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Coupling of Electromagnetic Field Computations with Particle Flow of Electrically Charged Particles

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Abstract

The particle-in-cell method is coupled with boundary-fitted coordinates in order to realistically model particle flow of electrically charged particles in technical, electromagnetic devices. Numerical algorithms describing the transition between the grid model and the mesh-free model are developed. Applications are presented in which these techniques have been successfully applied.

1 Introduction

Calculating electromagnetic effects by solving Maxwell's equation often requires the aid of computers. This is especially true when the system consists of complicated boundaries. Maxwell's partial differential equations describe the fields and the Lorentz equation expresses the motion of electrically charged particles in these fields. The electromagnetic fields determine the behavior of charged particles. The space charge of the particles themselves creates electromagnetic fields. These fields again influence the particles, and so on.

An attractive computational tool for numerically solving this nonlinear Maxwell-Lorentz problem is the particle-in-cell (PIC) method [1, 3]: A grid is introduced in order to compute the partial differential equations for the electromagnetic fields, and particles carrying electric charge and mass are advanced in these fields by solving the Lorentz equation. Originally, the PIC method was developed using uniform [3] grid zoning with grid lines parallel to the coordinate axis. However, with these concepts it was not possible to treat complicated technical devices without simplification of the geometry. In particular, when charged particles are created at slanted surfaces and accelerated in these technical devices, it is essential to carefully model the boundaries in the numerical approximation. Simplifications of parts of the geometry, e.g. at edges and curved parts of the electrodes, lead to artificial field-enhancement and, thus, to a distorted flow of particles.

To overcome these difficulties, two numerical methods have been coupled: Boundary-fitted coordinates are introduced to be able to treat the technical geometries, and the particle-in-cell method is used to describe the particle flow in electromagnetic fields in a self-consistent manner. On the discrete grid the field quantities are computed, whereas the particles are advanced in the physical space. Numerical algorithms describing the transition between the grid model and the mesh-free model were developed [5, 7].

The remainder of this article is as follows: In Section 2 the basic concept of the particle-in-cell method is introduced and in Section 3 that of boundary-fitted coordinates. The coupling between the PIC method and boundary-fitted coordinates is discussed in Section 4, presenting the interpolation and localization scheme in detail. Section 5 deals with applications in which these techniques have been successfully applied.

2 The particle-in-cell (PIC) method

Since particle flow in external and self-generated electromagnetic fields is to be modeled, the particle-in-cell particle method is applied. This method is successfully applied to electromagnetic problems where not only the applied electric and magnetic fields dominate the behavior of the simulation region but also the eigenfields induced by the flow of particles.

In order to effectively calculate the electric and magnetic forces acting upon the particles, a grid is defined in the computational area. On this discrete grid the fields are calculated. These fields are interpolated onto the particle position producing the forces acting upon the charged particles (Interpolation). With respect to the electric and magnetic forces on the particle position, each particle is transported further by solving the Lorentz equation (Particle Pushing). By means of the new position the particles have to be localized within the grid, computing the relative coordinates with respect to the cell the particle is located in (Localization). On the basis of the new phase space coordinates the charge and current densities can be calculated at the mesh points to serve as source terms for the next step of the field solver.

The advantage of this method is that the number of operations for the computation of the selfconsistent forces is only proportional to the number of particles. The drawback consists in the fact that the introduction of a grid produces a switching back and forth between a mesh-free model and a discrete model (see Fig. 1).

The particles used in the PIC method are so-called macro-particles. Each macro-particle represents an appropriate number of elementary particles of a specific type. A type of particles is characterized by the ratio between its specific charge and its mass. As the movement of elementary particles is to be simulated, each macro-particle moves like an elementary particle of the proper type. However, when determining the fields it must be taken into account that each macro-particle consists of many elementary particles.

3 Boundary-fitted coordinates

In order to compute discrete solutions of the electromagnetic fields in a technical device, partial differential equations have to be solved in a domain with complicated boundaries and mixed boundary conditions. In Fig. 2 an example for a discrete description of an L-shaped geometry with a boundary-fitted grid is shown. A boundary-fitted grid is logically equivalent to a monoblock grid (cf. Fig. 2b) and has therefore a regular data structure: Each interior grid point has an upper, a lower, a right, and a left neighboring point. Hence, they are well suited for finite difference schemes.

The computational grid is created numerically using the concept of Thompson [6]. The basic idea is the transformation of the physical area to a logical area. The boundary of the physical area is mapped onto the boundary of a rectangle. In this rectangle an equidistant grid is defined and transformed back to the physical area.

The grid system is computed by solving elliptic partial differential equations: Let $\xi(x,y)$, $\eta(x,y)$ be the mapping of the physical area in the (x,y)-plane onto the logical area in the (ξ,η)-plane given as the solution of the elliptic system

$$\Delta\xi(x,y) = P, \quad \Delta\eta(x,y) = Q$$

Then the inverse maps $x(\xi,\eta)$, $y(\xi,\eta)$ satisfy

$$\alpha x_{\xi\xi} - 2\beta x_{\xi\eta} + \gamma x_{\eta\eta} + J^2 x_\xi P + J^2 x_\eta Q = 0$$

$$\alpha y_{\xi\xi} - 2\beta y_{\xi\eta} + \gamma y_{\eta\eta} + J^2 y_\xi P + J^2 y_\eta Q = 0$$

where

$$J := x_\xi y_\eta - y_\xi x_\eta$$

and

$$\alpha := x_\eta^2 + y_\eta^2, \quad \beta := x_\xi x_\eta + y_\xi y_\eta, \quad \gamma := x_\xi^2 + y_\xi^2.$$

Solving the discretized Dirichlet problem leads to the grid points (x_{ij}, y_{ij}) in the physical space. With functions P and Q the density of interior lines can be controlled. Attraction and repulsion of grid lines towards specified points and lines can be achieved. Usually $P = 0$ and $Q = 0$ are chosen.

The advantages of elliptic grid generator systems are that the resulting grids are inherently smooth, the danger of overlapping of grid lines is small, and they can easily be adapted to general boundary configurations. Moreover, due to the logical structure of the grid, it is easy to adapt the mesh to the solution of the problem in order to obtain a better resolution of the numerical solution or to improve the grid in terms of smoothness and orthogonality or to handle physical effects where the boundary of the computational domain changes during the simulation.

4 Coupling the PIC method with boundary-fitted grids

The force acting upon the particles is determined by an interpolation from the fields calculated in the discrete model. Vice versa, to obtain the densities in the discrete model by means of the charge of the particles given in the mesh-free model, the particles must be localized within the grid. In the following, extended algorithms for interpolation, localization as well as particle pushing will be reported.

4.1 Interpolation

If a particle $P(\alpha_1, \alpha_2)$ is located in the unit square cell (I, J), $I = [0, 1] \times [0, 1]$, as shown in Fig. 3a the field u_p at the particle position is calculated from the fields $u_{i,j}$, $u_{i+1,j}$, $u_{i+1,j+1}$, $u_{i,j+1}$ given at the mesh points using the standard area-weighting method [1, 3]:

$$u_p = (1-\alpha_1)(1-\alpha_2)u_{i,j} + \alpha_1(1-\alpha_2)u_{i+1,j} + (1-\alpha_1)\alpha_2 u_{i,j+1} + \alpha_1\alpha_2 u_{i+1,j+1}$$

In order to be able to apply the area-weighting method in an arbitrary quadrangle as depicted in Fig. 3b proper interpolation weights have to be calculated. Geometrically the interpolation weight α_1 can be found by determining the line l_1 through point P intersecting line DC with the same ratio than line AB. In the same way, α_2 can be constructed by line l_2 intersecting line AD and BC with the same ratio. If S_{AB}, S_{BC}, S_{DC}, S_{AD} are these intersection points it holds

$$\alpha_1 = \frac{AS_{AB}}{AB} = \frac{DS_{DC}}{DC} \quad \text{and} \quad \alpha_2 = \frac{AS_{AD}}{AD} = \frac{BS_{BC}}{BC}$$

Let $P(x, y) \in V$ be the position of the particle inside cell (I, J) with corners $(x_{i,j}, y_{i,j})$, $(x_{i+1,j}, y_{i+1,j})$, $(x_{i+1,j+1}, y_{i+1,j+1})$, $(x_{i,j+1}, y_{i,j+1})$ (see Fig. 3b). The interpolation weights $(\alpha_1, \alpha_2) \in I^2$ are given by the following formulas:

$$\alpha_2 = \frac{-p + \sqrt{p^2 + q}}{x_{11}^s - 1} \text{ for } x_{11}^s \neq 1 \qquad \alpha_2 = \frac{y^s}{1 + x^s(y_{11}^s - 1)} \text{ for } x_{11}^s = 1$$

and

$$\alpha_1 = \frac{x^s}{1 + \alpha_2(x_{11}^s - 1)}$$

$$\text{with} \quad p = \frac{1}{2}[1 + x^s(y^s_{11} - 1) - y^s(x^s_{11} - 1)] \quad \text{and} \quad q = y^s(x^s_{11} - 1).$$

The quantities x^s and y^s are obtained from the matrix equation

$$\begin{pmatrix} x^s \\ y^s \end{pmatrix} = \begin{pmatrix} x_{10} - x_{00} & x_{01} - x_{00} \\ y_{10} - y_{00} & y_{01} - y_{00} \end{pmatrix}^{-1} \begin{pmatrix} x - x_{00} \\ y - y_{00} \end{pmatrix}$$

where the used subscripts are the abbreviation for: $(00) = (i, j)$, $(10) = (i + 1, j)$, $(01) = (i, j + 1)$ and $(11) = (i + 1, j + 1)$. A more theoretical treatment can be found in [5]. The proposed interpolation scheme together with the area-weighting method have the characteristical feature that linear functions are represented exactly.

4.2 Particle pushing

The equation of motion for charged macro-particles in electromagnetic fields are set up by the Lorentz force:

$$\mathbf{F} = \frac{d}{dt}(m\frac{d}{dt}\mathbf{x}) = q(\mathbf{E} + \frac{d}{dt}\mathbf{x} \times \mathbf{B}).$$

Since the macro-particles consisting of electrons reach velocities near the speed of light, the relativistic equation of motion must be solved:

$$\frac{d}{dt}(\mathbf{p}) = \frac{q}{m_0}(\mathbf{E} + \frac{\mathbf{p}}{\gamma} \times \mathbf{B}), \mathbf{p}(0) = \gamma(0)\mathbf{v}(0) \quad \text{and} \quad \frac{d}{dt}\mathbf{x} = \mathbf{v}, \mathbf{x}(0) = \mathbf{x}_0$$

with $m = m_0\gamma$ and m_0 being the rest mass of the particle. γ is the relativistic factor defined as

$$\gamma = \frac{1}{\sqrt{1 - (\frac{d}{dt}\mathbf{x})^2 / c^2}} \quad \text{and} \quad \mathbf{p}(t) := \gamma\frac{d}{dt}\mathbf{x} = \gamma\mathbf{v}(t).$$

4.3 Localization

In order to identify cells within a grid, the addresses in x- and y-direction of the left lower grid point of each cell are assigned to the cell as a pair of numbers (I, J). In an equidistant grid, the address of the cell, a particle with coordinates (x, y) is located in, is defined by

$$I = \text{INT}((x - x_1)/\Delta x) + 1 \quad \text{and} \quad J = \text{INT}((y - y_1)/\Delta y) + 1,$$

where (x_1, y_1) are the coordinates of the left lower corner point of the grid and Δx and Δy are the mesh-sizes in x- and y-direction, respectively. However, in boundary-fitted grids these formulas cannot be applied anymore.

For our applications, the interpolation scheme is also used in order to find the particle position with respect to the grid: After the new coordinates of the particle P have been computed, the interpolation weights (α_1, α_2) are determined by transforming the cell (I_0, J_0) the particle was located in at the previous time step. With knowledge of these interpolation weights (α_1, α_2) one can decide whether the particle still lies inside the same cell or whether it is outside the cell:

$(\alpha_1, \alpha_2) \in I^2 \iff$ Particle P still is inside cell (I_0, J_0).

$(\alpha_1, \alpha_2) \notin I^2 \iff$ Particle P has left cell (I_0, J_0).

In particular, when using an equidistant grid and under the condition that the particle can only move to a neighboring cell the following holds:

$\alpha_1 > 1, \alpha_2 > 1 \Longrightarrow$ Particle in cell $(I_0 + 1, J_0 + 1)$
$\alpha_1 \in I, \alpha_2 > 1 \Longrightarrow$ Particle in cell $(I_0, J_0 + 1)$
$\alpha_1 < 0, \alpha_2 > 1 \Longrightarrow$ Particle in cell $(I_0 - 1, J_0 + 1)$
$\alpha_1 > 1, \alpha_2 \in I \Longrightarrow$ Particle in cell $(I_0 + 1, J_0)$
$\alpha_1 \in I, \alpha_2 \in I \Longrightarrow$ Particle in cell (I_0, J_0)
$\alpha_1 < 0, \alpha_2 \in I \Longrightarrow$ Particle in cell $(I_0 - 1, J_0)$
$\alpha_1 > 1, \alpha_2 < 0 \Longrightarrow$ Particle in cell $(I_0 + 1, J_0 - 1)$
$\alpha_1 \in I, \alpha_2 < 0 \Longrightarrow$ Particle in cell $(I_0, J_0 - 1)$
$\alpha_1 < 0, \alpha_2 < 0 \Longrightarrow$ Particle in cell $(I_0 - 1, J_0 - 1)$.

However, when using a non-equidistant grid, it is of course not guaranteed that the particle is found by calculating the weights corresponding to the old cell addresses. When the particle has left the cell, this algorithm must be applied iteratively until the correct interpolation weights $(\alpha_1, \alpha_2) \in I^2$ are found. The applied particle search algorithm consists of four steps and reads as:

Search algorithm

Step 1 Let $(I, J) = (I_0, J_0)$ be the cell the particle was located in at the previous time step.

Step 2 Compute the interpolation weights (α_1, α_2) with respect to cell (I, J).

Step 3 Add the interpolation weights to the cell address: $(I + \alpha_1, J + \alpha_2)$.

Step 4 Set $(I, J) = (\mathrm{INT}(I + \alpha_1), \mathrm{INT}(J + \alpha_2))$.

Repeat steps 2 to 4 $k \in \mathrm{N}$ times.

The iteration parameter k depends on the structure of the grid. In case of an equidistant grid k can be chosen to be 1. (In this case, however, it is advisable to determine the cell in a direct manner.) Our experience indicates that usually $k = 3$ is sufficient.

4.4 Charge and current assignment

When the particles are pushed and localized within the grid, the new interpolation weights (α_1, α_2) have been computed with respect to the new cell. By means of the interpolation weights the charge (and current) densities can be computed on the grid points by taking into account the relative position of the particle within the cell:

$$\begin{aligned} \rho_{00} &= \rho_{00} + g_{00} \times q(i)/V_{00} \\ \rho_{10} &= \rho_{10} + g_{10} \times q(i)/V_{10} \\ \rho_{11} &= \rho_{11} + g_{11} \times q(i)/V_{11} \\ \rho_{01} &= \rho_{01} + g_{01} \times q(i)/V_{01} \end{aligned}$$

where $q(i)$ is the charge of the i-th macro-particle and V_{ij} being the volume assigned for node (i, j). The weights are given by

$$\begin{aligned} g_{00} &= (1 - \alpha_1) \times (1 - \alpha_2) \\ g_{10} &= \alpha_1 \times (1 - \alpha_2) \\ g_{11} &= \alpha_1 \times \alpha_2 \\ g_{01} &= (1 - \alpha_1) \times \alpha_2 \end{aligned}$$

5 Applications

Gyrotrons are capable of producing millimeter wave radiation at high average power levels in access of 1 MW with pulse lengths of several seconds. The properties of the electron beam injected into the interaction region are cruical to good performance of the tube. High power gyrotrons almost always use magnetron injection guns (MIGs) producing an annular electron beam in which the electrons execute small cyclotron orbits at a frequency required for cyclotron resonance interaction in a gyrotron. For a good interaction efficiency the perpendicular velocity should be as large as possible. A spread in perpendicular velocity results in a spread in axial velocity, and should be kept small as possible.

A numerical model of the electron gun investigated at the Karlsruhe Nuclear Research Center by Piosczyk [4] together with a boundary-fitted grid is drawn in Fig. 4a. Indicated are the cathode with grounded potential, the anode (80 kV) and the modulation anode (25 kV). The strength of the applied magnetic field in the cathode near area is about 0.2 T and increases up to 0.3 T. Since electron guns are rotationally symmetric, Fig. 4 shows the projection of the gun into the z-r plane.

In the simulation it is assumed that only the marked area at the cathode creates electrons by thermal emission with a total current of 25 A. This corresponds to an electric field strength at the cathode of 4100 kV/m. It should be noted that due to the importance of the emitting parts of the gun we chose a very fine resolution at the emitting cathode surface which is indicated in more detail in Fig. 4b.

For the numerical simulation, the time step is set to $dt = 5 \times 10^{-12}$ s. A stable stationary state is achieved after 2 000 time steps with about 3 000 electrons. The total simulation requires 10 min CPU time on an IBM 3090. For this steady-state, the trajectories of 3 sample electrons are computed in order to obtain an impression on the particle flow. Figures 5a and 5b show the movement in the (z, r)-plane and the (r, θ)-plane, respectively. A complete analysis of the results can be found in [2], where this model is applied to describe in detail the behavior of MIG guns. Moreover, a modified ray-trace version of the PIC model is used for the design and optimization of these MIG guns.

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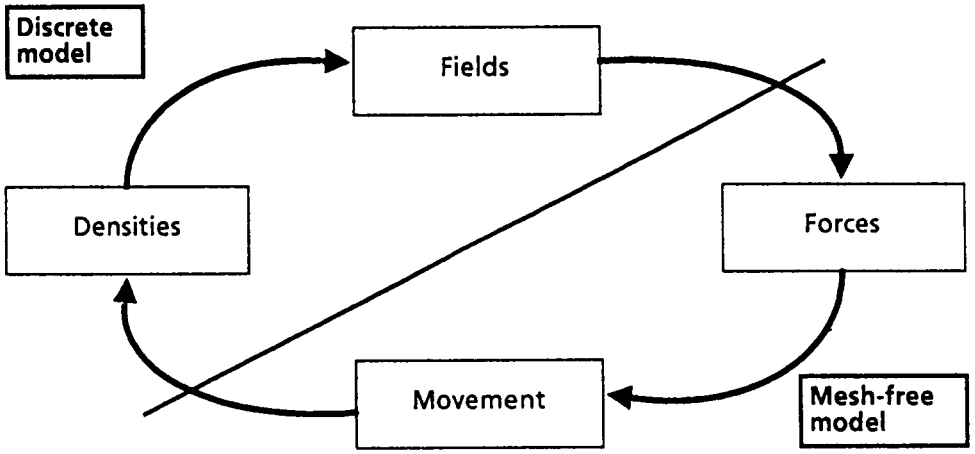

Figure 1: Iteration cycle of the particle-in-cell method.

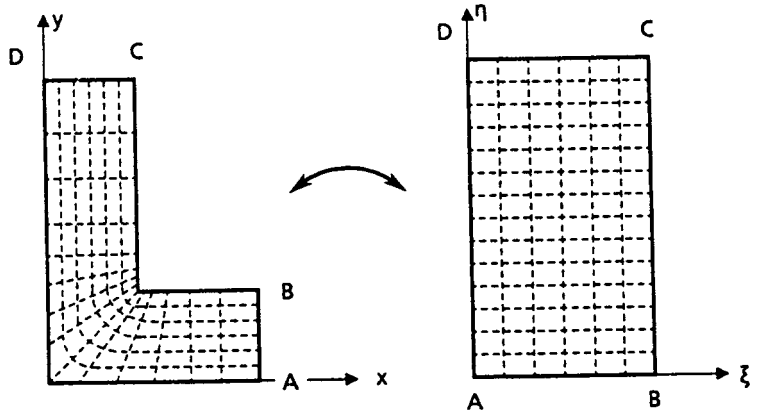

Figure 2: Discrete representation of an L-shaped geometry with a boundary-fitted grid. (a) physical grid, (b) logical grid.

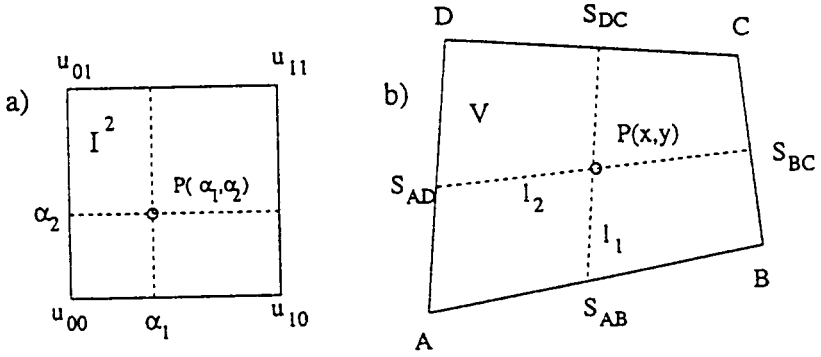

Figure 3: Geometrical interpretation of the interpolation weights (a) in the unit square cell and (b) in a quadrilateral cell.

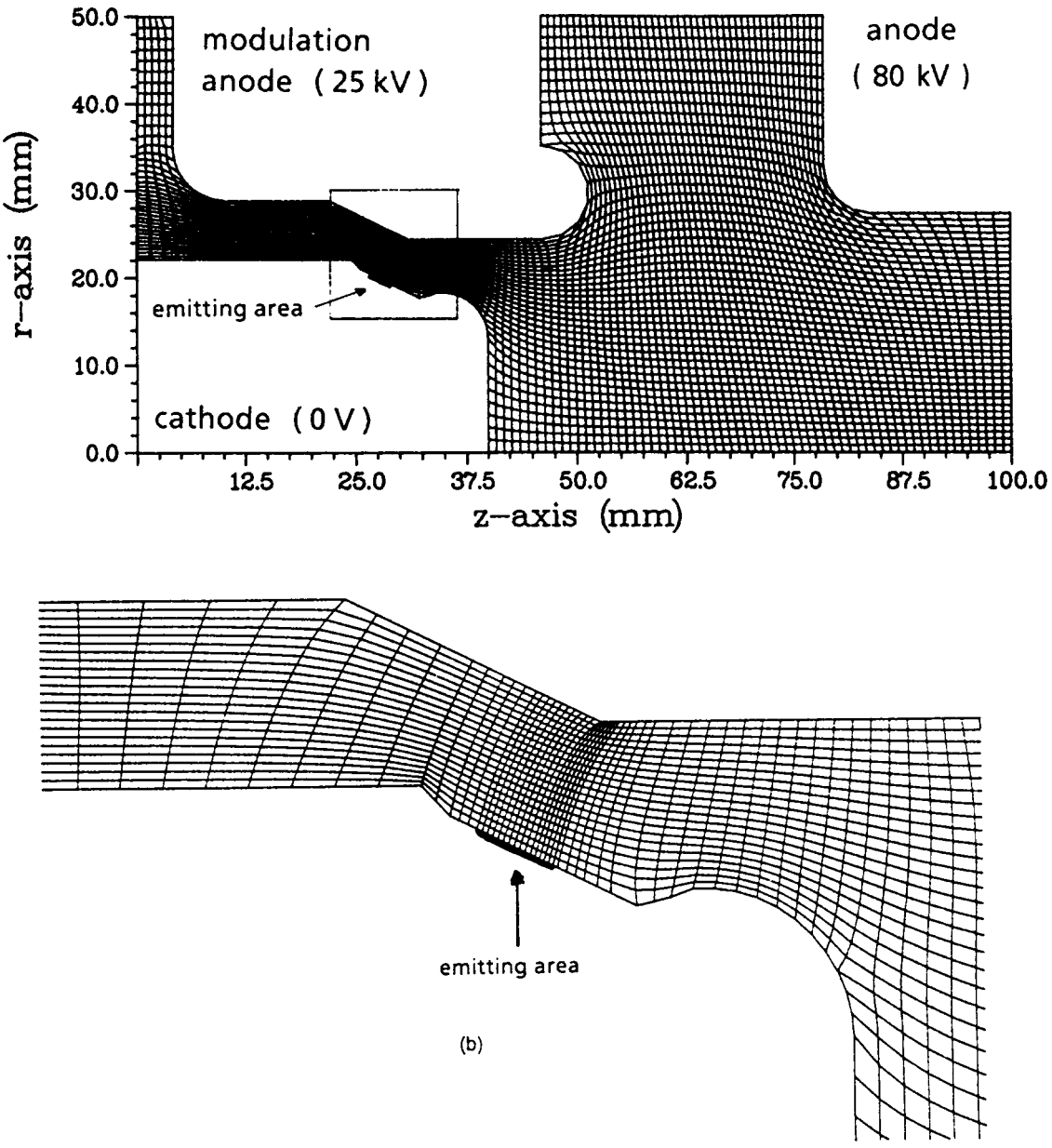

Figure 4: Numerical model of the MIG gun with a 120×51 boundary-fitted grid. (a) overall, (b) detailed.

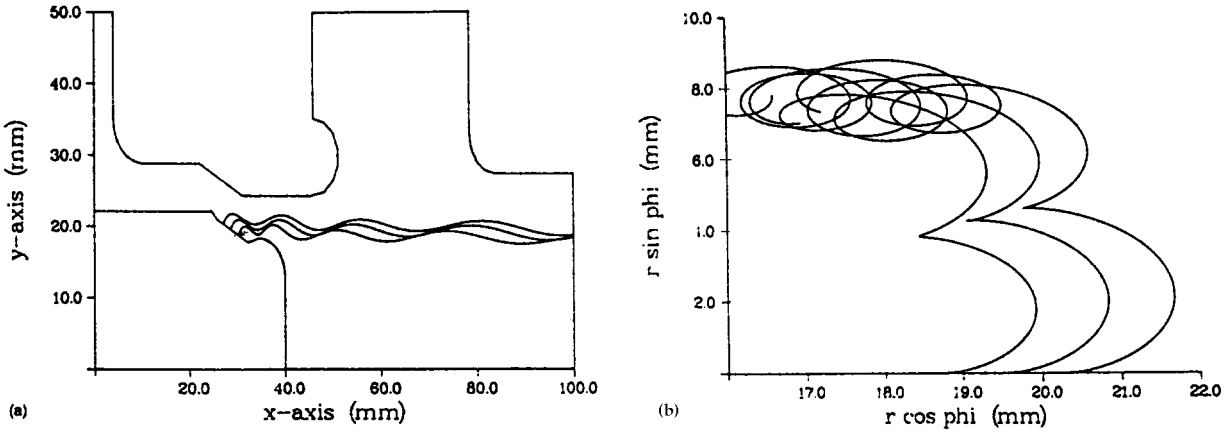

Figure 5: Single trajectories of electrons: (a) (z, r)-plane, (b) (r, θ)-plane.