ISSN 0915-633X

NATIONAL INSTITUTE FOR FUSION SCIENCE

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(Received - July 21, 1999)

NIFS-606 Aug. 1999

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RESEARCH REPORT
NIFS Series

NAGOYA, JAPAN

On the Two Weighting Scheme for δf Collisional Transport Simulation

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Abstract

The validity is given to the newly proposed two weighting δf scheme (Wang *et al.*, Ressearch Report of National Institute for Fusion Science **NIFS-588**, 1999) for collisional or neoclassical transport calculations, which can solve the drift kinetic equation taking account of effects of steep plasma gradients, large radial electric field, finite banana width, and the non-standard orbit topology near the axis. The marker density functions in weight equations are successively solved by using the idea of δf method and a hierarchy of equations for weight and marker density functions is otained. These hierarchy equations are solved by choosing an appropriate source function for each marker density. Thus the validity of the two weighting δf scheme is mathematically proved.

Keywords : Two weighting scheme, δf method, collisional transport, neoclassical transport, drift kinetic equation

1. Introduction

In recent fusion experiments, plasmas are often operated in parameter regimes beyond the valid scope of the conventional neoclassical theory[1] as seen in H-mode and ITB (Internal Transport Barrier) mode, in which assumptions for the neoclassical theory, $\rho_p \ll L_r$ and $M_p \ll 1$, are no longer valid, where ρ_p is poloidal Larmor radius, L_r is the radial gradient length of plasma parameters, and M_p is the poloidal Mach number. In such cases, effects of particle dynamics with finite orbit width, strong radial electric field, fast plasma rotation, large radial plasma gradients, and non-standard orbit topology near the magnetic axis are important for collisional transports. The works by Lin, Tang, and Lee [2,3] have first shown that the δf particle simulation [4-8], solving the drift ki-

netic equation, can be a powerful tool for such extended neoclassical transport calculations. However, they used the nonlinear weighting scheme [7] in which the distribution function f is used to fill the role of the marker density g in the weight equation. This nonlinear weighting scheme was initially derived for nonlinear gyrokinetic equation with nondiffusive motion. However, it can not be directly extended to the drift kinetic equation with diffusive motion due to Coulomb collision processes. Chen and White [9] have given a rigorous derivation of collisional δf algorithm by treating the weight as a new dimension of particle motion. The weight equation is closely related to how to add new particles to compensate particles lost through the diffusion process. However, the question how to evaluate g for weight calculation remained to be solved, although the precise estimation of g is essential for the δf method.

Recently, Wang *et al.* [10] have developed a new δf method to solve the drift kinetic equation, in which the collision scheme was much improved and the two weighting scheme was employed. A linear like-particle collision scheme, almost perfectly conserving the particle number, momentum, and energy has been given. The benchmark calculation of neoclassical transport using this collision scheme demonstrated increased accuracy in results, and the collision scheme by them seems to be most adequate for δf simulations. They showed that the nonlinear weighting scheme is ineffective and inaccurate for solving the drift kinetic equation because of a severe constraint that the relation $g = f$ must hold accurately in the simulation. Otherwise, correct results can not be guaranteed. However, it is generally difficult to impose this restriction on the simulation. They proposed a new scheme in which g is evaluated from its kinetic equation using the idea of δf method. The resultant weighting scheme consists of two weight equations and is more effective and accurate to solve the drift kinetic equation.

The purpose of the present paper is to give the mathematical basis for the validity of the two weighting scheme proposed by Wang *et al.* [10] for δf simulation studies of neoclassical or collisional transports.

2. Formulation of weight equations

The drift kinetic equation for a guiding center distribution function $f(\vec{x}, \vec{v}, t)$ in phase space $(\vec{x}, \vec{v})$ is given by [1],

$$\frac{\partial f}{\partial t} + (\vec{v}_{\parallel} + \vec{v}_d) \cdot \nabla f = C(f, f), \tag{1}$$

where $\vec{v}_{\parallel}$ is the velocity parallel to the magnetic field, $\vec{v}_d$ is the guiding center drift velocity, and C is the Coulomb collision operator. By separating f into two parts $f = f_0 + f_1$ with $\mid f_1 \mid \ll f_0$, the drift kinetic equation (1) becomes

$$\frac{\partial f_0}{\partial t} + \vec{v}_{\parallel} \cdot \nabla f_0 - C(f_0, f_0) = 0, \tag{2}$$

$$\frac{\partial f_1}{\partial t} + (\vec{v}_{\parallel} + \vec{v}_d) \cdot \nabla f_1 - C(f_1, f_0) = -\vec{v}_d \cdot \nabla f_0 + C(f_0, f_1). \tag{3}$$

The collision operator $C(f_1, f_1)$ has been neglected. A steady state solution to equation (2) is, for example, a Maxwellian distribution, $f_0 = f_M$. Since the drift term is retained, equation (3) can take the effect of finite orbit width into account.

We consider to solve the linearized equation (3) utilizing the δf method which differs from the full-f method only by considering particle weights to effectively treat the "source" term on the right hand side of equation (3). The conventionally used definition for the particle weight is $w = f_1/g$, where g is the

simulation particle distribution function (or marker density) evolving in phase space $(\vec{x}, \vec{v})$ [7,8]. This definition works well for nondiffusive particle motion in the Hamiltonian system, but causes difficulty in deriving the weight equation when particle motion is diffusive or stochastic due to, for example, Coulomb collisions [9]. In Ref.[9], the weight is treated as a new dimension of particle motion, in addition to the usual dimensions of $(\vec{x}, \vec{v})$ phase space. Simulation particles or markers are described by a marker distribution function, $F_M(\vec{x}, \vec{v}, w, t)$, in the extended phase space $(\vec{x}, \vec{v}, w)$.

The marker distribution function F_M obeys, in phase space $(\vec{x}, \vec{v}, w, t)$, the following kinetic equation :

$$\frac{D}{Dt}F_M + \frac{\partial}{\partial w}(\dot{w}F_M) = S_M(\vec{x}, \vec{v}, w, t). \quad (4)$$

where the notation D/Dt denotes, for an arbitrary function f_A,

$$\frac{D}{Dt}f_A \equiv \frac{\partial f_A}{\partial t} + (\vec{v_\parallel} + \vec{v_d}) \cdot \nabla f_A - C(f_A, f_0). \quad (5)$$

Since markers diffuse and some of them escape out of the plasma region or the simulation domain, a source S_M for markers should be introduced to control the marker population. The relation between f_1 and F_M is

$$f_1(\vec{x}, \vec{v}, t) = \int w F_M \, dw. \quad (6)$$

The marker distribution function or marker density in phase space $(\vec{x}, \vec{v})$ is given by

$$g(\vec{x}, \vec{v}, t) \equiv \int F_M(\vec{x}, \vec{v}, w, t) dw. \quad (7)$$

The weight equation is determined by requiring that equations (3), (4) and (6) are consistent with each other. The weight equation is determined as [9]

$$\dot{w} = \frac{1}{g}\left[-\int w S_M \, dw - \vec{v_d} \cdot \nabla f_0 + C(f_0, f_1)\right], \quad (8)$$

$$\frac{D}{Dt}g = \int S_M \, dw. \quad (9)$$

Note that equation (8) has been derived under the assumption that $\dot{w}$ does not depend on w itself. Equation (8), along with equations of motion in original phase space, represents the basic formalism for the δf method. It is noted that equations (8) and (9) clearly show the close relation between the weight w and the source S_M. Therefore, how accurately to evaluate g in equation (9) is the key point in the δf method.

If the banana width Δ_b is negligible compared to radial gradient lengths of plasma parameters, we can neglect the drift velocity $\vec{v_d}$ compared to $\vec{v_\parallel}$ in equations (3) and (5). Equation (3) becomes

$$\frac{\partial f_1}{\partial t} + \vec{v_\parallel} \cdot \nabla f_1 - C(f_1, f_0) = -\vec{v_d} \cdot \nabla f_0 + C(f_0, f_1). \quad (10)$$

This equation provides the starting point for conventional neoclassical transport analysis [1], in which $\rho_p \ll L_r$ and $M_p \ll 1$ are assumed. In this case, particles will remain on the same magnetic surface all the time as that of their initial locations. The particles never escape out of the simulation domain and new particles are not needed to be supplied. Therefore, $S_M = 0$ and we can set $g = f_0$ if $g(t = 0) = f_0$, since g and f_0 obey the same equation.

However, if we retain the drift velocity $\vec{v_d}$ in equations (3) and (9), particles diffuse out of their initial magnetic surface due to the drift motion and Coulomb collisions. Particles crossing the plasma boundary (the separatrix or the outermost closed surface) are lost out of the simulation domain. To keep the well populated particles in the plasma, new particles must be added into the plasma region or the simulation domain. In this case $S_M \neq 0$ and g and f obey different equations (Note that $Df/Dt = C(f_0, f_1) \neq \int S_M dw$). Accordingly, the nonlinear weighting scheme seems

difficult to be applied. This difficulty has been clearly illustrated in Ref.[10].

3. The hierarchy equations

We apply the idea of δf method to solving equation (9) for g. Splitting $g = g_0 + g_1$ with $\mid g_1 \mid \ll g_0$, we separate equation (9) into following two equations,

$$\frac{\partial g_0}{\partial t} + \vec{v_\parallel} \cdot \nabla g_0 - C(g_0, f_0) = 0, \tag{11}$$

$$\frac{\partial g_1}{\partial t} + (\vec{v_\parallel} + \vec{v_d}) \cdot \nabla g_1 - C(g_1, f_0) = -\vec{v_d} \cdot \nabla g_0 + \int S_M dw, \tag{12}$$

These equations are solved under the condition that $g_0 = f_0$ and $g_1 = 0$ at $t = 0$. We introduce another weight w_1 and a marker distribution function $G_M^{(1)}(\vec{x}, \vec{v}, w_1, t)$ in extended phase space $(\vec{x}, \vec{v}, w_1)$. Let $G_M^{(1)}$ obey the kinetic equation

$$\frac{D}{Dt} G_M^{(1)} + \frac{\partial}{\partial w_1}(\dot{w}_1 G_M^{(1)}) = \Omega_M^{(1)}(\vec{x}, \vec{v}, w_1, t), \tag{13}$$

with initial condition $G_M^{(1)}(t = 0) = f_0 \delta(w_1)$, and relate to g_1 through the following relation

$$g_1(\vec{x}, \vec{v}, t) = \int w_1 G_M^{(1)} dw_1. \tag{14}$$

Here a source term $\Omega_M^{(1)}$, like S_M in equation (4), is introduced to control the marker population. From the requirement that equations (12), (13) and (14) are consistent with each other, the equation for weight w_1 is determined as

$$\dot{w}_1 = \frac{1}{h^{(1)}} \left[- \int w_1 \Omega_M^{(1)} dw_1 - \vec{v}_d \cdot \nabla f_0 + \int S_M dw \right], \tag{15}$$

where the distribution function $h^{(1)}(\vec{x}, \vec{v}. t)$ is defined by

$$h^{(1)} \equiv \int G_M^{(1)}(\vec{x}, \vec{v}, w_1, t) dw_1, \tag{16}$$

and satisfies

$$\frac{D}{Dt} h^{(1)} = \int \Omega_M^{(1)} dw_1. \tag{17}$$

To determine the function $h^{(1)}$, we again employ the δf method to solve equation (17). Successively, we obtain, for $k = 2, 3, 4, \cdots$,

$$\frac{D}{Dt} G_M^{(k)} + \frac{\partial}{\partial w_k}(\dot{w}_k G_M^{(k)}) = \Omega_M^{(k)}(\vec{x}, \vec{v}, w_k, t), \tag{18}$$

$$\dot{w}_k = \frac{1}{h^{(k)}} \left[- \int w_k \Omega_M^{(k)} dw_k - \vec{v}_d \cdot \nabla f_0 + \int \Omega_M^{(k-1)} dw_{k-1} \right], \tag{19}$$

$$h^{(k)} \equiv \int G_M^{(k)} dw_k, \tag{20}$$

$$\frac{D}{Dt} h^{(k)} = \int \Omega_M^{(k)} dw_k. \tag{21}$$

Note that $\dot{w}_k$ is independent of w_k. Together with sets of equations (8), (9) for $\dot{w}$ and g, (15) and (17) for $\dot{w}_1$ and $h^{(1)}$, infinite sets of equations (19) and (21) for $k = 2.3, 4, \cdots$ form a hierarchy of weight and marker density equations. To obtain the objective weight w, it is necessary to trancate the chain of the hierarchy or sum up all the equations of the hierarchy.

4. Weights for markers

In the simulation, equation (4) for the distribution function F_M is solved by using a finite number of simulation particles or markers. The numerical representation of F_M is

$$F_M(\vec{x}, \vec{v}, w, t) = \sum_j \delta(\vec{x} - \vec{x}_j(t)) \delta(\vec{v} - \vec{v}_j(t)) \delta(w - w_j(t)), \tag{22}$$

where the index j represents the j-th marker. Each marker is pushed in extended phase space along the characteristics

$$\frac{d\vec{x}_j}{dt} = \dot{\vec{x}}_j, \quad \frac{d\vec{v}_j}{dt} = \dot{\vec{v}}_j, \quad \text{and} \quad \frac{dw_j}{dt} = \dot{w}_j. \tag{23}$$

From equations (6) and (7), f_1 is numerically represented as

$$f_1(\vec{x}, \vec{v}, t) = \sum_j w_j(t) \delta(\vec{x} - \vec{x}_j(t)) \delta(\vec{v} - \vec{v}_j(t)). \tag{24}$$

For the $j-$th marker, equation (24) can be expressed by

$$f_{1j} = w_j g_j. \tag{25}$$

Here f_{1j} and g_j are defined by

$$f_{1j} \equiv f_1(\vec{x}_j(t), \vec{v}_j(t), t), \tag{26}$$

$$g_j \equiv g(\vec{x}_j(t), \vec{v}_j(t), t). \tag{27}$$

It should be noticed that equation (25) is different from $w = f_1/g$ in continuous phase space $(\vec{x}, \vec{v})$, which is the original definition of the weight used in the Hamiltonian system. From equations (14) and (16), the relation $g_{1j} = w_{1j} h_j^{(1)}$ holds and the marker density g_j for the $j-$th marker can be written as

$$g_j = g_{0j} + w_{1j} h_j^{(1)}, \tag{28}$$

Likewise, for $k = 1, 2, 3, \cdots$,

$$h_j^{(k)} = h_{0j}^{(k)} + w_{k+1,j} h_j^{(k+1)}. \tag{29}$$

According to the assumption, $g_{0j} = h_{0j}^{(k)} = f_{0j}$ for all k. From equations (28) and (29), g_j can be written as

$$\begin{aligned} g_j &= f_{0j} + w_{1j}(f_{0j} + w_{2j} h_j^{(2)}) \\ &= (1 + w_{1j}) f_{0j} + w_{1j} w_{2j}(f_{0j} + w_{3j} h_j^{(3)}) \\ &= \cdots \\ &= (1 + w_{1j} + w_{1j} w_{2j} + w_{1j} w_{2j} w_{3j} + \cdots) f_{0j} \\ &\quad + w_{1j} w_{2j} w_{3j} \cdots h_j^{(\infty)}. \end{aligned} \tag{30}$$

Now we pay attention to the fact that the source terms $\Omega_M^{(k)}$'s can be chosen arbitrarily. On the other hand, the source term S_M should be selected so as to satisfy physics requirements under consideration. We choose $\Omega_M^{(k)}$'s as, for $k = 1, 2, \cdots$,

$$\int w_k \Omega_M^{(k)} dw_k = 0, \tag{31}$$

$$\int \Omega_M^{(k)} dw_k = (1 + \epsilon_k) \int S_M dw. \tag{32}$$

Here, we will assume that $\epsilon_1 \neq \epsilon_2 \neq \cdots$ and $| \epsilon_k | \ll 1$ for all k. By choosing $\Omega_M^{(k)}$'s as in equation (32), the marker densities can be approximated by

$$h^{(k)} = h^{(1)} + (\epsilon_k - \epsilon_1) h^{(1)} \simeq h^{(1)} + (\epsilon_k - \epsilon_1) f_0, \tag{33}$$

where $h^{(1)}$ of the second term on the right hand side was replaced by f_0, since the dominant term of $h^{(1)}$ is f_0. Taking account of equation (15) for $\dot{w}_1$, we can approximate $\dot{w}_k$, for $k = 2, 3, \cdots$, given by equation (19) to

$$w_k = w_1 + (\epsilon_k - \epsilon_1) f_0^2 \dot{w}_1 + \epsilon_{k-1} \frac{1}{f_0} \int S_M dw + O(\epsilon_k^2). \tag{34}$$

We estimate the third term on the right hand side of this equation, because this term may increase with time. For example, we choose S_M as

$$S_M = \nu(t) s(\vec{x}) f_0(\vec{v}) \delta(w - w_M), \tag{35}$$

where $\nu(t)$ is the injection rate of new markers, $s(\vec{x})$ is the spatial distribution of new markers, and $f_0(\vec{v})$ is the velocity distribution function for new markers. The markers are injected with the weight w_M. In this case, the second term in equation (34) is given by

$$\epsilon_k \frac{1}{f_0} \int S_M dw = \epsilon_k \nu(t) s(\vec{x}). \tag{36}$$

The time development of this term is roughly $\epsilon_k \nu s T_s$, where T_s is the simulation time. Since S_M has the same dimension as νf_0, $s(\vec{x})$ is of the order of unity and we can make νT_s of order unity, because ν corresponds to the loss rate of the plasma or collision frequency at the steady state. Now it is anticipated that the third term in equation (34) remains small during the simulation if $| \epsilon_k | \ll 1$ and that $w_k = w_1 + O(\epsilon_k)$ for $k = 2, 3, \cdots$.

Now we apply considerations above to the hierarchy equations. Equation (34) can hold for the $j-$th

marker and $w_{kj} = w_{1j} + O(\epsilon_k)$ for the j–th marker. The second term with $h_j^{(\infty)}$ on the right hand side in equation (30) vanishes because $\mid w_{kj} \mid < 1$ for all k. If we take, for example, $\epsilon_k = \varepsilon(-1)^{k-1}/k$ with $\mid \varepsilon \mid \ll 1$ (Note that $\sum_{k=1}^{\infty}(-1)^{k-1}/k$ =log2), the series with f_{0j} in equation (30) can converge to yield

$$g_j = (1+w_{1j}+w_{1j}^2+w_{1j}^3\cdots)f_{0j}+O(\varepsilon) = \frac{f_{0j}}{1-w_{1j}}+O(\varepsilon). \tag{37}$$

In the same way,

$$h_j^{(k)} = \frac{f_{0j}}{1-w_{1j}} + O(\varepsilon). \tag{38}$$

In the lowest order (we can choose ε as small as possible), we recover the previous two weighting equations [10] ;

$$\dot{w}_j = \frac{1-w_{1j}}{f_{0j}}\left[-\int wS_M\,dw - \vec{v}_d\cdot\nabla f_0 + C(f_0.f_1)\right]_j, \tag{39}$$

$$\dot{w}_{1j} = \frac{1-w_{1j}}{f_{0j}}\left[-\vec{v}_d\cdot\nabla f_0 + \int S_M\,dw\right]_j. \tag{40}$$

Thus, the validity of the two weighting δf scheme [10] for neoclassical study has been proved. Equations (39) and (40) represent a general and accurate weighting scheme. Now each simulation particle is assigned two weights, and the second weight w_1 is introduced to evaluate g (exactly saying, g_1) accurately. The new scheme elucidates the close relationship between the weight calculation and the way how to add new markers.

5. Summary

We have given a mathematical proof to the validity of the newly proposed two weighting scheme [10] for the collisional δf method by considering all the hierarchy equations. It should be remarked, however, that there may be other possible weighting schemes if $\Omega_M^{(k)}$'s are differently chosen.

Using the two weighting scheme and the new collision operator, Wang *et al.* [10] developed a δf simulation program code named "FORTEC" (Finite ORbit Transport study by an Extensive Code). In FORTEC they used a convenient choice for the marker source $S_M = \nu(t)s(\vec{r})f_0\delta(w)$. Then the weight equations are simplified to

$$\dot{w}_j = \frac{1-w_{1j}}{f_{0j}}\left[-\vec{v}_d\cdot\nabla f_0 + C(f_0,f_1)\right]_j, \tag{41}$$

$$\dot{w}_{1j} = \frac{1-w_{1j}}{f_{0j}}\left[-\vec{v}_d\cdot\nabla f_0 + \nu s f_0\right]_j. \tag{42}$$

Using FORTEC, they found [10,11,12] that the ion thermal diffusivity and parallel flow are largely reduced near the plasma center due to the non-standard orbit topology. It has also been shown that the ion thermal diffusivity decreases significantly when the density gradient becomes steep and the particle flux due to ion-ion like collisions, which vanishes in the conventional neoclassical theory, increases with decreasing density gradient scale.

Investigations on collisional or extended neoclassical transports are in progress considering effects of strong radial electric field, fast plasma rotation, and large gradients of density and temperature profiles.

Acknowledgment

The authors are thankful to Dr. S. Murakami for fruitful discussions. This work is supported by the Grand-in-Aid of the Ministry of Education, Science, Sports, and Culture (MOE), No. 10680479.

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