Parallel Direct Solver for the Finite Integration Technique in Electrokinetic Problems

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The finite integration technique allows the simulation of real-world electromagnetic field problems with complex geometries. It provides a discrete reformulation of Maxwell's equations in their integral form suitable for numerical computing. The resulting matrix equations of the discretized fields can be used for efficient numerical simulations on modern computers and can be exploited to use a parallel computing. In fact, by reordering the unknowns by the nested dissection method, it is possible to directly construct the lower triangular matrix of the Cholesky factorization with many processors without assembling the matrix system. In this paper, a parallel algorithm is proposed for the direct solution of large sparse linear systems with the finite integration technique. This direct solver has the advantage of handling singularities in the matrix of linear systems. The computational effort for these linear systems, often encountered in numerical simulation of electromagnetic phenomena by finite integration technique, is very significant in terms of run-time and memory requirements. Many numerical tests have been carried out to evaluate the performance of the parallel direct solver.

Index Terms—**Finite element methods, finite integration technique, linear systems, numerical analysis, parallel algorithms.**

I. Introduction

THE finite integration technique (FIT) [7]–[9] is one of the most successful numerical methods for the simulation of electromagnetic fields and of various coupled problems. This method is a consistent formulation for the discrete representation of Maxwell's equations on spatial grids. The key idea is to use the integral form in the discretization, rather than the differential form of Maxwells equations. By discretizing the integral form of Maxwell's equations on a pair of dual interlaced discretization grids, the finite integration technique generates so-called Maxwell's grid equations that guarantee the physical properties of computed fields and lead to a unique solution. The success of the FIT is probably due to two factors. First, it is an algorithm with a sound theoretical foundation including stability and orthogonality of numerically computed modes. Energy and charge conservation were demonstrated in a very early stage. Secondly, it is applicable not only in frequency but also in time domain, thus allowing the simulation of very large or very complex structures. The FIT, as the F.E.M [3], produces large systems which are usually solved by iterative or direct solvers [8]. The iterative solvers generate a sequence of approximate solutions. If the system is very sparse, these solvers are interesting because the utilization of memory is low. The Krylov subspace methods [8] are a powerful and widely used class of iterative solvers to solve the large and sparse linear systems. But it is should be noted that they may require a lot of iterations for convergence. So, a good preconditioner is necessary in order to improve the convergence rate and to get fast solutions. On the other hand, the direct solvers are important because of their generality and robustness. Indeed, for many cases, this is the method of choice because finding and computing a good preconditioner for an iterative solvers can be more expensive than using a direct method. These solvers compute factorization (Gauss for unsymmetric matrices, Cholesky for symmetric positive definite matrices [10]) and use the factors to solve the linear system. For sparse matrices these solvers involve much more complicated algorithms than for dense matrices. The main complication is due to the need of efficient handling of the fill-ins (zero entries turn into non-zero). These fill-ins are generated in the factors due to the factorization. For large systems the filling can be costly (CPU time) and require a very high storage capacity. Recently, the memory capacities have been increased and can accommodate a large full system. Moreover, as the CPU clock frequency stagnates, the number of processors increases to keep a constant acceleration of computing power. Nowadays, many new algorithms and software have emerged. They exploit new architectural features, such as memory hierarchy and parallelism. For example, the scientific libraries SuperLU [4] and Mumps [2] provide high performance solvers for very large sparse linear systems.

In this paper, the FIT is used to compute the electromagnetic phenomena. The system obtained has some priorities of regularity which can be used for the parallel computing. As the sizes of the problems increase and considering that the systems of equations need to be solved as efficiently as possible, it is necessary to exploit multiprocessors. Furthermore, in order not to use a large memory, the reordering technique (Nested Dissection [5]) is implemented to minimize the fill-ins during the factorization process. This technique keeps the regular structure of a matrix, with which it is easy to extract an efficient parallel computing without latency. The used of parallel direct solvers, provided by software libraries, is not interesting because they require the assembled matrix system. In addition, the matrix of the system should be nonsingular which requires a gauge condition. Due to these conditions, this paper proposes a parallel direct solver for FIT, in which the matrix systems can be assembled and factorized at the same time with a parallel performing.

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A strategy is proposed to automatically and properly treat the singularities in the factorized matrix.

II. The Finite Integration

The FIT generates exact algebraic analogues to Maxwell's equations, which guarantee that the physical properties of the fields are maintained in the discrete space. Moreover, it is necessary to define a dual mesh in order to construct the model. The local forms of Maxwell's equations are used on a set of primal and dual meshes. The primal mesh is composed of elements which are constructed using nodes, edges and facets. The dual mesh is introduced to define the necessary support for variables. For example, the discrete electric circulation is defined on the dual edges if the current density is defined across the primal facets and vice versa.

Maxwell's equations and the related material equations are transformed from the continuous to the discrete space by allocating electric and magnetic vector fields on the primal and the dual meshes. In this paper, both potential (scalar and vector) formulations of the electrokinetic problem are treated. In this case, the Maxwell's equations are

$$\boldsymbol{Curl}\boldsymbol{E} = 0 \tag{1}$$

$$\boldsymbol{Div}\boldsymbol{J} = 0 \tag{2}$$

with the electric field $\boldsymbol{E}$ and the current density $\boldsymbol{J}$.

At the first step, the electric vector potential formulation ($\boldsymbol{T}$-formulation) is used by considering $\boldsymbol{CurlT} = \boldsymbol{J}$. The electric field is discretized on the dual mesh then the circulation of electric field $\tilde{e}$ is defined by $\tilde{e} = \boldsymbol{E}.\tilde{l}$ with $\tilde{l}$ is the length of dual edge. The (1) can be solved by using the integral form [7]. On each dual facet the equation must be verified as

$$\sum_{i=1}^{4} \tilde{C}_i \tilde{e}_i = 0$$

The parameter $\tilde{C}_i$ shows the edges orientation. For all the dual facets, the incidence matrix (facet-edge) can be defined as the discrete operator $\boldsymbol{Curl}$ such as: $\tilde{C}\tilde{e} = 0$

In this case, the discrete behavior law is written as follows:

$$[j] = \left[[\tilde{l}]^{-1}[\sigma][S]\right][\tilde{e}] = [M_{fe}][\tilde{e}]$$

j represents the discrete form of the current density $\boldsymbol{J}$ such as $j = \boldsymbol{J}.S$ and S is the area of primal facet across by $\boldsymbol{J}$. $[\tilde{l}]$ is the diagonal matrix of dual edges length, $[S]$ is the diagonal matrix on area of primal facets and $[\sigma]$ denotes the matrix of electric conductivity such as $\boldsymbol{J} = \sigma.\boldsymbol{E}$. The obtained matrix M_{fe} is diagonal. The following linear system has to be solved:

$$C^T M_{ef} C T = C^T M_{ef} C^T T_s \tag{3}$$

The "$\boldsymbol{Curl}$"-matrix C is a topological matrix (has only elements 0, $+1$ or -1) and represents the edges-to-faces incidence matrix on the primary grid ($C = \tilde{C}^T$). $M_{ef} = M_{fe}^{-1}$ defines the mass matrix, the electrical vector potential and source are T and T_s respectively. The unknowns and source potentials are defined on primal edges. With this formulation a current density is imposed through the conductor by T_s [7].

For the scalar formulation (φ-formulation), $\boldsymbol{E}$ is defined on primal edges. With a similar process for scalar formulations, the final system will be

$$G^T M_{ne} G\varphi = G^T M_{ne} G^T \varphi_s \tag{4}$$

where G is the incidence matrix node-edge, M_{ne} represents the mass matrix, φ is the electrical scalar potential and φ_S is a scalar potential derived from source field (it allows to impose a voltage between two equipotential surfaces) [7]. This verifies the discrete form of the (2) with $\boldsymbol{E} = -\boldsymbol{Grad}\,(\varphi + \varphi_S)$. The potential φ is on the primal nodes and M_{ne} is obtained from

$$[\tilde{j}] = \left[[l]^{-1}[\sigma][\tilde{S}][e]\right] = [M_{ne}][e]$$

where $\tilde{j}$ represents the discrete form of the current density $\boldsymbol{J}$ on the dual mesh such as $\tilde{j} = \boldsymbol{J}.\tilde{S}$ and $\tilde{S}$ the area of the dual facet. With the help of a scalar potential source, a voltage between two electrodes can be imposed.

The matrices M_{ne} and M_{ef} are diagonal due to which the generated systems (3) and (4) have a regular structure.

The matrices $G^T M_{ne} G$ and $C^T M_{ef} C$ are symmetric positive semi-definite. For both formulations a gauge must be defined to solve the numerical systems (3) and (4) with a direct solver. For the φ-formulation just one unknown is fixed to zero. However a $\boldsymbol{T}$-formulation is classically gauged with a tree technique. In these conditions $G^T M_{ne} G$ and $C^T M_{ef} C$ will become symmetric positive definite matrices.

In this paper, it is proposed to use a practical approach to gauge these systems into the factorization.

III. Parallel Direct Solver

Solving large sparse linear systems is essential in numerous scientific domains. Several algorithms, based on direct methods, have been developed for parallel architectures [2], [4]. These solvers often have three distinct computational phases: analyze, factorize, and solve. The analysis phase (sometimes referred to the symbolic factorization or ordering step) determines a pivotal sequence and the data structures for the factorization. During the factorization phase, this sequence is used to compute the matrix factors. Forward elimination followed by a back substitution is performed during the solving phase using the stored factors.

In this section, a parallel direct solver is developed for the FIT using Cholesky factorization in the assembling of the singular system (3) and (4). This solver consists in three major steps: First, the problem is subdivided, with the nested dissection reordering, into a (small) number of loosely connected sub-problems. Secondly, the Cholesky algorithm is used into the assemblage; the factorized matrices of these sub-problems are directly assembled in parallel. This is also the case for the boundaries of the sub-problems. Lastly, a parallel resolution is used to obtain the solution. This solver is developed for multi-processor environments such as parallel machines or clusters.

A. Nested Dissection Method

The goal of the reordering techniques is to decrease the amount of fill-in and reduce the number of operations in the factorization and resolution of linear systems. The two most classical reordering methods used are the Minimum Degree [1] and the Nested Dissection [5]. The choice to use the nested dissection method comes from the fact that this technique allows, at first, more parallelism in the factorization than those using minimum degree techniques, but more importantly, it often produces better results.

Nested Dissection is a method of finding an elimination ordering. The algorithm uses a divide and conquer strategy on the

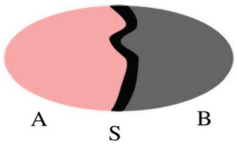

Fig. 1. 1 step of nested dissection.

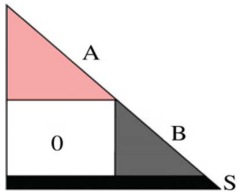

Fig. 2. Matrix structure.

graph of the matrix. The nested dissection approach is based on a recursive bisection of the graph of the matrix to be factorized. The basic idea of this method is the following: A first bisection is performed by selecting a set of vertices forming a separator. This separator is then removed from the original graph, and this generates a partition with two unconnected sub-graphs. The separator is chosen so that its size is as small as possible and that the sizes of the two delimited sub-graphs are equivalent. Each of the two sub-graphs is then bisected recursively following the same principle, until sub-graphs are successively generated with an indivisible size. The Nested Dissection reordering approach consists in ordering the unknowns of the sparse linear system in blocks such that the separator nodes receive a higher label than any of the nodes of the sub-graph. The recursion ends when the sub-graphs become too small. This analysis step produces an ordering matrix and an assembly tree. This assembly tree is then used to carry out the subsequent steps.

To illustrate this method, an example with a domain bisected by a single node separator (Fig. 1) is provided. The matrix system is split into the form shown in (Fig. 2)

The blocks A and B correspond to the sub-graphs, they are independent and are connected by S which corresponds to the node separator.

B. Assemblage and Factorization

The assemblage of the system (3) and (4) can be easily implemented element by element because the mass matrices M_{ef} and M_{ne} are diagonal respectively. The implementation of these systems mainly depends on the connectivity node-node for (3) and edge-edge for (4). The numerical factorization is performed by implicitly computing the lower triangular factor L of the sparse matrix system by using an assembly tree. This factorization is implemented into the assemblage. The factorization keeps the same block structure of the matrix provided by the Nested dissection. The lower triangular factor L, with a single node separator, is split into the following form:

$$L = \begin{bmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{bmatrix}$$

The blocks L_{11} and L_{22} correspond to the sub-graphs. These two sub-graphs are not joined by any edges for the reason that L_{21} is zero. Otherwise, L_{11} and L_{22} can be assembled in sparse and simultaneously. L_{33} is the block corresponding to the node separator and assembled in dense storage because the fill-in is completed. This process is always true for all sub-graphs and the node separators. Without reordering, the structure of L is shown in Fig. 3. When the reordering technique (Nested Dissection) of the nodes is used, the matrix L (Fig. 4) has less non-zero elements than without reordering. The matrix L (Fig. 4) can directly be generated in parallel because its block structure allows it.

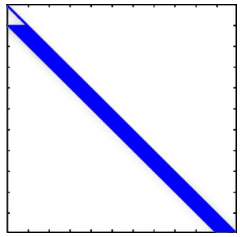

Fig. 3. Matrix without reordering.

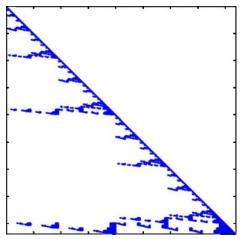

Fig. 4. Matrix system with reordering.

The Cholesky factorization [10] can only be used when the studied matrix system is symmetric positive definite. Here the systems (3) and (4) are positive semi-definite. In this paper, an approach is proposed to automatically detect singularities in these matrices: In the assemblage of L, if we found a near zero pivot at the kth row and column, the kth row and column are deleted and the kth unknown is fixed at zero. The resulting system is non singular but symmetric positive definite.

C. Resolution of Triangular Systems

Finally, the solution is computed by solving two triangular systems. $Ly = b$ is solved by forward elimination and followed by the resolution of $L^T x = y$ with backward substitution. These two substitutions are also parallelized because many set of unknowns are independents.

IV. Applications

In this paper, two current flow problems are treated to illustrate the efficiency of the proposed method. At first, a cylindrical cover connected to electric distribution wires is chosen as shown in Fig. 5. Because of the circular symmetry of the cylindrical cover, only 1/12 portion of this system is studied. The materials Almelec strand and metallic part are used. There are two parts ② and ④ which are coupled with the wire ① and ③. The conductivities from material ① to ④ are respectively 59.6 10^6 S/m, 59.6 10^6 S/m, 30.8 10^6 S/m and 30.8 10^6 S/m. ⑤ represents the contact resistances between the wire and the cylindrical covers (5250, 1163 and 2945 S/m).

To study this system, two meshes with orthogonal hexahedrons are used and the generated meshes are deformed to study the cylindrical geometries. The first mesh has 13662 nodes and 38097 edges brought 13226 unknowns for φ-formulation and 27960 unknowns for $\boldsymbol{T}$-formulation respectively. The second

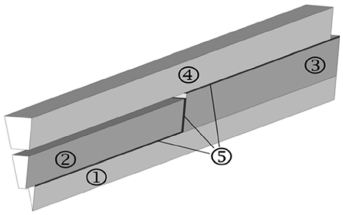

Fig. 5. 1/12 of cylindrical cover.

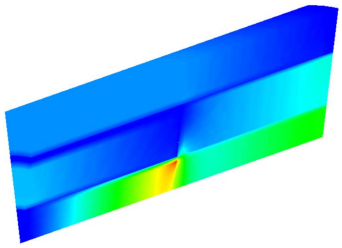

Fig. 6 Norm of the current density distribution.

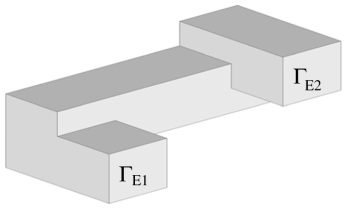

Fig. 7. Ordinary conductor.

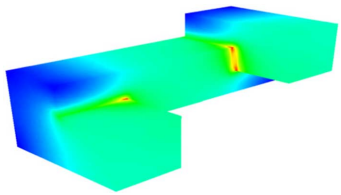

Fig. 8. Norm of the current density distribution.

mesh has 118767 nodes and 342886 edges with 117425 unknowns for the φ-formulation and 293466 unknowns for $\boldsymbol{T}$-formulation respectively. A voltage of 150 μV is imposed to allow a current of 1652 A with a power of 247.9 mW. Current distribution is shown in Fig. 6.

The second system shown in Fig. 7 is an example of an ordinary conductor. The conductivity is 59.6 10^6 $\mathrm{S/m}$. In this two meshes are used. The first mesh is composed of 136161 nodes and 400 160 edges (135279 unknowns for φ-formulation and 377 681 unknowns for $\boldsymbol{T}$-formulation) and the second mesh is composed of 450241 nodes and 1 332 240 edges (448319 unknowns for φ-formulation and 1281721 unknowns for $\boldsymbol{T}$-formulation). A voltage of 100 μV is imposed between the boundary conditions Γ_{E_1} and Γ_{E_2}. A current of 11.2 A and a dissipated power of 1.12 mW are obtained. The current density in this conductor is shown in Fig. 8.

To reach the efficiency of the parallel direct solver, both assemblage and resolution are executed on a cluster with 8 processors (two quad cores). The acceleration in accordance with the numbers of processors and the sequential time are shown in Table I and Table II. Higher parallel efficiency is obtained when the number of the unknowns is bigger, the scalability can reach 0.63 with 8 processors (Systeme2 Mesh2). For the coarse mesh the result of parallelization is not interesting because the setup time is small.

TABLE I
SPEED-UP AND SEQUENTIAL TIME OF THE PARALLEL DIRECT SOLVER SYSTEM 1

Number of processors	2	4	8	Seq. time
Mesh 1: 13 226 unknowns, φ form.	1.51	1.81	2.26	47 s
Mesh 2: 117 425 unknowns, φ form.	1.75	2.34	3.08	192 s
Mesh 1: 27 960 unknowns, $\boldsymbol{T}$ form.	1.69	1.98	2.56	68 s
Mesh 2: 293 466 unknowns, $\boldsymbol{T}$ form.	1.81	2.98	4.05	320 s

TABLE II
SPEED-UP AND SEQUENTIAL TIME OF THE PARALLEL DIRECT SOLVER SYSTEM 2

Number of processors	2	4	8	Seq. time
Mesh 1: 135 276 unknowns, φ form.	1.76	2.56	3.5	199 s
Mesh 2: 448 319 unknowns, φ form.	1.8	3.15	4.5	482 s
Mesh 1: 377 681 unknowns, T form.	1.85	2.70	4.2	465 s
Mesh 2: 1 281 721 unknowns, T form.	1.89	2.93	5.09	1256 s

V. CONCLUSION

A parallel direct solver based on a multi-threading technology and using a nested dissection method is implemented. This solver has been integrated into the assemblage of the systems for the FIT. This paper presents a block partitionable sparse matrix solver in which a matrix is divided into blocks. These blocks are assigned to different processors for parallel execution. The algorithm developed in this work exploits the sparsity at the block level as well as within a non-zero block and handles automatically and properly singularities in the studied system. The presented results demonstrate the efficiency of the proposed approach.

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