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Parallel software for Simulation of Emission Processes in Strong Electromagnetic Fields

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Abstract

The aim of this paper is development of parallel software for simulation of emission processes in strong electromagnetic fields. One of the modelling methods in this area is the smoothed particle method in combination with grid calculation of fields based on Maxwell's equations. In our work, for the axially symmetric geometry of a technical system, a numerical method for calculating the electron emission from the surface of metal cathodes is proposed. The technique uses the representation of large smoothed particles and implements electromagnetic field calculations on Cartesian spatial grids. Software realization focused on parallel computing. Testing of the approach confirmed its correctness and efficiency.

Keywords: parallel computing, electromagnetic fields, emission processes, smoothed particle method, Maxwell's equations.

1 Introduction

Steady worldwide demand for composite materials is demonstrated by various industries. The high rates of development of the market of polymer composite materials are determined by a wide range of their properties that exceed the properties of traditional materials, as well as a variable approach to creating a product, from modeling its structure, properties and shape to the choice of production technologies. Strict environmental policy, as well as the restriction and/or ban on dumps are factors constraining the growth of consumption of composites. For example, the aircraft, shipbuilding, automotive industries, traditional and green energy, etc. need various composite materials and technologies for their efficient and safe application. The latter is expressed in the requirements for product characteristics, regulations, cost thresholds. At the same time, price horizons for the production of new composite materials are determined, taking into account economic expediency. Note that the required new materials, the costs of their manufacture and application in various industries vary significantly. That is why composite materials can provide a wide range of technological and economic parameters.

Currently, the development and application of composite materials is carried out on the basis of a wide range of scientific and engineering studies, which are based on mathematical and computer modeling. This approach helps to produce effective technical and production solutions. Adequate mathematical and computer models make it possible to obtain accurate data on the properties of composites, their processing technologies, the shape and parameters of the final products.

One of the practical methods for obtaining and processing new composite materials is the impact on the substance of high-energy flows of charged particles. In this regard, generators of high-current ion and electron beams are being developed, as well as devices based on them (see for example [1]). Short-pulse generators of relativistic electron beams with a pulse duration in the range of micro- and nanoseconds, which do not destroy the structure of materials and are suitable for its comprehensive analysis, are currently most in demand. This technology is used both for laboratory research and in the production of special coatings for aerospace and automotive equipment.

In this paper, we study the problem of implementing devices that generate relativistic electron beams (REB) based on the field emission mechanism. The process of REB generation is accompanied by the formation of plasma. The aim of the work is to develop a computational technology and its software implementation for modeling emission processes in strong electromagnetic fields. The continuation of this work will be a numerical analysis of the interaction of particle beams with various media and materials. The computational technology under study includes the development of: (a) a mathematical model; (b) numerical methods for its analysis; (c) parallel algorithms and a set of programs for computing clusters and supercomputers; (d) a digital platform for conducting detailed numerical experiments. The novelty of the approach lies in the combination of the method of irregular grids and the method of particles, a new implementation of the model of particles in the form of clouds, a parallelization technique. To verify the developed numerical technique, we used data from [1-4]. Using the developed code, the emission process of relativistic electrons from the surface of a coaxial diode of real geometry was calculated.

2 Model and Methods

Field emission of relativistic electrons can be implemented in generators based on coaxial diodes with magnetic self-insulation. Let us consider one of the variants of such a generator, shown in Fig. 1. We will assume that the system is in a uniform magnetic field with induction B_z. The electron emission is initiated by a TE wave with amplitude E_0, coming from the left boundary. The REB arising in this case is amplified by the plasma layer generated at the preliminary stage by the anode-collector system.

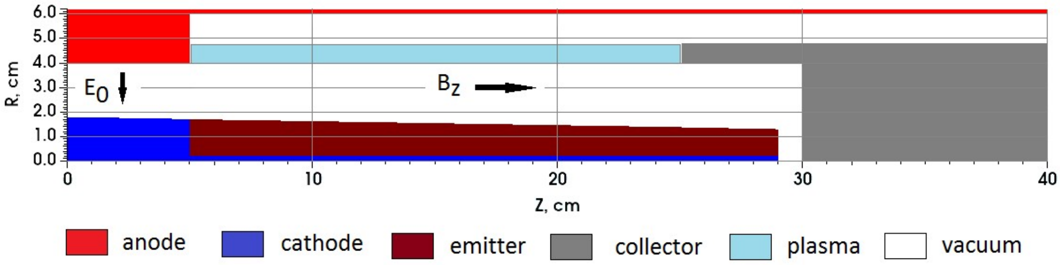

Figure 1. Coaxial diode with magnetic insulation.

The model is based on Maxwell's equations, which in SI, together with constitutive equations, have the form:

$$\begin{cases} \operatorname{div}\mathbf{D} = \rho, \quad \operatorname{div}\mathbf{B} = 0, \\ \operatorname{rot}\mathbf{E} = -\dfrac{\partial \mathbf{B}}{\partial t}, \quad \operatorname{rot}\mathbf{H} = \mathbf{j} + \dfrac{\partial \mathbf{D}}{\partial t}, \\ \mathbf{D} = \varepsilon_a \mathbf{E}, \quad \mathbf{B} = \mu_a \mathbf{H}. \end{cases} \tag{1}$$

Here $\mathbf{D}$ and $\mathbf{B}$ – electric and magnetic induction vectors, $\mathbf{E}$ and $\mathbf{H}$ – electric and magnetic field strength vectors, $\rho = \rho_- + \rho_+$ – bulk charge density, $\rho_- = q_- n_-$ and $\rho_+ = q_+ n_+$ – densities of negatively and positively charged particles, $q_- < 0$ and $q_+ > 0$ – particle charges, n_- and n_+ – volume concentrations of particles, $\mathbf{j} = \mathbf{j}_- + \mathbf{j}_+$ – total current density of the particles, $\mathbf{j}_- = \rho_- \mathbf{v}_-$ and $\mathbf{j}_+ = \rho_+ \mathbf{v}_+$ – current density of particles, $\mathbf{v}_-$ и $\mathbf{v}_+$ – average velocities of particles, $\varepsilon_a = \varepsilon\varepsilon_0$ and $\mu_a = \mu\mu_0$ – absolute dielectric and magnetic permeability of the medium, here μ_0 and ε_0 – magnetic and dielectric permittivity of vacuum, c – speed of light.

Equations (1) are considered in the region of the cylinder Ω, not occupied by the cathode Ω_C and anode Ω_A, that is $\Omega_D = \Omega / (\Omega_C \cup \Omega_A)$. Taking into account the constitutive equations and piecewise constants ε and μ from (1) we can obtain:

$$\begin{cases} \operatorname{div}(\varepsilon_a \mathbf{E}) = \rho, \quad \operatorname{div}\mathbf{B} = 0; \\ \operatorname{rot}\mathbf{E} = -\dfrac{\partial \mathbf{B}}{\partial t}; \quad \operatorname{rot}\left(\dfrac{1}{\mu_a}\mathbf{B}\right) = \mathbf{j} + \dfrac{\partial}{\partial t}(\varepsilon_a \mathbf{E}). \end{cases} \tag{2}$$

In this work, the method of smoothed particles for electrodynamics (SPE) is applied. It consists in the fact that instead of the classical equations of continuity and momentum, the equations of relativistic dynamics are used, written for individual charged particles.

$$\begin{cases} \dfrac{d\mathbf{r}_{\alpha,k}}{dt} = \mathbf{v}_{\alpha,k}, \quad \dfrac{d\mathbf{p}_{\alpha,k}}{dt} = q_{\alpha,k}\left(\mathbf{E} + \left[\mathbf{v}_{\alpha,k} \times \mathbf{B}\right]\right), \\ \mathbf{p}_{\alpha,k} = m_\alpha \mathbf{v}_{\alpha,k} \gamma_{\alpha,k}, \quad \gamma_{\alpha,k} = 1/\sqrt{1-\left(v_{\alpha,k}/c\right)^2}, \quad k = 1,\ldots,N_\alpha; \\ n_\alpha = \sum\limits_{k=1}^{N_\alpha} \delta\left(\mathbf{r} - \mathbf{r}_{\alpha,k}\right), \quad \rho_\alpha = \sum\limits_{k=1}^{N_\alpha} q_{\alpha,k} \delta\left(\mathbf{r} - \mathbf{r}_{\alpha,k}\right), \\ \mathbf{v}_\alpha = \dfrac{1}{N_\alpha} \sum\limits_{k=1}^{N_\alpha} \mathbf{v}_{\alpha,k}, \quad \mathbf{j}_\alpha = \sum\limits_{k=1}^{N_e} q_{\alpha,k} \delta\left(\mathbf{r} - \mathbf{r}_{\alpha,k}\right) \mathbf{v}_{\alpha,k}, \quad \mathbf{p}_\alpha = \dfrac{1}{N_\alpha} \sum\limits_{k=1}^{N_\alpha} \mathbf{p}_{\alpha,k}. \end{cases} \tag{3}$$

here $\mathbf{r}_{\alpha,k}$, $\mathbf{p}_{\alpha,k}$, $\mathbf{v}_{\alpha,k}$, $q_{\alpha,k}$ and m_α – radius-vector, momentum, velocity, charge and mass of the particle, $\gamma_{\alpha,k}$ – relativistic correction to speed, $v_{\alpha,k} = \left|\mathbf{v}_{\alpha,k}\right|$ – module of the particle speed, $\delta\left(\mathbf{r} - \mathbf{r}_{\alpha,k}\right)$ – the Dirac delta function describing the charge density of a particle of the sort α (e.g., $\alpha = "-"$ – for plasma electrons, $\alpha = "+"$ – for positively charged plasma ions), N_α – the number of particles of the kind α.

Equations (2) are solved using the grid method of finite volumes [5], which combines the explicit scheme FDTD [6, 7] for dynamic equations and the well-known "cross" scheme for the Poisson equation, solved by the iterative method [8]. Equations (3) are numerically implemented using the symmetric Adams scheme [8-10].

3 Parallel realization and results

Based on the developed numerical model, a parallel program was created using the ANSI C/C++ programming language and the MPI and OpenMP parallel computing standards. The parallelization technique is based on the domain decomposition method (DDM) [11, 12] and algorithms for dynamic load balancing of computers (DLB) [13]. Let's look at some details of parallel implementation.

1. The technique of parallelizing the FDTD scheme and solving the Poisson equation is related to the partition of the Cartesian cylindrical grid into compact domains of the same size. During calculations, each domain is attached to a specific MPI process, which sequentially performs calculations within four blocks of the dynamic algorithm.

The specificity of the chosen physical problem makes it possible to construct a simple and efficient partition of the computational domain only along the longitudinal coordinate z (Fig. 2). Therefore, in this case, precisely MPI technology is used in which each MPI process is located on a separate computing node of the cluster. This partition may be initially uniform (Fig. 2a). However, in the case of a complex real geometry, it is selected in accordance with the following criterion: the volume occupied by vacuum or plasma should be approximately the same for all MPI processes (Fig. 2b).

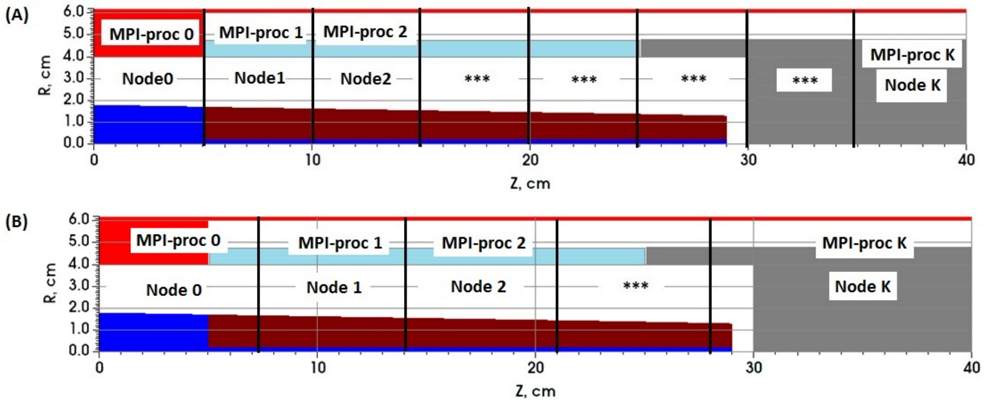

Figure 2. Variants of partitioning the volume of the computational domain into domains, which are processed by various MPI processes.

On each computing node (that is, in the area of responsibility of a specific MPI process), further parallelization is performed by starting computational threads. It is implemented using OpenMP technology. In the framework of computations on a grid, the uniform partitioning of grid nodes on threads is used. This is achieved by introducing a through linear numbering of the grid nodes. An important point in the effective use of parallelization on threads is the need for their one-time initialization at the very beginning of the calculation and attachment to a specific CPU core.

2. At each fixed moment of time (that is, at each step of the time cycle), not all domains can be occupied by particles. As a result, the used initial distribution of grid domains among between MPI processes turns out to be inefficient at the stage of calculating particle trajectories. In this situation, the transfer of particles from one computational domain to another is realized to speed up calculations. This takes into account: (a) the processes of emission (birth) of particles, (b) the natural migration of particles in accordance with the influence of an electromagnetic field, (c) the annihilation of particles on metal surfaces. If there are few particles in any domain (approximately 100), then one thread is used to calculate their trajectories. Otherwise, such a number of threads is used, which provides the maximum calculation speed. Since particles dynamically move from one domain to another for the above reasons (that is, they move from one MPI process to another MPI process), it becomes necessary to correct the computational load. This feature is implemented by the global dynamic load balancing algorithm. It involves measuring the calculation time of each cycle step in each MPI process and determining its average value, as well as the dispersion. The value of dispersion allows us to estimate the need for redistribution of particles among MPI processes. The transfer of particles from one MPI process to another is implemented using functions of asynchronous message passing.

3. The testing of the parallel algorithm was carried out on the emission problem discussed above and described in more detail in [4]. In calculations, the number of grid nodes and the emission factor responsible for the number of particles varied. High performance of acceleration and efficiency (the latter was 90-95%) were obtained with the number of parallel processes in the range of 1-256, at moderate dimensions of the grid model (the number of grid nodes is about 1 million) and at the number of particles is about 500,000. Testing was carried out on a supercomputer К60 Supercomputer Center of Collective Usage of the KIAM RAS.

4. The results of calculations of the REB development process in the absence and in the presence of plasma are presented in Figs. 3 and 4 (at the bottom of the figures there is a scale of values of the dimensionless electron density of the beam and plasma). As can be seen from the figures, electron emission starts sequentially from the left end of the emitter and moves along its entire surface. Moving away from the emitter, the electrons are accelerated by the field and either reach the anode or first break through the plasma layer and go to the anode. It can be seen that, in the second case, the beam electrons move the plasma electrons towards the anode. This was also observed in the experiments. It should be noted that the presence of the collector on the right side closes the circuit and stimulates secondary emission at the end of the cathode.

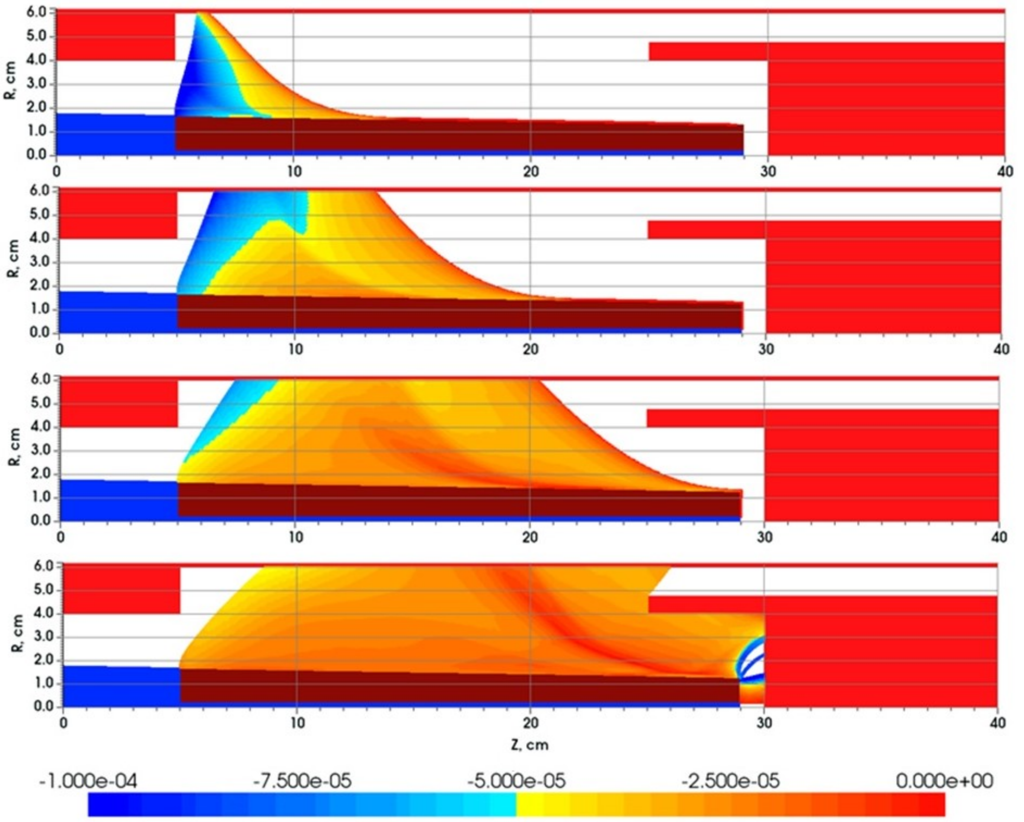

Figure 3. Electron density distributions at time moments t=0.5, 0.75, 1.0, 1.25 ns (arranged from top to bottom) under the absence of the plasma layer.

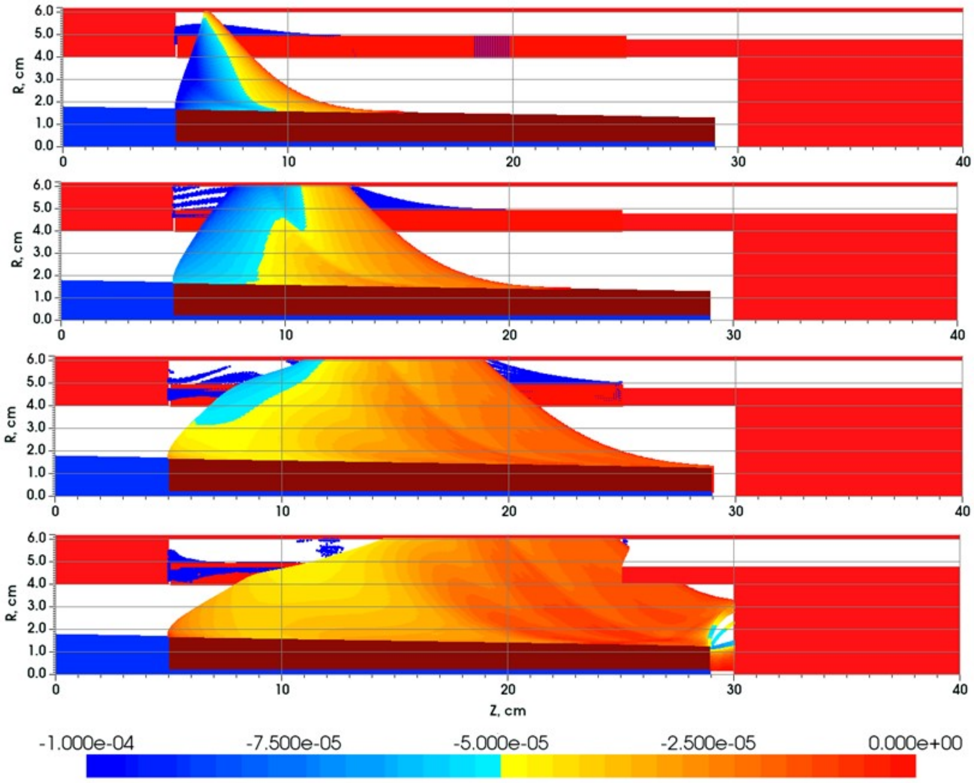

Figure 4. Electron density distributions at time moments t=0.5, 0.75, 1.0, 1.25 ns (arranged from top to bottom) under the presence of the plasma.

The time dependences of the total emission current are shown in Figure 5, 6. By the range of values, they correspond to the theoretical estimates and calculated data of work [4]. In the second case, some increase in the emission current is observed, stimulated by the presence of the plasma layer.

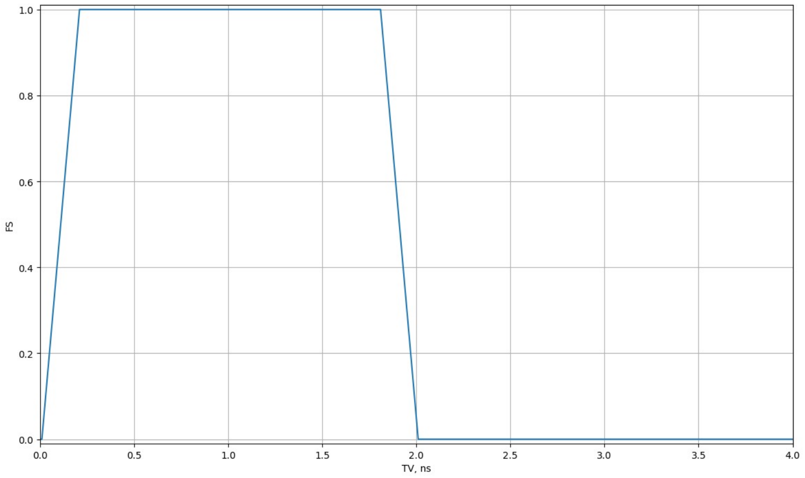

Figure 5. Time profile of the TE-wave.

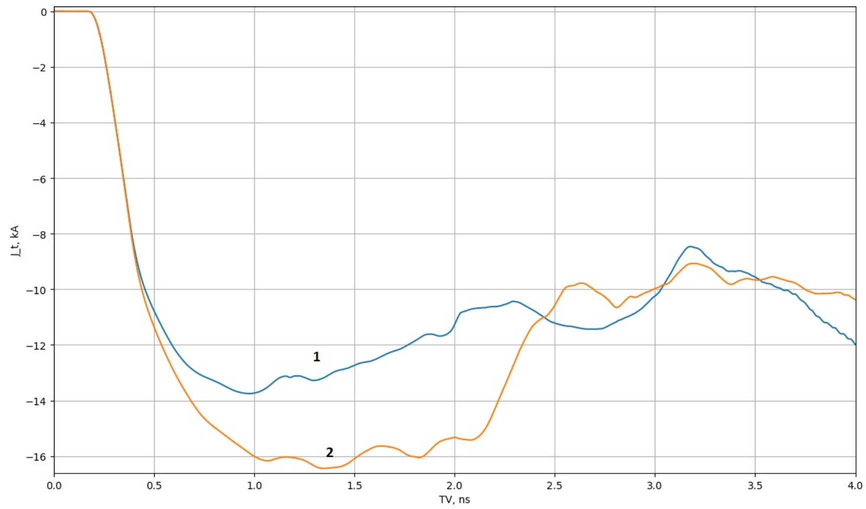

Figure 5. Dependences of the total emission current on time under a trapezoidal pulse of TE-wave modulation. Numbers 1 and 2 correspond to the calculation results under the absence and presence of the plasma layer.

4 Conclusions and Contributions

The problem of modeling emission processes in strong electromagnetic fields is considered. To solve it, a new computer model has been developed and its parallel software implementation has been carried out. The code was tested on the example of the problem of a coaxial diode with magnetic insulation and showed the effectiveness of numerical and parallel approaches. The realistic pictures of the emission process were obtained with the help of the developed code.

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