PRIAM/ANTIGONE : a 2D/3D Package for Accelerator Design

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Abstract

The status of the finite element package PRIAM/ANTIGONE, developed at LAL for electromagnetic engineering, is presented. A short review of the available capabilities of the package is given.

1 INTRODUCTION

The design of accelerators and detectors needs computing tools for solving the Maxwell's equations in two as well as in three dimensions. There exist for a long time different programs treating electromagnetic problems, which are based on finite difference methods. The finite difference methods are popular, mainly because they seem to be staightforward to implement. However they present some drawbacks as, for instance, the necessity of special treatments on the boundaries or the difficulty of moduling the density of the mesh of the computed structure.
Finite element methods do not present these drawbacks ; that is why they are more and more used in the electromagnetic domain. An other advantage of using these methods is the possibility of coupling electromagnetic calculations with mechanical, thermal or other calculations, where f.e.m. are widely implemented for a long time.
We present here the status of a package developed at LAL [1], PRIAM for 2D case and ANTIGONE for 3D, using Raviart-Thomas [2] and Nedelec [3] finite elements based on the properties of the operators *div* and *curl* involved in the Maxwell's equations and related to the well-known physical laws : Gauss's, Ampère's, Faraday's. Applications of the code are described by other authors in this conference [4].

2 THE FOUR VECTORS DESCRIBING THE ELECTROMAGNETIC FIELD

The electromagnetic field is characterized by four vector fields : $\vec{E}$, $\vec{D}$, $\vec{B}$, $\vec{H}$ satisfying the four Maxwell's equations :

$$\frac{\partial \vec{D}}{\partial t} + curl\, \vec{H} = \vec{j} \qquad (1)$$

$$\frac{\partial \vec{B}}{\partial t} + curl\, \vec{E} = 0 \qquad (2)$$

$$div\, \vec{D} = \rho \qquad (3)$$

$$div\, \vec{B} = 0 \qquad (4)$$

together with the constitutive relations :

$$\vec{D} = \varepsilon \vec{E}$$
$$\vec{B} = \mu \vec{H} \qquad (5)$$

ρ and $\vec{j}$ are respectively the charge and current density, ε and μ are permittivity and permeability of the medium.

When solving these equations on a bounded domain one has to take into account boundary conditions and, in the case of evolutive problems, initial conditions.
In applying numerical formulations one usually takes care of the continuity of the physical quantities as potential or fields. This point is important in presence of different media in the structure : the right continuities have to be ensured on the interfaces. The problem may be not trivial, if the choice of the numerical method is not adapted. Concerning the Maxwell's equations it is worth noting that only normal components of $\vec{D}$ and $\vec{B}$ and tangential component of $\vec{E}$ and $\vec{H}$ are continuous on interfaces between different media. In a similar manner the boundary conditions are of two types : perfectly conducting walls where tangential components of $\vec{E}$ and $\vec{H}$ vanish and symmetry boundaries where normal components of $\vec{D}$ and $\vec{B}$ vanish.

3 A MADE -TO-MEASURE FINITE ELEMENT FORMULATION

Take, for example, the electrostatic problem. The principle of a "classical" f.e.m. would be to search the potential under the form of a linear combination of well chosen basis functions (or interpolation functions) $w_i(x,y,z)$:

$$V(x,y,z) = \sum_{i=1}^{N} V_i\, w_i(x,y,z) \qquad (6)$$

the unknowns of the problem, V_i , beeing the values of potential on "nodes" of a mesh which can be irregular. N is the total number of these nodes. The formulation is consistent if the w's satisfy the following relations (if x_j, y_j, z_j are the coordinates of the node number j) :

$$w_i(x_j, y_j, z_j) = \delta_{ij}$$

(Kronecker's symbol)

The electrostatic problem may be solved, for example, by putting the above expression for V in Euler's equations of the electrostatic energy minimization problem (variational formulation) leading to a linear system for the V_i 's. If, for instance, the computational domain is meshed with tetrahedras (what we will assume from now on), the linear approximation consists of taking the vertices as nodes and the barycentric coordinates as basis fonctions. By this method we

get continuous potentials. The electric field derivated from this potential is not continuous, nor its tangential component on interfaces. In the following, this finite element will be called "P1".

There exist a little bit more sophisticated, so called "mixed" finite elements. Through this formulation, the calculated quantity is not only the potential but both $\vec{D}$ and V. $\vec{D}$ is searched under the form :

$$\vec{D}(x,y,z) = \sum_{i=1}^{N_d} \Phi_i \vec{N}_i(x,y,z) \qquad (7)$$

The unknowns Φ_i beeing now fluxes of $\vec{D}$ through the faces of the tetrahedras (in the case of linear approximation). Consequently the basis functions have to satisfy :

$$\iint_{F_j} \vec{N}_i . \vec{n}_j dS = \delta_{ij} \qquad (8)$$

This surface integral is taken over the face number j, $\vec{n}_j$ is the unit vector normal to that face, outgoing from the tetrahedron to which the basis vector function is related. For consistency reasons V is supposed to be constant in each tetrahedron.

These expressions are put, as before, in Euler's equations of a energy minimisation problem. There are at least two advantages in this approach arising from the fact that the unknowns of the problem are fluxes of $\vec{D}$, i.e. normal components of this vector: a) one can ensure strictly the Gauss's law when integrating on the surface of a tetrahedron, b) one get **automatically** the right continuity for normal component of $\vec{D}$ on interfaces between different media. In the following this finite element will be called "H(div)".

In a very similar manner one can define a finite element whose unknowns are circulations (instead of fluxes) along edges of tetrahedras, ensuring Faraday's and Ampère's laws on each of them and the right continuities of tangential components. These elements will be called "H(curl)".

Combining these three kinds of elements the PRIAM/ANTIGONE code solves specific electromagnetic problems (electrostatics, magnetostatics, eigenmodes...) as well as the full time domain Maxwell problem.

4 STATIC DOMAIN

Electrostatics

The package offers the possibility of using both P1 or H(div) elements. The first one is recommended when the user is interested in getting good values for the potential. The second one is well suited in presence of different kind of dielectric materials ; this is especially true when one is interested in getting values of capacities.

Magnetostatics

H(curl) element is used in solving the magnetostatic problem with $\vec{H}$ as unknown:

$$\begin{aligned} curl\,\vec{H} &= \vec{j} \\ div(\mu\vec{H}) &= 0 \end{aligned} \qquad (9)$$

Although not yet programmed in PRIAM/ANTIGONE an other formulation is possible using a H(div) element solving the problem with $\vec{B}$ as unknown:

$$\begin{aligned} div\,\vec{B} &= 0 \\ curl\frac{\vec{B}}{\mu} &= \vec{j} \end{aligned} \qquad (10)$$

The choice between the two possibilities depends on whether one wishes to ensure the right continuity on interfaces for $\vec{H}$ or for $\vec{B}$.

5 FREQUENCY DOMAIN

In the frequency domain the mixed finite elements provide very attractive results. The HF eigenmode problem for the electric field $\vec{E}$ is :

$$\frac{1}{\varepsilon} curl \frac{1}{\mu} curl\vec{E} = \omega^2 \vec{E} \qquad (11)$$

with the boundary condition on conducting walls :

$$\vec{E} \times \vec{n} = 0$$

Obviously the H(curl) element is very well suited in solving this problem. The formulation provides values of the circulation of $\vec{E}$ along the edges of the tetrahedras. So it is straightforward to get values of the fluxes of magnetic field $\vec{B}$ on the faces of the tetrahedras through the relation :

$$\iint_F \vec{B}.\vec{n}\,dS = \frac{-1}{i\omega} \iint_F curl\vec{E}.\vec{n}\,dS = \frac{-1}{i\omega} \oint \vec{E}\,d\vec{s} = C_1 + C_2 + C_3 \qquad (12)$$

C_1, C_2, C_3 beeing the previously calculated value of the circulation of E along the 3 edges of the face F. A very interesting property of the method is that it **does not provide any "spurious" (or "parasitic") mode** unlike more classical approaches. In these latter the phenomenon seems to be due to the fact that these formulations do not ensure the divergence free condition for $\vec{D} = \varepsilon\vec{E}$. The H(curl) element leads intrinsically to a divergence free $\vec{D}$.

The vector $\vec{H}$ is solution of the same eigenvalue problem as $\vec{E}$ (but with "dual" boundary conditions). Both formulations (in E and in H) are implemented in ANTIGONE (3D). It can be shown that H-formulation approximates the frequency by upper values whereas the E-formulation approximates it by lower values. In this manner we can get a range within lies the exact value. It worth noting that in the 2D case the H-formulation is equivalent to the method used in the well-known program SUPERFISH.

In PRIAM/ANTIGONE quasi-periodic boundary conditions are implemented in addition to the classical ones.

In the 2D case it is possible to get "transverse modes" (dipoles,quadrupoles etc.) for an axisymmetric geometry.

6 TIME DOMAIN

The use of the H(div) and H(curl) element for spatial discretization can be coupled with a time scheme for solving evolutive problems described by the equations (1) and (2) rewritten under the form :

$$\frac{\partial \vec{D}}{\partial t} = \vec{j} - curl\,\vec{H}$$
$$\frac{\partial \vec{B}}{\partial t} = -curl\,\vec{E} \qquad (13)$$

PRIAM/ANTIGONE use a "leap-frog" scheme.

given $(\text{curl } \vec{E})^{n-1/2}$ and $\vec{B}^{n}$ at the time step n, the time step n+1 consists in the following :

- calculate the time derivative of the circulations of $\vec{E}$ along edges of the tetrahedras (H(curl) element) ;
- $(curl\,\vec{E})^{n+1/2} = (curl\,\vec{E})^{n-1/2} + \Delta t \dfrac{\dot{C}_1 + \dot{C}_2 + \dot{C}_3}{V}$ on each tetrahedron (volume V) ;
- $\vec{B}^{n+1} = \vec{B}^{n} - \Delta t (curl\,\vec{E})^{n+1/2}$.

This scheme is used with the driving term $\vec{j}$ equal to 0 (travelling waves calculations) or equal to a given function (wake field calculations). If particles are present in the structure, the driving term has to be estimated as we will see below.
The Maxwell's equations (3) and (4) are automatically satisfied if they are at the initial time.
In the time domain absorbing boundary conditions ("open" boundaries) are implemented, in addition to usual ones.

7 SELF-CONSISTENT CALCULATION WITH PARTICLES

In presence of a charged particle beam, the particles contribute to the the driving terms ρ and $\vec{j}$. Such a beam is modelized by a set of macroparticles represented as Dirac distributions, so we have :

$$\rho = \sum_p q_p \delta(\vec{r} - \vec{r}_p)$$
$$\vec{j} = \sum_p q_p \delta(\vec{r} - \vec{r}_p)\vec{v}_p \qquad (14)$$

q_p, r_p, v_p beeing respectively the charge, position and velocity of the macroparticle p. The Maxwell's equations are solved for each time step by the above described space discretization and time scheme. In the finite element formulation the Dirac distributions for the driving terms occur inside integrals and are regularized from this fact.
In addition to the Maxwell's equations we have to take into account the Newton-Lorentz equations for each macroparticle :

$$\frac{d}{dt}(\gamma\vec{\beta}_p) = \frac{e}{mc}(\vec{E} + c\vec{\beta}_p \times \vec{B}) \qquad (15)$$

(e,m charge and mass of the considered kind of particle ; c light velocity, β_p ratio of the macroparticle velocity to c)
The time cycle of such a program consists of the following steps :

- solve the field equations (finite element method, here H(curl) element) with current positions and velocity of macroparticles ;
- from the field provided by the preceeding step, get the fields at the current positions of the macroparticles ;
- from these fields solve the Newton-Lorentz equation for each macroparticle (A Buneman-Boris algorithm is used) and update macroparticles positions and velocity.

The implementation includes the generation of particles at emitting surfaces following rectangular or gaussian pulse shape. Any shape is easily programmable.
Different initial conditions are available : electrostatic field, RF field etc. These fields are computed on the same mesh with the described above finite elements, avoiding any interpolation.

8 INTERFACES

The PRIAM/ANTIGONE package do not impose the use of determined mesh generators nor postprocessor. It can be interfaced with any finite element package or graphical software. At the moment interfaces with MODULEF, ANSYS, SYSTUS finite element mesh generators are available. Implement other interfaces is straightforward.
The code is written in standard FORTRAN-77 and therefore can be implemented on any system.

9 CONCLUSION

PRIAM/ANTIGONE offer a appreciable number of modules for solving the Maxwell's equations both in two and three dimensions, in static, frequency, time domains as well as in the particle coupled case. The package presents the advantage of using a consistent finite element formulation taking into account foundamental properties of the Maxwell's equation which can be interpreted in terms of continuities of field components.
Further developments are planed in the harmonic domain, especially S-matrix computation.

10 REFERENCES

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