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Energy and momentum preserving Coulomb collision model for kinetic Monte Carlo simulations of plasma steady states in toroidal fusion devices

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ABSTRACT

A kinetic Monte Carlo model suited for self-consistent transport studies is proposed and tested. The Monte Carlo collision operator is based on a widely used model of Coulomb scattering by a drifting Maxwellian and a new algorithm enforcing the momentum and energy conservation laws. The difference to other approaches consists in a specific procedure of calculating the background Maxwellian parameters, which does not require ensemble averaging and, therefore, allows for the use of single-particle algorithms. This possibility is useful in transport balance (steady state) problems with a phenomenological diffusive ansatz for the turbulent transport, because it allows a direct use of variance reduction methods well suited for single particle algorithms. In addition, a method for the self-consistent calculation of the electric field is discussed. Results of testing of the new collision operator using a set of 1D examples, and preliminary results of 2D modelling in realistic tokamak geometry, are presented.

1. Introduction

The most common tool for self-consistent transport modelling of edge plasmas in tokamaks is fluid modelling, like Ref. [1], where hydrodynamic (Braginskii [2]) model is used for plasma transport along the magnetic field, and an *ad hoc* ansatz (e.g., Bohm-like diffusivities) is used for the anomalous transport across the field. Such hydrodynamic modelling is numerically feasible, but there is strong evidence (both experimental and theoretical, see, e.g., a review paper [3]) that some effects which cannot be described in this framework (kinetic effects) play a significant role in transport phenomena.

One of the problems is the non-local nature of transport: under typical edge plasma conditions fluid equations are used somewhat outside their validity range. E.g., parallel heat flux in the divertor region is not a function of local temperature gradients only, but also contains contributions of the profile over several mean free path lengths. This problem is most pronounced for electron heat conduction, but there is some evidence that ion heat conduction and even parallel ion viscosity should be corrected as well, see Ref. [4]. Moreover, near the wall the distribution function can be very far from the Maxwellian – here the hydrodynamics can be applied in the sense of an order-of-magnitude-estimate at best. Another problem is the drift motion of particles – it is a non-trivial problem to take into account this phenomenon in the framework of

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fluid model [5–7]. This effect, which in particular leads to the dependence of divertor fluxes on the sign of the magnetic field, is important not only in tokamaks but also in stellarators [8,9]. In any case, it is impossible to distinguish passing and trapped particles in hydrodynamics – related effects, which are formally described by the anisotropic pressure tensor in Chew–Goldberger–Low form, are necessarily neglected in the MHD approach using an isotropic pressure in the closure of the energy equation. To treat such effects rigorously, a kinetic equation needs to be solved.

There are many attempts to improve the hydrodynamic models by means of kinetic corrections to the fluxes and (sometimes) boundary conditions, e.g. [10–12]. Here, the heat flux is calculated as an integral over the whole domain and is used in the fluid model afterwards. A related approach is hybrid modelling [13,14] – here fluid and strongly simplified kinetic equations are solved in turn (hydrodynamical profiles of density, velocity and temperature are used as a background to calculate kinetic fluxes and vice versa) until a common steady state reached. It should be noted that the very existence of this steady-state solution here can be questioned – in practice one uses much more simple "flux limiter" expressions instead [3].

There is an obvious need for a numerically feasible self-consistent kinetic model of plasma transport phenomena. One of the main challenges here is the dimensionality of the problem, which increases by two as compared to the fluid approach in case of the gyrokinetic (generally 5D) equation. In cases where dimensionality reduction is possible, such as in axisymmetric devices in the long mean free path limit (reduction to 3D by bounce-averaging) Vlasov–Fokker–Planck solvers can treat the problem efficiently. For finite collisionality, even in the axisymmetric tokamak (case considered here as an example) problem stays 4D and is therefore challenging for most methods in terms of memory requirements. (Another example of a 4D kinetic problem is the local solution of a drift kinetic equation at given flux surface in 3D magnetic geometries [15,16] where the memory requirements are also rather demanding.) Finally, in case of global solutions in 3D geometry (stellarators, tokamaks with external magnetic field perturbations) the problem is essentially 5D, and one has to rely on test particle (Monte Carlo) methods [17,18]. Further advances in the development of such methods which can be used for 3D magnetic geometries is the main purpose of this paper.

The first step in this direction should be a suitable Coulomb collision operator suitable for transport balance (steady state) problems with a phenomenological diffusive ansatz for the turbulent transport. During the last few decades there have been significant advances in the development of momentum and energy preserving Monte Carlo realizations of the collision operator for local problems (computation of neoclassical transport coefficients) as well as Particle in Cell (PIC) codes oriented at self-consistent modelling of the distribution function and electromagnetic fields involved in collective phenomena (plasma turbulence). These methods can, in principle, treat the Fokker–Planck collision operator accurately. The direct implementation of this operator – a self-consistent calculation of the drag and diffusion coefficients using the actual distribution function – is discussed in Ref. [19]. The authors overcome the difficulties in principle, but their approach remains too numerically extensive. An alternative approach – binary collisions – has been suggested by Takizuka and Abe [20]. This algorithm involves the pairing of scattering particles in each computational cell at random and then small-angle collisions are performed pairwise. This procedure naturally conserves particles, momentum and energy within each spatial cell, and has been generalized for weighted particles [21] and has been vectorized [22]. Now it is widely used in kinetic codes like VPIC [23] and ASCOT [24]. Nevertheless, the usage of the exact binary collisions for self-consistent transport modelling of fusion devices remains inordinately time consuming (see, e.g., Ref. [25]). The main difficulty here is the difference between the characteristic times (also called *stiffness*) of the problem: on the one hand, we need to follow the evolution of the system for the time of perpendicular (anomalous) transport, $\tau_\perp \sim a^2 D_\perp^{-1}$ (here a is the minor radius and $D_\perp$ is the anomalous perpendicular diffusion coefficient), which is hundreds of milliseconds. On the other hand, our time step is restricted by the electron collision time ($\sim 10^{-8}$ s at the edge of fusion devices). The requirement on the angle of scattering to be small adds another two orders of magnitude to the degree of stiffness. The transport time scale $\tau_\perp$, which has to be resolved in transport problems is much larger that the corresponding time scale in local problems (the longer of the collision time and the time for relaxation over the magnetic surface) or the turbulence saturation time typical for PIC modelling. For this reason, exact kinetic models like ASCOT [24] cannot produce profiles of plasma parameters by themselves – they must either assume background profiles or be used in combination with fluid codes like B2SOLPS5.0 [26].

One is therefore forced to sacrifice some accuracy in the description of collisions for the sake of efficiency. This has been done, e.g., in Refs. [27,28,25]. Jones et al. [27] introduced the concept of a "collisional field" – a Monte-Carlo-oriented Langevin formalism with velocity-space diffusion D and dynamical friction F coefficients independent of velocity. This shortcoming has been removed by Manheimer et al. [28] who calculated $D(v)$ and $F(v)$ using the actual distribution function; the only assumption was that the distribution of the "scatterer" particles is isotropic in its mean frame of reference. This procedure turns out to be quite noisy; the authors overcome this problem by averaging in space (along magnetic field lines). On the other hand, the assumption of a non-Maxwellian, but isotropic, distribution function is too restrictive. Therefore, in Ref. [25] a Maxwellian distribution has been assumed for the scatterer particles. Its parameters (density, drift velocity and temperature) are calculated by averaging over the particles populating the cell of interest. In addition, in order to avoid a systematic error which may appear in case where the conservation laws are fulfilled only statistically [29], the exact conservation of momentum and energy within the cell was enforced by correcting the velocities after the collisional scattering of test particles during a single time step.

As in Ref. [25], the approach of the present paper is also based on the (well known [30]) Monte Carlo model of collisional scattering by a Maxwellian background, but the momentum and energy conservation laws are enforced differently. In contrast to Ref. [25], parameters (temperature and fluid velocity) of the background Maxwellian are computed without averaging over the ensemble of test particles but evolve in time together with the test particle parameters in accordance