Monte-Carlo Simulation of Neoclassical Transport in Magnetic Islands and Ergodic Regions

Ryutaro KANNO1,2), Masanori NUNAMI3), Shinsuke SATAKE1), Hisanori TAKAMARU4), Yukihiro TOMITA1,2), Keisuke NAKAJIMA2), Masao OKAMOTO4) and Nobuyoshi OHYABU1,2)

1) National Institute for Fusion Science, Toki 509-5292, Japan
2) Department of Fusion Science, Graduate University for Advanced Studies, Toki 509-5292, Japan
3) Institute of Laser Engineering, Osaka University, Suita 565-0871, Japan
4) Department of Computer Science, Chubu University, Kasugai 487-8501, Japan

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1. Introduction

It is shown in Large Helical Device experiments that transport modeling based on only fluid description is insufficient to express edge transport phenomena in and around a magnetic island with lower collisionality. Furthermore, in recent tokamak experiments, it is found that the so-called stochastic diffusion theory based on “field line diffusion” overestimates the radial energy transport in collisionless edge plasma affected by resonant magnetic perturbations, though the perturbations induce a chaotic behavior in the field lines. These results imply that conventional modeling of edge transport should be reconsidered for a lower collisionality case. A simulation study of neoclassical transport in magnetic islands and ergodic regions is attempted for understanding the fundamental properties of such collisionless edge plasma. By using a drift kinetic equation solver without the assumption of nested flux surfaces (the KEATS code), it is possible to conduct the investigation. In this paper, we report the simulation study of ion transport in the ergodic region, neglecting the effects of an electric field and neutrals. The simulation results are interpreted through the discussion based on statistical studies.

Collisionless limit [6, 10], where α is a particle species, $v_{\text{th}}$ the thermal velocity, $D_{\text{mag}} = \sum q_i R_{\text{ex}} (2 \pi / n) B_t (m/n) B_t$ the magnetic diffusion coefficient, $R_{\text{ex}}$ the major radius of the magnetic axis, $q$ the safety factor, $\delta B_t$ the strength of the RMPs, and $B_t$ the toroidal component of the magnetic field. In collisionless edge ergodized plasma, the experimental thermal diffusivity $\chi_{\text{ex}}$ is inconsistent with the prediction of the stochastic diffusion theory $\chi_{\text{dl}} = v_{\text{th}} D_{\text{mag}} \chi_{\text{ex}} / \chi_{\text{dl}} \approx 1/10$ for electron thermal diffusivity [8]. Small RMPs cause complete suppression of the ELM events, and have a negligible effect on energy confinement.

The above experimental results for torus plasmas imply that conventional modeling of edge transport in magnetic islands and ergodic regions should be reconsidered for a lower collisionality case, and kinetic modeling is required for understanding stochastic transport in the ergodic region [11]. In order to understand fundamental properties of collisionless edge plasma in magnetic islands and ergodic regions, and to take a new look at the modeling of transport from the viewpoint of kinetic treatment, we attempt a simulation study of neoclassical transport in magnetic islands and ergodic regions. Here, even in the field line structure disturbed by the RMPs, Coulomb collision causes a transition between a passing particle orbit and a trapped particle orbit in toroidal and helical ripples.

author’s e-mail: kanno@nifs.ac.jp
(localized and/or blocked particle orbits) [12]; in the present paper we call it the neoclassical effect on transport phenomena. Recently, we developed a new transport simulation code without the assumption of nested flux surfaces; the KEATS code [13, 14]. The code is programmed by expanding the well-known Monte-Carlo particle simulation scheme based on the δf method [15–17]. By using the KEATS code, it is possible to execute the investigation. In this paper, we apply the KEATS code to a torus plasma having the ergodic region in the edge, and discuss the interpretation of the simulation results. Here, because of a limited computational time, we treat ions (protons) in our first numerical study of transport in the ergodic region. The details of the simulation model are briefly introduced in Sec. 2. In Sec. 3, the simulation results are shown. Finally, discussion and summary are given in Sec. 4.

2. Simulation Model

We consider that a guiding center distribution function of plasma \( f = f(t, x, v, \xi) \) is separated into an equilibrium-like background \( f_0 \) and a kinetic part \( \delta f \) of the distribution, \( f = f_0 + \delta f \), where the kinetic part \( \delta f \) is considered as a small perturbation from \( f_0 \). \( \xi = v_\parallel /v, \eta_i = v \cdot b, b = B/B, B = |B|, \) and \( B \) a magnetic field. The zeroth-order distribution function \( f_0 \) is given as a local Maxwellian distribution \( f_0 = f_M(x, v) = n(m/(2\pi T))^{3/2} \exp(-mv^2/(2T)) \), where \( m \) is the particle mass, \( n = n(x) \) the density, and \( T = T(x) \) the temperature. Applying the decomposition \( f = f_M + \delta f \) to the drift kinetic equation, we have the following equation of the kinetic part \( \delta f \):

\[
\frac{D}{Dt} \delta f = -\left\{ \frac{D}{Dt} f_M - C_T \delta f_M \right\},
\]

where the operator \( D/Dt \) defined as \( D/Dt := \partial/\partial t + (u_\parallel + v_\parallel) \cdot \nabla + a \cdot \partial/\partial v - C_T, \) \( u_\parallel = v_\parallel b \) the parallel velocity, \( v_\parallel \) the drift velocity of guiding center motion, and \( a \) the acceleration. In time-evolution of the \( \delta f \) part, the background \( f_M \) is assumed to be fixed because the background is in a quasi steady-state from the viewpoint of the \( \delta f \) part. The test particle collision operator \( C_T \) is given, for simplicity, as

\[
C_T = \frac{v_{\text{def}}}{2} \frac{\partial}{\partial \xi} \left( 1 - \xi^2 \right) \frac{\partial}{\partial \xi},
\]

and it can be implemented numerically by random kicks in velocity space, which represents the Coulomb scattering process, where \( v_{\text{def}} \) is the deflection frequency. Here, we should note the statistical accuracy of the operator \( C_T \) expressed by the Monte-Carlo method [18], especially around \( |\xi| \approx 1 \). The operator \( C_T \) is the field particle collision term, which represents local momentum conservation (\( C_T \) is needed to treat the parallel transport):

\[
C_F = v_{\text{def}} \frac{m}{T} v \cdot u_0.
\]

and \( u_0 \) is given as

\[
\int d^3 v v_{\text{def}} v \delta f = \int d^3 v v_{\text{def}} \frac{mv^2}{2T} f_M.
\]

In general, effects of an electric field and neutrals are important in edge transport, but in the present paper, these effects are neglected for simplicity. (The modeling of effect of a fluctuating field is discussed in Refs. [14, 19].)

To solve Eq. (1) by Monte-Carlo techniques, we adopt the two-weight scheme of the \( \delta f \) formulation [15–17]:

\[
\begin{align*}
\frac{Dg}{Dt} &= 0, \quad \frac{ Dw}{Dt} = -\frac{Dp}{Dt} + \frac{p}{f_M} C_T f_M, \quad \frac{Dp}{Dt} = \frac{p}{f_M} \frac{Df_M}{Dt}.
\end{align*}
\]

where \( g \) is the marker distribution function, \( w \) and \( p \) are the weight functions satisfying \( pg = f_M \) and \( aw = \delta f \). The Monte-Carlo simulation code, KEATS, is programmed in an Eulerian coordinate system, i.e., the so-called helical coordinates [5], and thus, the code does not need magnetic flux coordinates. Simulation results (e.g., estimation of the particle and energy fluxes) of the KEATS code for a case of a simple tokamak field agreed with the results of the “FORTEC-3D” code [16, 17], which is a drift kinetic equation solver and uses magnetic flux coordinates.

3. Simulation Results

For investigating radial transport in the ergodic region, we use a magnetic configuration formed by adding RMPs into a simple tokamak field with concentric circular flux surfaces, where the major radius of the magnetic axis \( R_{ax} = 3.6 \) m, the minor radius of the plasma \( a = 1 \) m, and the magnetic field strength on the axis \( B_{ax} = 4 T \). The unperturbed magnetic field is given by \( B_{ax} = -(B_{ax} R_{ax}/q)Z/R^2 \), \( B_{u} = B_{ax} R_{ax}/R \), and \( B_{p} = (B_{ax} R_{ax}/q)(R - R_{ax})/R^2 \) [20], where \( q \) is the safety factor and \( q^{-1} = 0.8 - 0.78(r/a)^4 \), and \( r = \sqrt{(R - R_{ax})^2 + Z^2} \). The RMPs causing resonance with, for example, the rational surfaces of \( q = m/n = 2/1, 3/1, 4/1, \ldots \) are numerically given by using the perturbation field generated by the island control coils of LHD [21–23], and the order of the strength is \( O(|dB_{ax}/B_{ax}|) \sim 10^{-3} \). The perturbation field is calculated from the Biot-Savart law applying filament currents in the island control coils shown in Fig. 2 of Ref. [23]. For example, the \( m/n = 1/1 \) component is created mainly by the dipole field generated by four pairs of the island control coils (two adjoining pairs are located at the opposite side (changing 180 degrees in the toroidal direction) of the other two pairs), and the \( m/n = 2/1 \) component is given mainly by the cusp field generated by the other two pairs, and so on. Here, each island control coil located above the torus is paired with the coil located just below it; the coil system consists of ten pairs of the coils located above and below the torus. The Poincaré plots of the magnetic field lines on a poloidal
cross section are shown in Fig. 1. The ergodic region appears in $r/a = 0.7 \sim 1$. In the KEATS code, the number of marker particles is $N_{MP} = 16,000,000$.

To investigate the effect of the existence of the ergodic region on the transport phenomena, we evaluate the energy flux of ions (protons) $Q_i$ for our first numerical study of the transport, because the evaluation of electron energy flux is highly time-consuming. The calculation time for ions is about 40 hr in real time to get the result with sufficient numerical accuracy by using a vector-parallel supercomputer SX-7, and the calculation time for electrons is estimated to be about 40 ($\approx \sqrt{m_i/m_e}$) times that for ions if the number of PEs (processing elements) is fixed, where 64 PEs are used in this paper.

The evaluation of the ion energy flux is carried out in the configuration having higher edge temperature $T_{edge} \sim 1$ keV at a center of the ergodic region. The temperature profile is given as $T_i = T_{ax}(0.02 + 0.98 \exp[-4(r/a)^2])$ with $T_{ax} \sim 2$ keV, which neglects the existence of the ergodic region. The density profile is homogeneous, $n_i = \text{const.} = 1 \times 10^{19}$ m$^{-3}$. The radial profile of the energy flux estimated from the KEATS computations is shown as red closed circles in Fig. 2; the maximum value of the effective radial-thermal-diffusivity $\chi_{eff}^i$ is estimated as $\chi_{eff}^i \approx 0.9$ m$^2$/s at $r/a \approx 0.8$, where $\chi_{eff}^i = \frac{Q_i^{(KEATS)}}{(n_i)|\partial T_i/\partial r|}$, and $Q_i^{(KEATS)}$ is the radial energy flux evaluated by the KEATS code. For simplicity, the radial energy fluxes are given by neglecting the existence of the ergodic region, because we have no magnetic coordinate system including several magnetic field structures as the core and ergodic regions. The energy flux $Q_i$ is averaged over a concentric circular shell region including all toroidal angles as if there were nested flux surfaces. Here, in the KEATS computations, the energy flux is given as [14]

$$Q_i(x) = \int d^3r \frac{m_i v_i^2}{2} (v_i + v_e) \delta f,$$  \hspace{1cm} (8)

where $\langle $ denotes the time-average, and the averaging time is longer than the typical time scale of $\delta f$ (both the orbit and collision times). It is confirmed that the energy flux evaluated by the KEATS code becomes quasi-steady after a sufficient amount of time.

The radial profile of the flux $Q_i^{(KEATS)}$ in Fig. 2 shows that the motion along a field line in the ergodic region is dominant in the transport for the lower collisionality case. As shown in Figs. 3 and 4, the radial transport is strongly affected by the existence of the ergodic region rather than...
4. Discussion and Summary

We have been developing a drift kinetic equation solver, KEATS, to study transport phenomena in the islands and ergodic regions. We apply the code to an edge disturbed by resonant magnetic perturbations under the assumption of neglecting effects of an electric field and neutrals, and find that the radial energy transport is strongly affected by the presence of the ergodic region rather than the magnetic islands. Detailed comparison between the simulation and the stochastic diffusion theory is needed, but it is left for future study.

Statistical properties of the guiding center orbits in the ergodic region are previously studied in monoenergetic test-particle simulations in detail [24]. Doubts over the validity of the stochastic diffusion theory for the collisionless limit has been reported. Furthermore, the analytical study of radial transport in Appendix supports this result. Therefore, we interpret that the strong energy flux in the lower collisionality region is not caused by “field line diffusion.” As shown in Ref. [24], a guiding center orbit in the ergodic region is not Brownian for a lower collisionality case, thus in the present paper the flux is used to study fundamental properties of the transport in the ergodic region, instead of the transport coefficient. We should note that in the stochastic diffusion theory, the ergodic region is assumed to be not bounded radially. There is a possibility that the application of the stochastic diffusion theory is not appropriate for estimating the transport coefficients in the radially bounded ergodic region with lower collisionality [24].

For a lower collisionality case, the transport is strongly affected by the existence of the ergodic region. The strong neoclassical flux causes time-evolution of the background described by the fluid equations. Further simulation study of the transport by simultaneously solving both the kinetic and fluid equations is needed for understanding of the collisionless edge ergodized plasma: the interim report of developing the KEATS code is written in Ref. [14].

The remainder of the problem is the evaluation of the electron energy flux. We are improving the KEATS code for reducing the calculation time. The simulation results will be reported in the near future.

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Appendix. Stochastic Analysis of Radial Transport in a Perturbed Field

In general, a fluid equation representing edge plasma transport in a steady-state corresponds to a stochastic differential equation described as $dX^i_t = \gamma U^i(X_t)\,dt + \epsilon^i\langle X_t \rangle dW^j_t$ and $i, j = 1, 2, 3$ [25, 26], where $\gamma$ is a constant (e.g., $\gamma = 5n/2$ for the heat balance equation if $n = \text{const}$.), $U = (U^1, U^2, U^3)$ a steady-state flow, $D^{ij} = \epsilon^i\epsilon^j\gamma$ a diffusion coefficient, $\gamma$ a metric coefficient, $X^i = (X^1, X^2, X^3)$ a diffusion process, and $W_j = (W^1_j, W^2_j, W^3_j)$ a Brownian process. It is assumed that a fluid is exposed to noise caused by resonant magnetic perturbations (RMPs), and that fluid particle motion is described by an Itô process $dY^i_t = \gamma U^i(t, \omega)\,dt + \epsilon^i(Y_t)\,dW^j_t$, instead of the process $X^i_t$, where the flow is represented as $\tilde{U}(t, \omega) = U(Y_t) + \text{“noise”}$ and satisfies the condition $P\{\int_0^t [U(s, \omega)]\,ds < \infty \text{ for all } t \geq 0\} = 1$. $P(A)$ denotes the probability of an event $A$, $\omega$ a fluid particle label, and “noise” a random function having zero mean and finite strength. (The definition of an Itô process is given in detail in Ref. [27].) It is known that an Itô process $Y_t$ coincides in law with a diffusion process $X_t$ if and only if $\mathbb{E}[\cdot|\mathcal{F}_t] = U(Y_t)$ [27], where $X_0 = Y_0 = x_0$ is a starting point of a fluid particle at $t = 0$, $\mathcal{F}_t$ is the $\sigma$-algebra generated by the set $\{Y_s; 0 \leq s \leq t\}$, and $\mathbb{E}[\cdot|\mathcal{F}_t]$ denotes the conditional expectation with respect to $\mathcal{F}_t$. This theorem means that the “noise” cannot cause diffusion in configuration space. We should reconsider the reason why the noise created by RMPs affect the radial transport.
Let us take the following collision operator:

$$C(f) = v_{\text{col}} \frac{\partial}{\partial u} \cdot \left\{ u f + \nu_{\text{th}} \frac{\partial f}{\partial u} \right\}, \quad (A.1)$$

where $v_{\text{col}} = v_{\text{col}}(x)$ is the collision frequency, $\nu_{\text{th}}$ the thermal velocity, and $u = U + u$ the velocity of a guiding center, and $U = U(x)$ the mean velocity [28]. The operator (A.1) is simpler, but is used only to get a rough idea of collisional effects [29]. We consider the motion of a guiding center along a field line for estimation of radially spreading the guiding centers by their parallel motions in a perturbed magnetic field. The guiding center motion exposed to the collisions (A.1) is given as an Ornstein-Uhlenbeck process:

$$dx = ud\tau = (U + u)dt, \quad (A.2)$$

$$du = -v_{\text{col}} d\tau + \sigma dW, \quad (A.3)$$

where $U = U(b), u = u(b), \sigma = \nu_{\text{th}} \sqrt{v_{\text{col}}}, W$ a Brownian process for the parallel direction, i.e., $dW_{\parallel} = \dot{b} dW$, $b = B/B$ the unit vector along a field line, and $B$ the unperturbed magnetic field. Here, the effects of toroidal and helical ripples are neglected for simplicity. The equations (A.2) and (A.3) are integrated respectively as

$$x = x_0 + \int_0^t (U + u) ds, \quad (A.4)$$

$$u = e^{-v_{\text{col}} t} u_0 + \int_0^t e^{-v_{\text{col}} (t-s)} \sigma dW_{\parallel}, \quad (A.5)$$

where $x_0$ and $u_0$ are the initial values at $t = 0$. Here, $\nu_{\text{th}}$ and $v_{\text{col}}$ are constant along a field line. The effect of a perturbation field on the motion is interpreted as noise on the motion along a field line of $B$. If the effect is expressed by a linear operator $\tilde{\theta} = \tilde{N} \theta$, then

$$dx = (v + \tilde{\theta}) d\tau = (v + \tilde{N} \theta) d\tau, \quad (A.6)$$

where $\tilde{N}$ is assumed to be smooth with respect to $t$. Recall that the statistical properties of neoclassical radial diffusion in a magnetic configuration having nested flux surfaces are confirmed through direct comparison with a Brownian process in configuration space given by tracing monoenergetic test particle orbits [30]. We consider the radial transport in the ergodic region through the same way, see also Ref. [24].

For the collisional limit $t \gg 1/v_{\text{col}}$ ($v_{\text{col}} \rightarrow \infty$), the diffusion (caused by the perturbation field) in configuration space is derived from Eq. (A.6)

$$dx \approx (1 + \tilde{N}) U dt + \frac{\nu_{\text{th}}}{v_{\text{col}}} (1 + \tilde{N}) dW_{\parallel}, \quad (A.7)$$

i.e., for the collisional limit, the diffusion in velocity space directly becomes the diffusion in configuration space (see the second term in the right-hand side of Eq. (A.7)). Note that the diffusion in configuration space originates from the collisions in velocity space. When the RMPs are added to the unperturbed magnetic field having nested flux surfaces, the parallel motion of a guiding center may cause radial fluctuation. If the noise $\tilde{\theta} = (\tilde{\theta}^1, \tilde{\theta}^2, \tilde{\theta}^3)$ is given as

$$\tilde{\theta}^i = \langle \tilde{N} \theta^i \rangle = \frac{\nu B_i}{B} \epsilon^{jik} \hat{v}_k \phi(t; i), \quad (A.8)$$

then the radial diffusivity $D_r = D_r |\delta B_i/B| \tilde{\theta}^i$ is obtained for the collisional limit, where $\phi$ is the unit vector for the poloidal direction, $\hat{v}_k$ the strength of the RMPs satisfying $|\delta B_i/B| \ll 1$, $B_i$ the toroidal component of $B$, $g = \det(g_{ij})$ the square of Jacobian, $\epsilon^{ijk}$ the Levi-Civita symbol, $\phi(t; i)$ the $i$th component of a zero mean random vector having a mean square of $E[\phi^2] = 1$ and being independent of $dW_{\parallel}$, and $D_r = \nu_{\text{th}}/v_{\text{col}}$ the parallel diffusivity [31]. Note that in the monoenergetic test-particle simulation [24], the radial behavior of the guiding center orbits for the collisional limit is observed numerically to be a standard diffusion process.

For the collisionless limit ($v_{\text{col}} \rightarrow 0$), the noise term $\tilde{N}(U + u_0)$, i.e., the motion along a field line, is dominant in the expression of the guiding center orbits. This noise term cannot cause diffusion in configuration space even if the ergodic region extends boundlessly, as shown in the first paragraph in this section; see also Refs. [14, 19, 27]. The radial transport should be treated in the framework of the theory based on the statistics of the guiding center motions exposed to the collisions in velocity space (i.e., the theory given by solving the drift kinetic equation), rather than the theory based on the “field line diffusion” without collisions. Note that it is not a trivial problem whether the radial flux in the ergodic region for a lower collisionality case can be estimated only by tracing monoenergetic test particle orbits, because the radial behavior of the test particle orbits is not a Brownian process [24]. Thus, in the present paper we employ the drift kinetic equation solver to obtain the distribution function of the guiding centers.

The above discussion shows that for a lower collisionality plasma ($t \leq 1/v_{\text{col}}$), the motions are not interpreted as the diffusion process predicted by the stochastic diffusion theory.


