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δf Monte Carlo computations of neoclassical transport in stellarators with reduced variance *

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In Ref. [1] a method with reduced variance in computations of mono-energetic transport coefficients which combines the standard δf method [2] with an algorithm employing constant particle weights and re-discretizations of the test particle distribution in phase space has been presented. This method is formally free of bias and allows simultaneous computations of bootstrap coefficient and diffusion coefficient. The linearized drift kinetic equation for the normalized perturbation of the distribution function $\hat{f}$ takes the following form if the total energy and the perpendicular adiabatic invariant are used as velocity space variables

$$\mathscr{L}_D \hat{f} \equiv \left(\frac{\partial}{\partial t} + \mathbf{V}_g \cdot \nabla - \mathscr{L}_C \right) \hat{f} = \dot{\psi} \equiv \mathbf{V}_g \cdot \nabla \psi \,, \tag{1}$$

where $\mathbf{V}_g$, and $\dot{\psi}$ are guiding center drift velocity and its contra-variant ψ-component, respectively, ψ is a flux surface label, $\mathscr{L}_C$ is the Lorentz collision operator, and the marker $\hat{f}$ is defined through the local Maxwellian distribution function f_M and the total distribution function f via $f = f_M - \hat{f}\partial f_M/\partial\psi$. In the following, instead of the total energy and the perpendicular invariant the velocity module v and the pitch parameter $\lambda = v_\parallel/v$ are used as velocity space variables. The mono-energetic radial diffusion coefficient and the normalized bootstrap coefficient, respectively, are given by

$$D_{\text{mono}} = -\frac{1}{\langle|\nabla\psi|\rangle^2} \left\langle \frac{1}{2} \int_{-1}^{1} \mathrm{d}\lambda\, \hat{f}\dot{\psi} \right\rangle, \qquad \lambda_{bb} = -\frac{3}{\rho_L B_0 \langle|\nabla\psi|\rangle} \left\langle \frac{1}{2} \int_{-1}^{1} \mathrm{d}\lambda\, \hat{f}\lambda B \right\rangle. \tag{2}$$

Here, ρ_L is the Larmor radius in the reference magnetic field B_0, B is the magnetic field module and $\langle A\rangle = \int \mathrm{d}\vartheta \int \mathrm{d}\varphi \sqrt{g} A / (\int \mathrm{d}\vartheta \int \mathrm{d}\varphi \sqrt{g})$ denotes the average over the volume between neighboring flux surfaces with ϑ and φ being the poloidal and the toroidal angles of flux coordinates and g is the metric determinant of flux coordinates $(\psi, \vartheta, \varphi)$. In the absence of a temperature gradient and a radial electric field the quantity λ_{bb} is linked to the equilibrium (bootstrap) current density $j_\parallel$ and the gradient of the pressure p by $\lambda_{bb} = -\left\langle j_\parallel B\right\rangle (c\,\langle|\nabla\psi|\rangle\, \mathrm{d}p/\mathrm{d}\psi)^{-1}$ if the mean free path l_c is put to a constant during the energy convolution. In the following D_{mono} is normalized by the plateau diffusion coefficient $D_{\text{plateau}} = \pi v \rho_L^2 (8\sqrt{2}\iota R)^{-1}$ where ι is the rotational transform and R is the major radius.

A variety of variance reduction methods developed mainly for Monte Carlo solutions of integral equations need a re-formulation of equation (1). If a steady state solution is looked for, $\hat{f}(t,\mathbf{z}) = \hat{f}(\mathbf{z})$, where $\mathbf{z} = (\vartheta, \varphi, \lambda)$, this leads to an integral equation for $F(\mathbf{z}) = (g(\mathbf{z}))^{1/2}\hat{f}(\mathbf{z})$

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which is given as $F(\mathbf{z}) = \int \mathrm{d}^3 z_0 K(\mathbf{z},\mathbf{z}_0) F(\mathbf{z_0}) + Q(\mathbf{z})$ where $Q(\mathbf{z})$ is a source term and the kernel $K(\mathbf{z},\mathbf{z}_0)$ is given by an expectation value which can be modeled in a standard way [3]. The solution of this equation can be presented as an expectation value of an integral along a stochastic orbit $F = \sum_{k=0}^{\infty} \mathscr{K}^k Q = C_0 \sum_{k=0}^{\infty} \overline{w_{(0)}\, \delta\left(\mathbf{z} - \mathbf{z}_{(k)}\right)}$, where $\mathbf{z}_{(k)}$ and $w_{(0)}$ are (random) test particle positions and weights and $C_0 = \int \mathrm{d}^3 z\, (g(\mathbf{z}))^{1/2}$. The averages (2) then are given by expectation values as

$$D_{\text{mono}} = -\frac{1}{\langle|\nabla\psi|\rangle^2} \sum_{k=0}^{\infty} \overline{w_{(0)}\, \dot{\psi}(\mathbf{z}_{(k)})}\,, \qquad \lambda_{bb} = -\frac{3}{\rho_L B_0 \langle|\nabla\psi|\rangle} \sum_{k=0}^{\infty} \overline{w_{(0)} \lambda_{(k)} B(\mathbf{z}_{(k)})}\,. \tag{3}$$

The method of constant test particle weights described by (3) has rather low variance for computations of D_{mono}, however, variance of λ_{bb} has a very unfavorable scaling with collisionality. Only the orbits originating in the boundary layer located in the velocity space around the trapped-passing boundary λ_{t-p} which is determined by the absolute maximum of the magnetic field on the flux surface contribute to λ_{bb}. This follows from the fact that the test particle weight $w_{(0)}$ depends on the coordinates of the starting point of the orbit but is independent of the sign of the starting pitch parameter $\lambda_{(0)}$. Test particles starting deeply in the trapped particle region produce almost no contribution to λ_{bb} because when they reach the passing region after many oscillations in the magnetic well, probabilities to be detrapped to the co-passing region with $\lambda > 0$ and to the counter-passing region with $\lambda < 0$ become weakly dependent on the starting point (and, therefore, on $w_{(0)}$) and are almost the same. Thus, contributions from such particles compensate each other statistically. Numerically this results in statistical compensation of large random numbers which introduces large variance in the computation. Therefore, in the long mean free path regime only trapped particles starting from the boundary layer whose detrapping probabilities essentially depend on the starting position and passing particles from this layer whose trapping probabilities also depend on the starting position can produce on average essential contribution to λ_{bb} (see Fig. 1).

In order to develop a formally "unbiased" method for computations it is convenient to split the source into "passing" and "trapped" sources $Q_p = \chi Q$ and $Q_t = Q - Q_p$ using $\chi = 0.5\{1 + \tanh[(|\lambda| - \lambda_{t-p})/\Delta\lambda]\}$, where λ_{t-p} is the pertinent trapped-passing boundary, and solve the problem with each source independently. Results for transport coefficients for these two sources are added up at the end. The problem with Q_p is solved with the standard method without using an annulus limiting the test particle motion. Since accumulation of large weights is avoided for this source, the convergence of the bootstrap coefficient is similar to that in a tokamak. For the treatment of the problem with Q_t one should notice the following. Particles with different signs of the weight detrapped from different magnetic wells quickly mix up in the close vicinity of the boundary layer so that each phase space volume element in this region contains both, particles with positive and negative weights if the number of test particles is large enough. The total weight in such a volume element which actually determines the distribution function being of relevance for the averages is smaller than the sum of the modulus of test particle weights contained in this element. Therefore a periodic re-discretization procedure which replaces all particles in the phase space volume element ("cell") with fewer particles which carry the total weight in this element would lead to a significant reduction in the test particle number. For the first iteration of this procedure (a detailed description is given in [1]) an algorithm with alternating weights is used. After the first iteration these test particle weights are divided by the number of steps so that test particles represent the discretized distribution used as a source within the second iteration. Starting from this second iteration, an algorithm with fixed test particle weights is used. Within each iteration, the test particles perform a number of steps corresponding to a time much smaller than collision time and large enough in order to fill the grid using a limited number of test particles. The source for the next iteration is computed by scoring weights on a grid. Due to annihilation of the weights on the grid and fixed module of the weight, the number of test particles needed for sampling the source term from the grid is decreasing with iterations and iterations are stopped when this number is below one, (see Fig. 2). Since source terms generated in this way are small in the passing and boundary region, particles are generated there with smaller weights and particles which enter the boundary layer from the trapped side are split in such a way that the number of test particles in the passing and trapped regions is of the same order. Results of computations with negligible radial electric fields stay in good agreement with results from NEO-2 a field line tracing code which computes transport coefficients for zero radial electric fields in arbitrary collisionality regimes [4], as shown in Figs. 3-5. In these figures, also results of computations with finite values of the electric field parameter are presented.

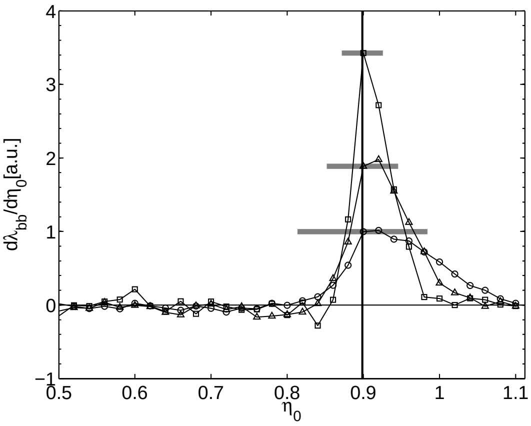

Fig. 1: Distribution $d\lambda_{bb}/d\eta_0$ of test particle contributions to λ_{bb} over the starting values of the normalized perpendicular invariant $\eta_0 = (1-\lambda_0^2)B_0/B(\mathbf{z}_0)$ for a tokamak with aspect ratio $R/r = 10$, where B_0 is a reference magnetic field. Collisionality parameters L_c/l_c are $1\cdot 10^{-2}$ (circles), $3\cdot 10^{-3}$ (triangles) and $1\cdot 10^{-3}$ (squares). The width of the boundary layer for each curve is indicated by a horizontal bar. The position of the trapped-passing boundary is shown by the solid vertical line.

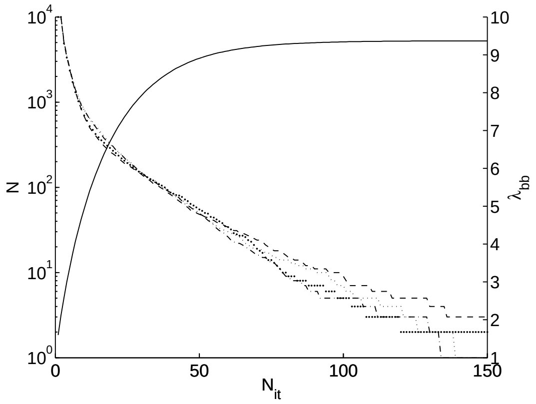

Fig. 2: Number of simulation particles N for four sub-runs (left axis, dashed lines) and final value of the bootstrap coefficient λ_{bb} computed from 40 sub-runs (right axis, solid line) versus number of iterations N_{it}. Here, 150 iterations approximately correspond to five collision times.

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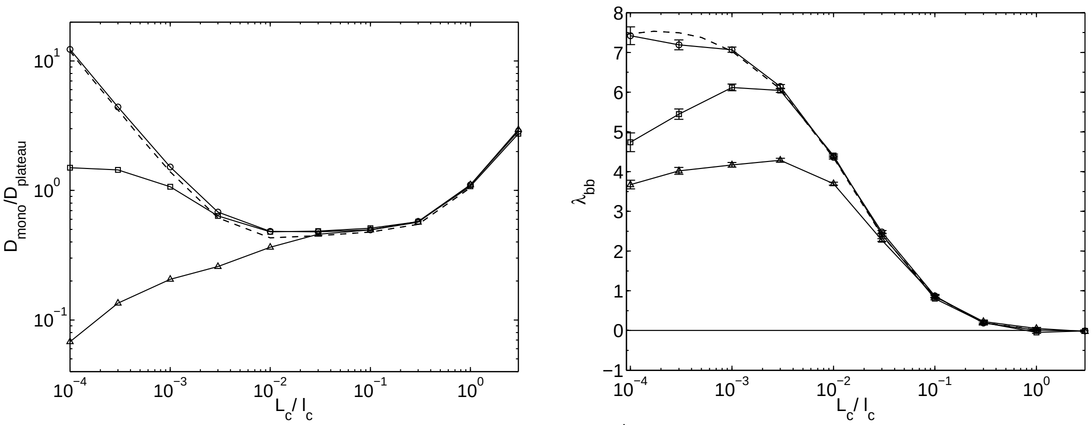

Fig. 3: Normalized diffusion coefficient $D_{\text{mono}}/D_{\text{plateau}}$ (left) and bootstrap coefficient λ_{bb} (right) for LHD with R=360 cm vs. collisionality parameter L_c/l_c at half plasma radius computed by NEO-MC (solid lines) and NEO-2 (dashed line) for $E_r/(vB) = 0$ (circles), $1 \cdot 10^{-4}$ (squares), $1 \cdot 10^{-3}$ (triangles).

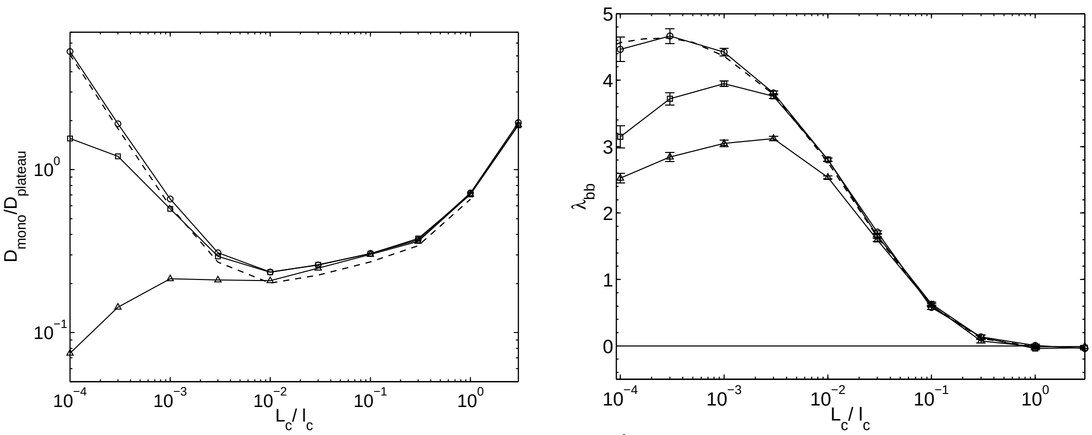

Fig. 4: Normalized diffusion coefficient $D_{\text{mono}}/D_{\text{plateau}}$ (left) and bootstrap coefficient λ_{bb} (right) for LHD with R=353 cm vs. collisionality parameter L_c/l_c at half plasma radius. Markers and line types are the same as in Fig. 3.

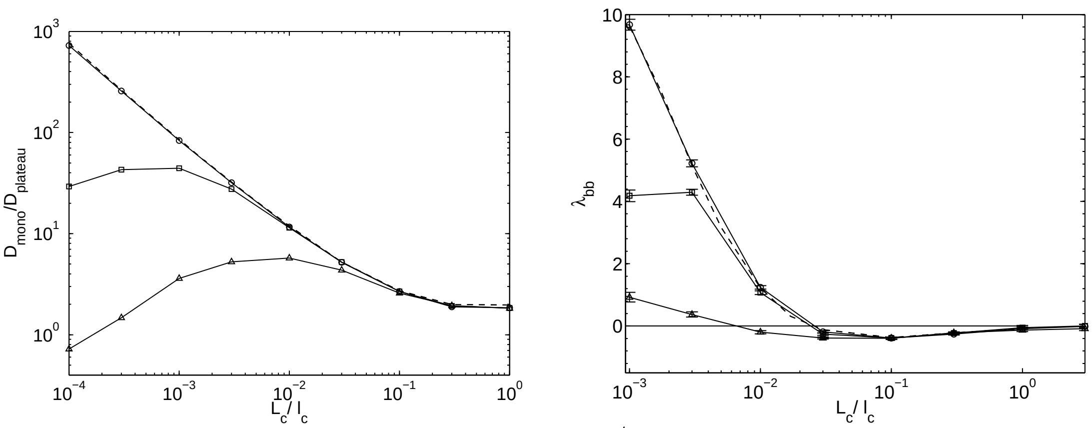

Fig. 5: Normalized diffusion coefficient $D_{\text{mono}}/D_{\text{plateau}}$ (left) and bootstrap coefficient λ_{bb} (right) for TJ-II standard configuration vs. collisionality parameter L_c/l_c at half plasma radius. Markers and line types are the same as in Fig. 3.