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Difference Schemes for the Time Evolution of Three-Dimensional Kinetic Equations

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This paper is devoted to the development of finite difference methods for the solution of problems involving the three-dimensional kinetic equation with a Coulomb collision operator. New conservative difference schemes are presented and analysed. The schemes include a new approximation for mixed derivatives and accurate treatment of internal separatrix layers. The main advantages of the new schemes are improved stability and accuracy which, for example, allows calculation of the ion distribution function in thermonuclear experiments for a wider range of parameters.

Key Words: conservative finite difference approximations; time evolved Fokker–Planck equation; kinetic physics.

1. INTRODUCTION

The three-dimensional kinetic equation with a Coulomb collision operator can be used, for example, to study the evolution of particle distribution functions in thermonuclear fusion tokamak experiments in the form of the three-dimensional Fokker–Planck equation [1–4]. This is the particular case we shall consider in this paper though the numerical techniques have wider applications, e.g. for physical problems that can be described by 3D parabolic equations, which include three phase space variables and time. Other codes using fully implicit difference schemes to solve the Fokker–Planck equation include those by Giruzzi [6], Westerhof *et al.* [7], and Shkarofsky *et al.* [8].

The tokamak is a torus configuration with a characteristically large magnetic field in the direction going the long way round (toroidally) and a smaller field going the short way

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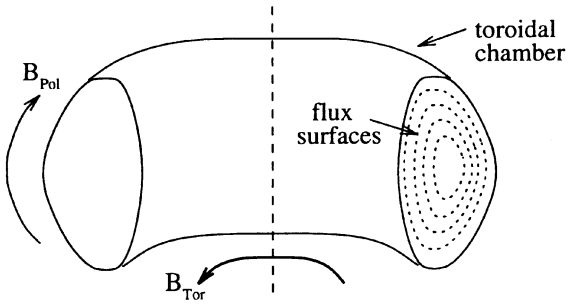

FIG. 1. Cross section of a tokamak showing the components of the magnetic field.

round (poloidally); see Fig. 1. The motion of charged particles in the torus is essentially a rapid gyration about a guiding centre with velocity parallel to the resulting helical field lines which map out nested flux surfaces. Due to the spatially varying magnetic field there exist two classes of particle, those that can pass through the high field on the inside edge of the flux surface and thus continue all the way round and those particles that become trapped on the low field side. Thus in velocity space there exists a separatrix between these particles called the trapped/passing boundary (TPB). The fast poloidal motion through the high and low field, the motion in the toroidal direction and the rapid gyration occur on time scales much shorter than those for the electromagnetic field variation and the problem can be reduced in dimension by averaging over the local coordinates of gyro angle, toroidal angle, and poloidal angle to give orbits characterised by three constants of the motion, v_0, θ_0, γ_0 (speed, a pitch-angle between the velocity vector and the magnetic field, and a flux surface radius) [4].

In what follows, u is the exact solution, f is the numerical solution, and z is the error between the two. In general the 3D kinetic equation for the distribution function u with the Coulomb collision operator has the form

$$\frac{\partial u}{\partial t} = \sum_{n,m=1}^{3} \mathcal{L}_{nm}[u], \tag{1}$$

where

$$\mathcal{L}_{nn}[u] = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^n} \left(A_{nn} \frac{\partial u}{\partial x^n} + B_n u \right) \tag{2}$$

for $m = n$ and

$$\mathcal{L}_{nm}[u] = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^n} \left(A_{nm} \frac{\partial u}{\partial x^m} \right) \tag{3}$$

for $m \neq n$.

Here $\sqrt{g}$ is the Jacobian term and A_{nm}, B_n are the coefficients representing collisions and also, in our case, external heating terms. The mixed derivative coefficients A_{nm} in (3) grow large due the anisotropic nature of the heating causing numerical problems in standard numerical schemes and thus a new method is proposed.

The outline of the paper is as follows: In Section 2 we describe the construction of the numerical grid on which these equations are solved. Section 3 introduces the difference

approximations under consideration and these are applied to the kinetic equation in Section 4. Theorems of existence and uniqueness of solutions to the equation are then discussed in Section 5 followed by stability and convergence theorems in Section 6. In Section 7 we show that the solution of the difference problem is positive semi-definite (as required for a distribution function) for certain conditions. Sections 8 and 9 give examples of applications and performance of the advanced difference schemes.

2. GRID CONSTRUCTION IN CONSTANTS OF MOTION COORDINATES

The principles of grid construction in terms of coordinates formed from the particle constants of motion should ensure good approximation of the distribution function on the boundaries and the enclosed area and also allow the calculation of integrals with an acceptable accuracy. The problem is formulated in an unlimited area of velocity space and it is important to take into account the fact that coefficients of the Coulomb collision operator behave differently in different parts of phase space with the proviso that they tend to zero at large speeds v_0.

In transition to the discrete problem for the averaged kinetic equation, it is necessary to approximate accurately the boundary conditions and conditions at the internal separatrix layer, so that the approximation of boundary conditions is not of lower order than that for the operators of the equation. For a Neumann problem (where the derivative of the grid function is specified at the boundary), or when on the boundary of phase space, the appropriate coefficient in the equation is degenerate, we shall use a so-called "flow grid" a half step from the appropriate boundary [1]. We shall also recede a half step from the separatrix. It is possible to construct an orthogonal grid on a plane (θ_0, γ_0). The separatrix for our problem lies in this plane, as illustrated in Fig. 2. For the Dirichlet problem (where the function is specified at the boundary) we shall use the usual grid with points on the boundary. The grid can be nonuniform.

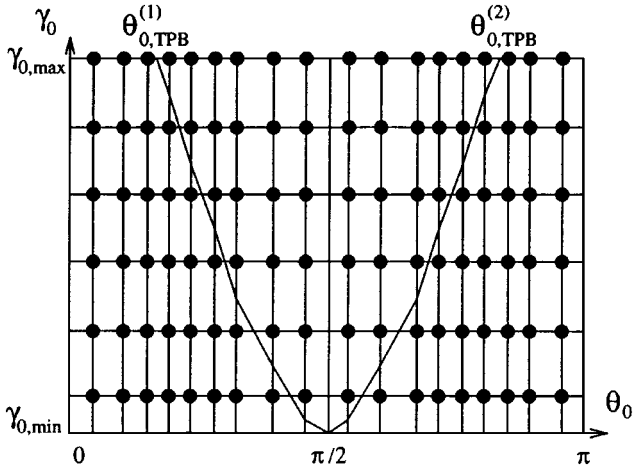

FIG. 2. A typical grid in the 2D plane showing an internal separatrix (TPB) for our problem. The boundary $\gamma_0 = \gamma_{0,\max}$ usually has a Dirichlet boundary condition (the function is zero). The other three boundaries have Neumann conditions (the flux through the boundary is zero).

We shall designate a grid variable x^n, $n = 1, 2, 3$, as

$$\bar{\omega}_n = \left\{x_i^n : x_i^n \in \left[x_{\min}^n, x_{\max}^n\right], i = 0, 1, \ldots, N_{x^n}, N_{x^n} + 1\right\},$$
$$\omega_n = \left\{x_i^n : x_i^n \in \left[x_{\min}^n, x_{\max}^n\right], i = 1, \ldots, N_{x^n}\right\}.$$

The nearest node of a grid in relation to the boundary of a separatrix layer is moved on a half-step. An example of a grid in a plane of variables (θ_0, γ_0) is presented in Fig. 2.

3. DIFFERENCE APPROXIMATION OF DIFFERENTIAL OPERATORS

Application of standard approximations without taking into account the specifics of a problem may mean that an unacceptable number of nodes on the difference grid is used in order to reach the required accuracy. Therefore we shall construct special approximations, taking into account a priori information about the behaviour of the distribution function.

The operator in Eq. (2) may be written as a sum of two components:

$$\begin{aligned}\mathcal{L}_{nn}[u] &= \frac{1}{\sqrt{g}}\frac{\partial}{\partial x^n}\left(A_{nn}\frac{\partial u}{\partial x^n} + \eta_n B_n u\right) + \frac{1}{\sqrt{g}}\frac{\partial}{\partial x^n}((1-\eta_n)B_n u)\\ &= \frac{1}{\sqrt{g}}\frac{\partial}{\partial x^n}\left(U_n\frac{\partial}{\partial x^n}(V_n u)\right) + \frac{1}{\sqrt{g}}\frac{\partial}{\partial x^n}((1-\eta_n)B_n u)\end{aligned} \tag{4}$$

with

$$U_n = A_{nn}\exp\left(-\int\frac{\eta_n B_n}{A_{nn}}dx^n\right), \quad V_n = \exp\left(\int\frac{\eta_n B_n}{A_{nn}}dx^n\right).$$

The function $\eta_n \in [0, 1]$ can be adjusted in order to raise the accuracy of the difference approximation. The integro-interpolation method [9] results in the approximation of the first component of the operator $\mathcal{L}_{nn}$,

$$\begin{aligned}\left(\Lambda_{nn}^{(1)}[f]\right)_i = \frac{1}{c_i\overline{h}_{x^n,i}}\Bigg[&U_{n,i+1/2}\left(\frac{V_{n,i+1}f_{i+1} - V_{n,i}f_i}{h_{x^n,i+1}}\right)\\ &- U_{n,i-1/2}\left(\frac{V_{n,i}f_i - V_{n,i-1}f_{i-1}}{h_{x^n,i}}\right)\Bigg]\end{aligned} \tag{5}$$

or

$$\begin{aligned}\left(\Lambda_{nn}^{(1)}[f]\right)_i = \frac{1}{c_i\overline{h}_{x^n,i}}\Bigg[&\frac{A_{nn,i+1/2}}{h_{x^n,i+1}}(\exp\{E_{n,i+1}\}f_{i+1} - \exp\{-E_{n,i+1}\}f_i)\\ &- \frac{A_{nn,i-1/2}}{h_{x^n,i}}(\exp\{E_{n,i}\}f_i - \exp\{-E_{n,i}\}f_{i-1})\Bigg], \quad x_i^n \in \omega_n,\end{aligned} \tag{6}$$

where f_i is the grid function, $i = 0, \ldots, N_{x^n} + 1$, $h_{x^n,i}$ is the grid-spacing, and $\overline{h}_{x^n,i}$ is the step between half-integer points of a grid,

$$\begin{aligned}E_{n,i} &= \frac{(\eta_n B)_{n,i-1/2}}{A_{nn,i-1/2}}\cdot\frac{h_{x^n,i}}{2}, \quad && i = 1, \ldots, N_{x^n},\\ c_i &= (\sqrt{g})_i, && i = 1, \ldots, N_{x^n},\\ \overline{h}_{x^n,i} &= \frac{h_{x^n,i+1} + h_{x^n,i}}{2}, && i = 1, \ldots, N_{x^n},\end{aligned}$$

The operator (5) or (6) approximates the first component of the operator (4) to second-order accuracy. This differencing gives an exact solution for the problem $\mathcal{L}_{nn} = 0$. In many kinetic problems the solution is close to the kernel of the operator over velocity (i.e., the distribution is close to a Maxwellian); therefore it is natural to expect improved accuracy for the full problem (2) when using (6). Numerous calculations have confirmed this.

Appropriate choice of the function η_n in (4) avoids overflow or loss of accuracy in using operator (6) in the case where $A_{nn} \ll B_n$. A suitable choice for the function η_n can be found by minimising the loss of accuracy in operator Λ_{nn}, when dealing with extreme values. We choose η_n from

$$\exp\left(\frac{(\eta B)_{n,i-1/2}}{A_{nn,i-1/2}}\frac{h_{x^n,i}}{2}\right)\Big/\exp\left(-\frac{(\eta B)_{n,i-1/2}}{A_{nn,i-1/2}}\frac{h_{x^n,i}}{2}\right) \le M_n,$$

and set it such that

$$\eta_{n,i-1/2} = \min\left\{\left|\frac{A_{nn,i-1/2}}{B_{n,i-1/2}}\right|\frac{\ln M_n}{h_{x^n,i}}, 1\right\},$$

which gives $0 \le \eta_n \le 1$ for $A_{nn} \ll B_n$ and $\eta_n = 1$ for $A_{nn} \sim B_n$. M_n can be related to the accuracy of the computer; e.g., $\log M_n$ can be equal to half the number of digits in the mantissa. For solutions f, close to the Maxwellian distribution, a choice of $\log M_n \sim 3$ in the velocity operator $n = 1$ and $\eta_n = 0$ for the other operators gives accurate numerical results on a modest grid.

For the second component $\mathcal{L}_{nn}$ in (4) it is possible to use well-known second-order approximations, e.g. centered differencing [9]. However, in the most complicated cases, when $A_{nn} \ll B_n$ and B_n changes sign, it can be better to apply an approximation with directed differences, taking into account the sign of B_n at each point on the grid so that

$$\begin{aligned}\left(\Lambda^{(2)}_{nn}[f]\right)_i = \frac{1}{c_i \bar{h}_{x^n,i}}[&((1-\eta_n)B_n)_{i+1/2}((1-\delta_{i+1/2})f_{i+1} + \delta_{i+1/2} f_i)\\ &- ((1-\eta_n)B_n)_{i-1/2}((1-\delta_{i-1/2})f_i + \delta_{i-1/2} f_{i-1})],\end{aligned} \tag{7}$$

with

$$\delta_{i-1/2} = \begin{cases} 0, & \text{if } B_{n,i-1/2} \ge 0,\\ 1, & \text{if } B_{n,i-1/2} < 0.\end{cases}$$

This approximation is obtained with the help of the integro-interpolation method. It has first-order error but improves the stability of calculations.

Finally the operator $\mathcal{L}_{nn}$ is approximated by the sum of (6) and (7),

$$(\Lambda_{nn}[f])_i = \left(\Lambda^{(1)}_{nn}[f]\right)_i + \left(\Lambda^{(2)}_{nn}[f]\right)_i. \tag{8}$$

For operators Λ_{nm} at $n \ne m$, apart from well-known approximations [9], we propose the following nonstandard 9-point approximation, which at each point of the grid uses not more than seven of nine possible nodes (see Fig. 3),

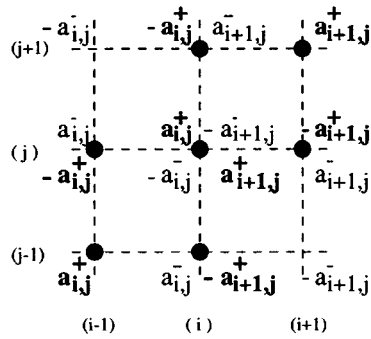

FIG. 3. Discretisation showing the seven nodes used if both $A_{nm,i-1/2,j}$ and $A_{nm,i+1/2,j}$ are positive.

$$
\begin{aligned}
(\Lambda_{nm}[f])_{ij} = \frac{1}{2c_{ij}\overline{h}_{x^n,i}}\Bigg[& \frac{a^+_{nm,i+1j}}{h_{x^m,j+1}}(f_{i+1j+1} - f_{i+1j}) + \frac{a^+_{nm,i+1j}}{h_{x^m,j}}(f_{ij} - f_{ij-1}) \\
& - \frac{a^+_{nm,ij}}{h_{x^m,j+1}}(f_{ij+1} - f_{ij}) - \frac{a^+_{nm,ij}}{h_{x^m,j}}(f_{i-1j} - f_{i-1j-1}) \\
& + \frac{a^-_{nm,i+1j}}{h_{x^m,j}}(f_{i+1j} - f_{i+1j-1}) + \frac{a^-_{nm,i+1j}}{h_{x^m,j+1}}(f_{ij+1} - f_{ij}) \\
& - \frac{a^-_{nm,ij}}{h_{x^m,j}}(f_{ij} - f_{ij-1}) - \frac{a^-_{nm,ij}}{h_{x^m,j+1}}(f_{i-1j+1} - f_{i-1j})\Bigg], \\
& \qquad \left(x^n_i, x^m_j\right) \in \omega_n \times \omega_m, \quad (9)
\end{aligned}
$$

where

$$
\begin{aligned}
a^+_{nm,ij} &= A^+_{nm}\left(x^n_{i-1/2}, x^m_j\right) = a^+_{ij}, \\
a^-_{nm,ij} &= A^-_{nm}\left(x^n_{i-1/2}, x^m_j\right) = a^-_{ij}, \\
A^+_{nm} &\equiv \frac{1}{2}[A_{nm} + |A_{nm}|] \geq 0, \\
A^-_{nm} &\equiv \frac{1}{2}[A_{nm} - |A_{nm}|] \leq 0.
\end{aligned}
$$

This approximation is obtained with the help of the integro-interpolation method. Its characteristic feature is that it takes into account the sign of A_{nm} and in some sense is an analogue of a directed difference. Such a discretisation of the operator ensures good conditioning of the equation matrix to give a unique solution as will be shown in Section 5. The operator $\Lambda_{nm}[f]$ approximates the initial operator (3) to second order.

We shall introduce the following notation:

$$
\hat{a}^1_{nm,ij} = \frac{a^+_{nm,i+1j}}{h_{x^m,j+1}}, \quad \hat{a}^2_{nm,ij} = \frac{a^+_{nm,i+1j}}{h_{x^m,j+1}} - \frac{a^-_{nm,i+1j}}{h_{x^m,j}}, \quad \hat{a}^3_{nm,ij} = -\frac{a^-_{nm,i+1j}}{h_{x^m,j}},
$$

$$
\hat{a}^4_{nm,ij} = \frac{a^+_{nm,ij}}{h_{x^m,j+1}} - \frac{a^-_{nm,i+1j}}{h_{x_m,j+1}}, \quad \hat{a}^6_{nm,ij} = \frac{a^+_{nm,i+1j}}{h_{x^m,j}} - \frac{a^-_{nm,ij}}{h_{x^m,j}},
$$

$$\hat{a}^5_{nm,ij} = \frac{a^+_{nm,i+1j}}{h_{x^m,j}} + \frac{a^+_{nm,ij}}{h_{x^m,j+1}} - \frac{a^-_{nm,i+1j}}{h_{x^m,j+1}} - \frac{a^-_{nm,ij}}{h_{x^m,j}},$$

$$\hat{a}^7_{nm,ij} = -\frac{a^-_{nm,ij}}{h_{x^m,j+1}}, \quad \hat{a}^8_{nm,ij} = \frac{a^+_{nm,ij}}{h_{x^m,j}} - \frac{a^-_{nm,ij}}{h_{x^m,j+1}}, \quad \hat{a}^9_{nm,ij} = \frac{a^+_{nm,ij}}{h_{x^m,j}}.$$

Note that as all coefficients $a^+_{nm,ij}$ are nonnegative, and the coefficients $a^-_{nm,ij}$ are nonpositive, then $\hat{a}^k_{nm,ij} \geq 0$, $k = 1, \ldots, 9$. This leads to improved stability properties for this approximation (9). Using $\hat{a}^k_{nm,ij}$ the expression for $\Lambda_{nm}[f]$ takes the form

$$(\Lambda_{nm}[f])_{ij} = \frac{1}{2c_{ij}\overline{h}_{x^n,i}}\big[\hat{a}^1_{nm} f_{i+1j+1} - \hat{a}^2_{nm} f_{i+1j} + \hat{a}^3_{nm} f_{i+1j-1} - \hat{a}^4_{nm} f_{ij+1}$$
$$+ \hat{a}^5_{nm} f_{ij} - \hat{a}^6_{nm} f_{ij-1} + \hat{a}^7_{nm} f_{i-1j+1} - \hat{a}^8_{nm} f_{i-1j} + \hat{a}^9_{nm} f_{i-1j-1}\big]. \quad (10)$$

(Here $\hat{a}^k_{nm} = (\hat{a}^k_{nm})_{ij}$ for all k.)

Neumann or Dirichlet boundary conditions can be immediately taken into account by well-known methods [9–11, 1] in the coefficients of operators (8), (10), retaining second-order accuracy. In some cases special boundary conditions are required near $v_0 = v_{0,\min}$. For example, Neumann or Dirichlet boundary conditions are usually not adequate at $v_0 = v_{0,\min}$ for modelling alpha particles in thermonuclear experiments. Zero flux at $v_0 = v_{0,\min}$ leads to a buildup of alpha particles with low energies, whereas in reality thermalized alpha particles (helium ash) would be removed from the plasma by processes which are difficult to model with kinetic codes. Setting the distribution function at $v_0 = v_{0,\min}$ to be zero would give too few alpha particles at $v_0 = v_{0,\min}$. The introduction of losses near $v_0 = v_{0,\min}$ would require knowledge of a loss coefficient. A very different approach was found to be adequate for the description of alpha-particle behaviour in experiments. This involves a boundary condition

$$\frac{1}{\sqrt{g}}\frac{\partial}{\partial x^n}\left[\sum_{m=1}^{3}\left(A_{1m}\frac{\partial u}{\partial x^m}\right) + B_1 u\right]\Bigg|_{v_0=v_{0,\mathrm{ash}}} = \begin{cases} \frac{1}{\sqrt{g}}\frac{\partial}{\partial x^n}\left[B_1 f^0_\alpha\right]\big|_{v_0=v_{0,\mathrm{ash}}}, & B_1 > 0, \\ 0, & B_1 \leq 0, \end{cases} \quad (11)$$

where $v_{0,\mathrm{ash}}$ is the speed at which particles are considered as lost to ash, $v_{0,\mathrm{ash}} > 0$. The whole problem is then formulated in $v_0 \in [v_{0,\mathrm{ash}}, \infty)$. Equation (11) allows particles to leave the solution domain and become "helium ash" $v_0 < v_{0,\mathrm{ash}}$ due to Coulomb friction, but it does not allow a flux into the solution domain from the cold particles.

Equation (7) with $\eta_n = 0$ can be used to approximate Eq. (11). Forward differencing allows the solution of the appropriate system of linear algebraic equations.

3.1. *Treatment of Separatrices in the Difference Operators*

This section is relevant to the particular case being considered which necessitates the use of a separatrix and can be ignored if internal boundaries are not of interest.

More challenging is the inclusion in the difference operators of additional conditions at an internal separatrix. For a solution of this problem we shall use the idea of the method of extending the grid outside the area [12]. We shall continue the grid from each area near

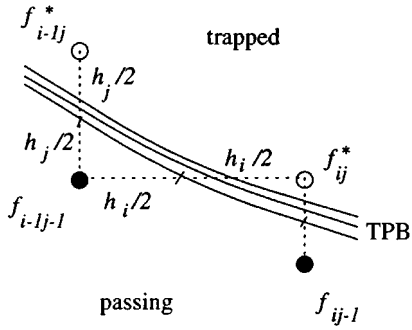

FIG. 4. An example of the extension of a grid outside of a passing particles region in a plane of variables (γ_0, θ_0). The ghost nodes are represented by empty circles.

a separatrix across the separatrix (see Fig. 4). We shall name new nodes as "ghost nodes" and designate values of the required function at these nodes by $f^*_k, k = 1, \ldots, n_g$, where n_g is the total number of introduced nodes. We shall require that n_g is greater than or equal to the number of conditions that have to be applied at the separatrix. With the help of ghost nodes and the initial grid nodes we approximate these conditions to a required order of accuracy. Let the number of used nodes of an initial grid be n_r, then the approximation of "conjunction" conditions, which connect initial and ghost nodes, can be written in the general form

$$\begin{aligned}
a_{11} f^*_1 + a_{12} f^*_2 + \cdots + a_{1n_g} f^*_{n_g} &= b_{11} f_1 + b_{12} f_2 + \cdots + b_{1n_r} f_{n_r} \\
a_{21} f^*_1 + a_{22} f^*_2 + \cdots + a_{2n_g} f^*_{n_g} &= b_{21} f_1 + b_{22} f_2 + \cdots + b_{2n_r} f_{n_r} \\
a_{31} f^*_1 + a_{32} f^*_2 + \cdots + a_{3n_g} f^*_{n_g} &= b_{31} f_1 + b_{32} f_2 + \cdots + b_{3n_r} f_{n_r}. \\
&\cdots
\end{aligned}$$

If the number of ghost nodes n_g is greater than the number of equations, we introduce additional relations to make the number of equations equal to n_g. The arbitrariness in compiling additional relations can be used, for example, to simplify the equations, improve the accuracy of the approximation, or ensure some behaviour required near the separatrix. The resulting system of linear algebraic equations can be written in the matrix form

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n_g} \\ a_{21} & a_{22} & \cdots & a_{2n_g} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n_g 2} & \cdots & a_{n_g n_g} \end{pmatrix} \begin{pmatrix} f^*_1 \\ f^*_2 \\ \vdots \\ f^*_{n_g} \end{pmatrix} = \begin{pmatrix} b_{11} \\ b_{21} \\ \vdots \\ b_{n_g 1} \end{pmatrix} f_1 + \cdots + \begin{pmatrix} b_{1n_r} \\ b_{2n_r} \\ \vdots \\ b_{n_g n_r} \end{pmatrix} f_{n_r}. \qquad (12)$$

By solving this system, we find a representation of grid function values at ghost nodes using values at nodes of the initial grid

$$f^*_k = \sum_{i=1}^{n_r} c_{ki} f_i, \quad k = 1, \ldots, n_g.$$

Now, substituting this expansion into the difference operator in place of values f^*_k, which occur near the separatrix, we arrive at an approximation which takes into account the

conjunction conditions and contains values of the grid function from nodes of the initial grid only.

It is important to note that, generally speaking, for each difference operator its own system (12) can be composed (e.g., for 3D kinetic problems in tokamaks, the trapped/passing boundary condition is discussed in [4]).

4. DIFFERENCE SCHEMES FOR KINETIC PROBLEMS

We shall consider a problem with a time-dependent and unknown function-dependent differential operator $\mathcal{L}$, cf. Eqs. (1)–(3),

$$\begin{cases} \dfrac{\partial u}{\partial t} = \mathcal{L}(t,u)[u] & \text{in } D \times (0, \mathtt{T}], \\ u = \varphi & \text{in } D \cup \Gamma_D \text{ at } t = 0, \\ l(t,u) = \psi & \text{on } \Gamma_D \times [0, \mathtt{T}]. \end{cases} \tag{13}$$

Here D is the range of phase variables, Γ_D is its boundary, and $0 \le t \le \mathtt{T}$. We shall represent operator $\mathcal{L}(t,u)$ as a sum of operators,

$$\mathcal{L}(t,u) = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3, \tag{14}$$

where

$$\begin{aligned} \mathcal{L}_1 &= \mu_1\mathcal{L}_{11} + \mu_2\mathcal{L}_{22} + \mathcal{L}_{12} + \mathcal{L}_{21} \\ \mathcal{L}_2 &= (1-\mu_2)\mathcal{L}_{22} + \mu_3\mathcal{L}_{33} + \mathcal{L}_{23} + \mathcal{L}_{32} \\ \mathcal{L}_3 &= (1-\mu_1)\mathcal{L}_{11} + (1-\mu_3)\mathcal{L}_{33} + \mathcal{L}_{13} + \mathcal{L}_{31}; \end{aligned}$$

$\mu_k \in [0,1]$ are weights.

Assume that difference approximations Λ_k, Λ_{nm} of operators $\mathcal{L}_k$, $\mathcal{L}_{nm}$, taking into account boundary conditions on the exterior boundaries and separatrices, are known.

For an approximate solution of problem (13) in time interval $t_{n-1} \le t \le t_{n+1}$ we shall use a two-cycle six-step splitting scheme,

$$\begin{aligned} \mathcal{B}\frac{f^{n-2/3} - f^{n-1}}{\tau} &= \Lambda_1^n\left(\lambda_1 f^{n-2/3} + (1-\lambda_1) f^{n-1}\right) \\ \mathcal{B}\frac{f^{n-1/3} - f^{n-2/3}}{\tau} &= \Lambda_2^n\left(\lambda_2 f^{n-1/3} + (1-\lambda_2) f^{n-2/3}\right) \\ \mathcal{B}\frac{f^{n} - f^{n-1/3}}{\tau} &= \Lambda_3^n\left(\lambda_3 f^{n} + (1-\lambda_3) f^{n-1/3}\right) \\ \mathcal{B}\frac{f^{n+1/3} - f^{n}}{\tau} &= \Lambda_3^n\left(\lambda_3 f^{n+1/3} + (1-\lambda_3) f^{n}\right) \\ \mathcal{B}\frac{f^{n+2/3} - f^{n+1/3}}{\tau} &= \Lambda_2^n\left(\lambda_2 f^{n+2/3} + (1-\lambda_2) f^{n+1/3}\right) \\ \mathcal{B}\frac{f^{n+1} - f^{n+2/3}}{\tau} &= \Lambda_1^n\left(\lambda_1 f^{n+1} + (1-\lambda_1) f^{n+2/3}\right) \end{aligned} \tag{15}$$

$$\Lambda_k^n = \Lambda_k(t_n, \tilde{f}^n), \quad k = 1, 2, 3,$$

with λ_k implicitness weights, $\tau = t_n - t_{n-1}$, and $\tilde{f}^n$, which affects the collisional coefficients in Λ_k^n, from the explicit step

$$\tilde{f}^n = f^{n-1} + \tau \Lambda\left(t_{n-1},\, f^{n-1}\right) f^{n-1}.$$

The system (15) can be rewritten in the more convenient form

$$\begin{aligned}
\left(\frac{1}{\tau}\mathcal{B} - \lambda_1 \Lambda_1^n\right) f^{n-2/3} &= \left(\frac{1}{\tau}\mathcal{B} + (1-\lambda_1)\Lambda_1^n\right) f^{n-1} \\
\left(\frac{1}{\tau}\mathcal{B} - \lambda_2 \Lambda_2^n\right) f^{n-1/3} &= \left(\frac{1}{\tau}\mathcal{B} + (1-\lambda_2)\Lambda_2^n\right) f^{n-2/3} \\
&\vdots \\
\left(\frac{1}{\tau}\mathcal{B} - \lambda_1 \Lambda_1^n\right) f^{n+1} &= \left(\frac{1}{\tau}\mathcal{B} + (1-\lambda_1)\Lambda_1^n\right) f^{n+2/3}.
\end{aligned} \tag{16}$$

A suitable choice for the grid function on the nth layer is $(f^{n+1} + f^{n-1})/2$.

The scheme (16) is conservative and approximate to second order over time and space if the operators $\mathcal{B}$ and Λ_k are conservative, have the second order of approximation on a spatial variable, and all $\lambda_k = 0.5$. Replacement of an explicit step, for example on $\tilde{f}^n = f^{n-1}$ is possible. It will result in a scheme of first-order approximation over τ, but will improve the stability.

General ideas of the splitting algorithms are discussed in, for example, Refs. [9, 10]. One of the new features in the proposed difference scheme is the inversion of a two-dimensional operator on each step, as

$$\begin{aligned}
\Lambda_1 &= \mu_1 \Lambda_{11} + \mu_2 \Lambda_{22} + \Lambda_{12} + \Lambda_{21} \\
\Lambda_2 &= (1-\mu_2)\Lambda_{22} + \mu_3 \Lambda_{33} + \Lambda_{23} + \Lambda_{32} \\
\Lambda_3 &= (1-\mu_1)\Lambda_{11} + (1-\mu_3)\Lambda_{33} + \Lambda_{13} + \Lambda_{31}.
\end{aligned}$$

The simultaneous inversion over two variables can be performed using, for example, Gaussian elimination for a sparse matrix. The required number of operations on, for example, the first step is $O(N_{x^1} N_{x^2}^2 N_{x^3})$, where N_{x^k} is the number of nodes of the grid in the kth direction and N_{x^2} is the bandwidth of the matrix. One of the basic advantages of such an approach is the possibility of implicit use in the scheme of operators with mixed derivatives, which makes the difference scheme more stable than with an explicit occurrence of mixed derivatives.

It is necessary to note that the decomposition of an operator in more simple operators can have drawbacks. For example, the two-dimensional operators may not retain the elliptic character of an initial three-dimensional operator. However, decomposition is necessary, as modern computer facilities do not yet allow us to carry out for large grids an inversion of an operator over three phase variables at once.

Previous work has investigated the properties of difference scheme (16) for positively semi-definite operators Λ_k in the Hilbert space of grid functions $L_{2,h}$ [10]. However, in the

kinetic equation the operators Λ_k can change sign because of the presence of first-order derivatives. Therefore, the standard results are not applicable. Also, from a physical point of view, for the problems under consideration, the properties of the numerical solution in Banach space $L_{1,h}$ are of interest, as, for example, $\| f \|_{L_{1,h}}$ is the difference analogue of particle density. Despite the complexities mentioned, for some classes of kinetic problems it has been possible to prove theorems on the existence and uniqueness of a solution of the difference problem with the help of some advancements to existing methods [9, 1]. It has also been possible to prove theorems about the stability and convergence of the difference scheme in Banach space $L_{1,h}$ and about the preservation of sign of the solution of the difference problem (e.g. required for a distribution function which should never be negative). The results are summarised in the following sections.

5. EXISTENCE AND UNIQUENESS OF THE SOLUTION OF THE DIFFERENCE PROBLEM

All equations in the system of Eqs. (16) have the same structure; therefore it is sufficient to investigate the existence and uniqueness of the solution to one of them, for example, the first,

$$\left(\frac{1}{\tau}\mathcal{B} - \lambda_1 \Lambda_1^n\right) f^{n-2/3} = \left(\frac{1}{\tau}\mathcal{B} + (1-\lambda_1)\Lambda_1^n\right) f^{n-1}, \tag{17}$$

$$\Lambda_1 = \mu_1 \Lambda_{11} + \mu_2 \Lambda_{22} + \Lambda_{12} + \Lambda_{21}.$$

To simplify we shall use the notation

$$\hat{f} \equiv f^{n-2/3}, \quad f \equiv f^{n-1}, \quad \lambda \equiv \lambda_1, \quad \Lambda \equiv \Lambda_1^n.$$

Then formula (17) becomes

$$\left(\frac{1}{\tau}\mathcal{B} - \lambda\Lambda\right)\hat{f} = \left(\frac{1}{\tau}\mathcal{B} + (1-\lambda)\Lambda\right) f. \tag{18}$$

For operator $\mathcal{B}$ we consider the operator

$$(\mathcal{B} f)_{ij} \equiv f_{ij} + \frac{e}{c_{ij}}(4 f_{ij} - f_{i-1j} - f_{i+1j} - f_{ij-1} - f_{ij+1}), \tag{19}$$

where e is a nonnegative constant factor which has the same dimensions as c_{ij}. The unit operator $\mathcal{B} \equiv \mathcal{I}$ is recovered for $e = 0$. With the help of a Taylor expansion around the point (i, j) it is possible to show that, if the function u has continuous derivatives to the required order, then $\mathcal{B}(\hat{f} - f)/\tau$ approximates derivative $\partial u/\partial t$ to first order over time and to second order over space (for a nonuniform grid the second order applies at some point that need not coincide with a grid point).

The following theorems of existence and uniqueness of the solution of the system of linear algebraic equations (18) are valid.

THEOREM 1. *Let the coefficients of the problem* (13) *satisfy the inequalities*

$$\begin{aligned}
&\frac{\mu_1}{\overline{h}_{x^1,i}}\frac{U_{1,i-1/2}}{h_{x^1,i}}V_{1,i-1} \geq \frac{1}{2}\left(\frac{\hat{a}^8_{12,ij}}{\overline{h}_{x^1,i}}+\frac{\hat{a}^6_{21,ij}}{\overline{h}_{x^2,j}}\right), \quad i=1,\ldots,N_{x^1}+1;\ j=1,\ldots,N_{x^2},\\
&\frac{\mu_1}{\overline{h}_{x^1,i}}\frac{U_{1,i+1/2}}{h_{x^1,i+1}}V_{1,i+1} \geq \frac{1}{2}\left(\frac{\hat{a}^2_{12,ij}}{\overline{h}_{x^1,i}}+\frac{\hat{a}^4_{21,ij}}{\overline{h}_{x^2,j}}\right), \quad i=0,\ldots,N_{x^1};\ j=1,\ldots,N_{x^2},\\
&\frac{\mu_2}{\overline{h}_{x^2,j}}\frac{U_{2,j-1/2}}{h_{x^2,j}}V_{2,j-1} \geq \frac{1}{2}\left(\frac{\hat{a}^6_{12,ij}}{\overline{h}_{x^1,i}}+\frac{\hat{a}^8_{21,ij}}{\overline{h}_{x^2,j}}\right), \quad i=1,\ldots,N_{x^1};\ j=1,\ldots,N_{x^2}+1,\\
&\frac{\mu_2}{\overline{h}_{x^2,j}}\frac{U_{2,j+1/2}}{h_{x^2,j+1}}V_{2,j+1} \geq \frac{1}{2}\left(\frac{\hat{a}^4_{12,ij}}{\overline{h}_{x^1,i}}+\frac{\hat{a}^2_{21,ij}}{\overline{h}_{x^2,j}}\right), \quad i=1,\ldots,N_{x^1};\ j=0,\ldots,N_{x^2},
\end{aligned} \tag{20}$$

and

$$\begin{aligned}
&\frac{\lambda}{c_{ij}}\left[\frac{\mu_1}{\overline{h}_{x^1,i}}\left(\frac{U_{1,i+1/2}}{h_{x^1,i+1}}(V_{1,i+1}-V_{1,i})-\frac{U_{1,i-1/2}}{h_{x^1,i}}(V_{1,i}-V_{1,i-1})\right)\right.\\
&\left.+\frac{\mu_2}{\overline{h}_{x^2,j}}\left(\frac{U_{2,j+1/2}}{h_{x^2,j+1}}(V_{2,j+1}-V_{2,j})-\frac{U_{2,j-1/2}}{h_{x^2,j}}(V_{2,j}-V_{2,j-1})\right)\right]\leq 0,\\
&\qquad\qquad i=1,\ldots,N_{x^1};\ j=1,\ldots,N_{x^2};
\end{aligned} \tag{21}$$

then the set of Eqs. (18) *with the unit operator* $\mathcal{B}\equiv\mathcal{I}$ *has a unique solution for any* $\tau>0$.

The conditions (20) mean that second-order derivative coefficients $\hat{a}_{nn}$ dominate the mixed derivative coefficients $\hat{a}_{nm}$, $n\neq m$. In general, if the conditions (20) are not valid, this theorem of existence and uniqueness can still be proved, but with a restriction on the time step. The proof of Theorem 1 will be done simultaneously with that of Theorem 2.

THEOREM 2. *Let the time step* τ *satisfy the conditions*

$$\begin{aligned}
&\frac{1}{\tau}\geq -\frac{\lambda}{e}\left(\frac{\mu_1}{\overline{h}_{x^1,i}}\frac{U_{1,i-1/2}}{h_{x^1,i}}V_{1,i-1}-\frac{1}{2}\left(\frac{\hat{a}^8_{12,ij}}{\overline{h}_{x^1,i}}+\frac{\hat{a}^6_{21,ij}}{\overline{h}_{x^2,j}}\right)\right),\\
&\qquad\qquad i=1,\ldots,N_{x^1}+1;\ j=1,\ldots,N_{x^2},\\
&\frac{1}{\tau}\geq -\frac{\lambda}{e}\left(\frac{\mu_1}{\overline{h}_{x^1,i}}\frac{U_{1,i+1/2}}{h_{x^1,i+1}}V_{1,i+1}-\frac{1}{2}\left(\frac{\hat{a}^2_{12,ij}}{\overline{h}_{x^1,i}}+\frac{\hat{a}^4_{21,ij}}{\overline{h}_{x^2,j}}\right)\right),\\
&\qquad\qquad i=0,\ldots,N_{x^1};\ j=1,\ldots,N_{x^2},\\
&\frac{1}{\tau}\geq -\frac{\lambda}{e}\left(\frac{\mu_2}{\overline{h}_{x^2,j}}\frac{U_{2,j-1/2}}{h_{x^2,j}}V_{2,j-1}-\frac{1}{2}\left(\frac{\hat{a}^6_{12,ij}}{\overline{h}_{x^1,i}}+\frac{\hat{a}^8_{21,ij}}{\overline{h}_{x^2,j}}\right)\right),\\
&\qquad\qquad i=1,\ldots,N_{x^1};\ j=1,\ldots,N_{x^2}+1,\\
&\frac{1}{\tau}\geq -\frac{\lambda}{e}\left(\frac{\mu_2}{\overline{h}_{x^2,j}}\frac{U_{2,j+1/2}}{h_{x^2,j+1}}V_{2,j+1}-\frac{1}{2}\left(\frac{\hat{a}^4_{12,ij}}{\overline{h}_{x^1,i}}+\frac{\hat{a}^2_{21,ij}}{\overline{h}_{x^2,j}}\right)\right),\\
&\qquad\qquad i=1,\ldots,N_{x^1};\ j=0,\ldots,N_{x^2},
\end{aligned} \tag{22}$$

and

$$\frac{1}{\tau} > \frac{\lambda}{c_{ij}}\left[\frac{\mu_1}{\overline{h}_{x^1,i}}\left(\frac{U_{1,i+1/2}}{h_{x^1,i+1}}(V_{1,i+1}-V_{1,i})-\frac{U_{1,i-1/2}}{h_{x^1,i}}(V_{1,i}-V_{1,i-1})\right)\right.$$
$$\left.+\frac{\mu_2}{\overline{h}_{x^2,j}}\left(\frac{U_{2,j+1/2}}{h_{x^2,j+1}}(V_{2,j+1}-V_{2,j})-\frac{U_{2,j-1/2}}{h_{x^2,j}}(V_{2,j}-V_{2,j-1})\right)\right],$$
$$i=1,\ldots,N_{x^1};\ j=1,\ldots,N_{x^2}, \quad (23)$$

then the set of Eqs. (18) *with operator* $\mathcal{B}$, *defined by* (19) *with* $e>0$, *has a unique solution.*

Before passing to a proof of Theorems 1 and 2 we make four remarks.

Remark 1. The theorems are formulated for the case $\eta_n = 1$. However, they are easily generalized for the case $\eta_n \neq 1$ (see Eq. (4)), and, if expression (7) is used to approximate the first derivatives, then less rigid restrictions on τ appear in Theorem 2.

Remark 2. Clearly, for any bounded coefficients of the equation, it is always possible to specify τ such that inequalities (22) and (23) are valid. If the right-hand side of any inequality is negative, that inequality should be excluded from consideration, as it does not impose restrictions on τ.

Remark 3. In the "worst" case, magnitudes in the right-hand side of (22) have order h^{-2}; nevertheless one may expect that the restriction on τ is weaker than in, e.g. explicit schemes, as is apparent from consideration of properties at every point of the grid. This supposition proves to be true by calculations.

Remark 4. As will be seen from the proof of the theorems, the "directed" approximation of mixed derivatives offered in the present work (Eq. (10)), gives "least" restriction on τ when compared with standard approximations.

The proofs of Theorems 1 and 2 are now done simultaneously. We shall consider a case when the boundary conditions at a separatrix change neither the approximation (in terms of number and place of grid points used) nor the properties of operator coefficients. (In general, conditions (20)–(23) can vary and the operator $\mathcal{B}$ may need to be changed.)

Proof. The set of Eqs. (18) can be written in the matrix form

$$T\hat{f} = Sf.$$

The matrices $T \equiv (\mathcal{B}/\tau - \lambda\Lambda)$ and $S \equiv (\mathcal{B}/\tau + (1-\lambda)\Lambda)$ have a banded structure; the nonzero elements, for a case when the boundary conditions at a separatrix do not change patterns of operators, fall only on three diagonal bands, each with a width of not more than three elements

$$\begin{pmatrix}
t_{11} & t_{12} & 0 & \cdots & t_{1N+1} & t_{1N+2} & 0 & \cdots & 0 & 0 & 0 \\
t_{21} & t_{22} & t_{23} & \cdots & t_{2N+1} & t_{2N+2} & t_{2N+3} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \ddots & \cdots & \vdots & \vdots & \ddots & \cdots & \vdots & \vdots & \ddots \\
\cdots & t_{kk-N-1} & t_{kk-N} & t_{kk-N+1}\cdots & t_{kk-1} & t_{kk} & t_{kk+1}\cdots & t_{kk+N-1} & t_{kk+N} & t_{kk+N+1} & \cdots \\
\cdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \cdots \\
\cdots & \cdots & 0 & 0 & 0\cdots & 0 & t_{PP-N-1} & t_{PP-N}\cdots & 0 & t_{PP-1} & t_{PP}
\end{pmatrix}.$$

Here $P = N_{x^1} N_{x^2}$ is the total number of points of a grid $\omega_1 \times \omega_2$ and N is the number of points over one of the directions (the band width is $3N$). For now let $N = N_{x^2}$. Values of indexes in t_{kl} are calculated using i, j as: $k = (i-1)N_{x^2} + j$, $i = 1, \ldots, N_{x^1}$, $j = 1, \ldots, N_{x^2}$; $l = (i'-1)N_{x^2} + j'$, where i', j' are nodes, included in the pattern of the operator Λ at point i, j.

According to the approximations (8), (10) of the differential operators, the elements of a matrix T are

$$t_{kk} = \frac{1}{\tau} + \frac{4e}{\tau c_{ij}} + \frac{\lambda}{c_{ij}} \left[\frac{\mu_1}{\overline{h}_{x^1,i}} \left(\frac{U_{1,i+1/2}}{h_{x^1,i+1}} + \frac{U_{1,i-1/2}}{h_{x^1,i}} \right) V_{1,i} \right.$$

$$\left. + \frac{\mu_2}{\overline{h}_{x^2,j}} \left(\frac{U_{2,j+1/2}}{h_{x^2,j+1}} + \frac{U_{2,j-1/2}}{h_{x^2,j}} \right) V_{2,j} - \frac{1}{2} \left(\frac{\hat{a}^5_{12,ij}}{\overline{h}_{x^1,i}} + \frac{\hat{a}^5_{21,ij}}{\overline{h}_{x^2,j}} \right) \right]$$

$$t_{kk-1} = -\frac{e}{\tau c_{ij}} - \frac{\lambda}{c_{ij}} \left[\frac{\mu_1}{\overline{h}_{x^1,i}} \frac{U_{1,i-1/2}}{h_{x^1,i}} V_{1,i-1} - \frac{1}{2} \left(\frac{\hat{a}^8_{12,ij}}{\overline{h}_{x^1,i}} + \frac{\hat{a}^6_{21,ij}}{\overline{h}_{x^2,j}} \right) \right]$$

$$t_{kk+1} = -\frac{e}{\tau c_{ij}} - \frac{\lambda}{c_{ij}} \left[\frac{\mu_1}{\overline{h}_{x^1,i}} \frac{U_{1,i+1/2}}{h_{x^1,i}} V_{1,i+1} - \frac{1}{2} \left(\frac{\hat{a}^2_{12,ij}}{\overline{h}_{x^1,i}} + \frac{\hat{a}^4_{21,ij}}{\overline{h}_{x^2,j}} \right) \right]$$

$$t_{kk-N} = -\frac{e}{\tau c_{ij}} - \frac{\lambda}{c_{ij}} \left[\frac{\mu_2}{\overline{h}_{x^2,j}} \frac{U_{2,j-1/2}}{h_{x^2,j}} V_{2,j-1} - \frac{1}{2} \left(\frac{\hat{a}^6_{12,ij}}{\overline{h}_{x^1,i}} + \frac{\hat{a}^8_{21,ij}}{\overline{h}_{x^2,j}} \right) \right]$$

$$t_{kk+N} = -\frac{e}{\tau c_{ij}} - \frac{\lambda}{c_{ij}} \left[\frac{\mu_2}{\overline{h}_{x^2,j}} \frac{U_{2,j+1/2}}{h_{x^2,j}} V_{2,j+1} - \frac{1}{2} \left(\frac{\hat{a}^4_{12,ij}}{\overline{h}_{x^1,i}} + \frac{\hat{a}^2_{21,ij}}{\overline{h}_{x^2,j}} \right) \right]$$

$$t_{kk-N-1} = -\frac{\lambda}{2c_{ij}} \left[\frac{\hat{a}^9_{12,ij}}{\overline{h}_{x^1,i}} + \frac{\hat{a}^9_{21,ij}}{\overline{h}_{x^2,j}} \right]$$

$$t_{kk-N+1} = -\frac{\lambda}{2c_{ij}} \left[\frac{\hat{a}^3_{12,ij}}{\overline{h}_{x^1,i}} + \frac{\hat{a}^7_{21,ij}}{\overline{h}_{x^2,j}} \right]$$

$$t_{kk+N-1} = -\frac{\lambda}{2c_{ij}} \left[\frac{\hat{a}^7_{12,ij}}{\overline{h}_{x^1,i}} + \frac{\hat{a}^3_{21,ij}}{\overline{h}_{x^2,j}} \right]$$

$$t_{kk+N+1} = -\frac{\lambda}{2c_{ij}} \left[\frac{\hat{a}^1_{12,ij}}{\overline{h}_{x^1,i}} + \frac{\hat{a}^1_{21,ij}}{\overline{h}_{x^2,j}} \right].$$

Matrix S has the same structure as matrix T, with elements s_{kl} differing from t_{kl} only in that before the square brackets the sign is opposite and the factor λ changes to $(1-\lambda)$.

We shall show that the matrix T is an M-matrix. A matrix $A = (a_{ij})$ is an M-matrix, if it is nondegenerate, $a_{ij} \le 0$ for all $i \ne j$ and $A^{-1} = (a^{-1}_{ij})$ is nonnegative, that is $a^{-1}_{ij} \ge 0$ [13]. Therefore, if T is an M-matrix, it is nondegenerate. Then for any right-hand side F there is a unique solution of the equation $T\hat{f} = F$, and thus also the set of equations (18).

To prove that T is an M-matrix it is enough to show that T has nonpositive nondiagonal elements and has strict diagonal dominance [13].

The nondiagonal elements of matrix T are $t_{kk-1}, t_{kk+1}, t_{kk-N}, t_{kk+N}, t_{kk-N-1}, t_{kk-N+1}, t_{kk+N-1}, t_{kk+N+1}$. The nonpositivity of $t_{kk-1}, t_{kk+1}, t_{kk-N}, t_{kk+N}$ follows from conditions (20) or (22), and nonpositivity of $t_{kk-N-1}, t_{kk-N+1}, t_{kk+N-1}, t_{kk+N+1}$ from the method of approximating the mixed derivatives, so that the first requirement for T to be an M-matrix is satisfied.

The final requirement is to check the elements of T for strict diagonal dominance, that is

$$|t_{kk}| > \sum_{\substack{l=1 \\ l\neq k}}^{P} |t_{kl}|, \quad k = 1, \ldots, P.$$

From (20) or (22)

$$\sum_{\substack{l=1 \\ l\neq k}}^{P} |t_{kl}| = \sum_{\substack{l=1 \\ l\neq k}}^{P} -t_{kl} = \frac{4e}{\tau c_{ij}} + \frac{\lambda}{c_{ij}} \left[\frac{\mu_1}{\overline{h}_{x^1,i}} \left(\frac{U_{1,i+1/2}}{h_{x^1,i+1}} V_{1,i+1} + \frac{U_{1,i-1/2}}{h_{x^1,i}} V_{1,i-1} \right) \right.$$
$$+ \frac{\mu_2}{\overline{h}_{x^2,j}} \left(\frac{U_{2,j+1/2}}{h_{x^2,j+1}} V_{2,j+1} + \frac{U_{2,j-1/2}}{h_{x^2,j}} V_{2,j-1} \right)$$
$$\left. - \frac{1}{2\overline{h}_{x^1,i}} \sum_{\substack{p=1 \\ p\neq 5}}^{9} (-1)^p \hat{a}^p_{12,ij} - \frac{1}{2\overline{h}_{x^2,j}} \sum_{\substack{p=1 \\ p\neq 5}}^{9} (-1)^p \hat{a}^p_{21,ij} \right].$$

Taking into account (21) or (23) and that

$$\sum_{\substack{p=1 \\ p\neq 5}}^{9} (-1)^p \hat{a}^p_{nm,ij} = \hat{a}^5_{nm,ij},$$

we obtain

$$\sum_{\substack{l=1 \\ l\neq k}}^{P} |t_{kl}| < \frac{1}{\tau} + \frac{4e}{\tau c_{ij}} + \frac{\lambda}{c_{ij}} \left[\frac{\mu_1}{\overline{h}_{x^1,i}} \left(\frac{U_{1,i+1/2}}{h_{x^1,i+1}} V_{1,i} + \frac{U_{1,i-1/2}}{h_{x^1,i}} V_{1,i} \right) \right.$$
$$+ \frac{\mu_2}{\overline{h}_{x^2,j}} \left(\frac{U_{2,j+1/2}}{h_{x^2,j+1}} V_{2,j} + \frac{U_{2,j-1/2}}{h_{x^2,j}} V_{2,j} \right)$$
$$\left. - \frac{1}{2\overline{h}_{x^1,i}} \hat{a}^5_{12,ij} - \frac{1}{2\overline{h}_{x^2,j}} \hat{a}^5_{21,ij} \right] = t_{kk} = |t_{kk}|.$$

Thus, T is an M-matrix and Theorems 1 and 2 are proved.

From Theorems 1 and 2, existence and uniqueness of the solution of the difference problem (16) follows. In a nonlinear case, when the coefficients of the equation depend on the function being solved for, the time step can become dependent on the number of the time layer (as it is probably necessary to select τ for each $\tilde{f}$). Therefore, for nonlinear problems this method of proof does not guarantee that it is possible to reach a given time with a finite number of steps. Thus in a nonlinear case, existence and uniqueness can only be proven for a small time interval using this method.

6. STABILITY AND CONVERGENCE

First, we shall prove the following theorem.

THEOREM 3. *Let T be an M-matrix, $\hat{f}$ be the solution of the equation $T\hat{f} = F_1$, and $\tilde{f}$ be the solution of the equation $T\tilde{f} = F_2$, with $|F_1| \le F_2$ valid for all the vector components. Then $|\hat{f}| \le \tilde{f}$.*

Proof. We shall consider a vector $v = \hat{f} + \tilde{f}$. It is the solution of the equation $Tv = V$, where $V = F_1 + F_2$. The vector V has nonnegative components,

$$V = F_1 + F_2 \ge F_2 - |F_1| \ge 0.$$

Further, as T is an M-matrix, it is monotonic [13]; that is, $Tv \ge 0$ implies $v \ge 0$. Then $-\tilde{f} \le \hat{f}$.

We shall consider $w = \hat{f} - \tilde{f}$. It is the solution of the equation $Tw = W$, where

$$W = F_1 - F_2 \le |F_1| - F_2 \le 0.$$

We similarly conclude that $w \le 0$ and therefore $\hat{f} \le \tilde{f}$. Then $|\hat{f}| \le \tilde{f}$, proving Theorem 3.

Next we consider a Banach space of grid functions $L_{1,h}$ with a norm

$$\|f\| = \sum_{i=1}^{N_{x^1}} \sum_{j=1}^{N_{x^2}} \sum_{k=1}^{N_{x^3}} |f_{ijk}| c_{ijk} \overline{h}_{x^1,i} \overline{h}_{x^2,j} \overline{h}_{x^3,k}. \tag{24}$$

In kinetic problems this may represent an integral over velocity space coordinates to give the density of particles in geometric space and therefore, for this particular norm, a study of stability and convergence properties is of importance.

THEOREM 4. *Let the coefficients of an initial problem* (13) *satisfy the inequalities* (20), (21). *Then in the Banach space of grid functions with norm* (24) *the scheme* (16) *with $\mathcal{B} = \mathcal{I}$ is absolutely stable for $\lambda_k = 1$, $k = 1, 2, 3$, and conditionally stable for $0 \le \lambda_k < 1$, $k = 1, 2, 3$. Also, if the exact solution u of a problem* (13) *in each of the areas divided by the separatrix has continuous derivatives and bounded derivatives of the required order, then the scheme* (16) *converges and has accuracy*

$$\|z^{n+1}\| = O(\tau^p + h^2), \quad n = 1, 3, 5, \ldots,$$

where $h = \max_{k=1,2,3} \max_{i=1,\ldots,N_{x^k}} h_{x^k,i}$ $p = 2$ for $\lambda_k = 1/2$, $k = 1, 2, 3$; $p = 1$ otherwise.

Proof. The error of solution of a difference problem is

$$z^n = f^n - u^n. \tag{25}$$

We shall note that at $n = 0$ (i.e., $t = 0$), and, for all n, at boundary points of a grid for a Dirichlet problem, $z^n = 0$.

We shall consider the first equation from (16). By substituting (25) in it with the appropriate time index, we obtain

$$\left(\left(\frac{1}{\tau}\mathcal{I} - \lambda\Lambda\right)\hat{z}\right)_{ijk} = \left(\left(\frac{1}{\tau}\mathcal{I} + (1-\lambda)\Lambda\right)z\right)_{ijk} + \psi^n_{ijk}, \tag{26}$$

where ψ_{ijk}^n is the error in approximating the first equation in a decomposed differential problem by use of the difference equation. In a proof of stability it is possible to consider ψ_{ijk}^n as some known right-hand side.

As well as Eq. (26), we shall consider the equation

$$\left(\left(\frac{1}{\tau}\mathcal{I}-\lambda\Lambda\right)\hat{w}\right)_{ijk}=\left(\left(\frac{1}{\tau}\mathcal{I}+(1-\lambda)\Lambda\right)|z|\right)_{ijk}+\left|\psi_{ijk}^n\right|. \tag{27}$$

If the scheme is not purely implicit, that is $\lambda<1$, it is necessary to impose a restriction on τ. We shall require that $1/\tau$ is not less than the maximum of the moduli of the diagonal coefficients of matrix $(1-\lambda)\Lambda$. In this case the right-hand side (27) will be nonnegative, as all elements of matrix $(\mathcal{I}/\tau+(1-\lambda)\Lambda)$ will be nonnegative. For the implicit scheme the restriction on τ is not required.

From Theorem 3, taking into account that $(\mathcal{I}/\tau-\lambda\Lambda)$ is an M-matrix, we find

$$0\le|z_{ijk}|\le w_{ijk}. \tag{28}$$

We sum Eqs. (27) with weight $c_{ijk}\overline{h}_{x^1,i}\overline{h}_{x^2,j}\overline{h}_{x^3,k}$. Since operator Λ is conservative, (a) the $\lambda\Lambda$ term on the left-hand side sums to zero for Neumann boundary conditions or positive terms for Dirichlet boundary conditions and (b) the $(1-\lambda)\Lambda$ term on the right-hand side sums to zero or results in nonpositive components. This gives

$$\sum_{i=1}^{N_{x^1}}\sum_{j=1}^{N_{x^2}}\sum_{k=1}^{N_{x^3}}\hat{w}_{ijk}c_{ijk}\overline{h}_{x^1,i}\overline{h}_{x^2,j}\overline{h}_{x^3,k}\le\|z\|+\tau\|\psi^n\|.$$

Then, using (28),

$$\|\hat{z}\|\le\|z\|+\tau\|\psi^n\|. \tag{29}$$

The inequality (29) means the first equation in (16) is stable. The stability of the remaining equations follows. Substituting an inequality of the form (29) in the inequality for the last equation of (16), we have

$$\|z^{n+1}\|\le\|z^{n-1}\|+\tau\sum_{l=1}^{6}\left\|\psi_l^n\right\|,\quad n=1,3,5,\ldots, \tag{30}$$

where ψ_l^n is the error in approximating the lth equation in a decomposed differential problem using the difference equation. Taking into account $\|z^0\|=0$, inequalities (30) give

$$\|z^{n+1}\|\le\frac{\mathrm{T}}{2}\max_{n'=1,\ldots,(n+1)/2}\sum_{l=1}^{6}\left\|\psi_l^{n'}\right\|,\quad n=1,3,5,\ldots, \tag{31}$$

where $\mathrm{T}=\tau(n+1)$. Equation (31) means the scheme (16) in the Banach space of grid functions with norm (24) is stable.

To prove the convergence of the difference scheme in Banach space we shall use a modification of an existing technique [9]. We shall present errors of approximation ψ_k^n as

$$\psi_l^n=\overset{\circ}{\psi}{}_l^n+\overset{*}{\psi}{}_l^n,\quad l=1,\ldots,6,\quad\sum_{l=1}^{6}\overset{\circ}{\psi}{}_l^n=0.$$

We shall for this purpose take

$$\overset{\circ}{\psi}{}_l^n = \mathcal{B}\left[\frac{\tau}{2}\left(\left(\frac{l}{m}-1\right)^2 - \left(\frac{l-1}{m}-1\right)^2\right)\frac{\partial^2 u^n}{\partial t^2}\right]$$
$$+ \Lambda_l\left[\lambda_l\tau\left(\frac{l}{m}-1\right)\frac{\partial u^n}{\partial t} + (1-\lambda_l)\tau\left(\frac{l-1}{m}-1\right)\frac{\partial u^n}{\partial t}\right], \quad l = 1, 2, 3,$$
$$\overset{\circ}{\psi}{}_{7-l}^n = -\overset{\circ}{\psi}{}_l^n, \quad l = 1, 2, 3, \ \ m = 3.$$

Then

$$\overset{*}{\psi}{}_l^n = -\mathcal{B}\left[\frac{u^{n+l/m-1} - u^{n+(l-1)/m-1}}{\tau} - \frac{\tau}{2}\left(\left(\frac{l}{m}-1\right)^2 - \left(\frac{l-1}{m}-1\right)^2\right)\frac{\partial^2 u^n}{\partial t^2}\right]$$
$$+ \Lambda_l\left[\lambda_l\left(u^{n+l/m-1} - \tau\left(\frac{l}{m}-1\right)\frac{\partial u^n}{\partial t}\right)\right.$$
$$\left. + (1-\lambda_l)\left(u^{n+(l-1)/m-1} - \tau\left(\frac{l-1}{m}-1\right)\frac{\partial u^n}{\partial t}\right)\right], \quad l = 1, 2, 3,$$
$$\overset{*}{\psi}{}_{7-l}^n = -\mathcal{B}\left[\frac{u^{n-(l-1)/m+1} - u^{n-l/m+1}}{\tau} + \frac{\tau}{2}\left(\left(\frac{l}{m}-1\right)^2 - \left(\frac{l-1}{m}-1\right)^2\right)\frac{\partial^2 u^n}{\partial t^2}\right]$$
$$+ \Lambda_l\left[\lambda_l\left(u^{n-(l-1)/m+1} + \tau\left(\frac{l}{m}-1\right)\frac{\partial u^n}{\partial t}\right)\right.$$
$$\left. + (1-\lambda_l)\left(u^{n-l/m+1} + \tau\left(\frac{l-1}{m}-1\right)\frac{\partial u^n}{\partial t}\right)\right], \quad l = 3, 2, 1, \ \ m = 3.$$

We shall present the error of solution as $z = \zeta + \xi$, where ζ satisfies the conditions

$$\mathcal{B}\frac{\zeta^{n+\frac{l}{m}-1} - \zeta^{n+\frac{l-1}{m}-1}}{\tau} = \overset{\circ}{\psi}{}_l^n, \qquad l = 1, 2, 3,$$
$$\mathcal{B}\frac{\zeta^{n-\frac{l-1}{m}+1} - \zeta^{n-\frac{l}{m}+1}}{\tau} = \overset{\circ}{\psi}{}_{7-l}^n, \quad l = 3, 2, 1,$$
$$\zeta^0 = 0.$$

Taking the sum of these equations we obtain

$$\mathcal{B}\zeta^n = \tau\sum_{l'=1}^{3}\overset{\circ}{\psi}{}_{l'}^n$$
$$\mathcal{B}\zeta^{n+1} = 0, \quad n = 1, 3, 5, \ldots;$$

that is, $z^{n+1} = \xi^{n+1}$ for $n = 0, 1, 3, 5, \ldots$ and

$$\zeta^{n+\frac{l}{m}-1} = \mathcal{B}^{-1}\left(\tau\sum_{l'=1}^{l}\overset{\circ}{\psi}{}_{l'}^n\right), \quad l = 1, 2, 3,$$
$$\zeta^{n-\frac{l-1}{m}+1} = \mathcal{B}^{-1}\left(\tau\sum_{l'=1}^{3}\overset{\circ}{\psi}{}_{l'}^n + \tau\sum_{l'=4}^{7-l}\overset{\circ}{\psi}{}_{l'}^n\right) = \mathcal{B}^{-1}\left(\tau\sum_{l'=1}^{7-l}\overset{\circ}{\psi}{}_{l'}^n\right), \quad l = 3, 2, 1.$$

(Note that $\mathcal{B}^{-1}$ exists, since $\mathcal{B}$ is an M-matrix.)

Then, substituting $z = \zeta + \xi$ in equations for z, we obtain a problem for ξ, distinguished from the problem for z only by the fact that ψ_l^n are substituted by

$$\tilde{\psi}_l^n = \overset{*}{\psi}_l^n + \Lambda_l \left[\lambda_l \mathcal{B}^{-1} \left(\tau \sum_{l'=1}^{l} \overset{\circ}{\psi}_{l'}^n \right) + (1-\lambda_l) \mathcal{B}^{-1} \left(\tau \sum_{l'=1}^{l-1} \overset{\circ}{\psi}_{l'}^n \right) \right], \qquad l = 1, 2, 3,$$

$$\tilde{\psi}_{7-l}^n = \overset{*}{\psi}_{7-l}^n + \Lambda_l \left[\lambda_l \mathcal{B}^{-1} \left(\tau \sum_{l'=1}^{7-l} \overset{\circ}{\psi}_{l'}^n \right) + (1-\lambda_l) \mathcal{B}^{-1} \left(\tau \sum_{l'=1}^{6-l} \overset{\circ}{\psi}_{l'}^n \right) \right], \quad l = 3, 2, 1.$$

From the stability of the difference scheme, an evaluation of the form of (31) for ξ is

$$\|\xi^{n+1}\| \le \frac{\mathrm{T}}{2} \max_{n'=1,\dots,(n+1)/2} \sum_{l=1}^{6} \left\| \tilde{\psi}_l^{n'} \right\|, \quad n = 1, 3, 5, \dots.$$

Taking into account the equality $\|z^{n+1}\| = \|\xi^{n+1}\|$, $n = 1, 3, 5, \dots$, we obtain, a priori, an evaluation for the error of solution,

$$\|z^{n+1}\| \le \frac{\mathrm{T}}{2} \max_{n'=1,\dots,(n+1)/2} \sum_{l=1}^{6} \left\| \tilde{\psi}_l^{n'} \right\|, \quad n = 1, 3, 5, \dots,$$

or, using the boundedness of partial derivatives,

$$\|z^{n+1}\| = O(\tau^p + h^2), \quad n = 1, 3, 5, \dots; \tag{32}$$

$p = 2$ at $\lambda = 1/2$; $p = 1$ otherwise. Equation (32) means the solution of the difference scheme will converge to the solution of the differential problem in Banach space with the norm (24). Theorem 4 is proved.

THEOREM 5. *Let τ satisfy the inequalities* (22), (23). *Then in the Banach space of grid functions with norm* (24) *the scheme* (16) *with an operator $\mathcal{B}$, defined by* (19) *with $e > 0$, is stable at $\lambda_k = 1$, $k = 1, 2, 3$. Also if the exact solution u of a problem* (13) *in each of the areas divided by a separatrix is smooth* (*i.e.*, *the derivatives to some order are continuous*), *the scheme* (16) *converges and has accuracy*

$$\|z^{n+1}\| = O\left(\frac{h^2}{\tau} + \tau + h^2 \right), \quad n = 1, 3, 5, \dots,$$

$h = \max_{k=1,2,3; i=1,\dots,N_{x^k}} h_{x^k,i}$.

Proof. In contrast to the proof of Theorem 4, the equation for the error here has the form

$$\left(\left(\frac{1}{\tau} \mathcal{B} - \Lambda \right) \hat{z} \right)_{ijk} = \left(\frac{1}{\tau} \mathcal{B} z \right)_{ijk} + \psi_{ijk}^n.$$

Consider equation

$$\left(\left(\frac{1}{\tau} \mathcal{B} - \Lambda \right) \hat{w} \right)_{ijk} = \left(\left| \frac{1}{\tau} \mathcal{B} z \right| \right)_{ijk} + \left| \psi_{ijk}^n \right|.$$

As before one can show that

$$0 \le |z_{ijk}| \le \hat{w}_{ijk}. \tag{33}$$

Summing the equations for w with weight $c_{ijk}\overline{h}_{x^1,i}\overline{h}_{x^2,j}\overline{h}_{x^3,k}$ and taking into account that operator Λ is conservative, we come to the inequality

$$\|\hat{w}\| + \sum_{i=1}^{N_{x^1}}\sum_{j=1}^{N_{x^2}}\sum_{k=1}^{N_{x^3}} e(4\hat{w}_{ijk} - \hat{w}_{i-1jk} - \hat{w}_{i+1jk} - \hat{w}_{ij-1k} - \hat{w}_{ij+1k})\overline{h}_{x^1,i}\overline{h}_{x^2,j}\overline{h}_{x^3,k}$$
$$\le \|z\| + \tau\|\psi^n\| + \sum_{i=1}^{N_{x^1}}\sum_{j=1}^{N_{x^2}}\sum_{k=1}^{N_{x^3}} e|4z_{ijk} - z_{i-1jk} - z_{i+1jk} - z_{ij-1k} - z_{ij+1k}|\overline{h}_{x^1,i}\overline{h}_{x^2,j}\overline{h}_{x^3,k}.$$

With grid functions $\hat{w}_{i+1jk}$ and z_{i+1jk} we shall construct continuously differentiable functions $\hat{w}$ and z with bounded partial derivatives of the second order. Then at some point

$$|4\hat{w}_{ijk} - \hat{w}_{i-1jk} - \hat{w}_{i+1jk} - \hat{w}_{ij-1k} - \hat{w}_{ij+1k}| \le M_1 h^2$$
$$|4z_{ijk} - z_{i-1jk} - z_{i+1jk} - z_{ij-1k} - z_{ij+1k}| \le M_2 h^2$$

and, hence,

$$\|\hat{w}\| \le \|z\| + Mh^2 + \tau\|\psi^n\| = \|z\| + \tau\left(M\frac{h^2}{\tau} + \|\psi^n\|\right).$$

Then, taking into account (33),

$$\|\hat{z}\| \le \|z\| + \tau\left(M\frac{h^2}{\tau} + \|\psi^n\|\right). \tag{34}$$

Substituting an inequality of the form (34) in an inequality for the last equation of scheme (16) and excluding $\|z^{n-1}\|$, we find

$$\|z^{n+1}\| = O\left(\frac{h^2}{\tau} + \max_{n'=1,\dots,(n+1)/2}\sum_{l=1}^{6}\left\|\psi_l^{n'}\right\|\right) = O\left(\frac{h^2}{\tau} + \tau + h^2\right),$$

$n = 1, 3, 5, \dots$, which proves the stability (in the sense that the error is limited) and convergence of scheme (16) at $h^2/\tau + \tau + h^2 \to 0$ in the Banach space of grid functions with norm (24). Theorem 5 is proved.

Remark 1. It is not possible to prove convergence for the case where h^2/τ is not small using this method (although it is possible to state the proximity of solutions of difference and differential problems for a small time interval). Moreover, in this case we failed to prove convergence using both methods of power inequalities and a priori estimations. However, the kinetic problems in many cases satisfy the inequalities (22), (23) for $\tau \sim h^{2-\varepsilon}$, $\varepsilon > 0$, and it is possible to choose, for example, $\tau = h^{2-\varepsilon}$, satisfying inequalities (22), (23), and $h^2/\tau \to 0$.

Remark 2. As well as analytic estimates, numerical study of the stability and convergence of scheme (16), including comparison with analytic solutions and with calculations from two-dimensional codes, has been carried out. Research has shown that, for the implicit scheme, the restrictions on τ and h^2/τ in Theorem 5, are probably a corollary of the method of proof. Violation of these restrictions at $\lambda_k = 1$ only resulted in negative values emerging in the solution at large x^1 (i.e., large speed), even for the case where $\mathcal{B} = \mathcal{I}$. However, the development of instability in the model problems being considered was not observed.

7. PRESERVATION OF THE SIGN OF THE SOLUTION OF THE DIFFERENCE PROBLEM

For our application the unknown function in the differential problem is the distribution function of particles, or, using the terminology of probability theory, a probability density. The distribution function must be nonnegative. An important question is whether the solution of the difference problem retains this property from one time layer to the next. The following theorems are valid.

THEOREM 6. *Let the coefficients of the problem* (13) *satisfy inequalities* (20), (21) *and let the initial condition be nonnegativity*, $f^0 \geq 0$. *Then at* $\lambda_k = 1, k = 1, 2, 3$, *for scheme* (16) *with* $\mathcal{B} = \mathcal{I}$,

$$f \geq 0, \tag{35}$$

for all whole and fractional time layers. If $0 \leq \lambda_k < 1, k = 1, 2, 3$, *the inequalities* (35) *are valid for some small* τ.

Proof. As before, the time-advancement equation for a new time-layer looks like

$$T\hat{f} = Sf,$$

where T is an M-matrix. Then T^{-1} exists,

$$\hat{f} = T^{-1}Sf,$$

and the elements of T^{-1} are nonnegative. Thus, if Sf has nonnegative components, $\hat{f}$ will be nonnegative.

At $\lambda_k = 1, k = 1, 2, 3$, the operator S is

$$S = \frac{1}{\tau}\mathcal{I}.$$

Therefore, if $f \geq 0$, $Sf \geq 0$ for any τ.

For $0 \leq \lambda_k < 1, k = 1, 2, 3$, the operator S is

$$S = \frac{1}{\tau}\mathcal{I} + (1 - \lambda_k)\Lambda_k.$$

In this case we shall require that $1/\tau$ is not less than the maximum of the moduli of the diagonal coefficients of matrix $(1 - \lambda)\Lambda_k, k = 1, 2, 3$. Then all elements of matrix $(\mathcal{I}/\tau + (1 - \lambda)\Lambda)$ will be nonnegative. Therefore, if $f \geq 0$, $Sf \geq 0$.

So from one time-layer to the next, the property of nonnegativity of f is maintained, proving Theorem 6.

THEOREM 7. *Let the initial condition be nonnegativity,* $f^0 \geq 0$. *Then the sum of the components of the solution of the difference scheme* (16) *is nonnegative*

$$\sum_{l=1}^{P} f_l \geq 0$$

for all whole and fractional time layers if $\eta_n = 0$ *in* (4).

Proof. The matrices $T = \mathcal{B}/\tau - \lambda\Lambda$ and $S = \mathcal{B}/\tau + (1-\lambda)\Lambda$ for $\eta_n = 0$ have the following property:

$$\sum_{k=1}^{P} t_{kl} = \frac{1}{\tau}, \quad \sum_{k=1}^{P} s_{kl} = \frac{1}{\tau}, \quad l = 1, \ldots, P.$$

Then

$$0 \leq \sum_{l=1}^{P} f_l \frac{1}{\tau} = \sum_{l=1}^{P} f_l \sum_{k=1}^{P} s_{kl} = \sum_{k=1}^{P} \sum_{l=1}^{P} s_{kl} f_l = \sum_{k=1}^{P} (Sf)_k$$
$$= \sum_{k=1}^{P} (T\hat{f})_k = \sum_{k=1}^{P} \sum_{l=1}^{P} t_{kl} \hat{f}_l = \sum_{l=1}^{P} \hat{f}_l \sum_{k=1}^{P} t_{kl} = \sum_{l=1}^{P} \hat{f}_l \frac{1}{\tau}$$

from which the theorem follows.

Remark 1. The restriction on τ in Theorem 6 is not a corollary of the method of proof. Calculations show that in "complicated" cases (with, for example, large mixed derivatives) the difference solution at some points can become negative. This occurs in the region of large x^1 (i.e., speed), where the values of the solution are very (exponentially) small. However, the sum of components of the solution remains nonnegative for any τ.

Remark 2. In considering the scheme (15) with equations of the form

$$\frac{\mathcal{B}\hat{f} - f}{\tau} = \Lambda \hat{f},$$

then the validity of Theorems 2 and 5 remains. By analogy to the proof of Theorem 6, it is possible to show that the solution of the difference problem will be nonnegative if the initial function is nonnegative.

8. CALCULATION OF BOOTSTRAP CURRENT

Toroidal plasmas exhibit a number of properties which are not observed in cylindrical plasmas. One of these is the existence of an additional electric current which is called the bootstrap current [14]. The bootstrap current is carried mostly by passing electrons. It appears due to temperature and density gradients and Coulomb collisions between passing and trapped electrons. The role of the bootstrap current increases with the plasma temperature. In hot plasmas this current is expected to play an important role, which could noticeably reduce the cost of a fusion power-plant.

The bootstrap current has been studied analytically by many authors. One of the most advanced analytic formulae is that obtained by Hirshman [15].

Besides their undoubted advantages, analytic formulae are only applicable in certain regions. In order to calculate the bootstrap current rigorously one has to solve the 3D kinetic equation (1) with special boundary conditions at the internal separatrix or TPB. These conditions involve step changes in the distribution function

$$(u\sqrt{g})_{tr,+} = (u\sqrt{g})_{+} + (u\sqrt{g})_{-}, \tag{36}$$

$$(u\sqrt{g})_{+} - (u\sqrt{g})_{-} = (u)_{tr,+}((\sqrt{g})_{tr,+} - (\sqrt{g})_{tr,-}) + \alpha\left(\frac{\partial u}{\partial \gamma_0}\right)_{tr,+} \tag{37}$$

and continuity of the flux normal to the TPB

$$\sum_{n=1,4,5}\left(\frac{j^{x^n}}{|\vec{\nabla}F|}\frac{\partial F}{\partial x^n}\right)_{+} + \sum_{n=1,4,5}\left(\frac{j^{x^n}}{|\vec{\nabla}F|}\frac{\partial F}{\partial x^n}\right)_{-} = \sum_{n=1,4,5}\left(\frac{j^{x^n}}{|\vec{\nabla}F|}\frac{\partial F}{\partial x^n}\right)_{tr,+}, \tag{38}$$

where "+" and "−" denote limits from regions of co- and counter-passing particles, "$tr, +$" and "$tr, -$" denote the same, but for trapped particles, the function α is the averaged width of the drift trajectory [4], the flux is given by

$$j_{\alpha}^{x^n} = \frac{1}{\sqrt{g}}\left(\sum_{m=1,4,5}\left(A_{nm}\frac{\partial u}{\partial x^m}\right) + B_n u\right) \tag{39}$$

and $F = 0$ is the equation for the boundary of the separatrix layer.

Equations (36)–(38) can be incorporated in the difference operators as discussed in Section 3.1, preserving particle conservation numerically.

Once the distribution function of the electrons is known, the bootstrap current density can be calculated using integral (22), given in [4].

The main aim of the calculations in this section was to compare numerical results with the analytic formula from [15] and to study the influence on the bootstrap current of different factors in the numerical approximation of the problem. For this purpose, at external boundaries, conditions of zero flux were used except at boundaries $v_{0,\min}$ and $\gamma_{0,\min}$, where the distribution function was set to a Maxwellian distribution. The initial distribution was also Maxwellian.

A toroidal plasma consisting of electrons and deuterium ($\beta = e, d$) was considered with magnetic field $B_0 = 5.8$ T, total current $I_p = 2$ MA and parabolic density, temperature and current density profiles

$$n_\beta(\gamma)/n_\beta(0) = \left(0.9\left(1 - (\gamma/\gamma_a)^2\right) + 0.1\right), \quad n_\beta(0) = 10^{20}\ \mathrm{m}^{-3},$$
$$T_\beta(\gamma)/T_\beta(0) = \left(0.9\left(1 - (\gamma/\gamma_a)^2\right) + 0.1\right), \quad T_e(0) = 15\ \mathrm{keV}, \quad T_d(0) = 1\ \mathrm{keV},$$
$$j(\gamma)/j(0) = \left(1 - (\gamma/\gamma_a)^2\right).$$

The ions were assumed to have a Maxwellian distribution. Circular cross-section magnetic flux surfaces were considered with major and minor radii of the torus $R_0 = 6$ m and $\gamma_a = 1$ m.

Figure 5 shows results of the numerical solution of the 3D kinetic equation (solid line) and analytical (dashed line) calculations using the formula from [15]. One can see satisfactory agreement.

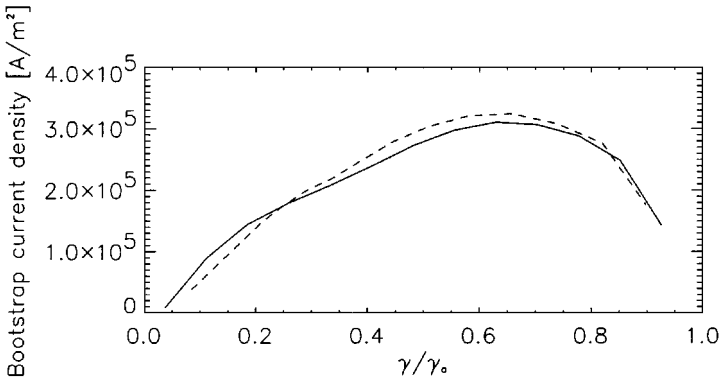

FIG. 5. Bootstrap current density. The solid line shows the numerical solution, the dashed line is the analytical result.

Several runs emphasised the importance of treating the TPB accurately. In particular, use of the usual condition of continuity of the distribution function instead of Eqs. (36) and (37) can give over 30% lower bootstrap current. It was also found that the mixed derivative $\mathcal{L}_{\theta_0\gamma_0}[u]$ and the nonlinear dependence of coefficients in the equation play an important role in formation of the bootstrap current.

9. CALCULATION OF HIGH ENERGY ION DISTRIBUTIONS

In this section we discuss some of the numerical difficulties of modelling high-energy ion behaviour in thermonuclear experiments and show how advanced approaches, described in the paper, can help for this application of kinetic codes.

In these problems, the B_n terms in the kinetic equation (1) can become dominant in comparison with the A_{nn} terms. Moreover, the coefficients B_{θ_0} and B_{γ_0} can change sign. In this complicated case it is appropriate to use approximation (7) with all $\eta_n = 0$. Another difficulty relates to the presence of the loss term and source in the kinetic equation

$$\frac{\partial u}{\partial t} = \sum_{n,m=1}^{3} \mathcal{L}_{nm}[u] - \frac{u}{\tau_{loss}} + S.$$

Losses can be large (i.e., τ_{loss} is small), so from the point of view of stability it is better to take it fully implicitly in the scheme. The source can have a delta-function-like dependence on phase space coordinates and requires use of a nonuniform grid and care in the transformation for local coordinates and calculation of integrals of S. The loss and the source terms can be spread between the first three equations in scheme (15) using weights which sum to unity and used symmetrically in the last three equations of (15).

In many advanced magnetic fusion devices it is important to take into account the deviations of drift trajectories from magnetic flux surfaces for high energy ions [4, 16]. This results in complicated formulae for A_{nn}, B_n, S, etc. (see [4]), which require the order of $O(N^5)$ arithmetic operations. The authors have developed fast algorithms for the calculation of trajectory-averaged coefficients—the presentation of these will be the subject of a later paper. Fast algorithms become extremely important, e.g. for alpha-particle simulations, since the coefficients are usually time dependent and have to be frequently updated during calculations.

The methods described in this paper were successfully used for the numerical simulation of alpha-particle behaviour in past and recent thermonuclear experiments on JET and TFTR [e.g. 16], allowing accurate calculation of the alpha-particle energy transferred to the background plasma and the accumulation of helium ash modelled using Eq. (11).

It is important to use Eq. (11) in the numerical scheme, otherwise the alpha-particle distribution at low speeds accumulates excessively.

In Ref. [16] results of the presented numerical scheme were compared with results of an alternative approach, based on a Monte-Carlo method. The global characteristics of the alpha particles, e.g. their heating of the background plasma appeared to be very close. However, the approach based on finite differences has noticeable advantages. In particular statistical noise is always present in Monte-Carlo methods, which can require unacceptably large numbers of alpha particles to produce smooth distribution functions [18]. The method based on the averaged 3D kinetic equation and finite differences allows one to obtain smooth distributions within a reasonable calculation time, which can be used not just for comparison with experimental measurements of particle distributions (e.g. to study MHD instabilities associated with fast particle distributions), but also as input to other codes.

10. CONCLUSIONS

Numerical methods for the solution of problems for multidimensional kinetic equations with the Coulomb collision operator have been developed. The approach used is based on the method of finite differences. Various conservative difference schemes for a numerical solution of mixed problems for the kinetic equation are presented and theoretically and numerically investigated. A series of difficulties, related to details of the operators of the kinetic equation which hamper application of the standard theorems of the theory of difference schemes, have been overcome. For some classes of coefficients of the equation, proofs have been presented of (a) theorems of existence and uniqueness of the solution of the discrete problem, (b) a theorem about absolute stability and convergence in the Banach space $L_{1,h}$ (related to the particle density in a kinetic problem), and (c) nonnegativity of the numerical solution. With some easing of the requirements on coefficients these theorems are proved with a restriction on the time step. The methods presented are successfully used in two of the most advanced kinetic codes, FPP-3D and BANDIT-3D, for modelling tokamak plasmas. The application to specific kinetic problems, i.e. the calculation of alpha-particle distributions and bootstrap currents, have been described.

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