

NUMERICAL CALCULATION OF NONSTATIONARY CHARGED-PARTICLE
BEAMS

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Algorithms are considered for the solution of nonstationary electronics problems which reduce to calculation of electromagnetic fields and numerical integration of the equations of motion of charged particles. It is assumed that at each moment of time the potential distribution is described by the Poisson equation. Field calculation is performed by finite-difference methods. For simulation of the space charge a modified "large particle" method is described. The KSI-BESM compilation system is discussed as a means of automation of the problem-solving process. Examples of problem solutions are offered.

1. In the design of electrovacuum devices, charged-particle accelerators, and other electrophysical apparatuses the formation of intense current flows with given properties in complex electromagnetic fields becomes of importance (see, for example, [1] and the literature cited therein).

In recent years significant progress has been made in the development of electromagnetic field computation algorithms for fields satisfying the Laplace or Poisson equations, calculation of charged-particle trajectories with consideration of space charge, and creation of programs for electronic computer calculation of complex electron-optical systems [2-16].

Calculation is reduced to solution of a self-congruent problem containing within itself field calculation, which is performed most often by finite-difference methods (although integral equation methods are also employed [11, 12]), and numerical integration of the equations of motion of the charged particles in the electromagnetic field.

For space-charge simulation the "large particles" method is used [7, 14], which in the case of stationary problems reduces to the more economical "current tube" or "filament" algorithm, described in detail, for example, in [2-8, 15, 16].

The effectiveness of practical problem calculation is strongly dependent on the degree of automation of the solution process, including initial data preparation, selection of economical algorithms, and presentation of results in a form convenient for processing. Some of these questions are considered in [6, 8-10].

In [16] a description is offered of the KSI-BESM compilation system for solution of a wide class of static electron-optical problems: calculation of beams of particles with various masses and charges is performed in two- or three-dimensional regions of practically arbitrary form, including media with various dielectric properties. Consideration of particle distribution over energies and angles, secondary emission, the influence of an external magnetic field, and relativistic effects is possible. Such a general formulation has various physicotchnical applications, for example, calculation of insulator construction, particle accelerators, electron tubes and guns, electron-optical converters, uhf electronic devices, etc.

The present study will describe algorithms for the solution of corresponding nonsta-

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tionary problems and means for automation of their computation in the KSI-BESM compilation system.

2. In solving nonstationary problems we make the following assumptions: a) the frequency and amplitude of variable electrode voltages are independent of particle space charge; b) the displacement currents are negligibly small in comparison to conduction currents; c) the "intrinsic" magnetic field created by the particle beam is negligibly small.

In this case the electric field potential φ satisfies the Poisson equation

$$\Delta\varphi(\mathbf{r}, t) = -4\pi\rho(\mathbf{r}, t) \quad (2.1)$$

where ρ is the space-charge density; t is the time; and \mathbf{r} is the point radius vector.

The motion of an individual particle with mass M_i and charge Z_i is described by the equation (we consider the nonrelativistic case)

$$\frac{d^2\mathbf{r}_i}{dt^2} = \frac{Z_i}{M_i} \left(-\nabla\varphi(\mathbf{r}_i, t) + \frac{1}{c} [\mathbf{v}_i \times \dot{\mathbf{B}}(\mathbf{r}_i, t)] \right) \quad (2.2)$$

where \mathbf{r}_i is the particle coordinate; $\mathbf{v}_i = d\mathbf{r}_i/dt$; c is the velocity of light; and \mathbf{B} is the induction of the "external" magnetic field. At the initial moment of time all elementary particles of one mass and charge located in a volume $\Delta\mathbf{r}$, and having velocities in the interval $\Delta\mathbf{v}$ are joined in one group, or "large particle." Its motion is described by an equation of the form of Eq. (2.2), where \mathbf{r}_i is the coordinate of the center of mass, and \mathbf{v}_i is the mean velocity of all elementary particles in one group.

If the computation region G is divided into subregions G_p with boundaries S_p and if Eq. (2.1) is integrated over each of the G_p , then after use of Green's formula we obtain for all p

$$\int_{S_p} \frac{\partial\varphi}{\partial\mathbf{n}} dS = -4\pi \int_{G_p} \rho d\mathbf{r} = -4\pi q_p \quad (2.3)$$

Below we will not construct numerical methods for Eq. (2.1), but for the equivalent system (2.3).

Then

$$q_p = \sum_i q_{ip} \quad (2.4)$$

where q_{ip} is the charge of the i -th large particle, referred to the volume G_p (summation is performed over all particles).

For the potential we consider boundary conditions of the following types:

$$\varphi|_{\Gamma_1} = g(\mathbf{r}, t) \quad (2.5)$$

$$\frac{\partial\varphi}{\partial\mathbf{n}} \Big|_{\Gamma_2} = 0 \quad (2.6)$$

$$\lambda_+ \frac{\partial\varphi}{\partial\mathbf{n}} \Big|_{\Gamma_3^+} = \lambda_- \frac{\partial\varphi}{\partial\mathbf{n}} \Big|_{\Gamma_3^-} \quad (2.7)$$

Here Γ_1 is the portion of the boundary Γ with given potential values (as a rule, the metal-electrode surfaces), Γ_2 are surfaces or lines of symmetry, and Γ_3 are divisions between media with differing dielectric constants.

In the presence of emitting boundary surfaces, aside from the initial data for the large particles located in the computation region at $t = 0$

$$\mathbf{r}_i|_{t=0} = \mathbf{r}_{i0}, \quad \mathbf{v}_i|_{t=0} = \mathbf{v}_{i0} \quad (2.8)$$

it is also necessary to set initial coordinates, velocities, and charge values for large particles entering into the region in subsequent time intervals. If at the emitter the current density is $\mathbf{j}(\mathbf{r}, \mathbf{V}, t)$, then from an elementary area ΔS_c during a time interval Δt we will "launch" particles with charge

$$q_k = \frac{1}{|\Delta\mathbf{V}|} \int_{\Delta S_k} \int_{\Delta\mathbf{V}} \int_{\Delta t} \mathbf{j}(\mathbf{r}, \mathbf{V}, t) dt d\mathbf{V} dS \quad (2.9)$$

where \mathbf{V} is the velocity of elementary particles entering from the corresponding interval ΔV . The current density \mathbf{j} is assumed a fixed function of \mathbf{r} , \mathbf{V} , t . A special class is represented by problems with current limited by space charge, where at zero initial particle velocities the current density on the emitter with potential $\varphi = 0$ is defined by

$$\mathbf{j}(\mathbf{r}, t) = c_1 \varphi^{3/2}(\mathbf{r} + d\mathbf{n}, t) d^{-2} \quad (2.10)$$

where c_1 is a known constant, and d is a value so small that at a distance d from the emitter equipotential lines may be considered "almost" parallel to its surface, and within this interval the solution is assumed to obey the three-halves law, Eq. (2.10).

We take into consideration problems with secondary emission, wherein on some surfaces a current density is given as a function of the current and velocity of incident "primary" particles, and also of the properties of the electrode material.

We will now consider the solution of the nonstationary problem. For the initial moment of time we find the potential distribution with density values and boundary conditions at $t = T_0 = 0$. Then in the field $\varphi(\mathbf{r}, 0)$, $\mathbf{B}(\mathbf{r}, 0)$ we calculate particle trajectories up to a moment $T_1 > T_0$ and the space charge introduced by these particles. Then for the charge distribution thus determined and boundary conditions at $t = T_1$, the function $\varphi(\mathbf{r}, T_1)$ is calculated, particle trajectories up to moment T_2 are calculated, etc. The process is continued up to a given $t = T$. During computation of the sequential interval $\Delta T_\nu = T_{\nu+1} - T_\nu$ as initial data we take the parameters of all particles calculated earlier at time $t = T_\nu$, and also parameters of particles which enter the computation region at this moment. If a particle passes beyond the limits of the region, it is excluded from further consideration. The error in such a representation of a nonstationary process is a value of the order of $o(\Delta T)$. If ΔT_ν is large compared to the characteristic time for change of problem parameters, then in each step T_ν iteration may be performed with respect to space charge, repeating the computation of trajectories and fields several times.

Potential field calculation will be performed by finite-difference methods in a rectangular (in the three-dimensional case, parallelepipedal) grid with piecewise-continuous steps. The Poisson equation with boundary conditions (2.5)-(2.7) is approximated by five-point (seven-point in three dimensions) difference equations, described in detail in [16, 17] and having, in general, a solution error of $o(h)$ (h being the maximum grid step). If the region has no internal boundaries, i.e., the medium is homogeneous, and the Neumann conditions are given only on boundaries parallel to the coordinate lines, the error is $o(h^2)$. The finite-difference Poisson equations are equivalent to an approximation of Eq. (2.3), while as G_k we take the cell of the difference grid. As an example, in Fig. 1 this is the region

$$\frac{x_i + x_{i-1}}{2} \leq x \leq \frac{x_i + x_{i+1}}{2}, \quad \frac{1}{2}(y_j + y_{j-1}) \leq y \leq \frac{1}{2}(y_j + y_{j+1})$$

while the equation has the form

$$\begin{aligned} (\Delta U)_{ij} = & \frac{h_j + h_{j-1}}{2h_{i-1}} U_{i-1j} + \frac{h_i + h_{i-1}}{2h_{j-1}} U_{ij-1} + \frac{h_j + h_{j-1}}{2h_i} U_{i+1j} \\ & + \frac{h_i + h_{i-1}}{2h_j} U_{ij+1} - \left(\frac{1}{h_i + h_{i-1}} + \frac{1}{h_j h_{j-1}} \right) \times \frac{(h_j + h_{j-1})(h_i + h_{i-1})}{4} U_{ij} = -f_{ij} = -4\pi q_{ij} \end{aligned} \quad (2.11)$$

Solution of the difference equations is performed by some iteration method, which may be represented in the form of a universal algorithm

$$U^{n+1} = U^n + H_n (\Delta U^n - f) \quad (2.12)$$

The matrix H_n defines the concrete algorithm, for example, for the explicit Peaceman-Rockford method having the form

$$H_n = \frac{2}{\tau} (E - \tau \Lambda_2)^{-1} (E - \tau \Lambda_1)^{-1} \quad (2.13)$$

where τ is the iteration parameter, and Λ_1 , Λ_2 are the lower and upper triangular matrices, $\Lambda_1 + \Lambda_2 = \Lambda$. More details of iteration methods employed are given in [16, 17].

The most effective algorithm for solution of difference equations is obviously that one employing a sequence of grids (see [17] and the literature cited therein), realized in the KSI-BESM system for two-dimensional problems with arbitrary boundary form and boundary conditions.

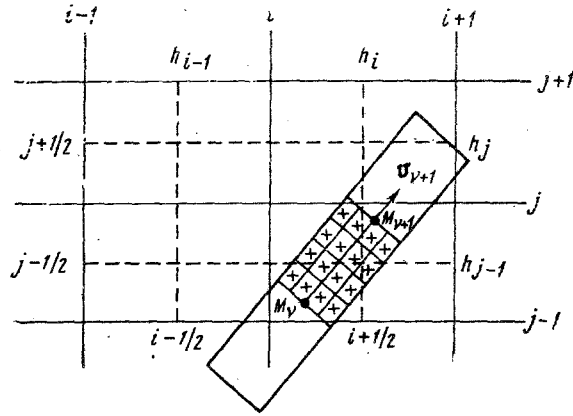


Fig. 1

Numerical integration of the equations of motion is performed, as in [14], by a stable system with second-order error. In the algorithm employed calculation of the right side is performed once in each step, not twice as in [14]:

$$\begin{aligned} \mathbf{v}_{n+1} &= \mathbf{v}_n + \beta \Delta t_n \left\{ -\nabla \varphi \left(\mathbf{r}_n + \frac{\Delta t_n}{2} \mathbf{v}_n \right) + \left[\frac{\mathbf{v}_{n+1} + \mathbf{v}_n}{2c} \mathbf{B} \left(\mathbf{r}_n + \frac{\Delta t_n}{2} \mathbf{v}_n \right) \right] \right\} \\ \mathbf{r}_{n+1} &= \mathbf{r}_n + \Delta t_n \frac{\mathbf{v}_{n+1} + \mathbf{v}_n}{2} \end{aligned} \quad (2.14)$$

Here the indices i are omitted for brevity, $\beta = Z/M$, Δt_n is the integration step ($\Delta t_n \leq \Delta T_v$). Potential gradients are calculated from the results of numerical solution of the Poisson equation at the grid nodes. The function $\mathbf{B}(\mathbf{r})$ is assumed given. A special case is the class of problems where magnetic-induction values are given along the axis or plane of symmetry, and are calculated at remaining points within the region from extension formulas.

We will examine the algorithm for space-charge computation in more detail. From an area ΔS of the emitting surface at some "middle" point M_0 at moment T_0 let there depart with a velocity v_0 an elementary particle, which over the time interval $\Delta T_1 = T_1 - T_0$ arrives at the point M_1 with velocity v_1 . We assume that at moment T_1 the charge of all particles of the velocity group with mean initial velocity v_0 leaving during the time ΔT_1 is located within a cylinder of volume $\Delta S M_0 M_1$. The value of this charge is equal to $\Delta T_1 I$ where I is the mean (over time ΔT_1) current value passing through the surface ΔS (if the "partial" current density $j(M_0, v_0, T_0)$, corresponding to elementary particles in the group with mean velocity v_0 is known, one can take $I = j(M_0, v_0, T_0) \Delta S$). The charge $\Delta T_1 I$ is distributed over cells G_k of the difference grid intersecting the volume $\Delta S M_0 M_1$, on the assumption that the value of j therein is constant. To do this we divide the base of the cylinder ΔS into N_1 equal areas, and the segment $M_0 M_1$ into N_2 intervals such that with the assumption of constant acceleration $(v_1 - v_0)/\Delta T_1$ a particle traverses the intervals in equal time intervals. Thus, we obtain $N_1 N_2$ volumes containing equal charges $\Delta T_1 I / N_1 N_2$, each of which we refer to that difference cell in which the corresponding volume's center lies. We then proceed further in an analogous manner. For example, at moment T_2 the previously considered charge $\Delta T_1 I$ is distributed over the volume of a cylinder with bases centered at M_2 and $M_{0,1}$, where M_2 and $M_{0,1}$ are the positions at T_2 of particles which departed at $t = T_1$ from the points M_1 and M_0 , respectively.

If at the initial moment there is already a space charge located within the calculation region, the large particles are defined as rectilinear cylinders with directions parallel to the corresponding mean elementary-particle velocities. In Fig. 1 for the two-dimensional case we schematically depict division of charges between sections with points M_v and M_{v+1} .

If the problem is stationary, i.e., boundary and initial conditions are time-independent, then the described process may be considered a performance of successive approximations to the solution. In particular, it is then possible to take $\Delta T = \infty$, i.e., the trajectories of all particles are calculated up to exit from the region, and the charge is considered distributed in current tubes ("filaments") whose forms are described by the

trajectories of the corresponding particles. For stationary problems selection of the iteration method by space charge is valuable (see, for example, [16]).

3. We will consider certain peculiarities of the KSI-BESM compilation system for calculation of nonstationary problems. The basic components of the KSI-BESM are language devices for description of the initial data and algorithms, a program library (module system), and a control complex.

An effective means of automating formulation of initial data is the PG language for description of two-dimensional boundary problems [18], which permits effective specification in convenient form of the configurations of multielectrode devices. The translator from PG language included in the KSI-BESM verifies validity of the input information, indicating any errors present.

The KSI-BESM module library contains a set of programs written in BESM-6 machine code and a catalog with information on the location and input parameters of all modules. The library contains a developed set of algorithm and service programs. The algorithm modules are distinguished by their functions, the form of the method employed, and that they also depend on the concrete form of the problem. For example, in the library there is a set of various iteration programs for solution of Poisson difference equations (point and block upper relaxation, longitudinal-transverse drive, variable triangle methods, etc.) with differing memory requirements and convergence rates for various problems. Independent modules are reserved for two- and three-dimensional variants, and also for absence or presence of space charge (i.e., the Laplace or Poisson equations). Analogously, for the other cumbersome part of the problem, trajectory calculation, algorithms for numerical integration of the equations of motion are realized in individual modules depending on the dimensionality of the problem, presence of a magnetic field, relativity effects, etc.

The service portion of the library, aside from control of input data, ensures printout of the results in useful form (potential, field intensity, current, etc., values, equipotential lines and trajectories, including graphic printout).

The operation of the compilation system is controlled by a modular programming language KSI [19], which contains operators for module rotation, information exchange with external computer components, library and archive formation, and also operators for arithmetical operations, control transmission, etc. The program in KSI language for solution of a concrete problem is transformed by the compiler to a control program, which then performs the calculation directly.

The KSI-BESM facilities permit computation in stages with storage of intermediate results in the archive, as well as computation of several variants of the problem.

The KSI-BESM library with catalog, PG translator, program compiler, and archive are contained on one magnetic tape. Each individual system module utilizes only one BESM-6 memory, and recourse to magnetic drums or tapes can be had when convenient by change of modules or completion of the computation.

The difference algorithms permit solutions of the Poisson equation on a rectilinear grid with piecewise constant steps and a number of nodes up to 10,000 in two dimensions and 7,000 in three dimensions. For the two-dimensional case, independent of the type of boundary problem, a sequence of coarser auxiliary grids may be utilized.

In the calculated region a varying quantity of emitting surfaces may be specified, including ones emitting "secondary" particles. The particles may be divided into an arbitrary number of energy or angular groups according to a distribution fixed by the user. Particle velocity and coordinate values found in solution of nonstationary problems are preserved either in the operative memory or on a magnetic drum. The maximum number of particles in the calculated region is ~7500 in two dimensions, ~5000 in three dimensions.

4. We will present some examples of calculation of nonstationary beams in electromagnetic fields.

The problem of interaction of a grouped electron flow with the high-frequency field of a planar diode in the high-amplitude regime was solved. The gap studied and particle beams are shown schematically in Fig. 2. The problem consists of calculating the motion of a monochromatic beam of length L , entering the gap with uniform velocity through the plane

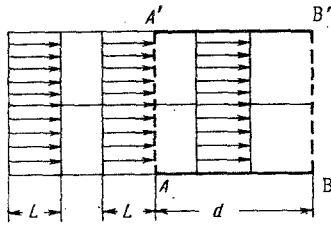


Fig. 2

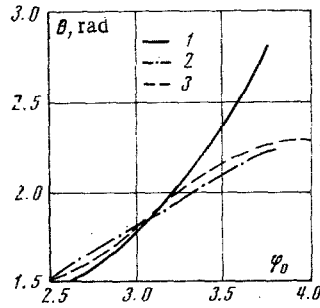


Fig. 3

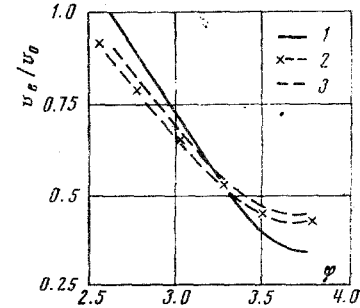


Fig. 4

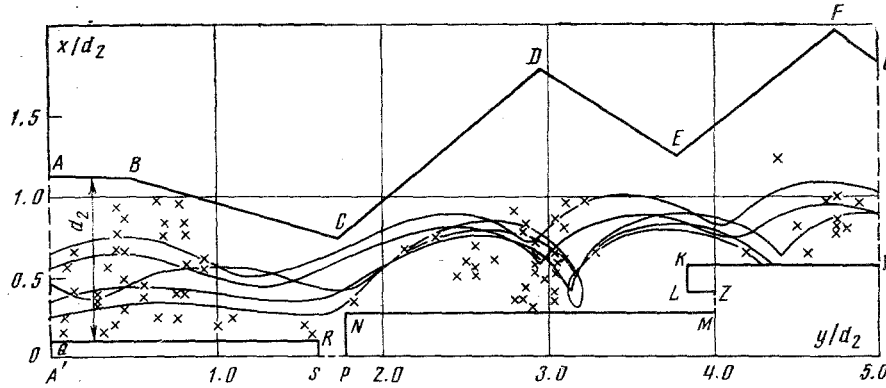


Fig. 5

AA', transparent to electrons, at a potential U_0 . At the output plane BB' of the gap a variable accelerating voltage $\varphi = U_m \sin(\omega t + \varphi_0)$, is applied, where φ_0 is the initial phase of the cluster in the gap $\omega = 2\pi\nu_0/5L$, ν_0 is the electron velocity at the gap input. On the planes AB and A'B' the condition $\partial\varphi/\partial n = 0$ is imposed. Calculations were performed for cluster precedence $p = I/U_0^{3/2} \approx 5 \cdot 10^{-6} a/b^{3/2}$ (I, beam current), initial phase $\varphi_0 = 150^\circ$ and statistical flight angle $\theta_0 = \omega d/\nu_0 = \pi/2$, where d is the gap width.

The cluster was simulated by 20 "large particles," released into the gap at intervals $\Delta T = L/20 \nu_0$. The field was calculated at the nodes of a uniform grid with $l = 40$ intervals across the gap width. Calculations were performed up to time $T = 100 \Delta T$.

Curves in Fig. 3 and Fig. 4 show the dependence of flight angle $\theta = \omega(T_L - T_0)$ and the ratio v_L/ν_0 on the electron entrance angle $\varphi + \omega T_0 + \varphi_0$ for a uhf oscillation amplitude $\xi = U/U_0 = 1.0$, where T_0 is the time of entrance of electrons into the system with velocity ν_0 ; T_L , ν_L are the time and velocity at exit from the system. Results of calculations obtained with the KSI-BESM system and the kinematic approximation (curves 2 in Figs. 3 and 4) practically coincide with corresponding theoretical data (curves 3 in Figs. 3 and 4) presented in [20]). Curves 1 in Figs. 3 and 4 correspond to calculation with consideration of space charge. As is evident from the graphs, space charge leads to acceleration of electrons in the forward portion of the cluster and braking of electrons at the cluster end (their flight angle increases).

A study was made of the electron flow-formation process in an electron optical system with braking.

The system geometry and electrode potentials are shown in Fig. 5. On the surfaces denoted by dashed lines the condition $\partial\varphi/\partial n = 0$ was imposed; on the line ABCDEFG — $\varphi = U_a$, on VKLZ — $\varphi = U_k$, on MNP — $\varphi = U_k$, on SPQ — $\varphi = U_{xk}$. The magnetic field H_0 was homogeneous and directed perpendicular to the plane of the diagram.

Through the system entrance plane AA' there periodically are introduced electron clusters which are represented as sets of large particles. The particles of each cluster are introduced into the region studied at identical time intervals $\Delta T = T_0/N$, where T_0 is the transit

time of a single cluster across AA'. Initial coordinate and velocity values of particles in the plane AA', and also values of the charges at each time moment, were set by the results of computing the preceding portion of the electron optical system. Calculations were performed for the following parameter values:

$$U_a / H_0^2 d_2^2 = 0.39 \text{ v/e} \cdot \text{cm}^3, \quad U_{x_k} = -0.075 U_a, \quad U_{k1} = 0 \\ U_{k2} = 0.15 U_a, \quad N = 24$$

The calculation region was covered by a rectilinear finite-difference grid with total of 2000 nodes. Figure 5 shows trajectories of electrons entering the region at time $T = 14 \Delta T$, calculated in the kinematic approximation. The same figure shows the distribution of large particles, denoted by crosses, at time $70 \Delta T$. Consideration of cluster space charge leads to settling of a portion of the particles in the first electron optical system section onto the cold cathode.

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