Evaluation of Monte Carlo Calculation Accuracy for α Particle Confinement Analysis in Heliotron Reactors^{*)}

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The GNET code is used to study α particle confinement with energy diffusion and pitch angle scattering in helical plasmas based on the Monte Carlo technique. The dependency of the accuracy of the distribution function on the number of test particles is studied. It is found that, as the number of test particles is increased, the shape of the velocity space distribution becomes smooth and the scattering of the energy loss fraction becomes small and converges to 5.06%.

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1. Introduction

In a heliotron reactor, the magnetic field is generated mainly by the coil current, and this system does not require a plasma current to produce a poloidal magnetic field. As a result, disruption due to the plasma current are avoided. However, the plasma behavior in three dimensional magnetic configuration -such as heliotron reactors- are more complex than in tokamaks. Several physics and technical problems remain to be studied, such as the behavior and confinement of high energy α particles in a helical plasma.

In heliotron systems, the magnetic field has two types of ripples, one is the helical ripple and the other is the toroidal ripple. An α particle trapped in a helical ripple is called a helical trapped particle. An α particle trapped in a toroidal ripple is called a toroidal trapped particle. An α particle which is trapped in neither the helical nor toroidal ripples is called a passing particle. Additionally, an α particle which transits between being a trapped particle and a passing particle is called a transition particle. These α particle motions cause complex orbits of trapped particles and enhance radial diffusion of energetic α particles.

In heliotron devices, when D-T experiments are performed, the confinement of high energy α particles is a very important issue. In order to keep a high plasma temperature, the high energy α particles must be confined until they thermalize. If high energy α particles are lost, not only is the heating power reduced, but the first wall would be damaged locally. Therefore, it is important to understand the behavior and the confinement of high energy α particles.

In this paper, the behavior of α particles are analyzed by using the Monte Carlo method. In this method, the resulting quantities are estimated using a finite number of test particles. Thus, statistical noise due to the finite number of test particles is inevitable. It is important to examine how many test particles are required to obtain a solution to the desired accuracy. However, the minimum number of particles necessary for an accurate evaluation of the α particle distribution in a helical magnetic configuration has not been well studied, previously.

In this paper, we have verified the dependence of the α particle distribution on the number of test particles assuming the helical type reactor extending the LHD [1] magnetic configuration.

2. Simulation Model

In this study, we assume the fusion reactor extending the LHD magnetic configuration. This magnetic configuration has the neoclassical transport optimized configuration in vacuum (the NC configuration), as shownin Fig. 1, which is based on the configuration $R_{ax} = 3.53$ m in LHD [2], where R_{ax} is the magnetic axis major radius. This reactor has a plasma volume of 1000 m³ and a magnetic field strength of 5 T.

The drift kinetic equation for the α particles in five dimensional phase space, with pitch angle and energy scattering, is described as follows :

$$\frac{\partial f}{\partial t} + (\vec{v}_{\parallel} + \vec{v}_{\perp}) \cdot \nabla f + \dot{\vec{v}} \cdot \nabla_{V} f = C^{\text{coll}}(f) + L^{\text{particle}}(f) + S_{\alpha}, \qquad (1)$$

where *f* is the distribution function of α particles, \vec{v}_{\parallel} is the velocity parallel to magnetic lines, \vec{v}_{\perp} is the drift velocity, C^{coll} is the linear Coulomb collision operator, L^{particle} is the loss from the last closed flux surface (LCFS), and S_{α} is the source term of the α particle generated by the fusion reaction. We solve equation (1) using the GNET (Global NEoclassical Transport) code [3], which uses a Monte Carlo technique to calculate the distribution function for the α

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Fig. 1 The flux contour for the NC configuration in the real coordinate. R is the major radius and Z is the minor radius in vertical direction.

particles.

In order to solve the drift kinetic equation (1), we introduce the Green function \mathcal{G} as follows :

$$\frac{\partial \mathcal{G}}{\partial t} + (\vec{v}_{\parallel} + \vec{v}_D) \cdot \nabla \mathcal{G} + \dot{\vec{v}} \cdot \nabla \vec{v} \mathcal{G} = C^{\text{coll}}(\mathcal{G}) + L^{\text{particle}}(\mathcal{G}), \qquad (2)$$

with the initial condition $\mathcal{G}(\vec{x}, \vec{v}, t = 0 | \vec{x}', \vec{v}') = \delta(\vec{x} - \vec{x}')\delta(\vec{v} - \vec{v}')$ and, $f = \int_0^t \mathcal{G}dt$. The function \mathcal{G} is evaluated using the equations of guiding center motion of test particles, which is expressed by the Hamiltonian of charged particles

$$H = \frac{1}{2}mv_{\parallel}^2 + \mu B(\psi, \theta, \phi) + q\Phi(\psi), \qquad (3)$$

in Boozer coordinates. In this study, the electrostatic potential Φ is assumed to be zero. In order to solve the equation of guiding center motion, the 6th-order Runge-Kutta method is used.

The linear Coulomb collision operator C^{coll} includes the operators of the pitch angle scattering and the energy scattering with background ions (deuterium and tritium) and electrons. These operators have been evaluated by Boozer and Kou-Petravic [4]. The former operator is

$$\lambda_n = \lambda_{n-1}(1 - \nu_d \tau) \pm \left[\left(1 - \lambda_{n-1}^2 \right) \nu_d \tau \right]^{1/2}, \qquad (4)$$

where $\lambda = v_{\parallel}/v$, $v_{\rm d}$ is the deflection collision frequency, τ is a time step, and subscripts *n* and *n* – 1 are numbers of time step. The symbol \pm means the sign is to be chosen randomly. The latter operator is described as the energy at time step *n*, E_n ,

$$E_{n} = E_{n-1} - (2\nu\tau) \left[E_{n-1} \left(\frac{3}{2} + \frac{E_{n-1}}{\nu} \frac{d\nu}{dE_{n-1}} E_{T} \right) \right]$$

$$\pm 2 \left[E_{T} E_{n-1} \left(\nu\tau \right) \right]^{1/2}, \qquad (5)$$





Fig. 2 The initial radial profile of α particles, for $n(0) = 2.0 \times 10^{20} \text{m}^{-3}$, with 50,000 test particles.

where ν is the collision frequency and $E_{\rm T}$ is thermal energy. The source term S_{α} is evaluated by using the fusion

reaction rate

S

$$\propto \int \int f_{\rm D}(v_{\rm D}) f_T(v_{\rm T}) \sigma(E) |v_{\rm D} - v_{\rm T}| \, \mathrm{d}v_{\rm D} \mathrm{d}v_{\rm T}, \quad (6)$$

where σ is a total fusion reaction cross-section, *E* is relative energy between deuterium and tritium, *n* is a radial profile of plasma density, and subscript D and T are deuterium and tritium respectively. f_D and f_T are the Maxwellian distribution function of deuterium and tritium respectively. *v* is dependant on the plasma temperature *T*. In this paper, *T* and *n* are taken to be

$$T(\rho) \text{ [keV]} = 9.5(1 - \rho^2) + 0.5,$$
 (7)

$$n(\rho) \ [10^{20} \text{m}^{-3}] = 1.9(1 - \rho^8) + 0.1,$$
 (8)

where ρ is a normalized minor radius. The initial radial profile of the α particles is plotted in Fig. 2 where the horizontal axis is the normalized plasma minor radius and the vertical axis is the number of particles distributed on each magnetic flux surface.

In this figure, $5 \times 10^4 \alpha$ particles are generated. We study the particle number dependency by using the number of α particles N_{α} from 10³ to 10⁵.

3. Simulation Results

We run the GNET code with a varying number of test particles, N_{α} , from 10^3 to 10^5 , until the α particle distribution reaches steady state. We study the *N* dependency of the α particle distribution in the helical type reactor extending the LHD magnetic configuration.

We first analyze the velocity-space distribution function of α particles. Figure 3 shows the velocity distribution of α particles in the plasma for various values of N_{α} . v_{\parallel} is the velocity parallel to the magnetic field and v_{\perp} is the velocity perpendicular to the magnetic field. The v_{\parallel} and



Fig. 3 Contour plots of the particle density in velocity space for the cases $N_{\alpha} = 2000$, 10, 000, and 50, 000. The contour levels are spaced logarithmically in the velocity space distribution.

Table 1 Deviation from the fitted lines.

N_{lpha}	$\theta = 90^{\circ}$	$\theta = 60^{\circ}$	$\theta = 30^{\circ}$
2000	1.01×10^{-3}	2.57×10^{-3}	1.06×10^{-2}
10000	2.63×10^{-4}	4.24×10^{-4}	2.66×10^{-3}
50000	1.09×10^{-4}	2.27×10^{-4}	6.98×10^{-4}
100000	6.87×10^{-5}	1.34×10^{-4}	7.55×10^{-4}

 v_{\perp} are normalized by $v_{1 \text{ M}}$, which is the α particle velocity of 1 MeV. There are 128 grid points in v_{\parallel} and 64 grid points in v_{\perp} . The distribution of low energy α particles becomes peaked by slowing down. It is found that the contours of the velocity space distribution becomes smooth as the number of test particles increases.

Next, we compare the velocity space distribution in the same pitch angle. Figure 4 shows the profile of the velocity space distribution at the specific pitch angle $\theta = 90^{\circ}$ for $N_{\alpha} = 2 \times 10^{3}$ and 10^{5} , where the distributions are normalized by the slowing down time, τ_{s} . The blue line shows a cubic fit to the data points. We can see that the velocity profiles become smooth as the number of test particles increases, and we see that the distribution converges. There is no clear difference of the velocity profiles between the 5×10^{4} and 10^{5} test particle cases. We show the deviation, σ_{α} , from the fitted curve (cubic functions) on Table 1. We



Fig. 4 The velocity profiles at the pitch angle $\theta = 90^{\circ}$ for each particle number case are normalized by the slowing down time τ_s . The blue line is the fitted curve. The lower sub-figures show the difference between each α particle distribution and the fitted curve.



Fig. 5 The energy loss fractions of α particle η_{loss} are calculated until α particles are thermarized for $N_{\alpha} = 1000 \sim 100,000$.

can see that σ_{α} becomes small when increasing of the number of particles and $\sigma_{\alpha} \leq 10^{-4}$ when $N_{\alpha} > 5 \times 10^{4}$. We conclude that the velicity-space distribution of α particles is well converged for $N_{\alpha} > 5 \times 10^{4}$.

Figure 5 shows the energy loss fraction of the α particles, η_{loss} , for several N_{α} . The energy loss fraction is defined as

$$\eta_{\text{loss}} = \frac{E_{\text{loss}}}{E_{\text{initial}}} \times 100, \tag{9}$$
$$E_{\text{loss}} = \int_{0}^{t} \int_{-v_{\parallel}}^{v_{\parallel}} \int_{0}^{v_{\perp}} \int_{V} L^{\text{particle}}(f) \mathrm{d}V \mathrm{d}v_{\perp} \mathrm{d}v_{\parallel} \mathrm{d}t,$$
$$E_{\text{initial}} = \int_{0}^{t} \int_{-v_{\parallel}}^{v_{\parallel}} \int_{0}^{v_{\perp}} \int_{V} S_{\alpha} \mathrm{d}V \mathrm{d}v_{\perp} \mathrm{d}v_{\parallel} \mathrm{d}t.$$

Table 2 Specs of 8 core Xeon (Cluster Node).

Computer name	vine	
Number of nodes	16	
	3.16 GHz (Intel Xeon	
CPU	Quadcore Dual) $\times 2$ / node	
Memory	16GB/ node	
HDD	73GB / node	



Fig. 6 The calculation time for each case. The calculation time increases linearly with the number of test particles. On the blue line, the calculations have not been optimized. On the green line, the calculations have been optimized.

When the particle number is small ($N_{\alpha} < 2 \times 10^4$), η_{loss} is not converged. When $N_{\alpha} > 3 \times 10^4$, η_{loss} converges to 5.06%. We see that 5×10^4 or more of test particles are necessary to accurately calculate η_{loss} .

However, we also have to consider the CPU cost for the calculation. We estimate the CPU time for the GNET code in each case Using the computer specs shown in Tabel 2. Each blade has 2 Quad Core CPUs and 16 GB memory. Figure 6 shows the calculation time for each case. The horizontal axis is the number of test particles, and the vertical axis is the calculation time per core. The blue line is the calculation time without optimization, and the green line is the calculation time with optimization, where the optimization option is specified in the compilation process. When we run GNET without optimization, the calculation time t_{ct} is t_{ct} [sec] ~ $2.2 \times N_{\alpha}$. When we run with optimization, the calculation time t_{ct} is t_{ct} [sec] ~ N_{α} . In the case of 5×10^4 particles, the calculation take about 14 hr.

4. Summary

We have studied the test particle number dependency of the accuracy of α particle distributions in a helical type fusion reactor using the drift kinetic equation solver code GNET. We vary the number of test particles, N_{α} : $10^3 \sim$ 10^5 . We have found that the contours of the velocity space distribution becomes smooth as the number of test particles increases. When $N_{\alpha} > 3 \times 10^4$, the variation of the energy loss fraction, η_{loss} , becomes very small and converges to 5.06%. We have seen that 5×10^4 or more test particles are necessary to accurately calculate η_{loss} . In the case of 5×10^4 particles, we need about 14 hours of CPU time on our Xeon cluster.

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