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Composition schemes for the stochastic differential equation describing collisional pitch-angle diffusion

L.J. Höök [a,b,*], T. Johnson [a]

[a] Department of Fusion Plasma Physics, School of Electrical Engineering, KTH, Sweden
[b] Division of Scientific Computing, Department of Information Technology, Uppsala University, Sweden

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ABSTRACT

Two new second order accurate Monte Carlo integration schemes are derived for the stochastic differential equation describing pitch-angle scattering by Coulomb collisions in magnetized plasmas. Here the pitch-angle is the angle between the magnetic field and the particle velocity vectors. Mathematically this collision process corresponds to diffusion in the polar angle of a spherical coordinate system. The schemes are simple to implement, they are naturally bounded to the solution domain and their convergences are shown to compare favourably against commonly used alternative integration schemes.

1. Introduction

Accurate numerical modelling of Coulomb collisions in guiding-centre following particle codes is of fundamental importance in many areas of plasma physics. Examples can be found in, e.g., neoclassical and turbulence transport models [1–3] and in the study of wall load due to toroidal magnetic field ripple [4]. When modelling these problems with particle codes it is common to separate the numerical integration of the guiding-centre orbits and the collisions, and to use higher order Runge–Kutta schemes for the orbit integration, while the order of the convergence of the collision integrator is low [1]. This ensures the conservation of orbit invariants, thus reducing the numerically induced transport. In comparison, a small numerical error in the collision integrator tends to cause a relatively modest error in the transport. Furthermore, this is a particularly efficient solution when the collisionality is low, like in the plateau and banana collisionality regimes, where the numerical error is likely to be dominated by the orbit tracing. The picture may however be quite different in the Pfirsch–Schlüter regime, where the time scales for the guiding centre orbit and the collisions are of the same order. Here the numerical error is a combination of the errors from integrating the orbits and the collisions, as well as an error from the separation of these two processes. In this regime the relatively large error from the collisions tends to dominate, thus requiring short time steps and massive computational resources to achieve convergence.

In this work we derive two new numerical schemes for the part of the collision operator that modifies the directions of the velocity vector without modifying the total velocity, the so called pitch-angle scattering. Mathematically, this type of scattering process is equivalent to isotropic diffusion on the sphere, a topic that has application in other fields of applied mathematics e.g. [5].

The outline of the paper is as follows. In Section 2 we give a brief overview on the guiding-centre drift equation with collisions. Section 3 presents the operator splitting method and the error from the separation of the orbit integrator and the collision integrator is discussed. Two new numerical schemes for the pitch-angle scattering process are derived in Section 4 based on the method of operator splitting. The new schemes are benchmarked in Section 5 and are followed by conclusions in Section 6.

2. Drift-kinetics with Coulomb collisions

The central result of this paper are the new numerical schemes for the modelling of diffusion on a sphere using a particle representation, as described in Section 4. While this scheme has application in many fields of applied mathematics, we have here chosen to study an application in plasma physics, more specifically, in guiding centre following codes with Coulomb collisions. The physics included in such codes can be described by the drift kinetic equation for the distribution function $f = f(\mathbf{R},$

* Corresponding author at: Department of Fusion Plasma Physics, School of Electrical Engineering, KTH, Sweden. Tel.: +46 706734576.
E-mail address: joh@kth.se (L.J. Höök).

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$\mathbf{v}, t)$, where $\mathbf{R}$ is the gyro centre position and $\mathbf{v}$ is the velocity

$$\frac{\partial f}{\partial t} + \mathcal{L}_0 f = \frac{\partial f}{\partial t} + \dot{\mathbf{R}} \cdot \nabla f + \dot{\mathbf{v}} \cdot \nabla_{\mathbf{v}} f = \mathcal{C}(f, f). \tag{1}$$

Here $\mathcal{C}$ is the collision operator, $\nabla_{\mathbf{v}}$ is the del-operator in velocity space, and $\dot{\mathbf{R}}$ and $\dot{\mathbf{v}}$ are the gyro centre drift velocity and acceleration, [6–8]. In general the Coulomb collision operator is a nonlinear operator depending on the Rosenbluth potentials [9], which are quite a challenge to model accurately. However, in many applications the collision operator can be approximated by $\mathcal{C}(f_M, f)$, where f_M is a Maxwellian distribution function. This simplifies the relevant derivatives of the Rosenbluth potentials to the analytical Chandrasekhar coefficients $\alpha(v), \beta(v), \gamma(v)$ [10] expressed in spherical coordinates (v, θ, ϕ), where $v = \|\mathbf{v}\|$, $\cos\theta = \mathbf{v} \cdot \mathbf{B}/(|\mathbf{v}||\mathbf{B}|)$, and ϕ is the gyro angle. The collision operator reduces to

$$\mathcal{C}(f_M, \cdot) = \frac{1}{v^2}\frac{\partial}{\partial v} v^2 \left[-\alpha(v) + \frac{1}{2v^2}\frac{\partial}{\partial v} v^2 \beta(v) \right] + \frac{1}{2v^2}\gamma(v)\mathcal{L} \tag{2}$$

and

$$\mathcal{L} = \frac{1}{2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \right) \right] \tag{3}$$

is the Lorentz operator, which is one half of the Laplace operator on the sphere. Even though this model is linear, some nonlinear effect can be accounted for by regularly recalculating the Chandrasekhar coefficients using temperatures and densities estimated from the test particle distribution [11]. In many applications the gyro angle dependence in (3) can be neglected, since it relaxes on the rapid time scale of the gyro period, leaving

$$\mathcal{L} = \frac{1}{2}\frac{\partial}{\partial\xi}(1-\xi^2)\frac{\partial}{\partial\xi} \tag{4}$$

with $\xi = \cos\theta, \xi \in \mathcal{D} = [-1, 1]$. Green's function for this operator can then be studied with the following reduced kinetic equation:

$$\frac{\partial \tilde{f}}{\partial t}(\xi, t) = \frac{1}{2}\frac{\partial}{\partial\xi}\left(1-\xi^2\right)\frac{\partial \tilde{f}}{\partial\xi}(\xi, t), \tag{5}$$

with the initial condition $\tilde{f}(\xi, 0) = \delta(\xi - \xi_0)$. Note that we have assumed $\gamma(v)/2v^2 = 1$, which correspond to a rescaling of the time, $\gamma(v)t/2v^2 \to t$. The general solution can be written explicitly in terms of the Legendre polynomials P_n,

$$\tilde{f}(\xi, t) = \sum_{n=0}^{\infty} \exp\left(-\frac{1}{2}n(n+1)t \right)\left(n + \frac{1}{2} \right) P_n(\xi_0) P_n(\xi). \tag{6}$$

The stationary solution ($\frac{\partial \tilde{f}}{\partial t} = 0$) is particularly simple:
$\frac{1}{2}\frac{\partial}{\partial\xi}\left(1-\xi^2\right)\frac{\partial \tilde{f}}{\partial\xi} = 0 \Rightarrow \tilde{f} = 1/2$, which is a flat distribution in $\mathcal{D}$.

3. Operator splitting

Operator splitting is a well-established method for the numerical integration of problems with great numerical complexity [12]. The central idea is to split the problem into several simpler problems. Consider the following example:

$$\frac{\partial f}{\partial t} = (\mathcal{A} + \mathcal{B})f, \qquad f(\cdot, t = 0) = f_0, \tag{7}$$

where $\mathcal{A}, \mathcal{B}$ are linear autonomous operators. The solution in terms of the exponential map is given by $f(\cdot, t) = \exp(\mathcal{A}t + \mathcal{B}t)f_0$. By assuming small times $t : \|\mathcal{A}t\| + \|\mathcal{B}t\| \ll 1$, the exponential map can be approximated by a product of maps, a so-called Lie–Trotter splitting [12]

$$\exp(\mathcal{A}t + \mathcal{B}t)f_0 = \exp(\mathcal{A}t)\exp(\mathcal{B}t)f_0 + \epsilon \tag{8}$$

where ϵ is the error. Note that this corresponds to solving (7) with the following sub-problems:

$$\frac{\partial h}{\partial t'} = \mathcal{B}h, \quad t' \in [0, t],\ h(\cdot, 0) = f_0 \tag{9}$$

$$\frac{\partial g}{\partial t'} = \mathcal{A}g, \quad t' \in [0, t],\ g(\cdot, 0) = h(\cdot, t). \tag{10}$$

The error is easily calculated for small time steps, $t \to \Delta t$

$$\epsilon = \frac{1}{2}\Delta t^2 ([\mathcal{B}, \mathcal{A}])f_0 + \mathcal{O}(\Delta t^3), \tag{11}$$

where $[\cdot, \cdot]$ is the commutator. The split described above concerns only PDEs. To construct the split for the corresponding SDE, there are two alternative approaches. One option is to first derive the SDE and then split the SDE in two parts. This is the method described in [13]. The alternative is to first split the PDE and derive the two SDEs; see Fig. 1.

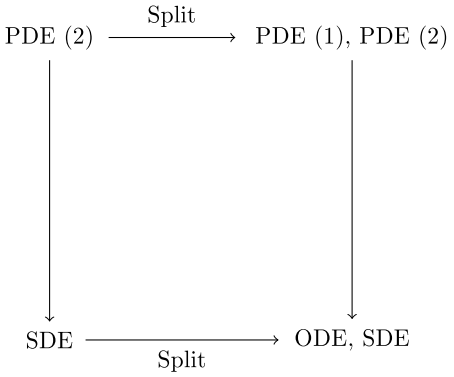

Fig. 1. Illustration of the two alternative approaches of splitting. In this paper we first split the PDE and derive the ODE and the SDE for each sub-problem. Note that the leading order derivative of the PDE is given in the parenthesis.

When the norm of the operators are comparable, the above splitting yields a local error of $\epsilon \sim \mathcal{O}(\Delta t^2)$ and a global error of $\sum \epsilon \sim \mathcal{O}(\Delta t)$, where the sum is over all time steps. To improve the convergence we have to turn to more advanced ways to split (7) [12].

A second order accurate splitting scheme is the well-known symmetric method according to Strang [14],

$$\begin{aligned} &\exp(\mathcal{A}\Delta t + \mathcal{B}\Delta t)f_0 \\ &\quad = \exp(\mathcal{A}\Delta t/2)\exp(\mathcal{B}\Delta t)\exp(\mathcal{A}\Delta t/2)f_0 + \epsilon. \end{aligned} \tag{12}$$

The symmetric splitting has a local error

$$\epsilon_{sym} = \frac{1}{2}\Delta t^2 \underbrace{([\mathcal{B}, \mathcal{A}] + [\mathcal{A}, \mathcal{A}] + [\mathcal{A}, \mathcal{B}])}_{=0} f_0 + \mathcal{O}(\Delta t^3).$$

This gives a global error of $\mathcal{O}(\Delta t^2)$. As an example, we can apply this result on the guiding-centre equation (1) to obtain the following second order composition:

$$\begin{aligned} \frac{\partial h_1}{\partial t} &= \mathcal{L}_o h_1, \quad t \in [0, \Delta t/2],\ h_1(\cdot, 0) = f_0 \\ \frac{\partial g}{\partial t} &= \mathcal{C}g, \quad t \in [0, \Delta t],\ g(\cdot, 0) = h_1(\cdot, \Delta t/2) \\ \frac{\partial h_2}{\partial t} &= \mathcal{L}_o h_2, \quad t \in [\Delta t/2, \Delta t],\ h_2(\cdot, \Delta t/2) = g(\cdot, \Delta t). \end{aligned} \tag{13}$$

Note that for the total error to be of second order, all three steps in (13) have to be integrated with at least second order accuracy.