Parallelization of a Constrained Three-Dimensional Maxwell Solver

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Summary. The numerical solution of very large 3D electromagnetic field problems are challenging for various applications in the industry. In this paper, we propose a nonoverlapping domain decomposition approach for solving the 3D Maxwell equations on MIMD computers, based on a mixed variational formulation. It is especially well adapted for the solution of the Vlasov-Maxwell equations, widely used to simulate complex devices like particle injectors or accelerators. This approach in particular leads to reuse without modification most of an existing sequential code.

1 Introduction

In order to simulate complex devices like particle injectors and accelerators, we need in some cases a full three-dimensional code for the solution of the Vlasov-Maxwell equations. A three-dimensional code [7] has been written for this purpose and has already been used for many applications (see [9]). This code solves the instationary Maxwell equations with continuous approximations of the electromagnetic field. The time-stepping numerical scheme is explicit thanks to a mass lumping procedure and leads to an efficient algorithm. Moreover, in order to handle precisely the conditions on the divergence of the fields, these are considered as constraints. They are dualized, using a Lagrange multiplier, which yields a saddle-point variational formulation. In this paper, we propose a domain decomposition approach for the parallelization of this constrained 3D Maxwell solver. This choice allows us to reuse a large part of the sequential code for the solution on each subdomain. We first recall the constrained wave equation formulation of Maxwell's equations. Then we introduce a adapted variational formulation, the continuity at the interfaces being imposed by duality using Lagrange multipliers. Next, we describe the discretization and derive a linear system suitable for multiprocessor solution. The preconditioned Uzawa algorithm used for the solution of this system is then described. And finally we present an exemple of numerical application.

2 Constrained Wave Equation Formulation

Let Ω be a bounded, open subset of \mathbb{R}^3 , and Γ its boundary. We denote by **n** the unit outward normal to Γ . Let c, ε_0 and μ_0 be respectively the light velocity, the dielectric permittivity and the magnetic permeability, the Maxwell equations in vacuum read:

$$\frac{\partial \overrightarrow{E}}{\partial t} - c^2 \nabla \times \overrightarrow{B} = -\frac{1}{\varepsilon_0} \overrightarrow{J}, \quad \nabla \cdot \overrightarrow{E} = \frac{\rho}{\varepsilon_0}, \tag{1}$$

$$\frac{\partial \vec{B}}{\partial t} + \nabla \times \vec{E} = 0, \qquad \nabla \cdot \vec{B} = 0, \tag{2}$$

where \overrightarrow{E} and \overrightarrow{B} are the electric and magnetic fields respectively. the charge and current densities ρ and \overrightarrow{J} satisfy the charge conservation equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \overrightarrow{J} = 0.$$
(3)

These quantities depend on the space variable \vec{x} and the time variable *t*. It is well known that when Maxwell's equations are used in a Particle in Cell code, as the continuity equation (3) is not generally satisfied numerically, special care needs to be taken so that the Poisson equation $\nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0}$ remains satisfied throughout the length of the computation [4]. The same problem occurs for the $\nabla \cdot \vec{B} = 0$ condition on some unstructured meshes when the divergence of a curl is not close enough to zero. If these constraints were not satisfied then spurious modes could polute the numerical solution. This problem was dealt with in [1] by using a constrained wave equation formulation of Maxwell's equations that we recall in the case of perfectly conducting boundary conditions. These are the only ones that we shall consider here, as the case of any artificial boundary is not an issue for the parallelization. The electric field is then computed using the following equations:

$$\frac{\partial^2 \overrightarrow{E}}{\partial t^2} + c^2 \nabla \times \nabla \times \overrightarrow{E} - \nabla p = -\frac{1}{\varepsilon_0} \frac{\partial \overrightarrow{J}}{\partial t}, \quad \nabla \cdot \overrightarrow{E} = \frac{\rho}{\varepsilon_0}, \tag{4}$$

together with the perfectly conducting condition $\overrightarrow{E} \times \overrightarrow{n} = 0$ on the boundary Γ , and the initial condition $\overrightarrow{E}(t=0) = \overrightarrow{E}_0$. Moreover, dealing with a second-order problem, we add an initial condition for $\partial_t \overrightarrow{E}$, directly obtained from (1) as t = 0. To enforce the divergence constraint on the electric field we have introduced the Lagrange multipliers p to dualize the constraint in (1). The treatment on the magnetic field is performed in the same way.

3 Variational Formulations

Let us first introduce a few notations. The bounded domain Ω is subdivided into N disjoint subdomains that we denote by Ω_i , $1 \le i \le N$. The boundary between

subdomains *i* and *j*, if not empty, will be denoted by Σ_{ij} and the whole internal boundary of subdomain *i* will be denoted by $\Sigma_i = \bigcup_j \Sigma_{ij}$. Moreover for a distribution $\mathbf{T} \in H^{-1/2}(\Sigma_{ij})^3$ and a function $\mathbf{f} \in H^{1/2}(\Sigma_{ij})^3$, $\langle T, f \rangle_{\Sigma_{ij}}$ denotes the corresponding duality product. Let us also recall the definitions of the functional spaces:

$$H(curl, \Omega) = \{ \overline{E} \in L^2(\Omega)^3, \nabla \times \overline{E} \in L^2(\Omega)^3 \}, H(div, \Omega) = \{ \overline{E} \in L^2(\Omega)^3, \nabla \cdot \overline{E} \in L^2(\Omega) \}, H_0(curl, \Omega) = \{ \overline{E} \in H(curl, \Omega), \ \overline{E} \times \overline{n} = 0 \text{ on } \Gamma \}.$$

In fact we are dealing with a time-dependant problem and we should include this dependency in the definition of the functionnal spaces. For sake of simplicity we will only assume that every formulations in the sequel hold for almost any *t* in the time interval $[0, \mathcal{T}]$. The variational formulation for the constrained equation of the electric field on the whole domain, is obtained first by multiplying the wave equation in (4) by $\vec{F} \in H_0(curl, \Omega) \cap H(div, \Omega)$ (denoted $H_0(curl, div, \Omega)$). Then integrating by parts over Ω , we get a first mixed variational formulation which is well posed since the well known inf-sup condition [3, 5] is fulfilled. Adding $c^2 \int_{\Omega} \nabla \cdot \vec{E} \nabla \cdot \vec{F} d\vec{x}$ to its LHS and $c^2/\varepsilon_0 \int_{\Omega} \rho \nabla \cdot \vec{F} d\vec{x}$ to its RHS, we get an augmented variational formulation which reads:

Find
$$(\vec{E}, p) \in H_0(curl, div, \Omega) \times L^2(\Omega)$$
 such that :

$$\frac{d^2}{dt^2} \int_{\Omega} \vec{E} \cdot \vec{F} \, d\vec{x} + c^2 \left(\int_{\Omega} \nabla \times \vec{E} \cdot \nabla \times \vec{F} \, d\vec{x} + \int_{\Omega} \nabla \cdot \vec{E} \, \nabla \cdot \vec{F} \, d\vec{x} \right) + \int_{\Omega} p \nabla \cdot \vec{F} \, d\vec{x}$$

$$= -\frac{1}{\epsilon_0} \frac{d}{dt} \int_{\Omega} \vec{J} \cdot \vec{F} \, d\vec{x} + c^2 / \epsilon_0 \int_{\Omega} \rho \nabla \cdot \vec{F} \, d\vec{x} \quad \forall \vec{F} \in H_0(curl, div, \Omega), \tag{5}$$

$$\int_{\Omega} \nabla \cdot \overrightarrow{E} q \, d \, \overrightarrow{x} = \frac{1}{\varepsilon_0} \int_{\Omega} \rho q \, d \, \overrightarrow{x} \quad \forall q \in L^2(\Omega).$$
(6)

This formulation is well posed as well. In order to get a Maxwell solver suitable for multiprocessor computation, we introduce a variational formulation, which allows to treat each subdomain Ω_i separately. The continuity conditions are expressed on the tangential and the normal part separately. The continuity conditions across the interfaces Σ_{ij} , i.e. between the different subdomains, are written as $[\vec{E} \times \vec{n}_i]_{\Sigma_{ij}} = 0$ and $[\vec{E} \cdot \vec{n}_i]_{\Sigma_{ij}} = 0$ where $[.]_{\Sigma_{ij}}$ is the jump across Σ_{ij} and \vec{n}_i the unit normal outward vector to Ω_i . Now, to handle these conditions, we enforce the continuity of the electric field by duality, introducing Lagrange multipliers on the subdomain interfaces. This method is similar in spirit to the dual Schur complement method as in [6]. A dualization procedure was also used in [2] to deal with continuity at material interfaces. We thus introduce the new unknowns λ_{ij} , which are the Lagrange multipliers of the above constraints. We define the functional space associated to the broken domain with no continuity requirement at the interfaces:

$$X_0 = \{ \overrightarrow{E} \in L^2(\Omega)^3, \overrightarrow{E}_{|\Omega_i} \in H(curl, \Omega_i) \cap H(div, \Omega_i), \overrightarrow{E} \times \overrightarrow{n} = 0 \text{ on } \Gamma \}.$$

Next we define the trace space on the internal boundaries

$$M = \left\{ \overrightarrow{\mu} \in \prod_{ij} (H^{1/2}(\Sigma_{ij}))^3; \ \exists \overrightarrow{F} \in H_0(curl, div, \Omega) \text{ with } \overrightarrow{F}_{|\Sigma_{ij}} = \overrightarrow{\mu}_{|\Sigma_{ij}} = \overrightarrow{\mu}_{ij} \right\}.$$

We shall decompose at any point of an internal boundary which is not shared by more than two subdomains any trace vector $\vec{\mu}$ in μ_n its normal component and $\vec{\mu}_T$ its tangential component. The orientation of \vec{n} is chosen so that the normal be outward for the subdomain with the smallest index. This decomposition is well defined almost everywhere on the internal boundary. We recall that the scalar components of the tangential traces of fields in $H(curl, \Omega_i)$ along Σ_{ij} , as well as the normal traces of fields in $H(div, \Omega_i)$ are defined in $H^{-1/2}(\Sigma_{ij})$. Then, the spaces $H^{1/2}(\Sigma_{ij})$ will be the natural functional spaces for these Lagrange multipliers $\vec{\lambda}_{ij}$. Then, from the augmented formulation (5)-(6) the new variational formulation defined on the whole broken domain Ω reads:

Find
$$(\vec{E}, p, \vec{\lambda}) \in X_0 \times L^2(\Omega) \times M$$
 such that :

$$\frac{d^2}{dt^2} \sum_i \int_{\Omega_i} \vec{E} \cdot \vec{F} \, d\vec{x} + c^2 \left(\sum_i \int_{\Omega_i} \nabla \times \vec{E} \cdot \nabla \times \vec{F} \, d\vec{x} + \sum_i \int_{\Omega_i} \nabla \cdot \vec{E} \, \nabla \cdot \vec{F} \, d\vec{x} \right) + \sum_i \int_{\Omega_i} p \nabla \cdot \vec{F} \, d\vec{x} + \sum_{ij} (\langle \lambda_n, [\vec{F} \cdot \vec{n}] \rangle_{\Sigma_{ij}} + \langle \vec{\lambda}_T, [\vec{F} \times \vec{n}] \rangle_{\Sigma_{ij}}) = -\frac{1}{\varepsilon_0} \frac{d}{dt} \sum_i \int_{\Omega_i} \vec{J} \cdot \vec{F} \, d\vec{x} + c^2 / \varepsilon_0 \sum_i \int_{\Omega_i} \rho \nabla \cdot \vec{F} \, d\vec{x} \quad \forall \vec{F} \in X_0, \qquad (7)$$

$$\sum_i \int_{\Omega_i} \nabla \cdot \vec{E} \, ad\vec{x} = \frac{1}{\varepsilon_0} \sum_i \int_{\Omega_i} \forall a \in L^2(\Omega), \qquad (8)$$

$$\sum_{i} \int_{\Omega_{i}} \nabla \cdot \vec{E} q d\vec{x} = \frac{1}{\varepsilon_{0}} \sum_{i} \int_{\Omega_{i}} \rho q d\vec{x} \quad \forall q \in L^{2}(\Omega), \quad (8)$$

$$\sum_{ij} (\langle \mu_n, [\vec{E} \cdot \vec{n}] \rangle_{\Sigma_{ij}} + \langle \vec{\mu}_T, [\vec{E} \times \vec{n}] \rangle_{\Sigma_{ij}}) = 0 \quad \forall \vec{\mu} \in M,$$
(9)

Following the strategy by Raviart and Thomas [8] it has been proven that this problem has a unique solution $(\vec{E}, p, \vec{\lambda})$ of which (\vec{E}, p) is the solution to the problem posed in the whole domain:

Theorem 1. Assuming that Ω is a convex polyhedron, problem (7)–(9) has a unique solution $(\vec{E}, p, \vec{\lambda}) \in X_0 \times L^2(\Omega) \times M$. Moreover, $(\vec{E}, p) \in H_0(curl, \Omega) \cap H(div, \Omega) \times L^2(\Omega)$ is the solution to the problem (5)–(6) and we have $\lambda_n = (\frac{c^2}{\epsilon_0}\rho - c^2\nabla \cdot \vec{E} - p)_{\Sigma_{ij}}, \ \vec{\lambda}_T = c^2(\nabla \times \vec{E})_{T|\Sigma_{ij}} \text{ on } \Sigma_{ij}.$

4 Space and Time Discretization

We assume that the domain Ω is first meshed with tetrahedra and then a mesh partitioner is used to subdivide the mesh into disjoint sub-meshes which correspond to the subdomains Ω_i , so that the intersection of the subdomains consists of faces of tetrahedra which coincide on each side. Following the method described in [1, 2], Taylor-Hood elements are used. For this purpose the coarse mesh of tetrahedra \mathcal{T}_{2h} is subdivided, each tetrahedron being subdivided into eight sub-tetrahedra to give the finer mesh \mathcal{T}_h . We shall denote by $(\varphi_k)_k$ the P^1 basis functions on the finer mesh and by $(\Psi_l)_l$ the P^1 basis functions associated to the coarser mesh. Let us also denote by $P_h^1(\Omega_i)$ the P^1 space defined on the fine mesh of Ω_i and $P_{2h}^1(\Omega_i)$ the P^1 space defined on the coarse mesh of Ω_i . We define $V_{hi} \subset P_h^1(\Omega_i)^3$ the finite dimensional space associated to $H_0(curl, \Omega_i) \cap H(div, \Omega_i)$ and $L_{2h} \subset P_{2h}^1(\Omega_i)$ the finite dimensional space associated to $L^2(\Omega_i)$ in the conforming finite element approximation, see [1] for more precisions. We can now introduce the finite dimensional space $T_{hij} = \{\vec{\tau} \in P_h^1(\Sigma_{ij})^3, \vec{\tau}(x) \cdot \vec{n}_i = 0\}$ for the discretization of the interfaces.

Then, we introduce the matrices associated to the different terms in the variational formulation. For the domain Ω_i , we denote by M_i the lumped mass matrix for vectors on the fine mesh and M_{2i} the lumped mass matrix corresponding to scalars on the coarse mesh. We denote by K_i the matrix corresponding to $c^2 \int_{\Omega_i} \nabla \times \vec{E}_i \cdot \nabla \times \vec{F}_i d\vec{x} + c^2 \int_{\Omega_i} \nabla \cdot \vec{E}_i \nabla \cdot \vec{F}_i d\vec{x}$, L_i the matrix corresponding to $\int_{\Omega_i} \nabla \cdot \vec{E}_i q_i d\vec{x}$ and R_{ij} the matrix corresponding to $\langle \vec{E}_i \cdot \vec{\mu}_{ij} \rangle$. Moreover for any matrix A, A^T denotes the transpose of A. In order to verify the discrete inf-sup condition, the electric field is approximated on the finer mesh \mathcal{T}_h (with the subscript h), whereas the Lagrange multiplier p is approximated on the coarser mesh \mathcal{T}_{2h} (with the subscript 2h). With this notation problem (7)–(9) discretized in space becomes

$$\frac{d^2}{dt^2} M_i \overrightarrow{E}_{hi}(t) + K_i \overrightarrow{E}_{hi} + L_i^T p_{2hi} + \sum_j \varepsilon_{ij} R_{ij}^T \overrightarrow{\lambda}_{hij} = -\frac{1}{\varepsilon_0} \frac{d}{dt} M_i \overrightarrow{J}_{hi}(t)$$
(10)

$$L_i \overrightarrow{E}_{hi}(t) = \frac{1}{\varepsilon_0} M_{2i} \rho_{2hi} \tag{11}$$

$$R_{ij}(\vec{E}_{hi} - \vec{E}_{hj}) = 0, \qquad (12)$$

with ε_{ij} defined by $\varepsilon_{ij} = 1$ if i < j and $\varepsilon_{ij} = -1$ if i > j. For time differentiation we choose an explicit centered scheme of order two (the leap-frog scheme), where Δt is the time-step and $t_n = n\Delta t$ are the discrete times. In order to enforce the constraints numerically the Lagrange multipliers are defined at the most advanced time steps. This yields, in each of the subdomain Ω_i , the following matrix problem which needs to be solved at each time step:

$$M_i \overrightarrow{E}_{hi}^{n+1} + L_i^T p_{2hi}^{n+1} + \sum_j \varepsilon_{ij} R_{ij}^T \overrightarrow{\lambda}_{hij}^{n+1} = \overrightarrow{F}_i^n$$
(13)

$$L_i \overrightarrow{E}_{hi}^{n+1} = \frac{1}{\varepsilon_0} M_{2i} \rho_{2hi}^{n+1}$$
(14)

$$R_{ij}(\overrightarrow{E}_{hi}^{n+1} - \overrightarrow{E}_{hj}^{n+1}) = 0, \qquad (15)$$

where \vec{F}_{i}^{n} contains all the terms being known at time t_{n+1} .

Let us now give an expression of the full linear system, involving all the subdomains. We denote $\vec{u} = (\vec{E}_1, p_1, \dots, \vec{E}_N, p_N)^T$ and $\vec{\lambda} = (\vec{\lambda}_{12}, \dots)^T$. Then the linear system to be solved has the form:

$$\begin{pmatrix} A \ R^T \\ R \ 0 \end{pmatrix} \begin{pmatrix} \overrightarrow{u} \\ \overrightarrow{\lambda} \end{pmatrix} = \begin{pmatrix} \overrightarrow{G} \\ 0 \end{pmatrix}$$
(16)

where

$$A = \begin{bmatrix} A_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & A_N \end{bmatrix}, \quad A_i = \begin{pmatrix} M_i & L_i^T \\ L_i & 0 \end{pmatrix}$$

and \vec{G} is the vector built up with the right-hand sides of (13) and (14). We chose to solve this system with an iterative algorithm, similar to the Uzawa algorithm. Noticing that we can eliminate the unknowns $(\vec{E}_1, p_1, ..., \vec{E}_N, p_N)$ in the system to get $RA^{-1}R^T \vec{\lambda} = RA^{-1}\vec{G}$, the Uzawa algorithm amounts to using a conjugate gradient algorithm on this latter system. The solution of this system involves the inversion of *A* which amounts to the local solution on each subdomain of the original constrained problem which was solved in the sequential code.

5 Solution of the Doubly Constrained System

In order to solve this doubly constrained system we shall use two embedded preconditioned Uzawa algorithms. The preconditioner of the outer Uzawa problem must be an approximate inverse of $RA^{-1}R^T$. We first remark that the columns of R corresponding to the degrees of freedom p_i are identically null. Therefore we have to find an approximate of $\tilde{R}\tilde{A}^{-1}\tilde{R}^T$ where \tilde{R} (resp. \tilde{A}) is the $N \times m$ (resp. $N \times N$) block submatrix extracted from R (resp. A) by eliminating the blocks related to the p_i 's. The analysis of the inner system yields that on each sub-domain *i*:

$$\tilde{A}_i = M_i^{-1} - M_i^{-1} L_i^T (L_i M_i^{-1} L_i^T)^{-1} L_i M_i^{-1}$$

The simplest preconditionner of the outer Uzawa problem is therefore defined as $P_{out} = \tilde{R}D\tilde{R}_T$ where *D* is a block diagonal matrix, each block D_i being a diagonal approximation of \tilde{A}_i . Noticing that $L_i M_i^{-1} L_i^T$ is the inner Uzawa operator we chose $D_i = diag(M_i^{-1} - M_i^{-1}L_i^T P_{in,i}^{-1}L_i M_i^{-1})$ with $P_{in,i}$ the preconditionner of the inner Uzawa problem. At every iteration of the outer Uzawa algorithm, we have to solve on each subdomain Ω_i the linear system:

$$\begin{cases} M_i \overrightarrow{E}_i + L_i^T p_i = \overrightarrow{b}_i \\ L_i \overrightarrow{E}_i = c_i \end{cases}$$

with the inner Uzawa algorithm. Note that, thanks to the chosen distribution of the matrix R, the outer Uzawa algorithm involves only local matrix vector products and reductions in addition to the local inner Uzawa solves.

6 Numerical Application

We present a classical test case related to the time evolution of a cavity resonant mode. We consider a cubic cavity enclosed in a perfect conductor in a cube of side equal to one. At time t = 0 we initialize the field components in the whole domain with the analytical expressions calculated at the initial time. Then the field values obtained at the final computational time $t = T_f$ can be compared with the exact solution. The cube is discretized by cutting each side into 16 pieces and then each resulting smaller cube into 6 tetrahedra. This gives us the coarse mesh. The associated fine mesh then consists of 196608 elements. We performed the domain decomposition by hand using the specificity of our mesh. The fields depicted on Fig. 1 enable us to verify visually that the results are correct, which is confirmed by comparison to the analytical results. The results are identical for the runs on different numbers of processors. We have also verified that even with an irregular partitionning such as those obtained with Metis the results are correct as well. In order to verify the ef-



Fig. 1. Components E_x and E_z computed on 4 processors

ficiency of the parallelization, we ran this test case on 1, 2, 4, 8 and 16 processors. Except, when going from 1 to 2 processors which does not give any improvement due to the overhead linked to the outer Uzawa the speed-up is proportional to the number of processors which corresponds to the optimal performance one can expect from the parallelization. For instance, for 300 time steps without diagnostics on an Origin 2000 with R10000 processors, the computation times are 6 min 27 s for one processor, 3 min 33 s for 4 processors and 53 s for 16 processors. However, these results about the efficiency of this parallelization algorithm must be assessed with regard to the accuracy achieved on the continuity of the solution at the interfaces and moreover to the error between the result on one processor and the results on several ones.

7 Conclusion

In this paper, we presented a nonoverlapping domain decomposition approach for solving the three-dimensional time-dependent Maxwell equations. It is constructed from a mixed variational formulation, as a constraint on the divergence is taken into account explicitely. For this purpose, it is especially well adapted for the solution of the Vlasov-Maxwell equations, widely used in the framework of plasma physics or hyperfrequency devices simulations. The domain decomposition methodology we chose to implement has the important asset, which led us to choose it, that it enables to reuse without modification most of the existing sequential code. It requires only to add an external Uzawa algorithm in order to enforce the continuity of the fields at the subdomain interfaces.

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