PRIAM : A SELF CONSISTENT FINITE ELEMENT CODE FOR PARTICLE SIMULATION IN ELECTROMAGNETIC FIELDS

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Abstract

A 2 1/2 dimensional, relativistic particle simulation code is described. A short review of the used mixed finite element method is given. The treatment of the driving terms (charge and current densities), initial, boundary conditions are exposed. Graphical results are shown.

Introduction

Future accelerators design needs numerical simulations taking into account the totality of the electromagnetic phenomena arising when ultrarelativistic bunches move in electromagnetic devices. These computations can be achieved only by somewhat sophisticated programs solving the complete Maxwell's and Newton-Lorentz equations by particle methods (i.e. coupling Eulerian and Lagrangian approaches).

We present here such a 2 1/2 particle code, PRIAM, developed at LAL (Orsay) and dedicated to the design of accelerator electromagnetic devices (RF-guns, accelerating cavities etc.). In PRIAM the particular choice is to use a "mixed" finite element method in solving the Maxwell's equations. This formulation, although quite unusual, is very well suited for the electromagnetic problem : the discrete unknowns related to the electric field **E** are not the nodal values but the circulations of **E** along edges of the elements (triangles) whereas the unknowns related to the magnetic field are values of B_φ constant on each triangle, in such a manner that some fundamental structural properties of the Maxwell's equations are preserved.

After a short review of the method (space and time discretization) some characteristics and facilities of the program will be described.

Aim of the program

The aim of the program is to simulate the dynamics of charged particles within time varying electromagnetic fields, in a self consistent manner. An axisymmetric geometry is assumed.

From symmetry a TM-mode has to be considered : the unknown functions are an electric vector field $\mathbf{E} = (E_z, E_r)$ together with a scalar field B_φ (azimuthal component). The Maxwell's equations are in this case :

$$\mathbf{curl}\ H_\varphi = \mathbf{j} + \frac{\partial \mathbf{D}}{\partial t} \qquad (1)$$

$$\mathrm{curl}\ \mathbf{E} = -\frac{\partial B_\varphi}{\partial t} \qquad (2)$$

$$\mathrm{div}\ \mathbf{D} = \rho \qquad (3)$$

+ initial and boundary conditions

E, **D**, B_φ, H_φ being bounded by the constitutive relations : $\mathbf{D} = \varepsilon\mathbf{E}$; $B_\varphi = \mu H_\varphi$.

The boundary condition is $\mathbf{E}\wedge\mathbf{n} = 0$ on conducting walls (**n** is a normal unit vector). On the axis $\mathbf{D}.\mathbf{n} = 0$ and $H_\varphi = 0$. On "open boundaries" some special (non reflecting) conditions have to be constructed.

The operator **curl** $w = (\frac{1}{r}\frac{\partial}{\partial r}(rw), -\frac{\partial w}{\partial z})$ operates from a scalar function to a vector one. The operator curl operates from a vector function to a scalar one : curl $\mathbf{p} = \frac{\partial p_r}{\partial z} - \frac{\partial p_z}{\partial r}$.

The driving terms **j** and ρ (current and charge densities) have to be calculated from Newton-Lorentz equation :

$$\frac{d}{dt}(\gamma\boldsymbol{\beta}) = \frac{e}{mc}(\mathbf{E} + c\boldsymbol{\beta}\wedge\mathbf{B}) \qquad (4)$$

In the dynamic calculations we consider the six components **E**, **B** in order to be able to take into account superimposed fields (focusing magnetic field etc.)

(c = light velocity ; $\boldsymbol{\beta} = (\beta_z, \beta_r) = \frac{\mathbf{v}}{c}$ with **v** = particle velocity ; $\gamma^{-1} = \sqrt{1-\boldsymbol{\beta}^2}$; e, m charge and mass of the particle)

Discretization of the Maxwell's equations

Space discretization

Let us consider a bounded computational domain Ω with a boundary $\Gamma = \Gamma_a \cup \Gamma_c \cup \Gamma_o$

(Γ_a : axis ; Γ_c : conducting boundary ; Γ_o open boundary)

The vector **E**, solution of the Maxwell's equations, belongs to the following functional space :

$$\mathcal{E} = \left\{\mathbf{p} ; \int_\Omega |\mathbf{p}|^2 < \infty, \int_\Omega |\mathrm{curl}\ \mathbf{p}|^2 < \infty, \mathbf{p}\wedge\mathbf{n} = 0 \text{ on } \Gamma_c\right\}$$

The scalar B_φ belongs to the following functional space :

$$\mathcal{B} = \left\{w ; \int_\Omega w^2 < \infty\right\}$$

curl operates from $\mathcal{E}$ to $\mathcal{B}$.

As well-known the quantity $\mathbf{E}\wedge\mathbf{n}$ is continuous at interfaces between different media (it is the case also for **B**.**n**, but it is obviously true here from symmetry).

In order to use a finite element method we can write a variational formulation of (1). Let **p** be any vector of $\mathcal{E}$, after multiplying both sides by **p**, integrating over Ω and applying the Green's formula we get the following problem :

find $\mathbf{E}\in\mathcal{E}$, $B_\varphi\in\mathcal{B}$ *such that for any* **p**:

$$\int_\Omega \varepsilon\frac{\partial \mathbf{E}}{\partial t}.\mathbf{p}\ r dr dz = \int_\Omega \frac{1}{\mu} B_\varphi\, \mathrm{curl}\ \mathbf{p}\ r dr dz - \int_\Omega \mathbf{j}.\mathbf{p}\ r dr dz + \int_{\Gamma_o} \frac{1}{\mu} B_\varphi \mathbf{p}\wedge\mathbf{n}\ r d\gamma \qquad (5)$$

with (2) and (3)

(in the following we will consider $\varepsilon = \varepsilon_0$; $\mu = \mu_0$)

The boundary integral is limited to the open boundary : indeed $\mathbf{p}\wedge\mathbf{n} = 0$ on Γ_c by definition of $\mathcal{E}$ and on the axis r = 0.

There exist finite element spaces having the same structural properties as $\mathcal{E}$ and $\mathcal{B}$ and allowing one to achieve the space discretization of the above variational formulation with so called "mixed finite elements". For PRIAM we used a "Nedelec"[1] triangular element (fig 1) : the electric field $\mathbf{E}$ is interpolated in each triangle by a vector with linear polynomial components :

$$\mathbf{E} \approx C_1(t)\,\mathbf{N}_1(z,r) + C_2(t)\,\mathbf{N}_2(z,r) + C_3(t)\,\mathbf{N}_3(z,r)$$

the $\mathbf{N}_i$'s being the linear basis functions and the degrees of freedom C_i (i.e. discrete unknowns of the formulation) being the circulations (tangential fluxes) of $\mathbf{E}$ along the edge n°i of the triangle. The coefficients of $\mathbf{N}_i$'s, which are of the form $(\alpha_i - \beta_i r, \gamma_i - \beta_i z)$ are calculated in ensuring the 9 conditions

$$\int_{\text{edge } j} \mathbf{N}_i \wedge \mathbf{n}_j \, d\gamma = \delta_{ij} \quad (\delta_{ij} = 0 \text{ if } i \neq j,\ 1 \text{ if } i = j).$$

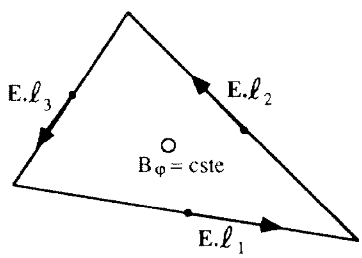

Fig. 1 : space discretization

This leads to an expression for $\mathbf{E}$ of the form : $\mathbf{E} \approx (\alpha_1 - \beta r, \alpha_2 + \beta z)$; $\alpha_1, \alpha_2, \beta$ being different on each triangle. In addition :

curl $\mathbf{E} \approx 2\beta = \frac{C_1 + C_2 + C_3}{S}$ on each triangle (S : area of the triangle)

The magnetic azimuthal field is interpolated by a constant function on each triangle.

curl $\mathbf{E}$ lies precisely in the functional space in which B_φ is interpolated. So the discretized form of the eq. (2) will be the strict application of the Faraday's law to the contour of the triangle : $C_1 + C_2 + C_3 = -\frac{\partial(B_\varphi S)}{\partial t}$. That is why, although none of the components E_z, E_r, B_φ is continuous passing from a triangle to another, these finite elements are nevertheless very performing, ensuring the continuity of $\mathbf{E} \wedge \mathbf{n}$ at interfaces.

Putting the linear expressions of $\mathbf{E}$ and B_φ in (5) and taking one after another $\mathbf{p} = \mathbf{N}_j$ we get a linear system to be solved with respect to the unknowns C_i.

Time discretization.

A "leap frog" time scheme is used : given $(\text{curl } \mathbf{E})^{n-1/2}\, B^n_\varphi$ at the time step n, the time step n + 1 consists in the following :

- inversion of the above linear system giving the time derivatives $C^n_{1t}, C^n_{2t}, C^n_{3t}$, on each triangle
- $(\text{curl } \mathbf{E})^{n+1/2} = (\text{curl } \mathbf{E})^{n-1/2} + \Delta t \cdot \frac{C^n_{1t} + C^n_{2t} + C^n_{3t}}{S}$
- $B^{n+1}_\varphi = B^n - \Delta t\,(\text{curl } \mathbf{E})^{n+1/2}$
- smoothing field values and solving Newton-Lorentz equation
- calculating new ρ and $\mathbf{j}$ as new driving terms starting from new particles positions and velocities

Continuity equation

The previous scheme treats Maxwell's equations (1) and (2). Taking into account eq. (3) is equivalent to ensure a charge continuity equation : $\text{div } \mathbf{j} + \frac{\partial \rho}{\partial t} = 0$.

Let $\tilde{\mathbf{E}}$ be the electric field as previously calculated ; a correction is searched under the form[2] $\mathbf{E}^* = -\,\mathbf{grad}\,\boldsymbol{\Phi}$ such that :

$$-\Delta\Phi = \frac{\rho}{\varepsilon_0} - \text{div } \tilde{\mathbf{E}}$$

this equation is solved by a classical P1-Lagrange finite element method.

Newton-Lorentz equation : macroparticles

The particles are represented as "macroparticles" carrying macroscopic charges q_p, which are assumed to be Dirac distributions :

$$\rho = \sum_p q_p\, \delta(\mathbf{r} - \mathbf{r}_p)$$

$$\mathbf{j} = \sum_p q_p\, \delta(\mathbf{r} - \mathbf{r}_p)\, c\, \beta_p$$

putting these expressions into the integrals of the right hand side of (5), we get the driving term of the linear system. The macroparticles are moved through the Newton-Lorentz equation. The latter is solved by a Boris-Buneman algorithm. For further information see, for example[3].

Boundary conditions

On conducting walls $\mathbf{E} \wedge \mathbf{n} = 0$; it means that the degrees of freedom (related to $\mathbf{E}$) are zero on these boundaries. This boundary condition is taken into account in dropping the corresponding nodes out of the linear system.

Concerning the open boundaries one has to express, the outgoing waves are not reflected. In our finite element formulation the most suited absorbing condition is $cB_\varphi = \mathbf{n} \wedge \mathbf{E}$; it can be put directly in the boundary integral of (5). This condition is absorbing for the outgoing waves at the first order with respect to the angle of incidence.

PRIAM allows one to take into account emitting boundaries (cathodes) : during the emitting phase a slice of macroparticles is emitted at each time step. The charge carried by each particle is weighted in order to get a constant or gaussian density (other shapes can be easily programmed).

Initial conditions

For numerical accuracy considerations it is much better to compute the initial (for example RF fields) or superimposed (focusing magnetic) fields on the same mesh, and with the same mixed finite element formulation : in this way the adequacy described above between discrete functional spaces and continuous spaces of the Maxwell's equations is preserved. Therefore a module has been developed for computing eigenmodes of resonant cavities[4]. A magnetostatic module will be soon available. Electrostatic fields can be taken into account directly by PRIAM.

Moreover any superimposed field can be programmed by the user.

Facilities of the program. Outputs

The program is being developed using MODULEF[5] facilities, in particular versatile mesh generators. Once the mesh has been provided, the user's data (boundaries, charge, pulse length, initial conditions etc.) are stored through a preprocessor and can be modified and reprocessed in a further run. A post processor allows one to analyze the outputs and to provide a set of graphics.

Figures (2, 3, 4, 5) show some graphical outputs related to the design of a LAL-RF gun[6]. A work made at CEA (Bruyères-le-Châtel)[7] compares the results of different programs in designing the ELSA project. This work and also results obtained at CERN[8] shows that PRIAM is in good agreement with programs using other approaches.

PRIAM is programmed in FORTRAN-77 under the norm GKS for the graphical modules.

Conclusion

The mixed finite element approach offers the advantage of combining the now well-known facilities of the usual finite element methods with a close approximation of the Maxwell's equations strictly preserving the laws of electromagnetism (Faraday's in our case) on each element of discretization. The formulation is very general and can be easily carried out in 3 dimensions.

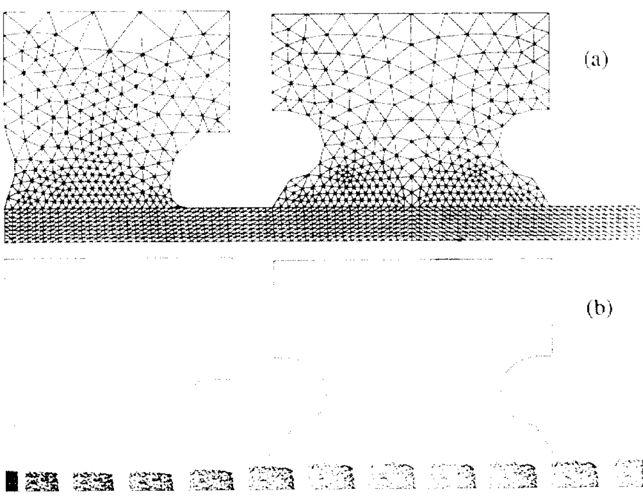

Fig. 2 : LAL-RF Gun simulation
(a) mesh
(b) behaviour of the single bunch

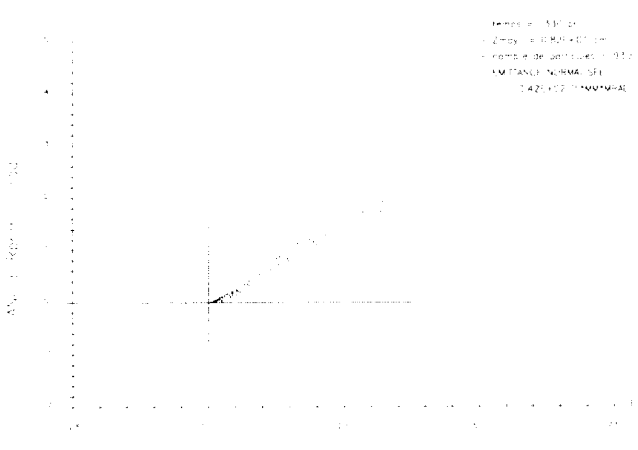

Fig. 3 : LAL-RF Gun simulation : (r, r') phase space at the exit of the gun

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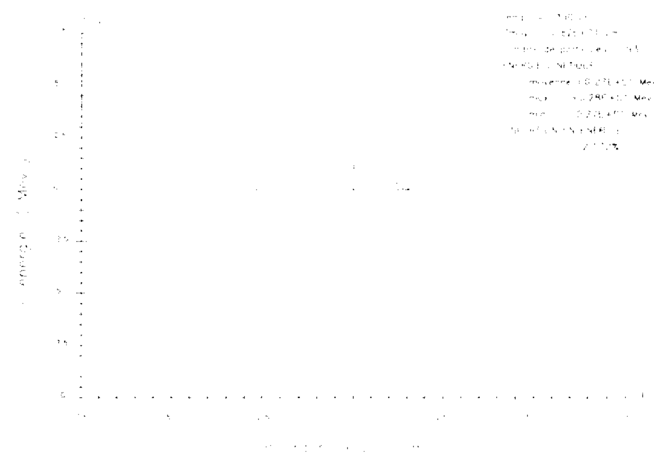

Fig. 4 : LAL-RF Gun simulation : z,E phase space at the exit of the gun

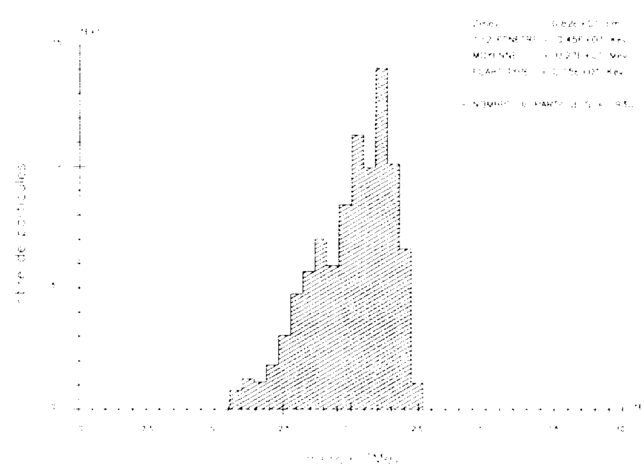

Fig. 5 : LAL-RF Gun simulation : z-histogram at the exit of the gun