Variance reduction in computations of neoclassical transport in stellarators using a δf method [*]

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In absence of radial electric field, mono-energetic transport coefficients are determined by the steady state solution of the linearized drift kinetic equation for the normalized perturbation of the distribution function $\hat{f}$ (marker),

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

where $v_\parallel$, $\mathbf{h}$, $\mathscr{L}_C$ and $\dot{\psi}$ are parallel velocity, unit vector along the magnetic field, Lorentz collision operator and co-variant ψ-component of the drift velocity, respectively. Here, ψ is a flux surface label, and a marker is defined through the local Maxwellian distribution function f_M and the total distribution function f via $f = f_M - \hat{f} \partial f_M / \partial \psi$. The mono-energetic radial diffusion coefficient and the normalized bootstrap coefficient, respectively, are given by

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

where $\lambda = v_\parallel / v$ is the pitch parameter, ρ_L is the Larmor radius in the reference magnetic field B_0, B is the magnetic field module and $\langle \dots \rangle$ denotes the average over the volume between neighboring flux surfaces. The quantity λ_{bb} is linked to the equilibrium (bootstrap) current density $j_\parallel$ and gradient of the pressure p by $\lambda_{bb} = - \langle j_\parallel B \rangle \left(c \langle |\nabla \psi| \rangle \, \mathrm{d}p/\mathrm{d}\psi \right)^{-1}$. 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 and R are the rotational transform and major radius, respectively.

In order to introduce the Monte Carlo operator it is convenient to re-write (1) in the integral form using a Green's function G defined by

$$\mathscr{L}_D \, G(t, \mathbf{z}, \mathbf{z}_0) = 0, \qquad G(0, \mathbf{z}, \mathbf{z}_0) = (g(\mathbf{z}_0))^{-1/2} \delta(\mathbf{z} - \mathbf{z}_0), \tag{3}$$

where $\mathbf{z} = (\vartheta, \varphi, \lambda)$ and g is a metric determinant of flux coordinates $(\psi, \vartheta, \varphi)$. This Green's function is normalized to 1, $\int \mathrm{d}^3 z \, (g(\mathbf{z}))^{1/2} G(t, \mathbf{z}, \mathbf{z}_0) = 1$. Thus, a formal solution to Eq. (1) is

$$\hat{f}(t, \mathbf{z}) = \int \mathrm{d}^3 z_0 \, (g(\mathbf{z}_0))^{1/2} \left(G(t - t_0, \mathbf{z}, \mathbf{z}_0) \hat{f}(t_0, \mathbf{z_0}) + \int\limits_{t_0}^{t} \mathrm{d}t' G(t - t', \mathbf{z}, \mathbf{z}_0) \dot{\psi}(\mathbf{z}_0) \right). \tag{4}$$

If a steady state solution is looked for, $\hat{f}(t,\mathbf{z}) = \hat{f}(\mathbf{z})$, Eq. (4) becomes an integral equation for $F(\mathbf{z}) = (g(\mathbf{z}))^{1/2} \hat{f}(\mathbf{z})$ given below also in the operator form,

$$F(\mathbf{z}) = \int d^3 z_0 K(\mathbf{z},\mathbf{z}_0) F(\mathbf{z}_0) + Q(\mathbf{z}) \equiv \mathscr{K} F + Q, \tag{5}$$

where $K(\mathbf{z},\mathbf{z}_0) = (g(\mathbf{z}))^{1/2} G(\Delta t,\mathbf{z},\mathbf{z}_0)$, Δt is the integration time step and

$$Q(\mathbf{z}) = \int d^3 z_0 \, (g(\mathbf{z}) g(\mathbf{z}_0))^{1/2} \int_0^{\Delta t} dt' G(t',\mathbf{z},\mathbf{z}_0) \, \psi(\mathbf{z_0}) \approx \Delta t \, (g(\mathbf{z}))^{1/2} \, \psi(\mathbf{z}). \tag{6}$$

Introducing the Monte Carlo operator, $\mathbf{Z}(\Delta t,\mathbf{z}_0)$, being the random position of a test particle starting at $\mathbf{z}_0$ after a single time step modeled in a standard way by the random change of λ in accordance with $\mathscr{L}_C$ and integration of particle drift equations, the kernel of the integral equation is given by an expectation value $K(\mathbf{z},\mathbf{z}_0) = \overline{\delta(\mathbf{z} - \mathbf{Z}(\Delta t,\mathbf{z}_0))}$. The solution of (5) by direct iterations can be presented as an expectation value of an integral along the stochastic orbit,

$$F = \sum_{k=0}^{\infty} \mathscr{K}^k Q = C_0 \sum_{k=0}^{\infty} \overline{w_0 \, \delta(\mathbf{z} - \mathbf{z}_k)}, \qquad \mathbf{z}_k = \mathbf{Z}(\Delta t,\mathbf{z}_{k-1}), \qquad w_0 = \Delta t \, \psi(\mathbf{z}_0), \tag{7}$$

where $C_0 = \int d^3 z \, (g(\mathbf{z}))^{1/2}$ and the random starting point $\mathbf{z}_0$ is chosen with the probability density $\overline{\delta(\mathbf{z} - \mathbf{z}_0)} = C_0^{-1} (g(\mathbf{z}))^{1/2}$. The averages (2) are given by expectation values as

$$D_{\text{mono}} = -\frac{1}{\langle|\nabla\psi|\rangle^2} \sum_{k=0}^{\infty} \overline{w_0 \psi(\mathbf{z}_k)}, \qquad \lambda_{bb} = -\frac{3}{\rho_L B_0 \langle|\nabla\psi|\rangle} \sum_{k=0}^{\infty} \overline{w_0 \lambda_k B(\mathbf{z}_k)}. \tag{8}$$

When $k\Delta t$ exceeds a few collision times, the correlation between $\mathbf{z}_k$ and w_0 is lost and, therefore, such terms in (8) tend to zero, e.g. $\overline{w_0 \psi(\mathbf{z}_k)} \to \overline{w_0} \ \overline{\psi(\mathbf{z}_k)} = 0$ because the expectation value $\overline{w_0} = C_0^{-1} \Delta t \int d^3 z \, (g(\mathbf{z}))^{1/2} \psi(\mathbf{z}) = 0$ due to Liouville's theorem. Thus, a finite sum over k is sufficient in (8). The method described by (8) has rather low variance in computations of D_{mono}, however, for λ_{bb} variance has a very unfavorable scaling with collisionality. Indeed, only the orbits originating in the boundary layer in velocity space of the width $\Delta\lambda \sim (L_c/l_c)^{1/2}$ where $L_c = 2\pi R/\iota$ and $l_c = v\tau_c$ are the connection length and mean free path, respectively, contribute to λ_{bb}. In addition, the contribution of a particle from the boundary layer is $\Delta\lambda$ times smaller than of a normal passing particle because of a higher trapping probability. Therefore, the variance in λ_{bb} scales for this method as $(l_c/L_c)^2$ in the long mean free path regime.

It should be noted that test particles at each step keep the same equilibrium distribution, $\overline{\delta(\mathbf{z} - \mathbf{z}_k)} = C_0^{-1} (g(\mathbf{z}))^{1/2}$. Therefore $\overline{w_0 \lambda_{k-j} B(\mathbf{z}_{k-j})} = \overline{w_j \lambda_k B(\mathbf{z}_k)}$ where $w_j = \Delta t \, \psi(\mathbf{z}_j)$, and

$$\sum_{k=0}^{\infty} \overline{w_0 \lambda_k B(\mathbf{z}_k)} = \lim_{k\to\infty} \overline{W_k \lambda_k B(\mathbf{z}_k)} = \lim_{K\to\infty} \frac{1}{K} \sum_{k=0}^{K} \overline{W_k \lambda_k B(\mathbf{z}_k)}, \qquad W_k = \sum_{j=0}^{k} w_j. \tag{9}$$

The procedure in (9) corresponds to a standard δf method [1] where the test particle weight W_k is an integral of ψ along a stochastic orbit. In a tokamak, the variance in λ_{bb} does not scale with the collisionality, and the required CPU time for this method scales linearly with

l_c/L_c. However, in stellarators variance in λ_{bb} again recovers the scaling $(l_c/L_c)^2$ because due to the non-zero bounce-averaged drift of trapped particles large contributions to W_k are acquired, which scale as $\dot{\psi}\tau_c$ and which are weakly correlated with the value of λ_k after they are detrapped. To overcome this problem, in Ref. [2] trapped particles with large W_k are replaced with particles with $W_k = 0$ which formally introduces some bias in the result.

For a formally "unbiased" method it is convenient to split the source in (5) into "passing" and "trapped" sources $Q_p = \chi Q$ and $Q_t = Q - Q_p$ using $\chi = \tanh\left((\lambda - \lambda_{t-p})/\Delta\lambda\right)$ where λ_{t-p} is a trapped-passing boundary. 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 (9) because accumulation of large weights is avoided there. For the problem with Q_t the formal solution to (5) is presented as $F = F_M + \Delta F_M$ where F_M satisfies a similar equation with a different source term, $F_M = \mathcal{K} F_M + Q_M$, and ΔF_M is known,

$$Q_M = \frac{1}{M} \sum_{k=0}^{M-1} \mathcal{K}^k Q, \qquad \Delta F_M = \sum_{k=0}^{M-1} \left(1 - \frac{k+1}{M}\right) \mathcal{K}^k Q. \tag{10}$$

ΔF_M is used only in averages (2) while Q_M is computed by scoring weights on the 3D grid. On the grid weights are partly annihilated. After the first such iteration, the module of the weight is fixed and then iterations are repeated formally putting $F = F_M$ and $Q = Q_M$ and applying the same procedure to the resulting integral equation. Due to annihilation and fixed module of the weight, the number of test particles needed for sampling the source term from the grid is decreasing and iterations are stopped when this number is below 1. The number of steps M for a single iteration is chosen to be much smaller than collision time and large enough in order to fill the grid using a limited number of test particles. 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 particles in the passing and trapped regions is of the same order. As a result, variance of this method is reduced to the scaling l_c/L_c. In addition, due to the decay of test particle number with iterations, the CPU time is also reduced and scales as $(l_c/L_c)^{3/2}$ for given accuracy which is much better than scaling $(l_c/L_c)^3$ of the standard δf method. Results of testing of the method for a few toroidal devices stay in good agreement with results of NEO-2, a field line tracing code which computes transport coefficients in arbitrary collisionality regimes [3], as shown in Figs. 1-3.

References

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[3] W. Kernbichler, S. V. Kasilov, G. O. Leitold, V. V. Nemov and K. Allmaier, *33rd EPS Conference on Plasma Physics, Rome, 19–23 June 2006*, ECA Vol. **30I** P-2.189 (2006)
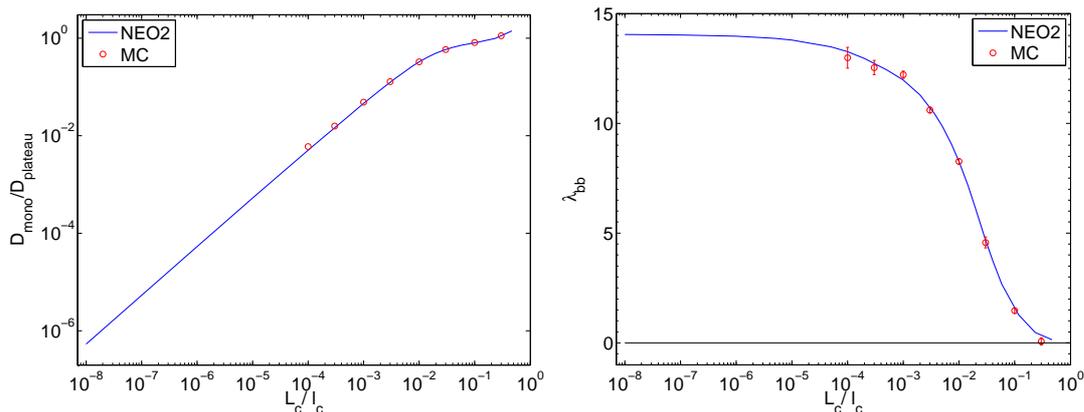
Figure 1: Normalized diffusion coefficient $D_{\mathrm{mono}}/D_{\mathrm{plateau}}$ (left) and bootstrap coefficient λ_{bb} (right) as functions of collisionality parameter L_c/l_c for a tokamak. The computation methods are indicated in the legend.
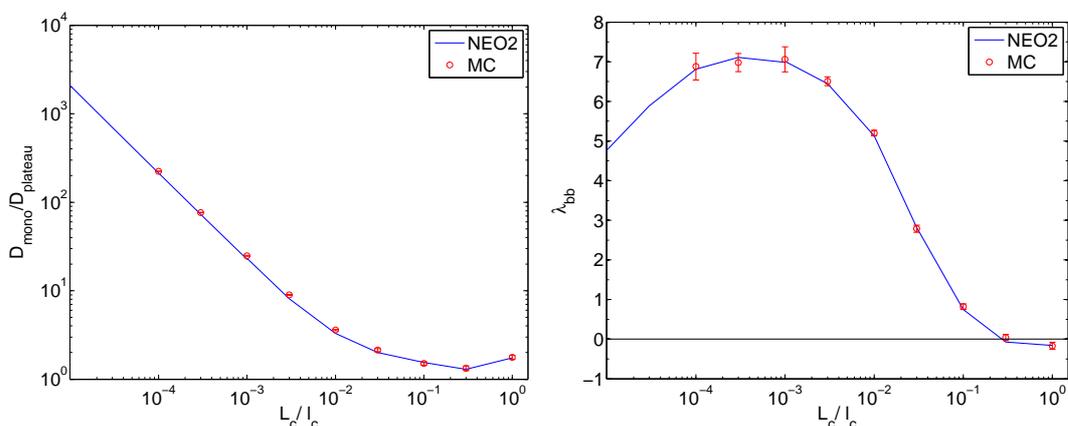
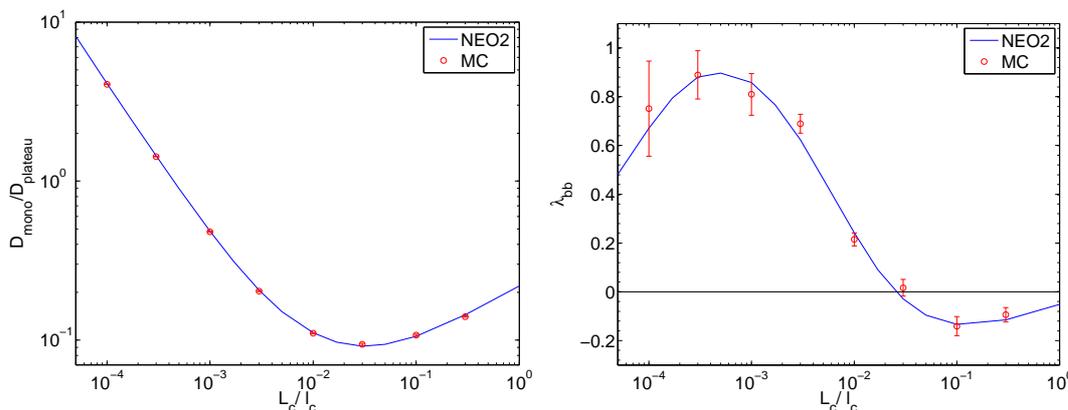Figure 2: The same as in Fig. 1 for LHD configuration with R=375 at half toroidal flux.

Figure 3: The same as in Fig. 1 for the standard configuration of W7-X at half toroidal flux.