Monte Carlo simulations for stellarators

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Introduction

For tokamaks the $\delta f$ Monte Carlo technique is a powerful method to study kinetic phenomena in plasmas, e.g. the bootstrap current [1, 2]. The idea of this approach depends on the determination of the deviation $\delta f$ from a Maxwellian. Starting from the drift kinetic equation, linearization yields a marker equation for the weights of test particles which contains the drift velocity. $\delta f$ methods show a significantly improved performance compared to full-$f$ Monte Carlo techniques.

In contrast to tokamaks the radial drift of ripple-trapped particles may result in a significantly enhanced radial transport in stellarators. In the $\delta f$ scheme this is reflected by the solution of the marker equation which lead to oscillating weights in the tokamak case, but to strongly increasing weights of the ripple-trapped particles in stellarators. This ripple-trapped contribution makes the application of the $\delta f$ Monte Carlo technique for stellarators a demanding problem for estimating the bootstrap current.

The $\delta f$ method

Numerical simulation of neoclassical processes has been greatly improved by the introduction of the $\delta f$ Monte Carlo technique, which consists of representing the equilibrium part of the plasma analytically, and using particle simulation to represent only deviations from the equilibrium.

Let’s consider the drift kinetic equation. Take the distribution function $f(\vec{x}, p, v, t)$ with $p = v_B/v$. Then

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + (\mathbf{v}_i + \mathbf{v}_d) \cdot \nabla f + p \frac{\partial f}{\partial p} + \mathbf{v} \frac{\partial f}{\partial v} = C(f)$$  \hspace{1cm} (1)

where $\mathbf{v}_i$ and $\mathbf{v}_d = \mathbf{v}_{E \times B} + \mathbf{v}_{\nabla B}$ are the drift velocities of the guiding center and $C(f)$ is a collision operator.

Linearization of $f$ yields $f = f_M + f_1$ where $f_M$ represents the Maxwellian as 0th order distribution function. This leads to an inhomogeneous equation for $f_1$

$$\frac{\partial f_1}{\partial t} + (\mathbf{v}_i + \mathbf{v}_d) \cdot \nabla f_1 + p \frac{\partial f_1}{\partial p} + \mathbf{v} \frac{\partial f_1}{\partial v} = - \frac{df_M}{dt} + C(f_1)$$  \hspace{1cm} (2)

where $f_M$ is considered as a steady-state distribution with $C(f_M) \approx 0$. 


The system of characteristic equations for the Hamiltonian part of the above equation contains now an additional equation the so called marker equation

\[ \frac{d}{dt} f_1 = - \frac{d}{dt} f_M. \]

In the case of a mono-energetic distribution \( f_M(\psi, v) \) in magnetic (Boozer) co-ordinates the density \( n(\psi) \), the temperature \( T(\psi) \) and the potential \( \Phi(\psi) \) are considered as constant on flux surfaces. In the neoclassical ordering, both terms with \( \frac{\partial f_1}{\partial \psi} \) and \( \frac{\partial f_1}{\partial v} \) are neglected with respect to the corresponding 0th order terms

\[
(v_1 + v_d) \cdot \nabla_{\theta, \psi} f_1 + p \frac{\partial f_1}{\partial p} - C(f_1) = - (v \nabla H)_{\psi} \left\{ \frac{n'}{n} + \frac{q \Phi'}{T} + \left( \frac{m v^2}{2T} - \frac{3}{2} \right) \frac{T'}{T} \right\} f_M. \tag{3}
\]

Being in this case the weighting function is

\[ w = - \int (v \nabla H)_{\psi} dt. \]

**Simulation results**

As a first step a Monte-Carlo technique following the ansatz of Boozer, Kuo-Petravic[3] with the additional marker equation was implemented. The simulation is performed by inserting test particles, or markers, at random locations on a designated flux surface and measuring dispersion on flux surfaces with respect to the simulation time which leads to an estimation of the mono-energetic particle transport coefficient.

To demonstrate the different behavior of the weights two stellarator cases and one tokamak case are compared. As stellarator examples the LHD (3.75 m standard configuration) and the Wendelstein 7-X (standard case) are compared. As an example for an elongated tokamak only the averaged toroidal curvature term in the \( |B| \)-Fourier spectrum of the W7-X configuration was taken into account.

In figure 1 the mono-energetic transport coefficient, normalized to the plateau value of the equivalent axisymmetric tokamak (with circular cross section), \( \Gamma_{11}^{*} \), is plotted as a function of the collisionality, \( \nu^{*} = \nu / v \cdot R / \lambda \), where \( v \) is the velocity of the mono-energetic test particles considered and \( \nu \) is the collision frequency. The flux surface at half of the plasma radius has been chosen. One can see that in the long-mean-free-path (\( \text{lmfp} \)) regime for a zero radial electric field the mono-energetic transport coefficient, \( \Gamma_{11}^{*} \), increases proportional to \( 1 / \nu \) Especially the LHD configuration shows an enhanced transport. That means that ripple-trapped particles rapidly move outwards leading to convection with decreasing collisionality.

Figure 2 shows the deviation from the Gaussian distribution in the \( \text{lmfp} \) regime. In the case of high collisionality the distribution of particles fits well to a Gaussian, but with low collisionality the particle distribution has a non Gaussian tail. This tail which represents the convective
losses is the reason for the failure of the standard $\delta f$ method determining the bootstrap current.

The code was benchmarked with various methods like the numerical solution of the ripple-averaged or the drift kinetic equation\cite{4}.

**Extended $\delta f$ approach**

The results of the $\delta f$ simulation for the bootstrap current from R. B. White\cite{5} showed that this approach did not work for stellarators in the \textit{lmfp} regime due to this strong convective losses. If we assume a zero radial electric field then the mono-energetic transport coefficients in the \textit{lmfp} increase proportional to $1/\nu$ whereas the coefficient for the bootstrap current is approximately constant. In this case especially ripple-trapped particles are strongly weighted, though they do not directly contribute to the bootstrap current.

A more sophisticated approach to estimate the transport coefficients in the \textit{lmfp} regime will be presented in the following. According to eq.(2) we separate the distribution function in one part with the radial drive and in another part with the parallel drive. Now we can write the linearized form of eq.(2) as

$$V (f_1 + g_1) − C (f_1 + g_1) = −(ν_{VB})_\psi \frac{df_M}{d\psi} + \frac{q}{TB} p v E_\parallel B_M.$$  \hspace{1cm} (4)$$

where $V$ represents the linearized Vlasov operator with $\dot{\psi}$ and $\dot{v}$ terms omitted. We split the
problem into two equations

\[ V(f_1) - C(f_1) = -(\nabla B)_\psi \frac{df_M}{d\psi} \]  

(5)

\[ V(g_1) - C(g_1) = \frac{q}{TB} p \nabla E \cdot B f_M \]

and get two marker equations

\[ w_f = \int (\nabla B)_\psi \, dt \]  

(6)

\[ w_g = \int p \, dt. \]

due to the two thermodynamic driving forces on the right hand side of the system (5).

The mono-energetic particle transport as well as the parallel conductivity coefficients are given by \( \langle \int \psi f_1 \, dp \rangle \) and \( \langle \int p g_1 \, dp \rangle \), respectively. These flux-surface-averaged coefficients can be calculated by applying the \( \delta f \) Monte Carlo technique directly to eqs. (5) and (6).

In the \( lmfp \) regime the distribution \( f_1 \) (\( g_1 \)) is mainly determined by it’s symmetric (asymmetric) part due to the symmetric (asymmetric) driving force on the right hand side of eq. (5). The coupling to the asymmetric (symmetric) part of \( f_1 \) (\( g_1 \)) is proportional to \( \nu^a \) and becomes extremely weak in the very \( lmfp \) regime. Consequently the “off-diagonal” coefficients, the bootstrap current (Ware pinch) coefficient given by \( \langle \int p f_1 \, dp \rangle \) (\( \langle \int \psi g_1 \, dp \rangle \)) are difficult to obtain by a straightforward \( \delta f \) Monte Carlo application to eqs. (5) and (6).

The “advanced” \( \delta f \) method for calculating the “off-diagonals” is based on good analytical estimation of the dominating parts of \( f_1 \) and \( g_1 \). Within the \( 1/\nu \)-regime, \( f_1 \) can be estimated by bounce-averaging eq. (5) for the trapped particles and integrating the collision term with respect to the magnetic moment (the passing particle distribution can be neglected). The disadvantage of this approach is related to the complex dependence of the trapped particle \( f_1 \) on the magnetic field topology. Solving the problem in 2nd order for \( g_1 \) is more promising. The asymmetric component of \( g_1 \) is only defined by the passing particles in the very \( lmfp \) limit which is easier to obtain. The Ware pinch coefficient can be calculated by the \( \delta f \) Monte Carlo by using the asymmetric estimate of \( g_1 \), and the bootstrap coefficient is obtained from the Onsager symmetry.

References