K. Mer-Nkonga et al., C. R. Physique 7 (2006).***

Keywords: Electromagnetic scattering; Domain decomposition; Integral equations; Fast multipole method; Parallel sparse direct solver

Mots-clés : Diffraction électromagnétique ; Décomposition de domaines ; Équations intégrales ; Méthode multipôle rapide ; Solveur direct creux parallèle

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Le calcul de la diffraction d'une onde électromagnétique à haute fréquence, par un obstacle hétérogène, est un problème très coûteux. Pour réaliser ce type de simulation avec un coût raisonnable, un code de calcul a été développé au CEA CESTA (code Odyssee), basé sur un couplage de méthodes et de solveurs originaux. Les méthodes ont été choisies selon des critéres de précision et de robustesse, et l'efficacité a été optimisée par des méthodes et des solveurs rapides, et par la parallélisation.

Pour prendre en compte d'une part l'obstacle et d'autre part le domaine de propagation infini, la modélisation du problème de diffraction est basée sur un couplage d'une discrétisation éléments finis des équations de Maxwell à l'intérieur du domaine hétérogène, et d'une équation intégrale posée sur la frontière extérieure à ce domaine.

Le couplage est réalisé par la méthode de décomposition de domaines de Després [2] ; les sous-domaines considérés ici sont concentriques (en « pelures d'oignons ») et on utilise un algorithme de type Gauss–Seidel relaxé où les sous-domaines sont résolus successivement du sous-domaine intérieur au sous-domaine extérieur [3,5,4]. cette configuration des sous-domaines permet d'accélérer la convergence.

L'équation intégrale considérée est l'équation intégrale de Després [6,7] ; cette équation a de bonnes propriétés de précision et de robustesse, en particulier par rapport à la convergence itérative. Le système est résolu par deux gradients conjugués imbriqués ou par un GMRES préconditionné. Les produits matrice-vecteurs sont accélérés par une méthode multipôle multiniveaux [8–10].

Dans les domaines intérieurs, les systèmes sont résolus par méthode directe parallèle à l'aide de la chaîne logicielle EMILIO, qui inclut le solveur PaStiX [11,12].

Les principales caractéristiques des méthodes considérées sont développées et des résultats numériques sur des objets complexes et de grande taille sont présentés.

1. Introduction

The numerical treatment of the scattering of an electromagnetic wave at high frequency by an inhomogeneous obstacle is very costly in terms of computational time and memory requirements. For this purpose, a coupling of original methods and solvers have been achieved using a numerical software, Odyssee, developed at CEA/CESTA. Our numerical strategy is guided by arguments of accuracy and robustness; moreover, the efficiency is improved by fast methods and solvers, and by parallelization. To take into account the inhomogeneous obstacle, together with the infinite domain of propagation, the modelling of the diffraction problem is based on a coupling of a finite element (FE) discretization of Maxwell's equations, and a Boundary Element Method (BEM) written on a boundary surrounding the inhomogeneous obstacle. The coupling of both formulations is achieved using a domain decomposition method (DDM).

The DDM is particularly attractive for the solution of a large problem: it is decomposed into several coupled subproblems that can be solved independently, thus reducing considerably the memory storage requirements. Two classes of methodologies may be identified. In the first (see, e.g., [1]), no iterations are required but the solutions may not be unique on account of the fact that these subproblems generally involve Dirichlet or Neumann boundary conditions. Methodologies of the second class [2–5] are based on an iterative DDM originally proposed in [2]: the fields in two adjacent subdomains are connected by a mixed boundary condition, termed transmission condition (TC), that ensures the uniqueness of the solutions and their convergence to the one of the original problem. If a particular, 'onion-like', partition of the computational domain into concentric subdomains circumscribing the object is performed, then the efficiency of the TCs is improved and, consequently, the number of iterations is reduced. In this case, a large number of redundant subproblem solutions are performed if the original Després's algorithm is employed, and these are suppressed if this algorithm is modified appropriately [3].

Scattering from a stealthy object, the bistatic Radar Cross Section (RCS) of which generally exhibits a very large angular dynamic range, can be accurately calculated only if an exact radiation condition, such as the EID (équation intégrale de Després) [6,7], is prescribed on the outer boundary of the whole computational domain. The EID is (weakly) coupled to the PDE formulation defined inside the outermost subdomain through the TC, so that the PDE and EID systems are solved independently at each DDM iteration, thus reducing considerably the complexity of the original problem [5,4]. In addition, since the matrices that are to be inverted in the EID are all Hermitian positive definite, the EID systems can be efficiently solved via a very simple double conjugate gradient (two imbricated conjugate

gradients) algorithm where the matrix–vector product can be further accelerated, in conjunction with considerable savings in memory, through the use of the MLFMA [8–10].

The corresponding numerical software is parallelized, each of the subproblems being solved successively. In the interior subdomains, the FE systems are solved with parallel sparse direct methods, using the software processing chain EMILIO (which includes the parallel sparse direct solver PaStix from INRIA) [11,12]. PaStix performs high performance sparse supernodal LDL^t or LL^t parallel factorization without pivoting for large sparse symmetric positive definite systems, and sparse supernodal LU parallel factorization with static pivoting for non-symmetric matrices having a symmetric pattern.

The main features of each method are given here, and numerical results with complex and large objects are presented.

2. A FE/BEM coupling with domain decomposition

Let Ω be a bounded domain with boundary Γ, and $\Omega_\infty = \mathbb{R}^3 \setminus \overline{\Omega}$. We consider the electromagnetic field (E, H) scattered by Ω. In the interior domain Ω, the relative electric permittivity ε and magnetic permeability μ can be anisotropic and variable functions, while in the exterior domain Ω_∞ we assume that $\varepsilon = \mu = 1$. The interior domain Ω is subdivided into P concentric subdomains Ω_i: $\Omega = \Omega_1 \cup \Omega_2 \cup \cdots \cup \Omega_P$, with $\partial\Omega_p = \Sigma_{p-1} \cup \Sigma_p$ for $p = 1, \ldots, P$, where $\Sigma_p = \partial\Omega_p \cap \partial\Omega_{p+1}$ and $\Sigma_P = \partial\Omega_P \cap \partial\Omega_{P+1} (= \partial\Omega_\infty) = \Gamma$. Σ_0 is the innermost surface of the computational domain on which a Leontovich boundary condition is prescribed. It is important to note that ε and μ may be discontinuous at the interfaces between the subdomains. The assumed (and suppressed) time dependence is $\exp(\mathrm{i}\omega t)$, and $k = 2\pi/\lambda = \omega/c$ is the wave number of the incident field (c is the speed of light). Let $\hat{n}_p$ denote the unit normal to Σ_p exterior to Ω_p, and let us define, for $q = p-1$, p [13]:

$$G^{\mathrm{out}}_{\Omega_p,\Sigma_q} = \hat{n}_q \times (E_p \times \hat{n}_q) - \frac{1}{\mathrm{i}k}(\mu^{-1}\nabla \times E_p) \times \hat{n}^{\mathrm{out}}_q$$
$$G^{\mathrm{in}}_{\Omega_p,\Sigma_q} = \hat{n}_q \times (E_p \times \hat{n}_q) - \frac{1}{\mathrm{i}k}(\mu^{-1}\nabla \times E_p) \times \hat{n}^{\mathrm{in}}_q$$

where $\hat{n}^{\mathrm{out}}_q$ (resp. $\hat{n}^{\mathrm{in}}_q$) is the normal to Σ_q, exterior (resp. interior) to Ω_p. We consider the following domain decomposition problem, with Després's like transmission conditions [2]:

Interior subdomains:

$$\begin{cases} k^2\varepsilon(x)E_p(x) - \nabla \times \big(\mu^{-1}(x)\nabla \times E_p(x)\big) = 0, \quad \nabla \cdot (\varepsilon E) = 0, \quad x \in \Omega_p \\ \hat{n}_q \times (E_p \times \hat{n}_q) - \dfrac{1}{\mathrm{i}k}(\mu^{-1}\nabla \times E_p) \times \hat{n}^{\mathrm{in}}_q = G^{\mathrm{in}}_{\Sigma_q} \quad \text{on } \Sigma_q, \text{ for } q = p-1, p \end{cases} \tag{1}$$

Exterior subdomain:

$$\begin{cases} \mathrm{i}kE(x) - \nabla \times H(x) = 0, \quad \mathrm{i}kH(x) + \nabla \times E(x) = 0, \quad x \in \Omega_\infty \\ \hat{n}_P \times (E_P \times \hat{n}_P) + H \times \hat{n}_P = G^{\mathrm{in}}_{\Sigma_P} \quad \text{on } \Sigma_P, \quad \lim\limits_{|x|\to\infty} \big((H \times \hat{x}) \times \hat{x} - E \times \hat{x}\big) = \mathrm{o}\left(\dfrac{1}{r}\right) \end{cases} \tag{2}$$

Interior problems are solved using a variational formulation of (1) and a discretization with $H(\mathrm{rot})$ edge finite elements, and the exterior problem is solved using Després's Integral Equation formulation (Section 3), discretized with $H(\mathrm{div})$ edge finite elements.

The (relaxed) DDM algorithm is defined as follows [3]. For $p = 1, \ldots, P+1$ and at iteration l, solve problem $\mathcal{P}^l_p$:

$$\begin{cases} E^l_p \text{ is the solution of the discrete variational problem in } \Omega_p \text{ with boundary conditions:} \\ (G^{\mathrm{in}}_{\Sigma_{p-1}})^l = (G^{\mathrm{out}}_{\Omega_{p-1},\Sigma_{p-1}})^l \\ (G^{\mathrm{in}}_{\Sigma_p})^l = \alpha_l (G^{\mathrm{in}}_{\Omega_p,\Sigma_p})^{l-1} + (1-\alpha_l)(G^{\mathrm{out}}_{\Omega_{p+1},\Sigma_p})^{l-1}, \quad \text{for } p \leqslant P \text{ with } \alpha_1 = 0,\ \alpha_l \in [0, 1/2],\ l \geqslant 2 \end{cases}$$

In G^{in} and G^{out}, the tricky computation of $\nabla \times E$ on the interfaces is avoided if these terms are computed recursively [3] (the corresponding complete algorithm is given in [5]). When this algorithm is employed, the number of redundant solutions of problems $\mathcal{P}^l_p$ that are being suppressed in Després's original one and yield identical values for E in Ω_{p+1} is equal to $(P+1)^2 + (P+1)(l-2)$ when $l \geqslant P+1$ [3]; note that the solution in Ω_1 is affected by the radiation

condition on Σ_P only if $l \geqslant P+1$. For the continuous problem, the convergence of this algorithm has been proved in [5]. Also, it has been shown [13] that the DDM algorithms reduce to particular iterative solutions of a more global linear system, defined for the whole computational domain Ω and where the unknowns are the quantities G^{in}, G^{out} defined on each side of the interfaces. In this approach, Després's (resp. the above) algorithm may be viewed as a kind of Jacobi (resp. Gauss–Seidel) iterative solution of this global system.

For the discrete problem, it can be shown that the algorithm converges by using the interface problem formalism with scattering operators $S_p : G^{\text{in}} \mapsto G^{\text{out}}$ of [13], which are shown to be contractions. The result is not classical for the operator S_∞ of a discretized integral equation. Indeed, it can be shown that the operator S_∞ of the discretized EID is a contraction: if $G^{\text{in}} = E_t + H \times n = -J + n \times M$, $G^{\text{out}} = E_t - H \times n = -G^{\text{in}} + 2n \times M$ (see Section 3 for notations), then we have:

$$\|S_\infty G^{\text{in}}\|^2 = \|G^{\text{out}}\|^2 + 2\left\| A_\infty \begin{pmatrix} J \\ M \end{pmatrix} \right\|_Z^2 \leqslant \|G^{\text{in}}\|^2$$

where $\|\gamma\|_Z^2 = \oint_{S^2} |\gamma(\hat{s})|^2$ and $\oint_{S^2}$ is used for integrals computed with a numerical quadrature.

3. Després's integral equations and the fast multipole method

3.1. Després's integral equations

The integral equations considered to model the exterior problem with a Léontovitch type Impedance Boundary Condition (IBC) on Γ, have been established by Després [6], considering the minimization of a quadratic functional with constraints, over the outgoing and incoming solutions of Maxwell's equations. Later, a paper by Collino and Després [7] established a relationship between Després's Integral Equations (EID) and standard formulations like EFIE and CFIE. Indeed, the EID are based on a particular combination of the Stratton-Chu representation formulae with the IBC on Γ, a decomposition of the Green kernel in real and imaginary parts, a symmetric positive operator for the imaginary part, and new unknowns $V = (J', M')$ (the Lagrangian multipliers of the minimization problem) which satisfy for the continuous problem $V = \sigma(J, M) = \sigma(n \times H|_\Gamma, -n \times E|_\Gamma)$ where σ is some constant. The equations obtained then read:

$$\begin{pmatrix} (1+\beta)\mathbb{I} + (\mathbb{A}^\infty)^* \mathbb{A}^\infty & -\mathbb{T}^* + \mathrm{i}\beta\mathbb{I} \\ \mathbb{T} - \mathrm{i}\beta\mathbb{I} & \beta\mathbb{I} + (\mathbb{A}^\infty)^* \mathbb{A}^\infty \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} + \mathbb{N}_R U = \begin{pmatrix} G \\ 0 \end{pmatrix}$$

where

$$U = \begin{pmatrix} \sqrt{\mathrm{i}} J \\ \sqrt{\mathrm{i}^{-1}} M \end{pmatrix}, \qquad \mathbb{T} = \begin{pmatrix} T_r & K_r - \frac{1}{2}\mathbf{n}\times \\ K_r - \frac{1}{2}\mathbf{n}\times & T_r \end{pmatrix}, \qquad (\mathbb{A}^\infty)^* \mathbb{A}^\infty = \begin{pmatrix} T_i & K_i \\ K_i & T_i \end{pmatrix}$$

$$\mathbb{A}_\infty U(\hat{s}) = a_\infty(u_1, \hat{s}) - \mathrm{i}\hat{s} \times a_\infty(u_2, \hat{s}), a_\infty(u, \hat{s}) = \frac{\mathrm{i}k}{4\pi} \int_{\Sigma_P} \hat{s} \times \big(u(x) \times \hat{s}\big) \mathrm{e}^{-\mathrm{i}kx.\hat{s}} \, \mathrm{d}\Sigma_P(x)$$

T_r, K_r (resp. T_i, K_i) are the real part (resp. imaginary part) of classical integral operators of Stratton–Chu representation formulae. We have $\mathbb{N}_R = 0$ if the reflection coefficient $R = (Z-1)/(Z+1) = 0$, or $Z = 1$, which is the case of the transmission condition in (2). Considering new unknowns $X = (X_+, X'_+, X_-, X'_-)$ where $(X_+, X_-) = \sqrt{\mathrm{i}}(u_2 - u_1, u_2 + u_1) = (M - \mathrm{i}J, M + \mathrm{i}J)$, one can obtain two weakly coupled systems, uncoupled when $R = 0$:

$$\begin{pmatrix} \mathbf{A}_+ & \mathbf{N}_+ \\ \mathbf{N}_- & \mathbf{A}_- \end{pmatrix} \mathbf{X} = \mathbf{G}, \quad \text{where } \mathbf{A}_\pm = \begin{pmatrix} I + D_\pm & B_\pm \\ -B_\pm^H & D_\pm \end{pmatrix} \text{ and } \mathbf{N}_\pm = \begin{pmatrix} R(I \pm \mathrm{i}n \times I) & 0 \\ 0 & 0 \end{pmatrix} \tag{3}$$

where $D_\pm = T_i \pm K_i$ is symmetric positive and $B_\pm = (T_r \pm K_r \pm \frac{1}{2}n\times)$. This latter formulation is used for the exterior problem (2). System (3) is discretized using the Nédélec or RWG edge-based finite elements.

3.2. Iterative solution of the EID

3.2.1. Solution with a double conjugate gradient

In the case of the transmission condition in (2) between subdomains Ω_N and Ω_∞, for which $R = 0$, systems with (X_+, X'_+) and (X_-, X'_-) are uncoupled. The system with $\mathbf{A}_+$ (resp. $\mathbf{A}_-$) can be solved independently by employing

two imbricated solvers with Hermitian positive definite matrices. An efficient iterative solver—a double conjugate gradient—is then used. Systems solved by the internal and external CG have a small condition number, slowly increasing with the wave number, as is shown theoretically in [7] for spherical scatterers (see Section 5 for complex numerical cases).

In the case of a monostatic RCS calculation, we have extended the CG method to the case of multiple right hand sides, following the construction of the MGCR by Soudais [14], and applied it to the context of the double conjugate gradient.

3.2.2. Solution with a preconditioned flexible GMRES

Problems where the materials can be modeled by an impedance boundary condition prescribed on the outermost boundary of object can be solved by employing solely an integral equation formulation. This implies that $R \neq 0$, in which case both systems in X_+, X_- are coupled and a third level of iteration is needed (e.g., a Jacobi method). Then, it may be more efficient to solve the global EID system (3) with a more general iterative method. We have considered a preconditioned flexible GMRES [15]. The preconditioning matrix is obtained using an approximation of matrices $\mathbf{A}_\pm$, in the form:

$$\tilde{\mathbf{A}}_\pm = \begin{pmatrix} \mathrm{Diag}(I + D_\pm) & \tilde{B}_\pm \\ -\tilde{B}_\pm^H & \mathrm{Diag}(D_\pm) \end{pmatrix}$$

where $\tilde{B}_\pm$ is a sparse approximation of $B_\pm$. We have considered for this approximation the matrix of near interactions of the FMM (see next section). At each iteration of FGMRES, the (sparse) system for preconditioning is solved by a conjugate gradient as in the previous section.

3.2.3. Comparison with other formulations for large size systems

We conclude Section 3.2 with some practical comparisons of the EID with other more classical formulations, first for the above mentioned FE-IE coupling ($R = 0$), and then for the more general case where $R \neq 0$ (Léontovitch IBC).

The system size of the EID ($4N$) is twice that of the CFIE. For the double CG solution, we have two levels of iterations, but no preconditioning is needed, and we have theoretical results of convergence. For a general Léontovitch IBC and a GMRES solution, we have eight matrix–vector products per iteration, since sub-systems with $\mathbf{A}_+$ and $\mathbf{A}_-$ in (3) are weakly coupled. This is twice that of the classical formulations implemented with the Léontovitch IBC [16]. However, as shown in the next section, the acceleration of the matrix–vector products with the fast multipole method can be more efficient than the one of matrix–vector products for classical integral formulations.

3.3. Parallel multilevel fast multipole method

The iterative solution of system (3) has a complexity of order $\mathrm{O}(N^2)$—the cost of matrix-vector products—which implies prohibitive costs for large size systems. The Fast Multipole Method (FMM) can than be applied to factorize matrices $D_\pm$, $B_\pm$ into products of sparse matrices. The FMM for acoustic or electromagnetic problems accelerates the calculation of far interactions using a suitable approximation of the Green kernel and a clustering of interaction *points* in multipole boxes [17].

The product $\mathbb{Z}\mathbb{J}$ is decomposed into near and far interactions: $\mathbb{Z}\mathbb{J} = (\mathbb{Z}\mathbb{J})^{\mathrm{near}} + (\mathbb{Z}\mathbb{J})^{\mathrm{far}}$. Far interactions are obtained using an approximation of the integral kernel. For the real part ($B_\pm$), we use the following approximation: if $x - y = d + X$ with $|d| < |X|$, we have:

$$G_r(x, y) = \frac{\cos(|x - y|)}{4\pi |x - y|} \simeq -\frac{k}{(4\pi)^2} \oint_{S^2} T_L(\hat{s}, X) \mathrm{e}^{\mathrm{i}kd\cdot\hat{s}} \, \mathrm{d}\omega_s$$

where

$$T_L(\hat{s}, X) = \sum_{l=0}^{L} (2l + 1)\mathrm{i}^l y_l(kX) P_l\left(\hat{X} \cdot \hat{s}\right)$$

is the transfer function, with $y_l(u)$ the spherical Bessel function of the second kind and $P_l(\theta)$ the Legendre polynomial of order l. For the imaginary part ($D_\pm$) we have:

$$G_i(x,y) = \frac{\sin(k|x-y|)}{4\pi|x-y|} \simeq \frac{k}{(4\pi)^2} \oint_{S^2} \mathrm{e}^{\mathrm{i}k(x-y)}\,\mathrm{d}\omega_s$$

The Multi-Level Fast Multipole Algorithm (MLFMA) is based on an octree and has a numerical complexity of $O(N \ln N)$ [8]. The MLFMA has been applied to the EID for Maxwell's equations in [9,10]. The global cost of MLFMA applied to matrices of the EID is less than for classical integral equations [9]: (i) $\mathbb{Z}^{\text{near}}$ reduces to a real matrix for $B_\pm$ and vanishes for $D_\pm$; (ii) Multipole to Local translations for $D_\pm$ are needed at only one level (the coarser one); (iii) The vector far-field $F_B(\hat{s})$ has at least two components in classical integral methods [18]; it is reduced to a scalar far-field for the EID.

The algebraic form of MLFMA reads:

$$\mathbb{Z}\mathbb{J} \simeq \mathbb{Z}^{\text{near}}\mathbb{J} + \mathbb{V}\left(\sum_l (\mathbb{A}^l)^T \mathbb{T}^l \mathbb{A}^l\right)\mathbb{V}^H\mathbb{J}$$

where products with $\mathbb{V}^H$, $\mathbb{A}^l$, etc., are made successively ($l = L_f, \ldots, L_c$ are the levels of the octree). The parallelization of MLFMA consists of the parallelization of all these products. For message passing based parallelization, it is based on a load-balanced distribution of multipole boxes on processors and overlapped communications during the aggregation (upward step $\mathbb{A}^l$), disaggregation (downward step $(\mathbb{A}^l)^T$) and translation step $\mathbb{T}^l$. We have obtained an efficiency of 73% on 40 processors for the Dassault-Aviation Cetaf with 5 millions of unknowns, which is rather similar to the efficiency obtained in [19].

4. Sparse direct solver EMILIO

Solving large sparse symmetric positive definite systems of linear equations is a crucial step in our application described above (Odyssee), as in many scientific and engineering applications. Consequently, many parallel formulations for sparse matrix factorizations have been studied and implemented. For our specific needs, we have developed (in collaboration with INRIA's research project: ScAlApplix) an industrial, robust and versatile software: EMILIO [12]. The goal of this software is to give efficient solution to the problem of the parallel solution of large sparse linear systems by direct methods (especially Cholesky–Crout factorization $A = LDL^t$ for symmetric matrices). In fact, software of the INRIA's project is called PaStiX [11] and its industrial version is called EMILIO, which includes in addition algorithms for the parallel assembly of the matrix in the context of the finite element method. In order to achieve efficient parallel sparse factorization, three pre-processing steps are required:

- *Ordering*. The ordering step computes a symmetric permutation of the initial matrix A such that the factorization process will exhibit as much concurrency as possible while incurring low fill-in. In our software, we use a tight coupling of the Nested Dissection and Approximate Minimum Degree (AMD) algorithms. The partition of the original graph into supernodes is achieved by merging the partition of separators computed by the Nested Dissection algorithm and the supernodes amalgamated for each subgraph ordered by Halo Approximate Minimum Degree.
- *Block symbolic factorization*. The block symbolic factorization step determines the block data structure of the factorized matrix L associated with the partition resulting from the ordering step. This structure consists of N column blocks, each of them containing a dense symmetric diagonal block and a set of dense rectangular off-diagonal blocks. One can efficiently perform such a block symbolic factorization in quasi linear memory space and computation time.
- *Block repartitioning and scheduling*. The block repartitioning and scheduling step refines the previous partition by splitting large supernodes in order to exploit concurrency within dense block computations, and which maps the resulting blocks onto the processors.

Concerning the parallel stage of the software, the three main steps are:

– *Parallel assembly*. The parallel assembly step, which consists in computing the elementary matrix of each element and adding this elementary matrix to the global matrix A. Since the global matrix is distributed, the parallel assembly is guided by two distributions: the distribution of the column blocks of the matrix (described above) and the distribution of the elements of the mesh (distribution computed just after the pre-processing steps). Every processor computes the elementary matrices of the elements assigned to it, and can add immediately the new coefficients in its local part of the global matrix (if the unknowns of the element are entirely local) or send contributions to the processors involved by the updates of the matrix.
– *Parallel sparse LDL^t factorization without pivoting*. We use this factorization in order to solve sparse systems with complex coefficients. The parallel solver is based on a supernodal fan-in approach and is fully driven by the algorithm which computes an efficient static scheduling of the block computations.
– *Parallel solution of the system*. The parallel solution of the system is also fully driven by the static scheduling step.

Therefore, these parallel steps have been designed to achieve a good computation time scalability and to reduce the memory overhead arising in the direct parallel methods. Moreover, in the context of SMP-nodes architectures, to fully exploit shared memory advantages, a relevant approach is to use a hybrid MPI-threads implementation of the solver. In this way, the communications within a SMP node can be advantageously substituted by direct access to shared memory between the processors in the SMP node using threads. In an earlier investigation, we have performed with PaStix a computation with some 10 million unknowns (corresponding to the size of one subdomain) on 64 processors IBM Power4 with 2 SMP nodes (32 processors per node), 64 Gigabytes RAM per node. The factorized matrix has 6.7×10^9 non-zero terms and has been factorized with 43 Tera operations in 400 seconds.

Our current research opens up new prospects of bridging the gap between direct and iterative methods. The goal is to provide a method which exploits the parallel blockwise technique used in the framework of high performance direct solvers. We want to extend these high-performance algorithms to develop robust parallel incomplete factorization based preconditioners for iterative solvers such as GMRES or Conjugate Gradient solvers.

5. Numerical results

For the test cases presented, simulations are performed on the terascale supercomputer of CEA (SMP nodes—Compaq AlphaServer ES45, processors EV68 at 1 GHz).

The first test case is a sphere-cone with different layers of materials (Fig. 1). The 3-dimensional mesh is composed of 6 subdomains, and some subdomain interfaces intersect a layer of material. There are three different materials in the volume, with characteristics: ($\varepsilon_1 = 2$, $\mu_1 = 1$), ($\varepsilon_2 = \mu_2 = 1$), ($\varepsilon_3 = 1 + \mathrm{i}$, $\mu_3 = (1 + \mathrm{i})/2$). The total amount of DoF is more than 10 million in the computational domain, and the biggest subdomain reaches 2 million DoFs. The number of elements on the outer boundary is 145 000. Only 7 global iterations of the DDM algorithm give us a solution with a good accuracy. We have used the sparse direct solver for each subdomain and the double conjugate gradient for the EID. A mean value of 30 iterations is needed at each DDM iteration for the EID. This case runs with 64 processors in 4 hours. On this example, we can see the efficiency of the direct solver PaStix: for problem sizes up to 2 million DoFs, we need less than 300 seconds to perform the solution in each subdomain. In Fig. 1 we compare the bistatic Radar Cross Section at 2 GHz obtained with Odyssee and that obtained with a 2D axi-symmetric software (SHFC). The 2-D mesh used for SHFC is shown in Fig. 1. The incident wave is perpendicular to the axis of the cone. The 2 curves match perfectly for the 2 polarizations of the incident waves.

The geometry of the second test case has the form of a stopper (Fig. 2). The purpose of this test case is to see the impact of the concave interfaces with singularities on the convergence of the DDM iterative algorithm [4]. The 3-dimensional mesh is composed of 4 subdomains, with a specific material in each subdomain: $\varepsilon_1 = 1 + \mathrm{i}$, $\varepsilon_2 = 2$, $\varepsilon_3 = 0.71(1 + \mathrm{i})$, $\varepsilon_4 = 0.5(1 + \mathrm{i})$, $\mu_i = \varepsilon_i$. An impedance boundary condition $Z = 1$ is imposed on the boundary. The total amount of DoFs is 5.63 million in the computational domain. The number of elements on the outer boundary is 120 000. 7 global iterations of the DDM algorithm give us a solution with a good accuracy. We have used the sparse direct solver for each subdomain and the double conjugate gradient for the EID. A mean value of 26 iterations is needed at each DDM iteration for the EID. This case runs with 64 processors in 2 hours and 20 min. In Fig. 2 we compare the bistatic Radar Cross Section at 1 GHz obtained with Odyssee and the one obtained with a 2D axi-

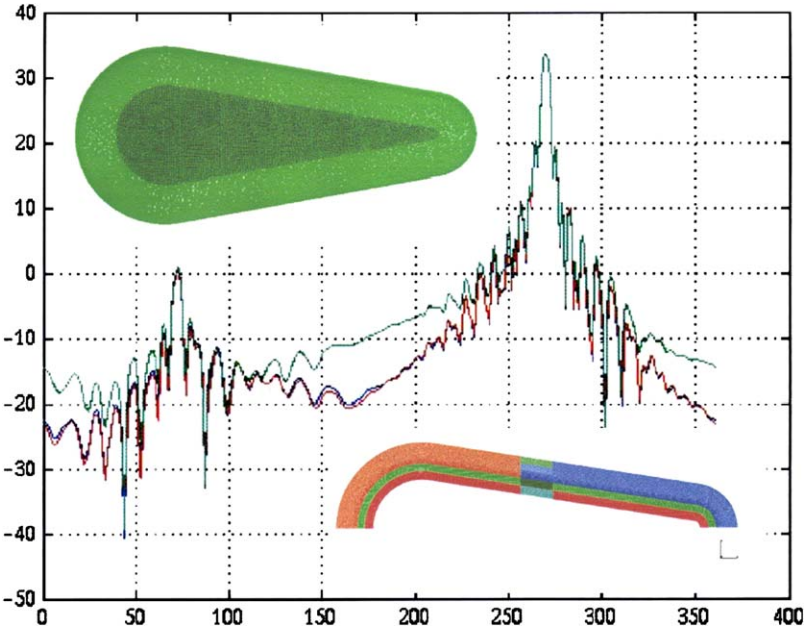

Fig. 1. Sphere-cone: 3-D and 2-D meshes, bistatic RCS (dB m^2) with Odyssee and SHFC.

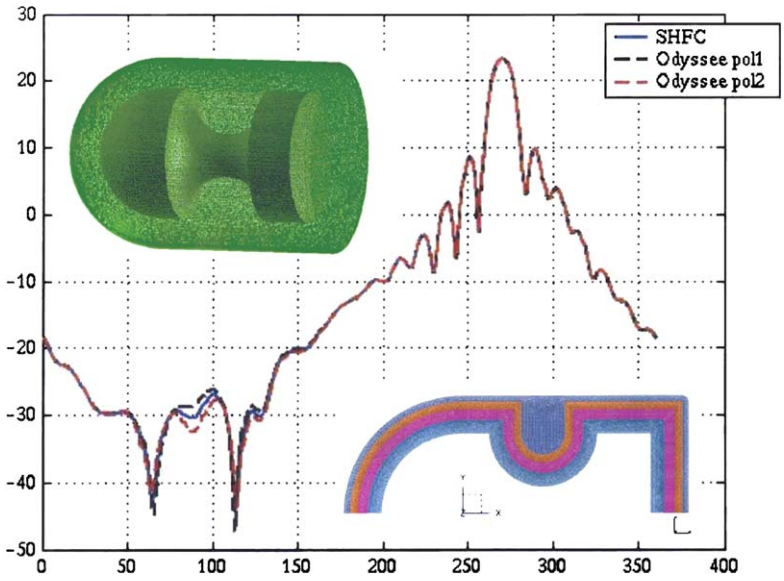

Fig. 2. Stopper: 3-D and 2-D meshes, bistatic RCS (dB m^2) with Odyssee and SHFC.

symmetric software (SHFC). The 2-D mesh used for SHFC is shown in Fig. 2. The incident wave is perpendicular to the axis of the cone. The 2 curves match well for the 2 polarizations of the incident waves.

6. Conclusion

We have presented a numerical strategy for electromagnetic scattering which efficiently couples a finite element discretization of the inhomogeneous part of the domain and a boundary integral method for the homogeneous unbounded exterior domain. The numerical results that have been presented illustrate the accuracy achieved on the RCS, and the efficiency of the iterative methods associated with the DDM and the EID. Moreover, the numerical complexity

has been further reduced by implementing a parallel multilevel fast multipole method for the iterative solution of the EID, together with an appropriate parallel sparse direct solver for the solution in the inner subdomains. Problems involving up to 10 million unknowns have been solved with six subdomains on 64 processors. In order to increase the numerical capabilities of the software, we have to further reduce the global cost of the EID solution, and to implement an hybrid parallelization that couples message passing and multi-threading. It is only in this context that computations involving 100 million unknowns with ten subdomains may be considered.

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