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On approximations of the charge transfer equation in semiconductor

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1. Introduction

In this paper the approximations of diffusion-convection equation, describing the charge transfer in semiconductors are concidered. In one-dimensional case this equation is the following:

$$-\frac{d}{dx}\, e^{-\alpha\varphi}\, \frac{du}{dx} = f, \qquad x \in [a, b]. \tag{1.1}$$

Here $\varphi(x)$ and $f(x)$ are known functions, electrostatic potential and source function, $\alpha = 1$ if (1.1) describes the transfer of positive charges (holes) and $\alpha = -1$ corresponds to the negative charge transfer (electrons). Below, we suppose $\alpha = 1$. On the boundary the Dirichlet or Neumann conditions are given.

The peculiarity of this equation is the existence of inner layers because of the locally strongly variable function $\varphi(x)$.

Equation (1.1) is the part of nonlinear equation system, describing electrophysical processes in the framework of the so called diffusion-drift model [1] in the stationary linearized case. For this system the flow density conservation lows are complited. That is why, it is naturally for deriving the difference analogues of equation (1.1) to use the integro-balanced approximation methods (box methods), for obtaining conservative schemes [2, 3].

The open question in the balanced methods theory is the construction of high order approximations. In paper [4] the set of integral-balanced approximations, giving each precision order under sufficient smoothnees of the flow, potential and the right-hand side of equation (1.1) in one-dimensional case are proposed.

In the article, these approximations are investigated and numerical comparision of difference schemes, derived with the help of them, and the widely used Sharfetter–Gummel scheme [5] is implemented. This scheme may be obtained, for example, by means of the Marchuk identity [2]. In our paper, Sharfetter-Gummel scheme is derived as particular case of balanced high precision approximations, this permites to obtain the error approximation estimate without the derivatives of unknown solution u.

In Section 2 the general principle of balanced difference schemes construction is described, and their approximation properties are investigated.

In Section 3 by means of Section 2 we construct some particular schemes, the Sharfetter–Gummel scheme, and the error approximation estimate in uniform norm under definite coefficients and right parts approximations is given.

In Section 4 the numerical experiments are described, and the schemes derived in Section 3 are compared.

2. Construction of balanced approximations

We define the flow $J(x) = -e^{-\varphi}\dfrac{du}{dx}$, then equation (1.1) may be rewritten in the following way:

$$\frac{dJ}{dx} = f. \tag{2.1}$$

After integrating $J(x)e^{\varphi}$ on the interval $[x_i, x_{i+1}]$, we obtain the equality

$$u_{i+1} - u_i = \int_{x_i}^{x_{i+1}} J(x)e^{\varphi}\,dx.$$

For approximation of integral on the right-hand side we use some quadrature formula, supposing that e^{φ} is the weight function. Then we have

$$\int_{x_i}^{x_{i+1}} J(x)e^{\varphi}\,dx = \int_{x_i}^{x_{i+1}} e^{\varphi}\,dx \cdot \sum_{k=1}^{n_i} \alpha_{i,k}J_{i,k} + \psi^{(1)}_{i+1/2}, \tag{2.2}$$

here n_i – quadrature nodes number, $J_{i,k} = J(x_{i,k})$, $x_i \le x_{i,k} \le x_{i+1}$ (so, the index k is the node number at the interval $[x_i, x_{i+1}]$), $\psi^{(1)}_{i+1/2}$ – approximation error of quadrature formula. Multiplier $\int_{x_i}^{x_{i+1}} e^{\varphi}\,dx$ is introduced for quadrature coefficients $\alpha_{i,k}$ to satisfy the normalisation condition

$$\sum_{k=1}^{n_i} \alpha_{i,k} = 1. \tag{2.3}$$

Then we approximate anyway the integral of e^{φ}:

$$\int_{x_i}^{x_{i+1}} e^{\varphi}\,dx = \tilde{p}_{i+1/2} + \psi^{(2)}_{i+1/2}, \tag{2.4}$$

where $\psi^{(2)}_{i+1/2}$ is the quadrature error. After substitution (2.4) to (2.2), we obtain

$$u_{i+1} - u_i = (\tilde{p}_{i+1/2} + \psi^{(2)}_{i+1/2}) \sum_{k=1}^{n_i} \alpha_{i,k} J_{i,k} + \psi^{(1)}_{i+1/2}.$$

Dividing the latter equality by $\tilde{p}_{i+1/2}$ we have

$$\frac{u_{i+1} - u_i}{\tilde{p}_{i+1/2}} = \sum_{k=1}^{n_i} \alpha_{i,k} J_{i,k} + \frac{\psi^{(2)}_{i+1/2}}{\tilde{p}_{i+1/2}} \sum_{k=1}^{n_i} \alpha_{i,k} J_{i,k} + \frac{\psi^{(1)}_{i+1/2}}{\tilde{p}_{i+1/2}}.$$

We use the analogous expression for the interval $[x_{i-1}, x_i]$, and after subtracting it from the previous one, we have the equation

$$\frac{u_{i+1} - u_i}{\tilde{p}_{i+1/2}} + \frac{u_{i-1} - u_i}{\tilde{p}_{i-1/2}} = \sum_{k=1}^{n_i} \alpha_{i,k} J_{i,k} - \sum_{k=1}^{n_{i-1}} \alpha_{i-1,k} J_{i-1,k} + \psi^J_i + \psi^p_i.$$

Here we note

$$\psi^J_i = \frac{\psi^{(1)}_{i+1/2}}{\tilde{p}_{i+1/2}} - \frac{\psi^{(1)}_{i-1/2}}{\tilde{p}_{i-1/2}}, \tag{2.5}$$

$$\psi^p_i = \frac{\psi^{(2)}_{i+1/2}}{\tilde{p}_{i+1/2}} \sum_{k=1}^{n_i} \alpha_{i,k} J_{i,k} - \frac{\psi_{i-1/2}}{\tilde{p}_{i-1/2}} \sum_{k=1}^{n_{i-1}} \alpha_{i-1,k} J_{i-1,k}. \tag{2.6}$$

Then we should group the flow differences for obtaining the equality

$$\frac{u_{i+1} - u_i}{\tilde{p}_{i+1/2}} + \frac{u_{i-1} - u_i}{\tilde{p}_{i-1/2}} = \sum_{l=1}^{m_i} \gamma_{i,l} (J_{i,l} - J_{i-1,l}) + \psi^J_i + \psi^p_i.$$

This may be done because quadrature coefficients $\alpha_{i,k}$ satisfy the normalization relaionship (2.3).

Replace the flow differences by the integrals of the right-hand side f. Equation (2.1) is integrated on the interval $[x_{i,l}, x_{i-1,l}]$:

$$J_{i,l} - J_{i-1,l} = -\int_{x_{i-1,l}}^{x_{i,l}} f(x)\, dx. \tag{2.7}$$

After substitution of the latter equality we receive:

$$\frac{u_{i+1} - u_i}{\tilde{p}_{i+1/2}} + \frac{u_{i-1} - u_i}{\tilde{p}_{i-1/2}} = -\sum_{l=1}^{m_i} \gamma_{i,l} \int_{x_{i-1,l}}^{x_{i,l}} f(x)\, dx + \psi^J_i + \psi^p_i. \tag{2.8}$$

Finally, approximating with satisfactory precision the rest integrals, we have the system of the difference equations

$$p_{i+1/2}\frac{u_{i+1}-u_i}{h_i}+p_{i-1/2}\frac{u_{i-1}-u_i}{h_{i-1}}$$
$$=\sum_{l=1}^{m_i}\gamma_{i,l}\sum_{k=1}^{r}q_{i,l,k}f(x_{i,l,k})+\sum_{l=1}^{m_i}\gamma_{i,l}\psi_{i,l}^{f}+\psi_i^{p}+\psi_i^{J},\ \ i=1,\ldots,n, \quad (2.9)$$

that is complited by equations that approximate boundary conditions. Here $p_{i\pm1/2}$ is ordinary definition of difference equation coefficients, $p_{i+1/2}=\frac{h_i}{\tilde{p}_{i+1/2}}$, $p_{i-1/2}=\frac{h_{i-1}}{\tilde{p}_{i-1/2}}$, $\psi_{i,l}^{f}$ is the approximation error of the integral $\int_{x_{i-1,l}}^{x_{i,l}}f(x)\,dx$, ψ_i^{J} and ψ_i^{p} are the approximation errors of the flow and coefficients defined above by formulae (2.5), (2.6).

3. Examples of difference schemes

3.1. Approximation properties of the Sharfetter–Gummel scheme

In formula (2.2), we replace the flow $J(x)$ by their value in the middle point of integration interval, denoted by $J_{i+1/2}$, i.e., we use the central rectangular quadrature formula:

$$\int_{x_i}^{x_{i+1}}J(x)e^{\varphi}\,dx=J_{i+1/2}\int_{x_i}^{x_{i+1}}e^{\varphi}\,dx+\psi_{i+1/2}^{(1)},$$
$$\psi_{i+1/2}^{(1)}=J'(\xi_1)\int_{x_i}^{x_{i+1}}(x-x_{i+1/2})e^{\varphi}\,dx.$$

We obtain the approximation of the integral of exponent $\tilde{p}_{i+1/2}$ from formula (2.4) by replacement the potential φ with the linear function $\tilde{\varphi}$ at the interval $[x_i,x_{i+1}]$ ($\tilde{\varphi}(x_i)=\varphi(x_i)$, $\tilde{\varphi}(x_{i+1})=\varphi(x_{i+1})$). In this case the integral of e^{φ} may be calculated exactly. So, we have the following approximation for the flow value at the point $x_{i+1/2}$:

$$J_{i+1/2}=\frac{u_{i+1}-u_i}{\int_{x_i}^{x_{i+1}}e^{\tilde{\varphi}}\,dx}+J_{i+1/2}\delta_i-\frac{\psi_{i+1/2}^{(1)}}{\int_{x_i}^{x_{i+1}}e^{\tilde{\varphi}}\,dx}, \quad (3.1)$$

where δ_i is the quantity of the order h_i^2, because $\delta_i\in(0,\psi_i^{(3)}(\eta_1))$, where

$$\psi_i^{(3)}(x)=\frac{(x-x_i)(x-x_{i+1})}{2}\varphi''(\eta_2),\qquad \xi_1,\eta_1,\eta_2\in(x_i,x_{i+1}).$$

The multiplier $\int_{x_i}^{x_{i+1}}(x-x_{i+1/2})e^{\varphi}\,dx$ has the second order with respect to h_i. This may be proved by using the theorem on averaging and the Taylor

expansion of exponent function. So, the complete error of approximation of $J_{i+1/2}$ may be estimated as

$$|\psi^J_{i+1/2}| + |\psi^p_{i+1/2}| \le \frac{h_i^2}{2}\Big(|J_{i+1/2}\varphi''(\eta_2)| + \frac{1}{4}|J'(\xi_1)\varphi'(\eta_3)|\Big),$$

where $\eta_3 \in (x_i, x_{i+1})$.

Finally, we have the difference equation

$$-\frac{u_{i+1}-u_i}{e^{\varphi_{i+1}}-e^{\varphi_i}}\frac{\varphi_{i+1}-\varphi_i}{h_{i+1}} - \frac{u_{i-1}-u_i}{e^{\varphi_{i-1}}-e^{\varphi_i}}\frac{\varphi_{i-1}-\varphi_i}{h_i} = \tilde{f}_i + \psi_i. \qquad (3.2)$$

Here $\tilde{f}_i$ is some approximation of the integral of the right-hand side, for example, $\tilde{f}_i = f(x_i)\cdot(h_i + h_{i+1})/2$.

After dividing equation (3.2) by the quantity h^l so that the right-hand side of (3.2) has the order $O(1)$, we obtain in the uniform norm that scheme (3.2) approximates differential equation (1.1) at nonuniform grid with the first order on h ($h = \max_i h_i$). In the case of uniform meshes the approximation order increases to the second order. It is interesting that the approximation estimate does not contain the derivatives of unknown solution, only the flow derivatives that are more smooth functions in practice.

In the paper [6] the questions of convergence were investigated. By means of power functions the first order of convergence for nonuniform grid and the second order for uniform one was proved in the uniform norm. The approximation error of flow $J_{i+1/2}$ was obtained in the following form:

$$|\psi_{i+1/2}| \le \frac{h_i^2}{2}\frac{e^{-\varphi_{i+1/2}}}{4}\Big(\frac{|u'''(\eta_4)|}{3} + |u'_{i+1/2}\varphi''(\eta_5)|\Big), \quad \eta_4, \eta_5 \in (x_i, x_{i+1}).$$

We see that the former estimate posesses the derivatives u''' and u'.

Let $u = e^{\varphi}$, then $J = -\varphi'$, and now we have the estimates

$$|\psi^J_{i+1/2}| + |\psi^p_{i+1/2}| \le \frac{h_i^2}{2}\Big(|\varphi'_{i+1/2}\varphi''(\eta_2)| + \frac{|\varphi''(\xi_1)\varphi'(\eta_3)|}{4}\Big),$$

and

$$|\psi_{i+1/2}| \le \frac{h_i^2}{2}\Big(|\varphi'_{i+1/2}\varphi''_{i+1/2}| + \frac{e^{\varphi(\eta_4)-\varphi_{i+1/2}}}{3}|(\varphi'(\eta_4))^3 + 3\varphi'(\eta_4)\varphi''(\eta_4) + \varphi'''(\eta_4)|\Big).$$

In the first estimate we have the additional terms posessing the third derivatives of φ and $(\varphi')^3$. So, we improve the constant in approximation error.

3.2. Schemes, derived by means of the Gauss and Markov quadratures

Now for approximation of the integral in formula (2.2) we use the Gauss and Markov quadratures (with different number of nodes); e^{φ} is considered as the weight function.

Under using the Gauss quadrature, coefficients $\alpha_{i,k}$ are calculated in the following way:

$$\alpha_{i,k} = \frac{c_{i,k}}{\int\limits_{x_i}^{x_{i+1}} e^{\varphi}\,dx}, \qquad c_{i,k} = \frac{\int\limits_{x_i}^{x_{i+1}} e^{\varphi}\Omega_{k,n_i}(x)\,dx}{\Omega^2_{k,n_i}(x_{i,k})}, \tag{3.3}$$

$$\Omega_{k,n_i}(x) = \frac{\omega_{n_i}(x)}{x - x_{i,k}}, \qquad \omega_{n_i}(x) = (x - x_{i,1}) \times \ldots \times (x - x_{i,n_i}).$$

Here $\omega_{n_i}(x)$ is the node polinomial. The quadrature nodes $x_{i,k}$ may be found from the following relations:

$$\int\limits_{x_i}^{x_{i+1}} e^{\varphi}\omega_{n_i}(x)q(x)\,dx = 0, \tag{3.4}$$

where $q(x)$ is the arbitrary polinomial of the degree less or equals to $n_i - 1$. The approximation error $\psi^{(1)}_{i+1/2}$ is the quantity of the order h^{2n_i+1}, $h = \max_i h_i$, really

$$\psi^{(1)}_{i+1/2} = \frac{J^{2n_i}(\eta_i)}{(2n_i)!} \int\limits_{x_i}^{x_{i+1}} e^{\varphi}\omega^2_{n_i}(x)\,dx, \quad \eta_i \in (x_i, x_{i+1}). \tag{3.5}$$

In equation (2.2) under application of the Markov quadrature with two fixed nodes, the rest quadrature nodes x'_l may be obtained from the relationship $\zeta_{n_i}(x'_l) = 0$, where $\zeta_{n_i}(x) = D^1_{n_i}/D^2_{n_i}$,

$$D^1_{n_i} = \begin{vmatrix} \omega_{n_i}(x) & \omega_{n_i}(x_i) & \omega_{n_i}(x_{i+1}) \\ \omega_{n_i-1}(x) & \omega_{n_i-1}(x_i) & \omega_{n_i-1}(x_{i+1}) \\ \omega_{n_i-2}(x) & \omega_{n_i-2}(x_i) & \omega_{n_i-2}(x_{i+1}) \end{vmatrix},$$

$$D^2_{n_i} = \begin{vmatrix} \omega_{n_i-2}(x_i) & \omega_{n_i-1}(x_{i+1}) \\ \omega_{n_i-2}(x_i) & \omega_{n_i-2}(x_{i+1}) \end{vmatrix}.$$

Quadrature coefficients are calculated by

$$\alpha_{i,l} = \frac{1}{\int\limits_{x_i}^{x_{i+1}} e^{\varphi}\,dx} \int\limits_{x_i}^{x_{i+1}} \frac{e^{\varphi}\zeta_{n_i}(x)}{(x - x'_i)\zeta'_{n_i}(x'_i)}\,dx,$$

and approximation error has the form

$$\psi_i^{(1)} = \frac{1}{\int\limits_{x_i}^{x_{i+1}} e^{\varphi}\,dx} \cdot \frac{J^{(2n_i-2)}(\eta_i)}{(2n_i)!} \int\limits_{x_i}^{x_{i+1}} \frac{e^{\varphi}\zeta_{n_i}^2(x)}{(x-x_i)(x-x_{i+1})}\,dx.$$

Here $\eta_i \in (x_i, x_{i+1})$. It is obvious that ψ_i^J is the term of the order h^{2n_i-2}.

After application of the quadrature formulae it is possible to group the flow divergences (relationship (2.3) is implemented). We obtain an equation of the form (2.9). The errors $\psi_{i,l}^f$ and ψ_i^p may be different (this depends on the method of coefficients and the right-hand side approximation), $\psi_i^J = O(h^{2n_i})$, that is the consequence of formulae (2.5) and (2.6).

So, under the increasing of integral approximation accuracy we can obtain the scheme of any approximation order (if functions J, φ and f are enough smooth). It is also important that we can use these constructions if J, f have the given jumps and the singularities with known *a priori* asymptotic behaviour are nearby the singular points.

We hope that because of high approximation order, these shemes will give higher order of solution accuracy than the Sharfetter–Gummel scheme when φ derivatives increase.

Below we describe three types of the difference schemes distinct by the method of flow approximation.

Scheme 1. Flow approximation by the Gauss formula with one node (Gauss1 scheme).

In accordance with formulae (3.4) the nodes $x_{i,1}$ may be calculated as $x_{i,1} = g_{i,1}/g_{i,0}$. Here

$$g_{i,k} = \int\limits_{x_i}^{x_{i+1}} e^{\varphi} x^k\,dx.$$

The coefficients $\alpha_{i,1}$ are equal 1 for every i. Equation (2.8) in this case is the following:

$$\frac{u_{i+1}-u_i}{\int\limits_{x_i}^{x_{i+1}} e^{\varphi}\,dx} + \frac{u_{i-1}-u_i}{\int\limits_{i-1}^{i} e^{\varphi}\,dx} = \int\limits_{x_{i-1,1}}^{x_{i,1}} f\,dx.$$

Under approximation of the rest integrals with definite accuracy we have the difference equation of the first approximation order on nonuniform mesh and of the second order on the uniform one.

Scheme 2. Flow approximation by the Gauss formulae with two nodes (Gauss2 scheme).

The quadrature nodes at each interval $[x_i, x_{i+1}]$ are derived as the solution to the algebraic equations system

$$\int_{x_i}^{x_{i+1}} e^{\varphi}(x - x_{i,1})(x - x_{i,2})\,dx = 0,$$
$$\int_{x_i}^{x_{i+1}} e^{\varphi}(x - x_{i,1})(x - x_{i,2})x\,dx = 0,$$

from which it follows that $x_{i,1}$ and $x_{i,2}$ satisfy the relationships

$$x_{i,1} + x_{i,2} = \frac{g_{i,2}g_{i,1} - g_{i,3}g_{i,0}}{(g_{i,1})^2 - g_{i,2}g_{i,0}},$$
$$x_{i,1}x_{i,2} = \frac{(g_{i,2})^2 - g_{i,1}g_{i,3}}{(g_{i,1})^2 - g_{i,2}g_{i,0}}.$$

From (3.3) we have relations for the coefficients $\alpha_{i,1}$ and $\alpha_{i,2}$:

$$\alpha_{i,l} = \frac{C_{i,l}}{g_{i,0}}, \quad l = 1, 2,$$
$$C_{i,1} = \frac{g_{i,2} - 2x_{i,2}g_{i,1} + (x_{i,2})^2 g_{i,0}}{(x_{i,1} - x_{i,2})^2},$$
$$C_{i,2} = \frac{g_{i,2} - 2x_{i,1}g_{i,1} + (x_{i,1})^2 g_{i,0}}{(x_{i,1} - x_{i,2})^2}.$$

The quantities $\gamma_{i,k}$ from (2.7) are determined by the equalities

$$\gamma_{i,1} = \alpha_{i,1}, \quad \gamma_{i,2} = \alpha_{i,4}, \quad \gamma_{i,3} = \alpha_{i,2} - \alpha_{i,4},$$

and equation (2.8) has the form

$$\frac{u_{i+1} - u_i}{\int_{x_i}^{x_{i+1}} e^{\varphi}\,dx} + \frac{u_{i-1} - u_i}{\int_{i-1}^{i} e^{\varphi}\,dx} = \gamma_{i,1} \int_{x_{i-1,1}}^{x_{i,1}} f\,dx + \gamma_{i,2} \int_{x_{i-1,2}}^{x_{i,2}} f\,dx + \gamma_{i,3} \int_{x_{i-1,2}}^{x_{i,1}} f\,dx.$$

After approximation of the rest integrals we have difference equation of the third approximation order for the nonuniform grid and of the fourth order for the uniform one.

Scheme 3. Flow approximation by the Markov formulae with three nodes (Markov3 scheme).

For construction of Scheme 2 we should calculate two intermediate nodes and approximate functions φ, f in these nodes; it leads to the additional

solution error. That is why it is interesting to compare this scheme with the scheme derived by using Markov's quadrature formula with two fixed nodes and one intermidiate. The order of approximation is the same as in Scheme 2, but it is necessary to approximate functions in one node only.

So, we use Markov's quadrature with the fixed nodes $(x_i,\ x_{i+1})$ and intermediate node x_i' that can be determined from the relationship $\zeta_3(x) = 0$, where

$$\zeta_3(x) = \frac{\begin{vmatrix} \omega_3(x) & \omega_3(x_i) & \omega_3(x_{i+1}) \\ \omega_2(x) & \omega_2(x_i) & \omega_2(x_{i+1}) \\ \omega_1(x) & \omega_1(x_i) & \omega_1(x_{i+1}) \end{vmatrix}}{\begin{vmatrix} \omega_2(x_i) & \omega_2(x_{i+1}) \\ \omega_1(x_i) & \omega_1(x_{i+1}) \end{vmatrix}}.$$

The quadrature coefficients are detemined in the following way:

$$\alpha_{i,l} = \frac{1}{g_{i,0}} \int_{x_i}^{x_{i+1}} \frac{e^{\varphi}\zeta_3(x)}{(x - x_i')\zeta_3'(x_i')}\, dx,$$

and approximation error has the form

$$\psi_i^J = \frac{1}{g_{i,0}} \cdot \frac{J^{(4)}(\eta_i)}{4!} \int_{x_i}^{x_{i+1}} \frac{e^{\varphi}\zeta_3^2(x)}{(x - x_i)(x - x_{i+1})}\, dx,$$

where $\eta_i \in (x_i, x_{i+1})$. It is obvious that ψ_i^J is the quantity of the fouth order with respect to h.

As in Schemes 1 and 2, we calculate the nodes and coefficients of quadrature using $g_{i,k}$. Equation (2.8) in this case is the following:

$$\frac{u_{i+1} - u_i}{\int_{x_i}^{x_{i+1}} e^{\varphi} dx} + \frac{u_{i-1} - u_i}{\int_{i-1}^{i} e^{\varphi} dx}$$

$$= \gamma_{i,1} \int_{x_{i-1}}^{x_i} f\, dx + \gamma_{i,2} \int_{x_{i-1}'}^{x_i'} f\, dx + \gamma_{i,3} \int_{x_i}^{x_{i+1}} f\, dx + \gamma_{i,4} \int_{x_{i-1}}^{x_{i-1}'} f\, dx + \gamma_{i,5} \int_{x_{i-1}'}^{x_i} f\, dx,$$

where

$$\gamma_{i,1} = \alpha_1^i, \quad \gamma_{i,2} = \alpha_2^i, \quad \gamma_{i,3} = \alpha_3^i, \quad \gamma_{i,4} = \alpha_1^{i-1} - \alpha_{i,1}, \quad \gamma_{i,5} = \alpha_3^i - \alpha_3^{i-1}.$$

Approximation order is the same as in Scheme 2.

4. Numerical comparison of balanced methods

Consider two model problems.

Problem 1. We seek a solution at the interval $[0, 1]$. Potential function and precise solution u are the following:

$$\varphi = qx, \quad u = e^{(q+1)x}.$$

In this case, the function f on the right-hand side of (2.1) and flow J are described as

$$f = -(q+1)e^x, \quad J = -(q+1)e^x.$$

In the experiments we consider the values of parameter $q = 2, 4, 8, 16$.

Problem 2. We seek a solution at the interval $[-0.5, 0.5]$. The potential and solution are the following:

$$\varphi = q\,\mathrm{arctg}(x), \quad u = e^{q\,\mathrm{arctg}(x)},$$

that provide the functions

$$f = \frac{2qx}{(1+x^2)^2}, \qquad J = -\frac{q}{1+x^2}.$$

Now $q = 2, 8, 16, 20, 27$.

On the boundary, the Dirichlet conditions are hold. For domain discretization we use the uniform mesh with the step $h = 1/2^k$, where k changes from 3 to 6 and nodes number n – from 9 to 65.

Under approximations described in Section 3, in one-dimentional case we have three-point equations systems, for its solving the sweeping method is used. All calculations are implemented with double precision.

In these problems, the flow is the more smooth function than the solution. Really, in Problem 1 we have:

$$u' = (q+1)e^{(q+1)x}, \quad J' = -(q+1)e^x,$$

in Problem 2:

$$u' = \frac{q}{1+x^2}e^{q\,\mathrm{arctg}(x)}, \quad J' = \frac{2qx}{(1+x^2)^2}.$$

Derivative of the potential φ linear depends on the parameter q. The global variation of φ is real even for maximum q in practice.

The aims of numerical experiments are, firstly, to show high approximation order of schemes derived in Section 3, secondly, to confirm the hypothesis about the higher efficiency of these schemes under greatest derivatives of φ (i.e., under growing parameter q) than the Sharfetter–Gummel scheme.

The methods are compared by the relative error of precise solution

$$\delta u = \max_i \left\{ \left| \frac{u_i^{\text{precise}} - u_i^{\text{difference}}}{u_i^{\text{precise}}} \right| \right\}.$$

Firstly, the problem of linear potential (Problem 1) is investigated. The quantities $g_{i,k}$ are calculated exactly, also we can compute exactly coefficients and the integral of the right-hand side. So, the errors $\psi_{i,l}^f$, ψ_i^p from formula (3.6) equal to zero, and the total approximation error is defined only by $\psi_{i,l}^J$.

The results of calculations are shown in Table 1. Here (and in all tables bellow) δu is given for different n, q in each square, and for four schemes: Sharfetter–Gummel scheme (the first line), Gauss1 scheme (second line), Gauss2 scheme (third line) and Markov3 (the fourth line).

Table 1. The problem with linear φ

n \ q	2	4	8	16
9	$1.3_{10}-3$ $2.6_{10}-4$ $2.3_{10}-8$ $2.1_{10}-5$	$3.7_{10}-3$ $4.1_{10}-4$ $3.6_{10}-8$ $3.7_{10}-6$	$1.0_{10}-2$ $5.8_{10}-4$ $5.0_{10}-8$ $5.5_{10}-6$	$2.4_{10}-2$ $6.4_{10}-4$ $5.6_{10}-8$ $6.6_{10}-6$
17	$3.3_{10}-4$ $6.6_{10}-5$ $1.4_{10}-9$ $2.3_{10}-7$	$9.4_{10}-4$ $1.0_{10}-4$ $2.2_{10}-9$ $4.3_{10}-7$	$2.6_{10}-3$ $1.5_{10}-4$ $3.3_{10}-9$ $7.3_{10}-7$	$6.3_{10}-3$ $1.8_{10}-4$ $4.0_{10}-9$ $1.0_{10}-6$
33	$8.3_{10}-5$ $1.7_{10}-5$ $9.0_{10}-11$ $2.4_{10}-8$	$2.4_{10}-4$ $2.6_{10}-5$ $1.4_{10}-10$ $4.6_{10}-8$	$6.5_{10}-4$ $3.8_{10}-5$ $2.1_{10}-10$ $8.2_{10}-8$	$1.6_{10}-3$ $4.8_{10}-5$ $2.6_{10}-10$ $1.2_{10}-7$
65	$2.1_{10}-5$ $4.2_{10}-6$ $5.1_{10}-12$ $2.3_{10}-9$	$5.9_{10}-5$ $6.5_{10}-6$ $7.7_{10}-12$ $4.9_{10}-9$	$1.6_{10}-4$ $9.6_{10}-6$ $1.4_{10}-11$ $8.6_{10}-9$	$4.0_{10}-4$ $1.2_{10}-5$ $1.6_{10}-11$ $1.3_{10}-8$

From Table 1 we can conclude that Schemes 1, 2, 3 calculate the solution more accurate and give smaller error under greatest q than Sharfetter–Gummel scheme. It is interesting that the error of Scheme 1 is less than error of Sharfetter–Gummel scheme in 4 times for small q and in 33 times for $q = 16$. Markov3 demonstrates here only third approximation order (theoratical estimate gives the fourth order), the other schemes confirme the results of Section 3: Sharfetter–Gummel and Gauss1 schemes have the second order, Gauss2 – the fourth one.

Now consider Problem 2. It is different from the first one because it is necessary to approximate quantities $g_{i,k}$, that gives an additional error in computation of quadrature nodes and coefficients.

In all experiments, we approximate the integrals of the right-hand side from (2.9) by the Simpson quadrature formulae, and the quantities $\tilde{p}_{i\pm1/2}$, $g_{i,k}$ in two ways:

1) by the Simpson formula;
2) by using the Gauss quadrature with four nodes of the 9th accuracy order.

The simple linear approximation of integrals $\int_{x_i}^{x_{i+1}} e^{\varphi} dx$ gives the big error ψ_i^p, therefore there is no sense to approximate flows accurately. Under the precise computation of the right-hand side of equation (2.9), the results are similar to the given below.

As in practicle problems, the functions φ, f are given by the values in mesh nodes, and it is necessary to derive their values in quadrature nodes. We must interpolate these functions at the intervals $[x_i, x_{i+1}]$. Under linear interpolation miscalculation is very great, that is why we suppose that the values of derivatives in mesh nodes are also known and we can interpolate φ, f by cube polinomials.

Results of calculations are shown in Table 2 under the first method of coefficients approximation and in Table 3 under the second one.

Table 2. Problem 2: Simpson's approximation of coefficients

n \ q	2	8	16	20	27
9	$9.0_{10}-4$ $1.9_{10}-4$ $2.8_{10}-6$ $2.0_{10}-6$	$8.7_{10}-3$ $8.9_{10}-4$ $3.1_{10}-4$ $3.1_{10}-4$	$1.8_{10}-2$ $4.5_{10}-3$ $3.7_{10}-3$ $3.7_{10}-3$	$2.3_{10}-2$ $9.1_{10}-3$ $8.2_{10}-3$ $8.2_{10}-3$	$2.9_{10}-2$ $2.4_{10}-2$ $2.3_{10}-2$ $2.3_{10}-2$
17	$2.2_{10}-4$ $4.8_{10}-5$ $1.8_{10}-7$ $1.3_{10}-7$	$2.2_{10}-3$ $1.9_{10}-4$ $1.9_{10}-5$ $1.9_{10}-5$	$5.3_{10}-3$ $4.7_{10}-4$ $2.6_{10}-4$ $2.6_{10}-4$	$6.6_{10}-3$ $8.3_{10}-4$ $6.1_{10}-4$ $6.1_{10}-4$	$8.9_{10}-3$ $2.1_{10}-3$ $1.9_{10}-3$ $1.9_{10}-3$
33	$5.6_{10}-5$ $1.2_{10}-5$ $1.1_{10}-8$ $8.2_{10}-9$	$5.4_{10}-4$ $4.4_{10}-5$ $1.2_{10}-6$ $1.2_{10}-6$	$1.3_{10}-3$ $7.3_{10}-5$ $1.9_{10}-5$ $1.7_{10}-5$	$1.7_{10}-3$ $9.8_{10}-5$ $3.9_{10}-5$ $3.9_{10}-5$	$2.4_{10}-3$ $1.9_{10}-4$ $1.3_{10}-4$ $1.3_{10}-4$
65	$1.4_{10}-5$ $3.0_{10}-6$ $7.1_{10}-10$ $5.1_{10}-10$	$1.4_{10}-4$ $1.1_{10}-5$ $7.7_{10}-8$ $7.8_{10}-8$	$3.4_{10}-4$ $1.5_{10}-5$ $1.1_{10}-6$ $1.1_{10}-6$	$4.4_{10}-4$ $1.7_{10}-5$ $2.5_{10}-6$ $2.5_{10}-6$	$6.2_{10}-4$ $2.4_{10}-5$ $8.0_{10}-6$ $8.0_{10}-6$

Here we can also see that Scheme 1 gives the greater accuracy than the Sharfetter–Gummel scheme. Under the greate q, the error of the Sharfetter–Gummel scheme is greater than the error of Gauss1 in four times under

Table 3. Problem 2: Gauss approximation of coefficients

n \ q	2	8	16	20	27
9	$9.0_{10}-4$ $1.9_{10}-4$ $2.6_{10}-6$ $1.6_{10}-5$	$8.9_{10}-3$ $6.6_{10}-4$ $1.8_{10}-5$ $4.4_{10}-5$	$2.0_{10}-2$ $7.4_{10}-4$ $3.8_{10}-5$ $3.6_{10}-5$	$2.6_{10}-2$ $7.1_{10}-4$ $4.6_{10}-5$ $2.8_{10}-5$	$3.5_{10}-1$ $6.0_{10}-4$ $5.5_{10}-5$ $1.8_{10}-5$
17	$2.2_{10}-4$ $4.8_{10}-5$ $1.7_{10}-7$ $1.8_{10}-6$	$2.2_{10}-3$ $1.7_{10}-4$ $1.1_{10}-6$ $5.6_{10}-6$	$5.4_{10}-3$ $2.2_{10}-4$ $2.5_{10}-6$ $6.2_{10}-6$	$6.9_{10}-3$ $2.2_{10}-4$ $3.2_{10}-6$ $5.9_{10}-6$	$9.6_{10}-3$ $2.2_{10}-4$ $4.3_{10}-6$ $5.3_{10}-6$
33	$5.6_{10}-5$ $1.2_{10}-5$ $1.1_{10}-8$ $1.8_{10}-7$	$5.6_{10}-4$ $4.3_{10}-5$ $7.1_{10}-8$ $6.3_{10}-7$	$1.3_{10}-3$ $5.7_{10}-5$ $1.6_{10}-7$ $7.9_{10}-7$	$1.8_{10}-3$ $5.9_{10}-5$ $2.1_{10}-7$ $8.2_{10}-7$	$2.5_{10}-3$ $6.1_{10}-5$ $2.8_{10}-7$ $8.2_{10}-7$
65	$1.4_{10}-5$ $3.0_{10}-6$ $6.6_{10}-10$ $1.8_{10}-8$	$1.4_{10}-4$ $1.1_{10}-5$ $4.5_{10}-9$ $6.8_{10}-8$	$3.4_{10}-4$ $1.4_{10}-5$ $1.0_{10}-8$ $9.0_{10}-8$	$4.4_{10}-4$ $1.5_{10}-5$ $1.3_{10}-8$ $9.5_{10}-8$	$6.2_{10}-4$ $1.6_{10}-5$ $1.8_{10}-8$ $1.0_{10}-7$

small q, and approximately in 22 times under the greater q. The results of calculations by Schemes 2 and 3 in the case of the first method of coefficients approximation are nearly the same, and Scheme 3 has the preference under more precise approximation of $\tilde{p}_{i\pm1/2}$ and $g_{i,k}$.

For all experiments we can conclude:

- all schemes confirm theoretical estimates, only Scheme 3 (flow approximation by the Markov formula) showes lower approximation order;
- schemes constructed by the Gauss quadrature formulae for flow approximation gives more accurate solution than the Sharfetter–Gummel scheme under greater gradients of potential;
- under the same approximation order, Scheme 1 (Gauss1) gives smaller error than the Sharfetter–Gummel scheme, and Scheme 2 (Gauss2) is "better" than Scheme 3 (Markov3).

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