## Conservative Finite-Difference Scheme and Two-Stage Iteration Process of its Realization for the 2D Problem of Semiconductor Plasma Generation by Femtosecond Pulse

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**Abstract.** In this paper we develop conservative finite-difference schemes (FDS) for the process of femtosecond pulse interaction with semiconductor. This process is described by the set of 2D dimensionless differential equations concerning concentrations of both free electrons and ionized donors, and potential of electric field, induced by laser pulse and laser beam intensity changing. The electron mobility, electron diffusion, nonlinear dependence of absorption coefficient on semiconductor characteristics are taken into account also.

For the problem under consideration we have constructed and compared two conservative FDS. One of them is based on the well known split-step method, the second one is based on the original two-stage iteration process. We paid the special attention to the 2D Poisson equation solution. This equation is solved by using an additional iteration process. Thus, to solve the problem under consideration it is necessary to achieve a convergence of two iteration processes.

As follows from computer simulation provided by us, the criterion choice for the iteration process convergence can significantly affect on the equations solution accuracy. We used the criterion based on assessment of an absolute and relative error of the solution obtained on iterations. This criterion is also used for Poisson equation solving. However, the iteration convergence criterion, based on discrepancy estimating, is more effective for using in this case.

Computer simulation results showed that the developed conservative FDS on the base of two-stage iteration process is an effective tool for investigation of complicated modes of semiconductor characteristics changing.

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## 1 Introduction

Investigation of a laser radiation interaction with semiconductor is very modern problem because semiconductors are widely used in many applications such as optoelectronics devices (see, for example [1-22]). Among them we would stress an optically bistable element, based on using various nonlinear responses of semiconductor, exposed by a laser radiation. As it is well-known, the optical bistability (OB) is very promising phenomenon for the creation and developing of all-optical data processing. This phenomenon characterizes by existence of a hysteresis loop for semiconductor characteristics. This results in two stable states appearing: upper and low states for the same value of the incident optical pulse intensity. Realization of one of them depends on initial conditions for the problem. Thus, the problem has not the unique steady state solution if an OB occurs. Moreover, under certain conditions, the problem solution can become unstable and complicated oscillating regimes of semiconductor characteristics changing develop.

OB phenomenon accompanies also by many various nonlinear effects occurring in semiconductor. So, we face to necessity of computing very complicated regimes. For example, developing of the helical wave for electron-hole plasma was demonstrated in [23-24] if a semiconductor is placed in the external electric field. For computer simulation of these complicated nonlinear non-stationary processes it is necessary to use especially developed finite-difference schemes (FDS) which possessing such properties as conservatism, stability to initial condition perturbation and stability to round-off errors. Of course, at developing the FDS, the main question is the difference solution proximity to the solution of the differential problem. However, if we provide a computer simulation during long-time interval in comparison with characteristic times of processes under investigation, we have to take into account accumulation of rounding errors at computer simulation. If the FDS possesses property of stability to rounding errors accumulation, then this FDS possesses the property of asymptotic stability [25]. Construction of such FDS is an urgent problem. For example, in [26] there is at least one sample of using FDS which doesn't provide asymptotic stability property. To avoid this influence one has to use extraordinary small grid steps.

One of the well-known approaches for computer simulation of multi-dimensional equations is the split-step method using [27-32]. However, in [33] we had shown that this method possesses some disadvantages for the problem under consideration and it is stimulated us to develop a new FDS for computer simulation of this problem. In the present paper we continue our research in this direction. Below we paid our main attention to solving the Poisson equation with respect to the electric field potential. The aim is a choice of an iteration process termination criterion for high computation accuracy achievement at long time interval (about 1000 dimensionless units). For this purpose we have to develop a FDS, which possess the asymptotic stability property.

## 2 Statement of 2D problem

The process under consideration is described by the following set of 2D dimensionless differential equations [34-36]:

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = \gamma(n-N), \quad 0 < x < L_x, \quad 0 < y < L_y, \quad t > 0, \tag{2.1}$$

$$\frac{\partial n}{\partial t} = D_x \frac{\partial}{\partial x} \left( \frac{\partial n}{\partial x} - \mu_x n \frac{\partial \varphi}{\partial x} \right) + D_y \frac{\partial}{\partial y} \left( \frac{\partial n}{\partial y} - \mu_y n \frac{\partial \varphi}{\partial y} \right) + G(N, n) - R(N, n), \quad (2.2)$$

$$\frac{\partial N}{\partial t} = G(N,n) - R(N,n), \quad \frac{\partial I}{\partial y} + \delta_o \delta(N,n)I = 0.$$
(2.3)

Above the following notations are introduced. Function *n* denotes a free electron concentration in the conductivity zone of a semiconductor; *N* is a concentration of ionized donors. Function  $\varphi$  describes a dimensionless electric field potential. *I* is the intensity of laser radiation propagating along the *y* axis. The coordinate *x* is a coordinate that is transverse to the laser pulse propagation direction. Variables *x*, *y* are dimensionless spatial coordinates and  $L_x$ ,  $L_y$  denote their maximal values, correspondingly. Variable *t* denotes dimensionless time, its maximal value is equal to  $L_t$ . Coefficients of electron diffusion  $D_x$ ,  $D_y$  and coefficients of electron mobility  $\mu_x$ ,  $\mu_y$  are non-negative constants. Parameter  $\gamma$  depends, in particular, on the maximal achieving concentration of free charged particles,  $\delta_0$  denotes a maximal semiconductor absorption coefficient of laser energy.

Light energy absorption coefficient  $\delta(N,n)$  can be approximated by different ways in dependence of physical experiment conditions. Below we consider its following approximation

$$\delta(N,n) = (1-N)e^{-\psi(1-\xi n)}, \quad \psi, \xi > 0, \tag{2.4}$$

which is close to one of the experimental dependencies [34] corresponding to the concentration OB existence. This dependence takes into account the Burstein-Moss effect: dynamic saturation of the excited energy levels in the conduction band and depletion of donor levels. The functions G and R, describing generation and recombination of free charged particles in the semiconductor, are given by the formulas

$$G(N,n) = q_0 I\delta(N,n), \quad R(N,n) = \frac{nN - n_0^2}{\tau_p},$$
 (2.5)

where  $n_0$  is an equilibrium value of the free electron concentration and ionized donor concentration,  $\tau_p$  characterizes a recombination time of free electron.  $q_0$  is a maximal intensity of the incident laser pulse, its profile is Gaussian one along the *x*-coordinate

$$I|_{y=0} = \exp\left(-\left(\frac{x - 0.5L_x}{0.1L_x}\right)^2\right)(1 - \exp(-10t)).$$
(2.6)

Boundary conditions (BC) for the set of equations (2.1) are written below if an electric current is absent through the semiconductor faces and if a semiconductor is placed in the external electric field:

$$\left( \frac{\partial n}{\partial x} - \mu_x n \frac{\partial \varphi}{\partial x} \right) \Big|_{x=0,L_x} = \left( \frac{\partial n}{\partial y} - \mu_y n \frac{\partial \varphi}{\partial y} \right) \Big|_{y=0,L_y} = 0,$$

$$\frac{\partial \varphi}{\partial x} \Big|_{x=0,L_x} = -E_x, \quad \frac{\partial \varphi}{\partial y} \Big|_{y=0,L_y} = -E_y.$$

$$(2.7)$$

But it should be stressed, that in the present paper we provide computer simulation with  $E_x = E_y = 0$ . In this case, the problem solution is symmetrical concerning the laser beam centre. So, it is important feature for an accuracy estimating for the FDS.

Initial conditions for the charged particle concentrations depend on the BC for the set of equations. If an external electric field is non-zero we have to solve an additional stationary problem for initial distribution of the semiconductor characteristics. If the external electric field is absent then the initial conditions are written in the following manner:

$$n|_{t=0} = N|_{t=0} = n_0, \quad \varphi|_{t=0} = 0, \quad I|_{t=0} = 0.$$
 (2.8)

For the problem (2.1)-(2.8) the law of charge conservation takes place:

$$Q(t) = \int_{0}^{L_{y}} \int_{0}^{L_{x}} (n(x,y,t) - N(x,y,t)) dx dy = 0.$$
(2.9)

Difference analogue of this invariant has to be valid for the difference problem. We follow this invariant for the FDS construction. If the difference analogue for the invariant (2.7) conserves, then our FDS is a conservative one. This property shouldn't be loosen due to the accumulation of a computing error even for computation on long time interval. So, our aim is to construct the conservative FDS with the asymptotic stability property.

## 3 Finite-difference schemes

To solve the problem (2.1)-(2.8) we have constructed a FDS. Below we describe it briefly. With this aim let us introduce in the domain

$$\bar{G} = \{0 \le x \le L_x\} \times \{0 \le y \le L_y\} \times \{0 \le t \le L_t\},\$$

the uniform grids in time and space

$$\Omega = \omega_x \times \omega_y \times \omega_t, \quad \Omega' = \omega_x \times \omega_y \times \omega'_t, \quad \Omega'' = \omega_x \times \omega'_y \times \omega'_t, \\ \omega_x = \{x_i = ih_x, i = \overline{0, N_x}, h_x = L_x / N_x\}, \quad \omega_y = \{y_j = jh_y, j = \overline{0, N_y}, h_y = L_y / N_y\},$$

$$\omega_{y}' = \left\{ y_{j}' = (j - 0.5)h_{y}, j = \overline{0, N_{y} + 1}, h_{y} = L_{y}/N_{y} \right\}, \quad \omega_{t} = \left\{ t_{k} = k\tau, k = \overline{0, N_{t}}, \tau = L_{t}/N_{t} \right\}, \\ \omega_{t}' = \left\{ t_{k}' = (k + 0.5)\tau, k = \overline{0, N_{t} - 1}, \tau = L_{t}/N_{t} \right\}.$$

Let's define grid functions  $n_h$ ,  $N_h$ ,  $\varphi_h$  on  $\Omega$  by the following way:

$$n_{ijk} = n(x_i, y_j, t_k), \quad N_{ijk} = N(x_i, y_j, t_k), \quad \varphi_{ijk} = \varphi(x_i, y_j, t_k).$$

Functions  $\bar{n}_h$ ,  $\bar{N}_h$ ,  $\bar{\varphi}_h$  are defined on the grid  $\Omega'$  shifted on time:

$$\bar{n}_{ijk} = n\left(x_i, y_j, t'_k\right), \quad \bar{N}_{ijk} = N\left(x_i, y_j, t'_k\right), \quad \bar{\varphi}_{ijk} = \varphi\left(x_i, y_j, t'_k\right).$$

Function  $I_h$  is defined on the grid  $\Omega''$  shifted additionally on spatial coordinate y:  $I_{ijk} = I(x_i, y'_i, t'_k)$ .

For brevity, below we used the following index-free notations:

$$\begin{split} f &= f_i = f_{ijk} , \quad f_{i\pm 1} = f_{i\pm 1jk}, \quad f_{j\pm 1} = f_{ij\pm 1k}, \\ f_{i\pm 0.5} &= 0.5 \left( f_{ijk} + f_{i\pm 1jk} \right), \quad f_{j\pm 0.5} = 0.5 \left( f_{ijk} + f_{ij\pm 1k} \right), \quad \hat{f} = \hat{f}_i = f_{ijk+1}, \\ \stackrel{0.5}{f} &= f_i = 0.5 \left( f_i + \hat{f}_i \right) = 0.5 \left( f + \hat{f} \right), \end{split}$$

where *f* is one of the grid functions  $n_h$ ,  $N_h$ ,  $\varphi_h$ .

$$I_i = I_{ijk}, \quad I_{i\pm 1} = I_{i\pm 1jk}, \quad \hat{I}_i = I_{ij+1k}, \quad \stackrel{0.5}{I}_i = 0.5 (I_i + \hat{I}_i).$$

For the FDS construction we also use the following notations:

$$\begin{split} R &= \left(nN - n_0^2\right) / \tau_p, \quad \hat{R} = \left(\hat{n}\hat{N} - n_0^2\right) / \tau_p, \quad \stackrel{0.5}{R} = 0.5(R + \hat{R}), \quad \bar{R} = \left(\bar{n}\bar{N} - n_0^2\right) / \tau_p, \\ G &= q_0 \stackrel{0.5}{I}\delta, \quad \hat{G} = q_0 \stackrel{0.5}{I}\delta, \quad \stackrel{0.5}{G} = 0.5(G + \hat{G}), \quad \bar{G} = q_0 \stackrel{0.5}{I}\bar{\delta}, \\ \delta &= (1 - N)\exp\left(-\psi(1 - \xi n)\right), \quad \hat{\delta} = (1 - \hat{N})\exp\left(-\psi(1 - \xi \hat{n})\right), \\ \bar{\delta} &= (1 - \bar{N})\exp\left(-\psi(1 - \xi \bar{n})\right), \quad \stackrel{0.5}{\delta} = 0.5(\delta + \hat{\delta}). \end{split}$$

The first and the second differential derivatives are defined in standard way and notated as follows:  $f_x$ ,  $f_{\bar{x}}$ ,  $f_{\bar{x}x}$ ,  $f_y$ ,  $f_{\bar{y}y}$ ,  $f_{\bar{y}y}$ ,  $f_t$ . We use also the following notation for BC writing:

$$f_{x,ij} = \frac{f_{i+1j} - f_{ij}}{h_x}, \quad f_{\bar{x},ij} = \frac{f_{ij} - f_{i-1j}}{h_x}, \quad f_{y,ij} = \frac{f_{ij+1} - f_{ij}}{h_y}, \quad f_{\bar{y},ij} = \frac{f_{ij} - f_{ij-1}}{h_y}.$$

Laplace difference operator is stated in the standard way:  $\Lambda f = f_{\bar{x}x} + f_{\bar{y}y}$ . For brevity, we introduce another finite-difference operators:

$$\mathcal{L}_{\bar{x}x}(n)\varphi = \frac{\mu_x}{h_x}(n_{i+0.5}\varphi_x - n_{i-0.5}\varphi_{\bar{x}}), \\ \mathcal{L}_{\bar{y}y}(n)\varphi = \frac{\mu_y}{h_y}(n_{j+0.5}\varphi_y - n_{j-0.5}\varphi_{\bar{y}}).$$

Let's notice that the FDS conservatism means a validity of a difference analogue for the conservation law. At the integral (2.9) computation we use trapezoid rule, which possesses the second order of accuracy

$$Q(t_k) = \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} c_{ij} h_x h_y \left( n_{ijk} - N_{ijk} \right),$$

$$c_{ij} = \begin{cases} 1/4, \quad i = 0, j = 0; \quad i = 0, j = N_y; \quad i = N_x, j = 0; \quad i = N_x, j = N_y; \\ 1/2, \quad i = 0, j = \overline{1, N_y - 1}; \quad i = N_x, j = \overline{1, N_y - 1}; \\ 1/2, \quad i = \overline{1, N_x - 1}, j = 0; \quad i = \overline{1, N_x - 1}, j = N_y; \\ 1, \quad i = \overline{1, N_x - 1}, j = \overline{1, N_y - 1}. \end{cases}$$
(3.1)

We follow this invariant validity because it is an important characteristic of a FDS efficiency. For the problem under consideration the asymptotic stability property violation can be caused by conservatism property violation (invariant (3.1) value increases in time) or in the obtained solution symmetry violation. It should be stressed that the corresponding conservative FDS for 1D problem was developed in [33]. Let us notice that in our computer simulation we compute the invariant (3.1) in inner grid nodes because of an optical radiation presence at two boundaries of the domain.

For numerical solution of the problem (2.1)-(2.8) we approximate the initial-boundary problem by the set of nonlinear finite-difference equations. For their resolvability the various iteration processes are used.

#### 3.1 Finite-difference scheme on the base of split-step method (FDS 1.1)

As it is well known, the split-step method is widely used for solution of such problems. Therefore, we firstly apply this method for computer simulation. But this method has some significant disadvantages as it will be shown below. Nevertheless, to stress advantages of a conservative FDS, we will compare the computer simulation results obtained on these methods.

Using the standard version of this method we write below the following finitedifference <u>FDS 1.1</u>

$$\frac{\bar{n} - n}{0.5\tau} = D_x (\bar{n}_{\bar{x}x} - \mathcal{L}_{\bar{x}x}(n)\varphi) + D_y (n_{\bar{y}y} - \mathcal{L}_{\bar{y}y}(n)\varphi) + G - R,$$
(3.2)
$$\Lambda \bar{\varphi} = \gamma (\bar{n} - \bar{N}), \quad i = 1, \cdots, N_x - 1, \quad j = 1, \cdots, N_y - 1, \quad k \ge 0,$$

$$\frac{\bar{N} - N}{0.5\tau} = G - R, \quad i = 0, \cdots, N_x, \quad j = 0, \cdots, N_y, \quad k \ge 0,$$

with corresponding BC and initial conditions:

$$\bar{\varphi}_{x,0j} = \bar{\varphi}_{\bar{x},N_xj} = 0, \quad \bar{n}_{x,0j} = \bar{n}_{\bar{x},N_xj} = 0, \quad j = 0, \cdots, N_y,$$

$$\bar{\varphi}_{y,i0} = \bar{\varphi}_{\bar{y},iN_y} = 0, \quad \bar{n}_{y,i0} = \bar{n}_{\bar{y},iN_y} = 0, \quad i = 0, \cdots, N_x,$$

$$n_{ij0} = N_{ij0} = n_0, \quad \varphi_{ij0} = 0, \quad I_{ij0.5} = 0, \quad i = 0, \cdots, N_x, \quad j = 0, \cdots, N_y,$$

$$(3.3)$$

and

$$\frac{n-\bar{n}}{0.5\tau} = D_x(\bar{n}_{\bar{x}x} - \mathcal{L}_{\bar{x}x}(\bar{n})\varphi) + D_y(\hat{n}_{\bar{y}y} - \mathcal{L}_{\bar{y}y}(\bar{n})\varphi) + \bar{G} - \bar{R},$$
(3.4)
$$\Lambda \hat{\varphi} = \gamma(\hat{n} - \hat{N}), \quad i = 1, \dots, N_x - 1, \quad j = 1, \dots, N_y - 1, \quad k \ge 0,$$

$$\frac{\hat{N} - \bar{N}}{0.5\tau} = \bar{G} - \bar{R}, \quad i = 0, \dots, N_x, \quad j = 0, \dots, N_y, \quad k \ge 0,$$

$$\frac{\hat{I} - I}{h_y} + \delta_0 \stackrel{0.5}{\delta} \stackrel{0.5}{I} = 0, \quad i = 0, \dots, N_x, \quad j = 1, \dots, N_y - 1, \quad k \ge 0,$$

with corresponding BC and initial conditions:

$$\hat{\varphi}_{x,0j} = \hat{\varphi}_{\bar{x},N_x j} = 0, \quad \hat{n}_{x,0j} = \hat{n}_{\bar{x},N_x j} = 0, \quad j = 0, \cdots, N_y,$$

$$\hat{\varphi}_{y,i0} = \hat{\varphi}_{\bar{y},iN_y} = 0, \quad \hat{n}_{y,i0} = \hat{n}_{\bar{y},iN_y} = 0, \quad i = 0, \cdots, N_x,$$

$$I_{i0k} = \exp\left(-\left(\frac{x_i - 0.5L_x}{0.1L_x}\right)^2\right) (1 - \exp(-10t_k)), \quad k = 0, \cdots, N_t, \quad i = 0, \cdots, N_x.$$
(3.5)

Using the standard differential derivatives expansion in a Taylor series, it is easy to proof

**Theorem 3.1.** <u>FDS 1.1</u> (3.2), (3.4) possesses the second order of approximation on spatial coordinates and on time coordinate in inner grid nodes concerning the point  $(x_i, y_j, t'_k)$  on sufficient smooth solution of the problem (2.1)-(2.8). BC (3.3), (3.5) possess the first order of approximation.

For brevity we omit the proof of the Theorem 3.1.

The BC (3.3), (3.5) are approximated with the first order on spatial coordinates to achieve the FDS conservatism property validity. Necessity of such BC approximation was considered in [33] for 1D case, and could be easily generalized for 2D case.

**Theorem 3.2.** <u>FDS 1.1</u> *is a conservative one if the BC are approximated with the first order on spatial coordinates.* 

*Proof.* We can write down the following sum from the equations concerning free electron and ionized donor concentrations:

$$\sum_{i=1}^{N_x - 1} \sum_{j=1}^{N_y - 1} (n_t - N_t)$$

$$= \sum_{i=1}^{N_x - 1} \sum_{j=1}^{N_y - 1} (D_x \bar{n}_{\bar{x}x} - 0.5 D_x \mathcal{L}_{\bar{x}x}(n) \varphi - 0.5 D_x \mathcal{L}_{\bar{x}x}(\hat{n}) \hat{\varphi})$$

$$+ \sum_{i=1}^{N_x - 1} \sum_{j=1}^{N_y - 1} \left( D_y \overset{0.5}{n_{\bar{y}y}} - 0.5 D_y \mathcal{L}_{\bar{y}y}(n) \varphi - 0.5 D_y \mathcal{L}_{\bar{y}y}(\hat{n}) \hat{\varphi} \right).$$
(3.6)

Let's calculate the sums entering the right part of equality (3.6):

$$\sum_{i=1}^{N_x-1} \bar{n}_{\bar{x}x} = \frac{1}{h_x^2} \sum_{i=1}^{N_x-1} (\bar{n}_{i-1} - 2\bar{n} + \bar{n}_{i+1}) = \frac{1}{h_x} (\bar{n}_{\bar{x},N_xj} - \bar{n}_{x,0j}),$$

$$\sum_{i=1}^{N_x-1} \mathcal{L}_{\bar{x}x}(\hat{n})\hat{\varphi} = \mu_x \sum_{i=1}^{N_x-1} \left( \hat{n}_{i+0.5} \frac{\hat{\varphi}_{i+1} - \hat{\varphi}_i}{h_x^2} - \hat{n}_{i-0.5} \frac{\hat{\varphi}_i - \hat{\varphi}_{i-1}}{h_x^2} \right)$$

$$= -\mu_x \hat{n}_{0.5j} \frac{\hat{\varphi}_{1j} - \hat{\varphi}_{0j}}{h_x^2} + \mu_x \hat{n}_{N_x-0.5j} \frac{\hat{\varphi}_{N_xj} - \hat{\varphi}_{N_x-1j}}{h_x^2}.$$

Other sums are calculated in the same way. Thus we receive:

$$\sum_{i=1}^{N_{x}-1} \sum_{j=1}^{N_{y}-1} (n_{t}-N_{t})$$

$$= \frac{D_{x}}{h_{x}} \sum_{j=1}^{N_{y}-1} (\bar{n}_{\bar{x},N_{x}j}-\bar{n}_{x,0j}) + \frac{D_{y}}{h_{y}} \sum_{i=1}^{N_{x}-1} (n_{\bar{y},iN_{y}}+\bar{n}_{\bar{y},iN_{y}}-n_{y,i0}-\bar{n}_{y,i0})$$

$$+ \frac{D_{x}\mu_{x}}{2h_{x}} \sum_{j=1}^{N_{y}-1} (n_{0.5j}\varphi_{x,0j}+\hat{n}_{0.5j}\hat{\varphi}_{x,0j}-n_{N_{x}-0.5j}\varphi_{\bar{x},N_{x}j}+\hat{n}_{N_{x}-0.5j}\hat{\varphi}_{\bar{x},N_{x}j})$$

$$+ \frac{D_{y}\mu_{y}}{2h_{y}} \sum_{i=1}^{N_{x}-1} (n_{i0.5}\varphi_{y,i0}+\hat{n}_{i0.5}\hat{\varphi}_{y,i0}-n_{iN_{y}-0.5}\varphi_{\bar{y},iN_{y}}+\hat{n}_{iN_{y}-0.5}\hat{\varphi}_{\bar{y},iN_{y}}). \quad (3.7)$$

At BC approximation with the first order as we do in (3.3), (3.5), then right part of (3.7) is equal to zero. Thus **FDS 1.1** is a conservative one.

However, at carrying out the computer simulation we have found, that this FDS isn't applicable for the problem solution during long time interval: it does not possess the asymptotic stability property and, as a consequence, the invariant (3.1) value does not conserve (see Fig. 1, dash line). Therefore, we modified this method and added an iteration process for FDS resolution (see below). Therefore, for our investigations we prefer to use modified finite-difference **FDS 1.2**.

# 3.2 Modified finite-difference scheme on the base of split-step method (FDS 1.2)

The modified FDS on the base of split-step method is write in following manner:

$$\frac{\bar{n} - n}{0.5\tau} = D_x (\bar{n}_{\bar{x}x} - \mathcal{L}_{\bar{x}x}(n)\varphi) + D_y (n_{\bar{y}y} - \mathcal{L}_{\bar{y}y}(n)\varphi) + G - R,$$

$$\frac{\hat{n} - \bar{n}}{0.5\tau} = D_x (\bar{n}_{\bar{x}x} - \mathcal{L}_{\bar{x}x}(\hat{n})\hat{\varphi}) + D_y (\hat{n}_{\bar{y}y} - \mathcal{L}_{\bar{y}y}(\hat{n})\hat{\varphi}) + \hat{G} - \hat{R},$$
(3.8)

$$\begin{split} &\Lambda \hat{\varphi} = \gamma \left( \hat{n} - \hat{N} \right), \quad i = 1, \cdots, N_x - 1, \quad j = 1, \cdots, N_y - 1, \quad k \ge 0, \\ &\frac{\hat{N} - N}{\tau} = \overset{0.5}{G} - \overset{0.5}{R}, \quad i = 0, \cdots, N_x, \quad j = 0, \cdots, N_y, \quad k \ge 0, \\ &\frac{\hat{I} - I}{h_y} + \delta_0 \overset{0.50.5}{\delta} \overset{I}{I} = 0, \quad i = 0, \cdots, N_x, \quad j = 1, \cdots, N_y - 1, \quad k \ge 0. \end{split}$$

BC and initial conditions are defined in (3.3), (3.5). It is easy to see a validity of two theorems formulated below.

**Theorem 3.3.** <u>FDS 1.2</u> (3.8) possesses the second order of approximation on spatial coordinates and on time coordinate in inner grid nodes concerning the point  $(x_i, y_j, t'_k)$  on sufficient smooth solution of the problem (2.1)-(2.6). BC (3.3), (3.5) possess the first order of approximation.

**Theorem 3.4.** <u>FDS 1.2</u> *is a conservative one if the BC are approximated with the first order on spatial coordinates.* 

We omit a proof of the Theorem 3.4, as it is similar to the proof of the Theorem 3.2.

Because the FDS (3.8) is nonlinear one, the following iteration process for solving the equation concerning a free electron concentration on the upper time layer is used. At the first step we calculate the function  $\bar{n}$  on additional semi-layer of time. Then we carry out calculation of the functions on the upper time layer. To do this we have to compute a donor concentration, and free electron concentration, and the electric field potential, as well as the beam intensity on each of iteration. Thus, we use an iteration process:

$$\frac{\bar{n}-n}{0.5\tau} = D_x \left(\bar{n}_{\bar{x}x} - \mathcal{L}_{\bar{x}x}(n)\varphi\right) + D_y \left(n_{\bar{y}y} - \mathcal{L}_{\bar{y}y}(n)\varphi\right) + G - R,$$
(3.9)
$$\frac{\bar{n}-\bar{n}}{0.5\tau} = D_x \left(\bar{n}_{\bar{x}x} - \mathcal{L}_{\bar{x}x}(\overset{s}{\hat{n}})\overset{s}{\hat{\varphi}}\right) + D_y \left(\overset{s+1}{\hat{n}}_{\bar{y}y} - \mathcal{L}_{\bar{y}y}(\overset{s}{\hat{n}})\overset{s}{\hat{\varphi}}\right) + \overset{s}{\hat{G}} - \overset{s}{\hat{R}},$$

$$\Lambda^{\overset{s+1}{\hat{\varphi}}} = \gamma \left(\overset{s+1}{\hat{n}} - \overset{s+1}{\hat{N}}\right), \quad i = 1, \cdots, N_x - 1, \quad j = 1, \cdots, N_y - 1, \quad k \ge 0,$$

$$\frac{\overset{s+1}{\hat{N}-N}}{\tau} = \overset{s}{G} - \overset{s}{R}, \quad i = 0, \cdots, N_x, \quad j = 0, \cdots, N_y, \quad k \ge 0,$$

$$\frac{\overset{s+1}{\hat{I}-I}}{h_y} + \delta_0 \overset{s+1}{\delta} \overset{s+1}{I} = 0, \quad i = 0, \cdots, N_x, \quad j = 1, \cdots, N_y - 1, \quad k \ge 0.$$

For finite-difference equations (3.9) the BC are written in the form:

$$\hat{\phi}_{x,0j}^{s+1} = \hat{\phi}_{\bar{x},N_xj}^{s+1} = 0, \quad \bar{n}_{x,0j} = \bar{n}_{\bar{x},N_xj} = 0, \quad j = 0, \cdots, N_y,$$

$$\hat{\phi}_{y,i0}^{s+1} = \hat{\phi}_{\bar{y},iN_y}^{s+1} = 0, \quad \hat{n}_{y,i0}^{s+1} = \hat{n}_{\bar{y},iN_y}^{s+1} = 0, \quad i = 0, \cdots, N_x,$$

$$I_{i0k} = \exp\left(-\left(\frac{x_i - 0.5L_x}{0.1L_x}\right)^2\right) (1 - \exp(-10t_k)), \quad k = 0, \cdots, N_t, \quad i = 0, \cdots, N_x.$$

$$(3.10)$$

As an initial approach of the functions for the iterative process, their values, calculated on a previous time layer, are undertaken:

$$\hat{n} = n, \quad \hat{N} = N, \quad \hat{\phi} = \varphi, \quad \hat{I} = I.$$
 (3.11)

Criterion of the iteration process convergence is given by the following expressions:

$$\begin{vmatrix} s+1\\ \hat{n} - \hat{n} \end{vmatrix} \leq \varepsilon_1 \begin{vmatrix} s\\ \hat{n} \end{vmatrix} + \varepsilon_2, \quad \begin{vmatrix} s+1\\ \hat{N} - \hat{N} \end{vmatrix} \leq \varepsilon_1 \begin{vmatrix} s\\ \hat{N} \end{vmatrix} + \varepsilon_2, \quad (3.12)$$
$$\begin{vmatrix} s+1\\ \hat{\phi} - \hat{\phi} \end{vmatrix} \leq \varepsilon_1 \begin{vmatrix} s\\ \hat{\phi} \end{vmatrix} + \varepsilon_2, \quad \begin{vmatrix} s+1\\ \hat{I} - \hat{I} \end{vmatrix} \leq \varepsilon_1 \begin{vmatrix} s\\ \hat{I} \end{vmatrix} + \varepsilon_2, \quad \varepsilon_1, \varepsilon_2 > 0, \quad i = 0, \cdots, N_x, \quad j = 0, \cdots, N_y.$$

We supposed, that we found out the problem solution on the upper time layer if the inequalities (3.12) are satisfied for all functions and for all grid nodes simultaneously.

For the practice it is very important that the following theorem is valid.

**Theorem 3.5.** <u>FDS 1.2</u> *is a conservative one on each of iterations if BC are approximated with the first order on spatial coordinates.* 

However, computer experiments have shown, that <u>FDS 1.2</u> doesn't provide asymptotic stability property under certain conditions (see below the computer results). This is caused by two factors. The first one is an iteration process using to solve the resulting difference equations. The second one is a consequence of a electric current flow on *x*-coordinate in Eq. (3.8): we use a free electron concentration at different time layers. Regard to this, in the present paper we constructed another conservative FDS.

#### 3.3 Symmetrical finite-difference scheme (FDS 2)

Below on the base of Crank-Nicolson method we develop another FDS – it is a symmetric one and it looks in following manner:

$$\frac{\hat{n}-n}{\tau} = D_x \, \overset{0.5}{n_{\bar{x}x}} + D_y \, \overset{0.5}{n_{\bar{y}y}} + \overset{0.5}{G} - \overset{0.5}{R} \\ - \frac{D_x}{2} \left( \mathcal{L}_{\bar{x}x}(\hat{n})\hat{\varphi} + \mathcal{L}_{\bar{x}x}(n)\varphi \right) - \frac{D_y}{2} \left( \mathcal{L}_{\bar{y}y}(\hat{n})\hat{\varphi} + \mathcal{L}_{\bar{y}y}(n)\varphi \right), \quad (3.13)$$

$$\begin{split} &\Lambda \hat{\varphi} = \gamma \left( \hat{n} - \hat{N} \right), \quad i = 1, \cdots, N_x - 1, \quad j = 1, \cdots, N_y - 1, \quad k \ge 0, \\ &\frac{\hat{N} - N}{\tau} = \overset{0.5}{G} - \overset{0.5}{R}, \quad i = 0, \cdots, N_x, \quad j = 0, \cdots, N_y, \quad k \ge 0, \\ &\frac{\hat{I} - I}{h_y} + \delta_0 \overset{0.50.5}{\delta} \overset{I}{I} = 0, \quad i = 0, \cdots, N_x, \quad j = 1, \cdots, N_y - 1, \quad k \ge 0, \end{split}$$

with corresponding BC and initial conditions

.

$$\begin{aligned} \hat{\varphi}_{x,0j} &= \hat{\varphi}_{\bar{x},N_xj} = 0, \quad \hat{n}_{x,0j} = \hat{n}_{\bar{x},N_xj} = 0, \quad j = 0, \cdots, N_y, \\ \hat{\varphi}_{y,i0} &= \hat{\varphi}_{\bar{y},iN_y} = 0, \quad \hat{n}_{y,i0} = \hat{n}_{\bar{y},iN_y} = 0, \quad i = 0, \cdots, N_x, \\ I_{i0k} &= \exp\left(-\left(\frac{x_i - 0.5L_x}{0.1L_x}\right)^2\right) (1 - \exp(-10t_k)), \quad k = 0, \cdots, N_t, \quad i = 0, \cdots, N_x, \\ n_{ij0} &= N_{ij0} = n_0, \quad \varphi_{ij0} = 0, \quad I_{ij0.5} = 0, \quad i = 0, \cdots, N_x, \quad j = 0, \cdots, N_y. \end{aligned}$$
(3.14)

**Theorem 3.6.** <u>FDS 2</u> (3.13) possesses the second order of approximation on spatial coordinates and on time coordinate in inner grid nodes concerning the point  $(x_i, y_j, t'_k)$  on sufficient smooth solution of the problem (2.1)-(2.8). BC (3.14) possess the first order of approximation.

**Theorem 3.7.** <u>FDS 2</u> *is a conservative one if BC are approximated with the first order on spatial coordinates.* 

We omit a proof of the Theorem 3.7, as it is similar to the proof of the Theorem 3.2.

We solve the obtained set of nonlinear difference equations by means of the original two-stage iteration process. Below the first stage of the iteration process with the correspondingly BC is written:

$$\frac{\hat{n}^{s+1}}{\tau} = D_x \frac{\hat{n}^{s+1}}{\hat{n}_{\bar{x}x}} + D_y \frac{\hat{n}^{s}}{\hat{n}_{\bar{y}y}} + \frac{\hat{n}^{s}}{G} - \frac{\hat{n}^{s}}{R} - \frac{D_x}{2} \left( \mathcal{L}_{\bar{x}x} \left( \hat{n} \right) \hat{\phi} + \mathcal{L}_{\bar{x}x} (n) \varphi \right) - \frac{D_y}{2} \left( \mathcal{L}_{\bar{y}y} \left( \hat{n} \right) \hat{\phi} + \mathcal{L}_{\bar{y}y} (n) \varphi \right), \quad (3.15)$$

$$\Lambda \hat{\phi}^{s+1} = \gamma \left( \hat{n}^{s+1} - \hat{N} \right), i = 1, \cdots, N_x - 1, \quad j = 1, \cdots, N_y - 1, \quad k \ge 0,$$

$$\frac{\hat{N}^{s+1}}{\tau} = \hat{G} - \hat{R}, \quad i = 0, \cdots, N_x, \quad j = 0, \cdots, N_y, \quad k \ge 0,$$

$$\frac{\hat{n}^{s+1}}{h_y} + \delta_0 \hat{\delta} \hat{I} = 0, \quad i = 0, \cdots, N_x, \quad j = 1, \cdots, N_y - 1, \quad k \ge 0.$$

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BC and initial conditions for Eq. (3.13) on iterations are the following

$$\hat{\varphi}_{x,0j}^{s+1} = \hat{\varphi}_{\bar{x},N_xj}^{s+1} = 0, \quad \hat{n}_{x,0j}^{s+1} = \hat{n}_{\bar{x},N_xj}^{s+1} = 0, \quad j = 0, \cdots, N_y,$$

$$\hat{\varphi}_{y,i0}^{s+1} = \hat{\varphi}_{\bar{y},iN_y}^{s+1} = 0, \quad i = 0, \cdots, N_x,$$

$$I_{i0k} = \exp\left(-\left(\frac{x_i - 0.5L_x}{0.1L_x}\right)^2\right) (1 - \exp(-10t_k)), \quad k = 0, \cdots, N_t, \quad i = 0, \cdots, N_x.$$

$$(3.16)$$

The second stage is:

with corresponding BC and initial conditions on the (s+2) iteration

$$\hat{\phi}_{x,0j}^{s+2} = \hat{\phi}_{\bar{x},N_xj}^{s+2} = 0, \quad j = 0, \cdots, N_y,$$

$$\hat{\phi}_{y,i0}^{s+2} = \hat{\phi}_{\bar{y},iN_y}^{s+2} = 0, \quad \hat{n}_{y,i0}^{s+2} = \hat{n}_{\bar{y},iN_y}^{s+2} = 0, \quad i = 0, \cdots, N_x,$$

$$I_{i0k} = \exp\left(-\left(\frac{x_i - 0.5L_x}{0.1L_x}\right)^2\right) (1 - \exp(-10t_k)), k = 1, \cdots, N_t, \quad i = 0, \cdots, N_x.$$

$$(3.18)$$

It is very important to pay attention that for the finite-difference <u>FDS 2</u> we check the criterion of iteration convergence only after we make both iteration stages:

$$\begin{vmatrix} s+2 & s \\ \hat{n} & -\hat{n} \end{vmatrix} \leq \varepsilon_1 \begin{vmatrix} s \\ \hat{n} \end{vmatrix} + \varepsilon_2, \quad \begin{vmatrix} s+2 & s \\ \hat{N} & -\hat{N} \end{vmatrix} \leq \varepsilon_1 \begin{vmatrix} s \\ \hat{N} \end{vmatrix} + \varepsilon_2, \quad \begin{vmatrix} s+2 & s \\ \hat{P} & -\hat{P} \end{vmatrix} \leq \varepsilon_1 \begin{vmatrix} s \\ \hat{P} \end{vmatrix} + \varepsilon_2, \quad (3.19)$$
$$\begin{vmatrix} s+2 & s \\ \hat{I} & -\hat{I} \end{vmatrix} \leq \varepsilon_1 \begin{vmatrix} s \\ \hat{I} \end{vmatrix} + \varepsilon_2, \quad \varepsilon_1, \varepsilon_2 > 0, \quad i = 0, \cdots, N_x, \quad j = 0, \cdots, N_y.$$

If these inequalities are not valid for any functions and for any grid points simultaneously, then we repeat our calculations. As the initial approach for iteration process the equalities (3.11) are used.

As one can see, the main difference between the finite-difference <u>FDS 1.2</u> and the finite-difference <u>FDS 2</u> consists in approach for solution of the nonlinear equation concerning the free electron concentration. At the finite-difference <u>FDS 1.2</u> construction we have based on the summary approximation principle. On the contrary, for <u>FDS 2</u> we use the iteration process and don't use the additional semi-layer on time axis. The following theorem takes place.

**Theorem 3.8.** <u>FDS 2</u> is a conservative one on each of iterations if BC are approximated with the first order on spatial coordinates.

Let us note, that the <u>FDS 2</u> conservatism on each iteration is very important property for the asymptotic stability validity.

#### 3.4 Additional iteration process for the Poison equation

One more complexity, appearing at solving the problem (2.1)-(2.8), is caused by the solution of the 2D Poisson equation

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = \gamma(n - N), \quad 0 < x < L_x, \quad 0 < y < L_y.$$
(3.20)

Obviously, if this equation has zero-value BC, then for its solution one can apply the method of Fast Fourier Transform. However, in more general case this method cannot be used. In connection with this we arrange another iteration process for the Poisson equation solving. Moreover, our computer simulation showed, that an accuracy of the Poisson equation solution, which can be estimated also by using the discrepancy

$$\Psi(\varphi) = \Lambda \varphi - \gamma(n - N), \quad i = 1, \cdots, N_x - 1, \quad j = 1, \cdots, N_y - 1, \quad (3.21)$$

influences significantly on the problem (2.1)-(2.8) solution. The main question is: what criterion of the iteration process stopping is necessary to apply for the iteration process convergence estimation? To solve Eq. (3.20) with arbitrary BC we have to arrange additional iteration process in a such way, that we have to solve only the 1D problem. Taking into account a linearity of Eq. (3.20) we use the split-step method in this case. For this purpose we introduce an additional auxiliary grid function *F* on the spatial grid  $\bar{\Omega} = \omega_x \times \omega_y$ , which is governed by the problem:

$$F^{0} = \stackrel{s}{\hat{\varphi}}, \quad \frac{F^{p+1} - F^{p}}{\bar{\tau}} = F^{p+1}_{\bar{x}x} + F^{p}_{\bar{y}y} - \gamma \begin{pmatrix} s+1 & s+1 \\ \hat{n} & -\hat{N} \end{pmatrix}, \quad (3.22)$$

$$\frac{F^{p+2} - F^{p+1}}{\bar{\tau}} = F^{p+1}_{\bar{x}x} + F^{p+2}_{\bar{y}y} - \gamma \begin{pmatrix} s+1 & s+1 \\ \hat{n} & -\hat{N} \end{pmatrix}, \quad i = 1, \cdots, N_{x} - 1, \quad j = 1, \cdots, N_{y} - 1.$$

$$F_{x,0j} = F_{\bar{x},N_{x}j} = 0, \quad F_{y,i0} = F_{\bar{y},iN_{y}} = 0.$$

Here  $p = 0, 1, 2, \cdots$  is the number of iteration, parameter  $\bar{\tau}$  is the iteration step, which is not equal to time grid step  $\tau$ . The functions *n* and *N* are taken on the upper layer in time coordinate (here for brevity we consider only the additional iteration process for the first stage (3.15) of iteration process for the finite-difference **FDS 2**, as for the second stage (3.17) this additional process constructed in the same way). For solving obtained difference equation we use Thomas algorithm on each iteration of the process (3.22). The convergence estimation of this additional iteration process is based on one of the following criterion:

$$\begin{vmatrix} p^{+2} & p \\ F & -F \end{vmatrix} \le \varepsilon_3 |F^p| + \varepsilon_4, \quad \varepsilon_3, \varepsilon_4 > 0, \quad i = 1, \cdots, N_x - 1, \quad j = 1, \cdots, N_y - 1, \tag{3.23}$$

which is similar to (3.12) or the criterion of the discrepancy (3.21) assessment:

$$\left|F_{\bar{x}x}^{p+1} + F_{\bar{y}y}^{p+2} - \gamma \begin{pmatrix} s+1 & s+1 \\ \hat{n} & -\hat{N} \end{pmatrix}\right| \le \varepsilon_5, \quad \varepsilon_5 > 0, \quad i = 1, \cdots, N_x - 1, \quad j = 1, \cdots, N_y - 1.$$
(3.24)

If the solution, obtained on the p+2 iteration, satisfies to the chosen criterion, then it is the Poisson equation solution for s+1 iteration with respect to the concentration of free electrons and ionized donors:  $\hat{\varphi}^{s+1} = F^{p+2}$ .

## **4** Computer simulation results

We estimate the efficiency of various FDS, used for the problem (2.1)-(2.8) solution, by the following criteria: accuracy of the invariant (3.1) conservation, symmetry of obtained solution in the case of corresponding initial conditions. We also compare the obtained results to the previous results obtained for the problem under consideration in 1D case. Opportunity of using the large grid step on time coordinate without the solution accuracy loosing is an important advantage of the FDS, obviously, because it is very actual question for multidimensional non-stationary problems modelling. Below we discuss computer simulation results for the following set of the parameters:

$$\delta_0 = 2, \quad q_0 = 1.5, \quad D_x = D_y = 10^{-5}, \quad \gamma = 10^3, \quad n_0 = 0.01, \quad \mu_x = 1, \quad \mu_y = 1, \quad (4.1)$$
  
 $\psi = 2.553, \quad \xi = 3, \quad \tau_v = 1, \quad L_x = L_y = 1.$ 

The grid steps for spatial coordinates are equal to  $h_x = h_y = 0.01$ . We use the criterion (3.23) for the iteration process convergence at the Poisson equation solving.

From Fig. 1 it follows that the <u>FDS 1.1</u> is not a conservative one: value of invariant (3.1) increases fastly in time. So, it should be stressed, that this FDS doesn't provide validity of the physical conservation law. As for the <u>FDS 1.2</u> and the <u>FDS 2</u> we see that the invariant (3.1) conserves with high accuracy. Nevertheless, one can see small increasing



Figure 1: Time evolution of the invariant Q(t) calculated with grid steps and iteration process parameters  $\tau = 5 \cdot 10^{-4}$ ,  $\bar{\tau} = 10^{-4}$ ,  $\varepsilon_1 = 10^{-5}$ ,  $\varepsilon_2 = 10^{-7}$ ,  $\varepsilon_3 = 10^{-5}$ ,  $\varepsilon_4 = 10^{-7}$  using the <u>FDS 1.1</u> (dash line), the <u>FDS 1.2</u> (solid line) and the <u>FDS 2</u> (dot line).

of its value with time growing. This is a consequence of iteration process presence. Obviously, the solution is obtained with certain accuracy because of occurring of iteration process.

As it is follows from the formula (2.6), the Gaussian profile is chosen for the incident pulse and it is symmetric relatively to the centre of x-axis. Respectively, the problem solution should possess a symmetric distribution on this coordinate in any time moment. We follow this feature for all FDS under consideration.

One can see apparently from Fig. 2 (a, d, j, m) that the computer simulation results are the same till certain time moment for all FDS. However, with time increasing, the solutions, obtained using **FDS 1.1** and **FDS 1.2**, lose their symmetry (Fig. 2 b, e). It is not possible to correct this shortcoming by decreasing the grid step on time axis  $\tau$  at constant grid steps on spatial: for the **FDS 1.1**  $\tau$  decreasing leads to anomalous increasing in iteration number (more than 400), which is necessary to achieve the Poisson equation solution. Obviously, this is unacceptable for the practice. Under using the **FDS 1.2** we see improvement of the results with  $\tau$  decreasing. However, we don't still achieve completely solution symmetry (Fig. 2 h). The further time increasing leads to essential deviation of obtained distributions (Fig. 2 c, f, i) from symmetrical distribution in *x*-coordinate. This demonstrates essential influence of the time grid step on the solution, obtained using the FDS developed on the base of the split-step method, and necessity of small grid steps using. It means that the property of asymptotic stability of the FDS is absence. If we use the **FDS 2** it does not occur: the solution is symmetrical even for calculations providing with rather big step  $\tau = 10^{-3}$  (Fig. 2 j–o).

This demonstrates the advantage of the proposed <u>FDS 2</u> on the base of the two-stage iteration process.



Figure 2: Free electron concentration distribution calculated for parameters  $\varepsilon_1 = \varepsilon_3 = 10^{-5}$ ,  $\varepsilon_2 = \varepsilon_4 = 10^{-7}$ ,  $\overline{\tau} = 10^{-4}$  at using the <u>FDS 1.1</u> with  $\tau = 10^{-3}$  (a, b, c), the <u>FDS 1.2</u> with  $\tau = 10^{-3}$  (d, e, f) and with  $\tau = 5 \cdot 10^{-4}$  (g, h, i) the <u>FDS 2</u> with  $\tau = 10^{-3}$  (j, k, l) and with  $\tau = 5 \cdot 10^{-4}$  (m, n, o).

	t = 0.1	t = 0.5	t = 1	t=2	t = 100	t = 500	t = 1000	
$ au = 10^{-3}$								
FDS 1.1	0.00071	0.01573	0.061	9.034	33.838	84.907	140.011	
FDS 1.2	0.00152	0.01798	0.04682	0.14079	0.31716	0.33261	0.33354	
<u>FDS 2</u>	0.000014	0.00012	0.00023	0.00017	0.00018	0.00043	0.00028	
$\tau = 5 \cdot 10^{-4}$								
FDS 1.1	0.00035	0.00786	0.0308	4.58	-	-	-	
FDS 1.2	0.00075	0.00897	0.02339	0.07026	0.15858	0.16645	0.16833	
FDS 2	0.000007	0.00007	0.00007	0.00013	0.00048	0.00026	0.00015	
$\tau \!=\! 5 \!\cdot\! 10^{-6}$								
<u>FDS 1.2</u>	0.000007	0.00009	0.00024	-	-	-	-	

Table 1: The discrepancy accuracy  $|\Psi(\varphi)|$  evolution in time at using the criterion (3.23) and iteration parameters  $\varepsilon_1 = \varepsilon_3 = 10^{-5}$ ,  $\varepsilon_2 = \varepsilon_4 = 10^{-7}$ ,  $\bar{\tau} = 10^{-4}$ .

Below we discuss an influence of calculation accuracy of the electric field potential distribution on the problem solution. For this purpose we calculate the discrepancy accuracy changing in time if we use the criterion (3.23) for the iteration process (3.20). As one can see from the Table 1, the discrepancy  $\Psi(\varphi)$  achieves a high accuracy and its value doesn't practically increase in time if we use the FDS 2 for our calculations. Small increasing of the discrepancy value at time moment  $t = 10^3$  is caused by an iteration process presence. Obviously, it brings some mistake in the problem solution as well as round off errors. However, if the FDS possesses an asymptotic stability property, these errors introduced in solution don't increase. In the contrary, the FDS 1.2 does not provide conservation of  $\Psi(\varphi)$  value: its value increases monotonously with time increasing. To achieve a satisfactory accuracy of  $\Psi(\varphi)$  at the <u>FDS 1.2</u> using (the same order of the accuracy, corresponding to the FDS 2) using we have to decrease grid step  $\tau$  by three order less in comparison with the <u>FDS 2</u> using (see, for example, the discrepancy for t=1). However, such grid step decreasing leads to unacceptable computer simulation time increasing. That's why, a value of the discrepancy  $\Psi(\varphi)$  is absent in the Table 1 for **FDS 1.1** and FDS 1.2 on big time moments.

Regarding the <u>FDS 1.1</u> it should be stressed that this FDS does not provide the discrepancy conservation (it means that the discrepancy increases in time) and we have to make too many number of iterations (more than 400) to achieve the iteration process convergence. Moreover, after certain time moment, the discrepancy value changes less than  $10^{-7}$  after 50 iterations.

Thus, the finite-difference <u>FDS 2</u> has obvious advantages in comparison with two other FDS if one need to make a computer simulation during long time interval or if a problem solution possesses a strong gradient in one of spatial coordinates or in time.

However, we found out certain of parameter set, at which this FDS with the criterion (3.23) does not provide the discrepancy  $\Psi(\varphi)$  conservation with rather high accuracy de-



Figure 3: Free electron concentration distribution calculated for parameters  $\tau = 10^{-3}$ ,  $\varepsilon_1 = 10^{-4}$ ,  $\varepsilon_2 = 10^{-6}$ ,  $\bar{\tau} = 10^{-4}$  using the <u>FDS 2</u> and the iteration process (3.20) with the criterion (3.23) ( $\varepsilon_3$ ,  $\varepsilon_4$ ) = ( $10^{-3}$ ,  $10^{-5}$ ) (a), ( $\varepsilon_3$ ,  $\varepsilon_4$ ) = ( $10^{-5}$ ,  $10^{-7}$ ) (b) or with the criterion (3.24)  $\varepsilon_5 = 5 \cdot 10^{-3}$  (c),  $\varepsilon_5 = 10^{-3}$  (d) time moment t = 1000.



Figure 4: Dependence of discrepancy accuracy preservation from iteration process convergence for parameters  $(\varepsilon_3, \varepsilon_4) = (10^{-3}, 10^{-5})$  (1),  $(\varepsilon_5) = (5 \cdot 10^{-3})$  (2),  $(\varepsilon_5) = (10^{-3})$  (3),  $(\varepsilon_3, \varepsilon_4) = (10^{-5}, 10^{-7})$  (4).

spite the fact that the condition (3.23) is satisfied. Let us stress, that a computation error accumulation at electric field potential calculation leads to the problem solution symmetry breaking. Therefore we control the accuracy of function  $\varphi$  calculation by means of the discrepancy  $\Psi(\varphi)$ . As one can see from Fig. 3, at high accuracy of  $\Psi(\varphi)$  (less than  $10^{-3}$ ) calculation, the free electron concentration distribution is symmetrical (Figs. 3b, 3d), but the solution symmetry is broken if  $\Psi(\varphi)$  increases (Figs. 3a, 3c).

In Fig. 4 one can see dependence of a discrepancy  $\Psi(\varphi)$  accuracy on parameters  $\varepsilon_3$ ,  $\varepsilon_4$ ,  $\varepsilon_5$ . Other parameters are the same, as for Fig. 3. We can see high correlation between the discrepancy  $\Psi(\varphi)$  accuracy and the solution symmetry violation.

Now let's investigate the iteration process convergence for the Poisson equation. Computer simulations results, obtained using the <u>FDS 2</u>, for the criterion (3.23) and

	$\left F^{p+2}-F^{p}\right \leq \varepsilon_{3}\left F^{p}\right +\varepsilon_{4}$		$ F_{\bar{x}x}^{p+2} + F_{\bar{y}y}^{p+2} - \gamma \binom{s+1}{n} - \frac{s+1}{N}  \le \varepsilon_5$						
	$\varepsilon_3 = 10^{-3}, \\ \varepsilon_4 = 10^{-5}$	$\varepsilon_3 = 10^{-5}, \ \varepsilon_4 = 10^{-7}$	$\varepsilon_5 = 5 \cdot 10^{-3}$	$\varepsilon_5 = 10^{-3}$					
t=1									
I stage ( $ \Psi(\phi) $ ; $N_p$ )	$(6,5 \cdot 10^{-4};1)$	$(10^{-4};10)$	$(1,5\cdot 10^{-3};1)$	$(6,5 \cdot 10^{-4};1)$					
II stage ( $ \Psi(\varphi) $ ; $N_p$ )	$(5,8 \cdot 10^{-4};1)$	$(1,2 \cdot 10^{-4};1)$	$(1,5\cdot 10^{-3};1)$	$(5,8 \cdot 10^{-4};1)$					
t = 10									
I stage ( $ \Psi(\phi) $ ; $N_p$ )	$(2 \cdot 10^{-2}; 1)$	$(5,2\cdot 10^{-4};26)$	$(3,3\cdot 10^{-3};3)$	$(9 \cdot 10^{-4};7)$					
II stage ( $ \Psi(\varphi) $ ; $N_p$ )	$(8,1\cdot 10^{-3};1)$	$(5,6\cdot 10^{-4};1)$	$(3 \cdot 10^{-3}; 1)$	$(8,2 \cdot 10^{-4};1)$					
t=100									
I stage ( $ \Psi(\phi) $ ; $N_p$ )	$(3,8 \cdot 10^{-2};1)$	$(3,3\cdot 10^{-4};20)$	$(3,4\cdot 10^{-3};3)$	$(9,7 \cdot 10^{-4};6)$					
II stage ( $ \Psi(\varphi) $ ; $N_p$ )	$(6,3 \cdot 10^{-3};1)$	$(2,1\cdot 10^{-4};1)$	$(3,5\cdot 10^{-3};1)$	$(7,3 \cdot 10^{-4};1)$					
t = 1000									
I stage ( $ \Psi(\phi) ;N_p$ )	$(2,8\cdot 10^{-2};1)$	$(3,3\cdot 10^{-4};13)$	$(2,1\cdot 10^{-3};3)$	$(7,3\cdot 10^{-4};6)$					
II stage ( $ \Psi(\phi) $ ; $N_p$ )	$(5,\overline{4\cdot 10^{-3};1})$	$(3,\overline{1\cdot 10^{-4};1})$	$(1,\overline{5\cdot 10^{-3};1})$	$(5,\overline{7\cdot 10^{-4};1})$					

Table 2: Discrepancy  $\Psi(\varphi)$  accuracy changing in time and number of iterations  $N_p$  for the iteration process (3.20) convergence achieving obtained on the first stage of the iteration process (3.13)-(3.16) for different time moments t at using the criterion (3.23) or (3.24) with  $\tau = 10^{-3}$ ,  $\varepsilon_1 = 10^{-4}$ ,  $\varepsilon_2 = 10^{-6}$ ,  $\bar{\tau} = 10^{-4}$ .

(3.24), are shown in the Table 2, because other FDS are essentially worse for our problem solution. It should be noted, that the difference between obtained results if we use different criteria for the iteration process (3.22) convergence, are shown at early time points and they increase eventually. As we can see from the Table 2, under certain iteration parameters (for example, rather small values of  $\varepsilon_3$ ,  $\varepsilon_4$ ,  $\varepsilon_5$ ) the iteration convergence criterion choice does not influence on the discrepancy accuracy conservation and on performance of the iterative process (3.22) convergence. However, with  $\varepsilon_3$ ,  $\varepsilon_4$ ,  $\varepsilon_5$  increasing, the criterion (3.24) seems more effective, because its using allows to calculate  $\Psi(\varphi)$  with higher accuracy under the same condition. As for calculations with using the criterion (3.23), it should be noted that at rather small values of the iteration parameters  $\varepsilon_3$ ,  $\varepsilon_4$ , the achievement of enough small  $\Psi(\varphi)$  values is possible. However for this purpose it is required bigger number of iterations, than in the case of using the criterion (3.24).

One of the ways for iteration process property improvement, known in literature [25], is the regularization method. As example, we apply this method for the <u>FDS 2</u> in combination with the criterion (3.24) by adding the following summand to the right part of equation concerning the free electrons concentration in (3.15)-(3.18):

$$v_x \begin{pmatrix} s+1 & s \\ n & -n \end{pmatrix}, \quad v_x = const.$$

In some cases, using such kind of the regularization, it is possible to do a computation with large grid steps. Moreover, computer experiments demonstrated that the best results are reached at  $v_x = 0$  for the problem under consideration, which is equivalent to the **FDS 2**. One needs to stress that for  $v_x \neq 0$  we obtain the same solution of the problem, but it takes more computational time due to iteration number increasing for the process (3.22).

## 5 Conclusions

In this paper the advantages of the FDS on the basis of the two-stage iteration process are demonstrated using computer simulation. One of its main advantages consists in property of the asymptotic stability. Thus, it is possible to provide a computation on long time interval without the conservatism property losing. Another feature of this iteration process consists in the conservatism property of the FDS on each of iterations.

We proposed new estimation to construction for the iterative process accuracy with respect to the solution of the Poisson equation concerning the electric field potential, induced by laser pulse. It is based on the criterion of the discrepancy accuracy estimation. This allows to calculate the electric field potential with high accuracy and with good high-speed performance. Accuracy of the electric field potential calculation influences in a strong way on the problem solution. If this accuracy is not high enough, then the problem solution can lose its symmetry.

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