A MIXED FINITE ELEMENT METHOD FOR PARTICLE SIMULATION IN LASERTRON

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Summary

A particle simulation code is being developed with the aim to treat the motion of charged particles in electromagnetic devices, such as Lasertron. The paper describes the use of mixed finite element methods in computing the field components, without derivating them from scalar or vector potentials. Graphical results are shown.

1. Introduction

Because of the high intensity of the Lasertron bunched beam, the space charge forces and the wake fields are to be taken into account. The electromagnetic fields and the particle distribution interact strongly. The computer simulations of these phenomena are "naturally" derived from "particle methods", using both Eulerian and Lagrangian descriptions[1,2,3,4]. In this paper we describe a work in progress : the program PARADE. In the program PARADE, the equations of motion are integrated by classical methods. In solving the field equations mixed finite element methods are used. By using these formulations we avoid derivating the field components from any scalar or vector potential : the fields are directly computed (more precisely their fluxes). In the case of the Maxwell's equations the mixed finite element methods can be interpreted by means of the physical laws such Gauss's, Faraday's etc...

The particle motion in a field represented by the Poisson's equation (hence including the space charge effects) is completely treated in the code. The resolution of the time dependent Maxwell's equations are being implemented.

2. Poisson's Equation

When the particles are non-relativistic, their velocities are negligible in comparison with the propagation velocity of the electromagnetic fields, these later can be considered as static at each time step. They are described by the Poisson's equation.

In order to simplify the notations we present here the case of the plane symmetry. In the code both cylindrical and plane symmetries are treated.

Let be Ω the computational domain, with boundary Γ, Γ_0 the fixed potential boundaries (cathode, anode, focusing electrode etc...), Γ_1 the Neumann boundaries, $(\Gamma = \Gamma_0 \cup \Gamma_1)$ the Poisson's equation is :

$$\begin{cases} -\Delta U = \dfrac{\rho}{\epsilon_0} \\ U = U_0(x,y) \quad \text{on } \Gamma_0 \\ \overrightarrow{gradU}.\vec{n} = 0 \quad \text{on } \Gamma_1 \end{cases} \tag{1}$$

$\rho(x,y)$ is the charge density at the location (x,y), $\vec{n}$ is the unit vector normal to the boundary Γ.

Mixed variational formulation

The principle of this formulation is to take as unknowns two functions : the scalar function U and the vector function $\vec{E}$ related by the constraint $\vec{E} = -\overrightarrow{gradU}$. Hence the problem (1) becomes :

Find a pair $(\vec{E}, U)$ such that :

$$\begin{cases} (a) \quad \vec{E} = -\overrightarrow{gradU} \\ (b) \quad div\vec{E} = \dfrac{\rho}{\epsilon_0} \end{cases} \tag{2}$$

$$U = U_0 \text{ on } \Gamma_0 \qquad \vec{E}.\vec{n} = 0 \text{ on } \Gamma_1$$

After multiplying (2-a) and (2-b) respectively by the "test functions" $\delta\vec{E}$ (electric virtual field) and δU (virtual potential), integrating over Ω and applying the Green's theorem, the following relations are verified for any δU and $\delta\vec{E}$ (such that $\overrightarrow{\delta E}.\vec{n} = 0$ on Γ_1) :

$$\begin{cases} (a) \quad \int_\Omega \vec{E}.\overrightarrow{\delta E} - \int_\Omega U div\overrightarrow{\delta E} = -\int_{\Gamma_0} U_0(\overrightarrow{\delta E}.\vec{n}) \\ (b) \quad \int_\Omega div\vec{E}\delta U = \dfrac{1}{\epsilon_0}\int_\Omega \rho\delta U \end{cases} \tag{3}$$

$$\vec{E}.\vec{n} = 0 \quad on\ \Gamma_1$$

By applying the Green's theorem to (3-a) we have :

$$\int_\Omega \vec{E}.\overrightarrow{\delta E} + \int_\Omega \overrightarrow{gradU}.\overrightarrow{\delta E} - \int_\Gamma U\overrightarrow{\delta E}.\vec{n} = -\int_{\Gamma_0} U_0(\overrightarrow{\delta E}.\vec{n}) \tag{4}$$

By comparing (3-a) and (4), (2-a) can be obtained as Euler's equation with the "natural" boundary condition $U = U_0(x,y)$ on Γ_0. A similar result is immediate for (3-b) and (2-b). Hence we have the following weak formulation of the problem (2) : *find a pair of functions $(\vec{E}, U)$ such that the relations (3) are verified for any δU and $\overrightarrow{\delta E}$ ($\overrightarrow{\delta E}.\vec{n} = 0$ on Γ_1).* The solution $(\vec{E}, U)$ is to be searched in functional spaces with the following properties

$$\int_\Omega U^2 < \infty \qquad (space\ L^2\ (\Omega))$$

$$\int_\Omega |\vec{E}|^2 < \infty, \int_\Omega |div\vec{E}|^2 < \infty \qquad (Sobolev\ space\ H(div, \Omega))$$

and $\vec{E}.\vec{n} = 0$ on Γ_1 (essential boundary condition). The test functions are to be taken in these spaces.

The solution $(\vec{E}, U)$ makes the following Lagrangian stationary :

$$\mathcal{L}(\vec{E}, U) = \frac{1}{2}\int_\Omega |\vec{E}|^2 + \int_{\Gamma_0} U_0(\vec{E}.\vec{n}) - \int_\Omega U(div\vec{E} - \frac{\rho}{\epsilon_0})$$

One recognizes the minimization problem of a "complementary energy" under the constraint $div\vec{E} - \frac{\rho}{\epsilon_0} = 0$, U being nothing other but a Lagrange's multiplicator.

Discretization

The domain Ω is covered with a triangular mesh. Inside each triangle U is approximated by a constant function U^h (the value at the barycentre), $\vec{E}$ is approximated by a polynomial vector function $\vec{E}^h$:

$$E_x^h = \alpha_1 + \beta x \qquad E_y^h = \alpha_2 + \beta y$$

The used finite elements are schematized on fig.1. The degrees of freedom related to $\vec{E}$ are the fluxes of $\vec{E}$ through the triangle sides. They are supported by nodes located at the middle of the sides.

$$\vec{E}^h = \phi_1 \vec{N}_1(x,y) + \phi_2 \vec{N}_2(x,y) + \phi_3 \vec{N}_3(x,y)$$

The $\vec{N}_i$'s are the basis polynomials such that : $\int_{a_j} \vec{N}_i . \vec{n_j} = \delta_{ij}$. One notices that this interpolation yields :

$$div\vec{E}^h = \frac{\phi_1 + \phi_2 + \phi_3}{S}$$

(where S is the area of the triangle). Therefore the Gauss's law is verified on each triangle. In other words, if the exact solution is such that $div\vec{E} = 0$, then the interpolated function verifies $div\vec{E}^h = 0$ too. This interpolation ensures the continuity of the flux of $\vec{E}$ through the boundaries of the triangles. The later property is characterized by saying that this mixed finite element is conforming in $H(div)$. This type of element was first introduced in different papers of Frayes De Veubeke. P.A. Raviart and J.M. Thomas [5,6] used these elements for solving second order equations in two dimensions (1977). We developed an axisymmetrical version for our program.

On the whole domain Ω one has :

$$\vec{E}^h = \sum_{i=1}^{N_e} \phi_i \vec{N}_i \qquad U^h = \sum_{j=1}^{N_v} U_j M_j$$

N_e : number of nodes located on the boundaries of the triangles

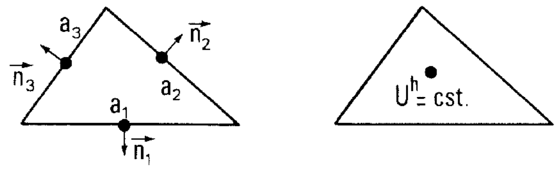
N_v : number of nodes located at the barycentres

M_j is the basis function such that $M_j = 1$ on the triangle j, $M_j = 0$ elsewhere.

Putting these expressions into the relations (3) and taking the basis polynomials as test functions one obtains a system of linear equations of the form :

$$\begin{bmatrix} A & B \\ {}^tB & 0 \end{bmatrix} \begin{bmatrix} \Phi \\ U \end{bmatrix} = \begin{bmatrix} U' \\ Q \end{bmatrix}$$

A penalization method leads to the factorization of a symmetric, positive definite matrix.



(a) Interpolation of $\vec{E}$ (conforming in $H(div)$) (b) Interpolation of U

Fig. 1 : Discretization of the Poisson's equation

Coupling the FEM to the particle motion

This coupling is achieved through the following steps :

(a) From the initial spatial distribution of the superparticles the density ρ is calculated by counting the superparticles in each triangle. By integrating with respect of equations (3) we obtain the RHS of the above matrix equation.

(b) The field equations are solved by the described above method. The results are fluxes of $\vec{E}$.

(c) From the calculated fluxes the field $\vec{E}$ acting on each particle is interpolated and the motion equations are solved for one time step (we used a Leap-frog-scheme). The iteration is continued with the new particle positions.

First results

Fig.(2.a) shows the mesh used for a LAL-Lasertron simulation. One can see advantages of the finite element methods in describing odd boundaries, locally mesh refining etc... Fig.(2-b) shows the bunch behaviour in the accelerating space. One can observes the space charge phenomena and the focusing effect of the Wehnelt. One notices some numerical fluctuations, due to a relatively coarse field interpolation from calculated fluxes. This later will be improved in the near future.

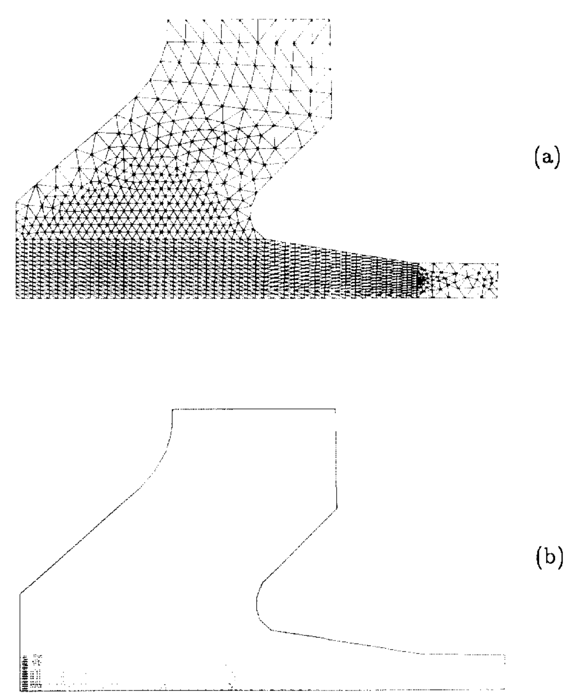


Fig. 2 : Behaviour of a single bunch in the accelerating region (initial radius : 5mm, Q = 1,9 nc, V = 330 kV). The bunch is represented every 50 ps.

3. Time Dependent Maxwell's Equations

For the Lasertron, an axisymmetrical TM mode is to be considered, from symmetry ; the field components are : $\vec{E} = (E_z, E_r, 0)$, $\vec{B} = (0, 0, B_\varphi)$. In this case, the Maxwell's equations can be written :

$$\begin{cases} (a)\ curl\vec{E} + \dfrac{\partial B_\varphi}{\partial t} = 0 \\ (b)\ c\vec{u}rlB_\varphi - \dfrac{1}{c^2}\dfrac{\partial \vec{E}}{\partial t} = \mu_0 \vec{j} \\ (c)\ div\vec{E} = \dfrac{\rho}{\epsilon_0} \end{cases} \quad (5)$$

$$\vec{E} \times \vec{n} = 0 \text{ on conducting walls}$$

It is easy to see that the condition 5-c is automatically satisfied if it is at the initial time $t = 0$ and if there is no charge creation.

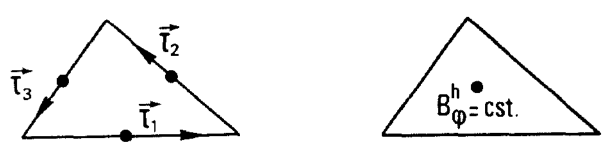
We can use mixed finite elements in order to find a pair consisting of a scalar function B_φ and a vector function $\vec{E} = (E_z, E_r)$. A variational formulation is : *Find a pair* $(\vec{E}, B_\varphi)$ *such that :*

$$\begin{cases} \displaystyle\int_\Omega \frac{\partial \vec{E}}{\partial t}\overrightarrow{\delta E} - \frac{1}{c^2}\int_\Omega B_\varphi curl\overrightarrow{\delta E} = -\frac{1}{\epsilon_0}\int_\Omega \vec{j}\cdot\overrightarrow{\delta E} \\ \displaystyle\int_\Omega curl\vec{E}\delta B + \int_\Omega \frac{\partial B_\varphi}{\partial t}\cdot\delta B = 0 \\ \text{for any } \overrightarrow{\delta E},\ \delta B \end{cases}$$

$\vec{E}$ and $\vec{\delta E}$ are to be taken in $H(curl, \Omega)$ with $\vec{E} \times \vec{n} = 0$, $\vec{\delta E} \times \vec{n} = 0$ on the conducting boundaries. B_φ and δB are to be taken in $L^2(\Omega)$. $H(curl, \Omega)$ is defined in the same way as $H(div, \Omega)$, replacing *div* by *curl*.

In our code we are developing an axisymmetrical version of such a mixed element, first introduced by Nedelec[7], represented on figure 3. This conforming in $H(curl)$ element ensures the continuity of the "tangential" fluxes. Inside each triangle, $\vec{E}$ is interpolated by $\vec{E}^h$:

$$E_z^h = \alpha_1 - \beta r \qquad\qquad E_r^h = \alpha_2 + \beta z$$



(a) Interpolation of $\vec{E}$ (conforming in $H(curl)$) (b) Interpolation of B_φ

Fig. 3 : Discretization of the time dependent Maxwell's equations

The degrees of freedom are the tangential fluxes. We have:

$$curl\vec{E}^h = \frac{(\vec{E}.\vec{\ell})_1 + (\vec{E}.\vec{\ell})_2 + (\vec{E}.\vec{\ell})_3}{S}$$

Putting this relation into (5.a) we obtain the Faraday's law on the triangle. Figure 4 shows the fields generated by a Gaussian bunch passing through a Lasertron output cavity at the speed of light. (An alternating explicit time-scheme was used).

4. The Club MODULEF

Our program developments are achieved using MODULEF facilities.

Club MODULEF[8] was created in 1974 to bring together French and foreign universities, as well as industrial companies with the goal of designing and implementing a modular portable finite element program package. Exchange among members of the club is purely of a scientific (hence noncommercial) nature. Additional members are welcome. The requirements for joining are an interest in and need for finite element procedures and a desire to participate in the improvement and maintenance of a high quality package. For more information write to M. Bernadou at INRIA-Rocquencourt, B.P. 105, 78153 LE CHESNAY, France.

5. Conclusion

The mixed finite element method is very well suited for electrodynamic equations. It allows one to introduce the advantages of finite element methods in the particle simulation programs : use of standard algorithms, easy implementation of the boundary conditions, versatile mesh generation, locally refining etc...

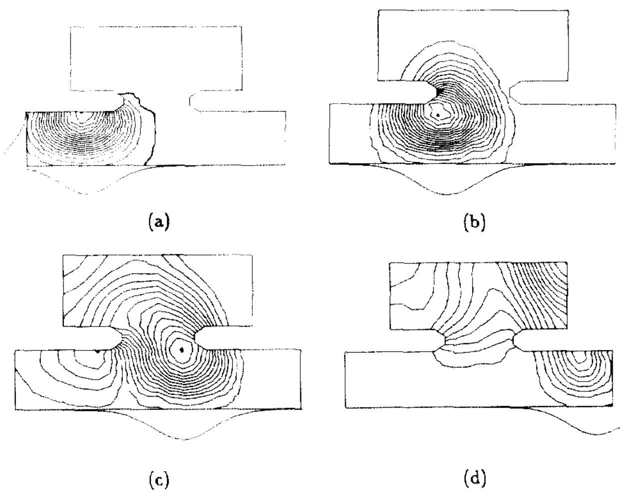


Fig. 4 : Fields generated by a Gaussian bunch ($\sigma_z = 0.25cm$; $\sigma_r = 0.18cm$) passing through an axisymmetrical cavity (*lines* $rB_\varphi = cst$).

References

[1] W.B. Herrmannsfeldt "Computer simulation of the Lasertron" SLAC/AP-41, April 1984.

[2] W.B. Herrmannsfeldt "Lasertron simulation with a two-gap cavity" SLAC/AP-41, April 1985.

[3] H. Nishimura "Particle simulation code for non-relativistic electron bunch in lasertron" in Proceedings of the 1984 Linear Accelerator Conference GSI, Darmstadt, May 1984 pp.165-167.

[4] T. Shintake "FCI-Field charge interaction program" KEK Preprint 84-15, Nov. 1984.

[5] P.A. Raviart, J.M. Thomas, "A mixed finite element method for 2nd order elliptic problems". In D.A. Eckmann B. (eds). Mathematical aspects of finite element methods. Lectures Notes 606 Springer Berlin (1977).

[6] J.M. Thomas, Thesis Paris (1977).

[7] J.C. Nedelec, "Mixed finite element in R^3", Numerische Mathematik 35 1980 pp.315-341.

[8] M. Bernadou et al., MODULEF "A modular finite element library" INRIA (Rocquencourt, 1986).