Application of the stochastic mapping technique to modeling the distribution function in stellarator geometry

Winfried Kernbichler1, Sergei V. Kasilov2, Martin F. Heyn1

1 Institut für Theoretische Physik, Technische Universität Graz, Petersgasse 16, A–8010 Graz, Austria
2 Institute of Plasma Physics, National Science Center “Kharkov Institute of Physics and Technology”, Ul. Akademicheskaya 1, 310108 Kharkov, Ukraine

Introduction

The stochastic mapping technique (SMT) is a Monte-Carlo (MC) method to solve the drift-kinetic equation in the long mean free path regime. SMT is based on the fact that in this regime the drift particle orbits are only slightly modified by collisions during the time needed to pass the characteristic magnetic field scale along the field lines. In a stellarator, in general, this is one magnetic field period. In conventional MC methods the stochastic particle orbits have to be followed everywhere in phase space. In the SMT approach however, only the footprints of the stochastic orbits are traced on Poincaré cuts, which are surfaces defined by the fact that the parallel gradient of the magnetic field module is zero there. This gives a significant gain in the computational speed because the integration of test particle orbits between the cuts is replaced by an interpolation on the map. For a simple magnetic field model the code is two orders of magnitude faster than a conventional one and this ratio even increases with increasing magnetic field complexity.

Regular and stochastic mapping

The position of the footprint on a particular cut labelled with index m is described by a set of 4 parameters \( u^i \) where \( u^{1,2} = x^{1,2} \) are the spatial coordinates of the footprint on the minimum-B surface and \( u^3 = p, \ u^4 = \lambda \) are the momentum module and pitch, respectively. Without collisions, each new footprint of a drift orbit, \( (m', u') \) (bold face here denotes the full set of variables), is determined by the Poincaré map, \( m' = \mathbf{M}_m(u), \ u'^i = U^i_m(u) \), where \( \mathbf{M}_m(u) \) gives the index of the next cut to be passed by the drift orbit. This can be one of two neighboring cuts for a passing particle or the same cut for a trapped one. The quantity \( U^i_m(u) \) gives the coordinates on this next cut. This map is also called below a regular map, because it is completely determined by the solution of the equations of particle drift motion. In the presence of weak collisions the map has to include a small random perturbation of the particle coordinates \( \delta u^i_m(u) \) which describe the effect of collisions, \( m' = \mathbf{M}_m(u + \delta u_m(u)), \ u'^i = U^i_m(u + \delta u_m(u)) \). Such a mapping therefore becomes stochastic. Those random perturbations to the regular Poincaré map have been obtained from the drift-kinetic equation in Ref. [1]. Also in this reference, the drift kinetic equation has been transformed to an integral equation describing the conservation of the particle flux density \( \Gamma_m \) through the Poincaré cuts. In the case of a stationary problem it can be written in the following form,

\[
\Gamma_{m'}(u') = \sum_m \int d^4u \left\langle \delta_{m', \mathbf{M}_m(u + \delta u_m(u))} \delta \left[u' - U^i_m(u + \delta u_m(u))\right] \right\rangle \left[ (1 - \tilde{\nu}_m(u)) \Gamma_m(u) + Q_m(u) \right], \tag{1}
\]

This work was partly supported by the Association EURATOM-OEAW under contract number ERB 5004 CT 96 0020.
Here $\Gamma_m = dN/2\pi d^4u \, dt = J_m f$, where $dN$ is the number of particles passing through the element of the cut area $d\alpha_m$ during the time $dt$ due to their drift motion. This quantity is proportional to the distribution function $f$ where the Jacobian $J_m$ is given in the next section.

In the case of a time dependent problem, the dimension of the map has to be increased because a time variable $\tau^3 = t$ should be included into the set of parameters $\tau^i$. The map for this time variable is given by $U^3_m(\mathbf{u}) = \tau^3 + \tau_{0m}(\mathbf{u})$ where $\tau_{0m}$ is the so-called “bounce-time”. It is defined as time for the transition from one cut to another (passing particles) or for the return to the same cut (trapped particles). The map of this variable is strictly regular. With this change the form of equation (1) is preserved.

The random perturbations $\delta\mathbf{u}_m$ depend also on a set of random numbers $\xi_i$ that satisfy the following requirements, $\langle \xi_i \rangle = 0$ and $\langle \xi_i \xi_j \rangle = \delta_{ij}$, where $\langle \ldots \rangle$ means the average over those numbers. Also the following requirements for the covariance and the deviation have to be satisfied,

$$\langle \delta u^i_m \delta u^j_m \rangle = 2D^{ij}_m(\mathbf{u}), \quad \langle \delta u^i_m \rangle = \mathcal{F}_m^i(\mathbf{u}).$$

Here $D^{ij}_m$, $\mathcal{F}^i_m$, $\varrho_m$ and $\mathcal{Q}_m$ are obtained by integration of the velocity space diffusion coefficients, of the components of the friction force, and of the particle sink and source rate, respectively, along the regular orbits (see [1]). The particular form of $\delta u^i_m$ is $\delta u^i_m = \alpha^{ij}_m \xi_j + \mathcal{F}_m^i$ where $\alpha^{ij}_m$ satisfies the relation $\alpha^{ik}_m \alpha^{jl}_m \delta_{kl} = 2D^{ij}_m$.

The solution of the integral equation (1) is obtained as an average over an ensemble of Markov chains,

$$\Gamma_m(\mathbf{u}) = \langle \sum_{k=1}^{\infty} w_k \delta_{m,m_k} \delta (\mathbf{u} - \mathbf{u}_k) \rangle$$

(3)

where $(\mathbf{m}_k, \mathbf{u}_k)$, $w_k$ (here $k = 0, 1, 2, \ldots$) are the subsequent positions of the footprint and the statistical weight of the test particles, respectively. For such a construction of the Markov chain, the initial footprint, $(\mathbf{m}_0, \mathbf{u}_0)$, is generated randomly with a probability density $p^{(Q)}_m(\mathbf{u}) = \mathcal{Q}_m(\mathbf{u})/w_0$ where the initial statistical weight $w_0$ is defined through $\sum_m \int d^4u \, p^{(Q)}_m(\mathbf{u}) = 1$.

Then each next footprint, $(\mathbf{m}_{k+1}, \mathbf{u}_{k+1})$, is obtained from the previous one, $(\mathbf{m}_k, \mathbf{u}_k)$, with the help of the stochastic mapping procedure described above. Before each mapping however, the particle weight $w_{k+1}$ is put to $w_k$ with a probability $1 - \varrho_m$ or is put to zero with a probability $\varrho_m$. In the latter case, the Markov chain is terminated. This standard procedure to solve integral equations is realized numerically in two stages. First, the regular map, $M_m$, $U_m$, and the parameters of the stochastic processes, $\tilde{D}^{ij}_m$, $\tilde{\mathcal{F}}_m^i$, $\tilde{\varrho}_m$, $\tilde{\mathcal{Q}}_m$ are precomputed numerically and stored on a rectangular mesh. Then, during the actual MC run, Markov chains are built just using interpolation between the stored data and, of course, standard random numbers. Such a procedure is, on one hand, much faster than conventional MC but, on the other hand, requires, especially in case of a stellarator, a huge amount of storage (4D). This demand for memory is usually much higher than the available computer memory. A solution to this problem is given in the next sections. In addition, in stellarator geometry the topology of the minimum-B surfaces is rather complex and requires a special coordinate system for an automatic parametrisation.

**Local magnetic coordinate systems**

In order to describe minimum-B surfaces in a stellarator, in each magnetic field period, numbered with $n$, a separate local magnetic coordinate system $(x^{1}_{(n)}, x^{2}_{(n)}, x^{3}_{(n)})$ is used, where the first two coordinates satisfy the magnetic differential equation $\mathbf{h} \cdot \nabla x^{1,2}_{(n)} = 0$. Here
\( h = B / B \) is a unit vector along the magnetic field. These coordinates are linked with the cylindrical variables \((R, \varphi, Z)\) through the characteristics of the magnetic differential equation, \(X^1(R, \varphi, Z; \varphi')\) and \(X^2(R, \varphi, Z; \varphi')\), which satisfy the magnetic field line equations,

\[
\frac{\partial X^1}{\partial \varphi'} = \frac{h^h(X^1, \varphi', X^2)}{h^h(X^1, \varphi', X^2)}, \quad \frac{\partial X^2}{\partial \varphi'} = \frac{h^h(X^1, \varphi', X^2)}{h^h(X^1, \varphi', X^2)},
\]

and the initial conditions \(X^1(R, \varphi, Z; \varphi) = R\), \(X^2(R, \varphi, Z; \varphi) = Z\). With this follows,

\[
x^i_{(n)} \equiv X^i(R, \varphi, Z; \varphi_n), \quad i = 1, 2; \quad x^3_{(n)} = \varphi - \varphi_n,
\]

where \(\varphi_n = 2\pi n / N\) and \(N\) is the number of field periods. A particular coordinate system is used between the “reference” cut \(\varphi = \varphi_n\) and the next “reference” cut \(\varphi = \varphi_{n+1}\). In other words, a particle position is described by the projection of its actual position along the magnetic field lines to the “reference” cut and by the toroidal distance from this cut. Different local coordinate systems are linked to each other through the magnetic field map

\[
x^i_{(n\pm 1)} = X^i_{\pm}(x^1_{(n)}, x^2_{(n)}), \quad i = 1, 2, \quad x^3_{(n\pm 1)} = x^3_{(n)} \mp 2\pi / N,
\]

where \(X^i_{\pm}(x^1, x^2) \equiv X^i(x^1, 0, x^2; \pm 2\pi / N)\). In any magnetic field topology, such multiple magnetic coordinate systems allow to separate the drift particle motion from the fast parallel motion which by definition leaves the coordinates \(x^{1,2}_{(n)}\) unchanged. Thus the artificial cross-field transport arising from numerical errors can be avoided. Those errors usually arise during integration of the magnetic field for particles moving strictly along the magnetic field. If local magnetic coordinates are used, such transport can only appear due to errors in the variable change, which is done with the help of the magnetic field map. For this reason, the magnetic field map is stored on a fine mesh and interpolated with the help of bicubic splines which can provide the necessary accuracy. Similar multiple magnetic coordinate systems have been also used in Ref. [2].

The Poincaré cuts are those surfaces \(x^3_{(n)} - x^3_{m} = 0\) where \(x^3_{m}\) satisfies the condition for an extremum,

\[
B'(x^1_{(n)}, x^2_{(n)}, x^3_{m}) = 0, \quad B'(x^1_{(n)}, x^2_{(n)}, x^3_{(n)}) \equiv h \cdot \nabla B = h^3 \frac{\partial B}{\partial x^3_{(n)}},
\]

and \(m = (n, m)\) is a set of two indices where index \(m\) enumerates solutions to (7) within the period \(n\) starting from the reference cut. Of course, due to particle trapping within magnetic wells only minima are relevant here. The Jacobian \(J_m\) takes a rather simple form, \(J_m = p^3 \lambda \hat{B}_v(x^1_{(n)}, x^2_{(n)}, 0) / (m_e \gamma B(x^1_{(n)}, x^2_{(n)}, x^3_{m}))\) where \(m_e\) and \(\gamma\) are electron mass and relativistic factor, respectively, and \(\hat{B}_v\) is a physical toroidal component of the magnetic field. Labeling of the cuts with the vector index \(m\) removes ambiguities in the definition of the cuts. However, it introduces artificial boundaries everywhere where one of the cuts intersects the reference cut \((B'(x^1_{(n)}, x^2_{(n)}, 0) = 0 \) or \(B'(x^1_{(n)}, x^2_{(n)}, 2\pi / N) = 0\)) in addition to the natural boundaries where the minimum-B surface ends (see Fig.1).

**Mapping in local magnetic coordinates**

In the absence of particle cross-field drift the unperturbed map \(U^i_{m}(u)\) becomes rather simple. The spatial coordinates stay unchanged, \(U^{1,2}_{m}(u) = u^{1,2} \equiv x^{1,2}_{(n)}\), if the starting and the end cut
The effects of the magnetic and electric drift result in small displacements of the footprint relative to the Lamor radius, \( \Delta x^{1,2} = \Delta x^{1,2}_E + \Delta x^{1,2}_B \). With this, the maps can be written as

\[
U^{1,2}_m(u) = u^{1,2} + \Delta x^{1,2}_m(u), \quad U^{1,2}_m(u) = X^{1,2}_m(u^{1} + \Delta x^{1}_m(u), u^{2} + \Delta x^{2}(u))
\]

for the two cases described above, respectively.

Here it is assumed that the electrostatic potential \( \Phi \) is constant along the magnetic field, \( \Phi = \Phi(x^{1}_{(n)}, x^{2}_{(n)}) \). In the limit of small Larmor radii the displacement due to the magnetic drift,

\[
\Delta x^{1,2}_B = \int_0^{t_m} dt \nu^{1,2}_B,
\]

scales linearly with the momentum module \( v^3 = p \). Here \( v^{1,2}_B \) is the drift velocity in absence of an electric field. The displacement due to the electric drift is proportional to \( 1/p \),

\[
\Delta x^{1,2}_E = -\frac{c\tau_{nm}}{B_v} \frac{\partial \Phi}{\partial x^{2}_{(n)}}, \quad \Delta x^{2}_E = \frac{c\tau_{nm}}{B_v} \frac{\partial \Phi}{\partial x^{1}_{(n)}},
\]

because \( \tau_{nm} \propto 1/p \). Therefore it is not necessary to store this dependence of the unperturbed map, and storage of \( U^{1,2}_m(u) \) becomes 3-dimensional, because only the dependencies on the spatial coordinates \( u^{1,2} \) and on pitch \( u^4 = \lambda = p_{\parallel}/p \) have to be stored. In addition, the remaining components of the regular map, \( U^{2,3}_m(u) \) and \( U^{4,5}_m(u) \), are obtained using the conservation of the magnetic moment and of the total energy and need only a 2D storage of the magnetic field module on the Poincaré cuts. Thus, usage of the local magnetic coordinates reduces the amount of necessary storage to amounts reasonable on modern workstations. Moreover, simple scaling of \( \Delta x^{1,2}_E \) with \( \Phi \), Eq. (10), would allow for iterations with changing electrostatic potential during an MC run without need for reloading the maps.

**Treatment of Coulomb collisions**

In the present version of the code, the effect of Coulomb collisions described by the deviation \( \mathcal{D}^{\lambda\nu}_m \) and the variance \( \mathcal{E}^{\lambda\nu}_m \) is taken into account only in the velocity space. This allows to describe in a correct way only the strongest particle transport effects coming from the magnetic field asymmetry. For the suprathermal particles of interest here, this treatment of Coulomb collisions is good, whereas for thermal particles the distortion of the background plasma distribution becomes more important. Assuming the scattering background plasma to be an isotropic Maxwellian, the effect of collisions is described by two components of the variance tensor, \( \mathcal{D}^{\lambda\nu}_m = D^{\lambda\nu}_m \tau_{nm} \) and \( \mathcal{D}^{\lambda\nu}_m = D^{\lambda\nu} \Lambda_m \), where \( D^{\lambda\nu} \) and \( D^{\lambda\nu} \) are components of the Coulomb diffusion tensor over momentum module and pitch angle. These components depend only on the momentum module. Also the bounce time \( \tau_{nm} \) and the geometry dependent quantity \( \Lambda_m \) just scale inversely with \( p \). The components of the deviation \( \mathcal{F}^{\lambda\nu}_m \) have a similar simple structure. Thus, the storage requirement for the “stochastic” parameters of the map is also reduced to 3D, because complex dependencies of deviation and variance on the momentum module can be factorized. Tests of the mapping procedure for the description of collisional transport in the...
“Uragan-3M” torsatron [3] showed that the SMT code and a direct MC code gives close results (see Fig.2).

Figure 1. Cross section of the cuts in the plain $Z = \text{const}$. Bottom and top straight lines are the reference cuts, solid curves are the minimum-B cuts, dotted lines are the maximum-B surfaces. Different colors of minimum-B cuts correspond to different values of the cut index $m$ (topologically the same cut surface is split by artificial boundaries into regions with different cut index $m$). The point where minimum-B and maximum-B surfaces merge is the "natural" end of the minimum-B cut.

Quasilinear effects of ECRH

In addition to Coulomb collisions, quasilinear effects of rf-heating are also responsible for diffusion in velocity space. This sort of diffusion often can be described using an analytical model and, therefore, does not cause immediate storage problems. This is the case, especially if one considers 2nd harmonic X-mode ECRH assuming that the rf field amplitude is highly localized in space and has a Gaussian shape along the magnetic field lines, $E \propto \exp\left(-\frac{1}{2} \alpha_s s^2\right)$, where $s$ is the distance along the field line and $\alpha_s$ is the inverse area of the beam. In this case, the variance and deviation of the particle energy after one pass through the beam is given as

$$
\bar{D}_{QL}^E = \frac{\pi \epsilon E - k^2 B_{\text{res}}^2 p^4}{2 \mu_0^2 \omega^2 \alpha B^2} \exp(-\eta), \quad \eta = \frac{m_0^2 \omega^2}{\alpha_1 p^2} \left( \gamma - \frac{B}{B_{\text{res}}} - \frac{k_{||} p_{||}}{m_0 \omega} \right)^2, \quad (11)
$$

$$
\mathcal{F}_{QL}^E = \left( \frac{\partial}{\partial \mathcal{E}} + \frac{1}{B_{\text{res}}} \frac{\partial}{\partial \mu} \right) \bar{D}_{QL}^E, \quad (12)
$$

with $\mathcal{E}, \mu$ the energy and magnetic moment, $p_{\perp}, p_{||}$ the perpendicular and parallel momentum in the beam center, $E^-$ the right-polarized component of the wave electric field, $B$ the magnetic field in the beam center, $B_{\text{res}} = m_0 c / 2 \omega$, $\omega$ the wave frequency, $k_{\perp}, k_{||}$ the perpendicular and parallel wave number. With (11) and (12) known, the components of $\bar{D}_{m}^i$ and $\mathcal{F}_{m}^i$ have the simplest form if $\mathcal{E}$ and $\mu$ are used as velocity space variables,

$$
\bar{D}_{m}^j = \beta^j \beta^i \bar{D}_{QL}^E, \quad \mathcal{F}_{m}^i = \beta^i \mathcal{F}_{QL}^E, \quad \beta^E = 1, \quad \beta^\mu = \frac{1}{B_{\text{res}}}. \quad (13)
$$
The nonlinear effects during the wave-particle interaction will reduce the energy absorption by particles passing the beam with small velocity. In order to describe this reduction qualitatively, \( D_{QG}^{\infty} \), is replaced by the model coefficient

\[
[D_{QG}^{\infty}]^4 = \frac{D_{QG}^{\infty}}{\sqrt{1 + (\alpha D_{QG}^{\infty})^2}} \quad \alpha = \frac{\partial^2 \eta}{\partial \varepsilon^2}.
\]  

(14)

Such a model assumes 'heating out of resonance'. In this model the energy gain of particles passing through the beam is assumed to stop when the particle diffuses out from the resonance zone \((\eta \gg 1)\) due to the rf-interaction. Using in addition to SMT a \( \delta f \)-scheme for a separate description of suprathermal particles and thermal particles [4], the electron distribution function can be resolved by a MC computation within a reasonable computation time (see Figures 3-6).

The computation is performed for a medium size stellarator with \( l=2 \), five magnetic field periods, \( R = 2 \) m, \( B = 2.5 \) T, and a constant plasma density \( n_e = 10^{19} \) m\(^{-3}\) and temperature \( T_e = 3 \) keV. A localized ECRH beam with \( P = 100 \) kW and \( \alpha_1 = 2.5 \times 10^3 \) m\(^{-2}\) is assumed to be perpendicularly injected into the magnetic field minimum. The variation of the beam amplitude due to absorption is not taken into account. The distribution of the absorbed power over the poloidal cross section is shown in Fig. 3. The cold resonance position is exactly on the magnetic axis. One magnetic surface is shown and three points (1, 2, 3) are indicated, where the distribution function is reconstructed. The direction of the electron drift is downwards.

In Fig. 4 the total distribution function is shown for point 1 (inside the absorption region). The formation of a quasilinear plateau can be observed mainly in the passing particle region. The perturbed distribution function in Fig. 5 corresponds to the point below the beam (in the direction of the drift). It is formed mainly by ripple trapped particles, which contribute to convective particle and energy losses. In turn, the perturbed distribution function above the beam (Fig. 6) is formed mainly by passing particles detrapped in the lower region of the configuration. Note that despite the peaked perturbed distribution function \( \delta f \), the total distribution function for this parameter set has negative derivatives over perpendicular energy everywhere.

**Summary**

The stochastic mapping technique is a Monte Carlo method for the solution of the quasilinear drift kinetic equation which allows to resolve the distribution function in a stellarator. This method is much faster than a conventional Monte Carlo method, it requires however a huge amount of computer memory. The usage of multiple local magnetic coordinate systems takes the memory requirement down to a reasonable level and allows for a computation on usual workstations. The method has been benchmarked against the conventional MC method. Up to now it was applied to modeling the suprathermal electron distribution function during ECRH in stellarator geometries where the magnetic field module has not more than one minimum on the field line within a field period. The method described here can be used to model the effects of suprathermal particles (electrons and ions) generated by rf-heating, such as nonlocal convective energy losses, generation of the ambipolar electric field due to convective transport of suprathermals, and current drive.
References