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Geometric integrator for charged particle orbits in axisymmetric fusion devices

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ABSTRACT

A semi-analytical geometric integrator of guiding centre orbits in an axisymmetric tokamak is described. The integrator preserves all three invariants of motion up to computer accuracy at the expense of reduced orbit accuracy and it is roughly an order of magnitude more efficient than a direct solution of the equations of guiding centre motion with a standard high order adaptive ODE integrator.

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1. Introduction

An evaluation of the distribution function and/or its moments by direct modelling of particle orbits is widely used in plasma physics (see, e.g., codes like EUTERPE [1,2] or ASCOT [3]). An efficient algorithm for calculation of trajectories of charged particles in complex (quasi-)stationary magnetic and electric fields is one of the key issues in such codes because of the high number of test particle orbits required to minimize the statistical error of such calculations, which scales inversely with the square root of the number of test particles. This issue is especially important for global transport modelling (e.g., see Ref. [4]) where the profiles of plasma parameters are calculated self-consistently from test particle trajectories, which have to be traced over the profile relaxation (confinement) time.

Within transport modelling, computation of stochastic test particle orbits [5] requires the solution of guiding centre equations [6,7], which is usually performed with help of general-purpose ODE integrators. In case of axisymmetric systems (tokamaks) the guiding centre motion is fully integrable, because there exist three integrals of motion, which fully determine each orbit in the 5D phase space: The total energy w, magnetic moment μ and the canonical toroidal angular momentum p_φ, respectively are given by

$$w = \frac{m(v_\perp^2 + v_\parallel^2)}{2} + e\Phi, \qquad \mu = \frac{mv_\perp^2}{2B}, \qquad p_\varphi = mv_\parallel \frac{B_\varphi}{B} + \frac{e}{c}A_\varphi, \tag{1}$$

with electrostatic potential Φ, magnetic field module B, co-variant toroidal component of the magnetic field B_φ, co-variant toroidal component of the vector potential A_φ, speed of light c, particle charge e, mass m, perpendicular velocity $v_\perp$, and parallel velocity $v_\parallel$. An accurate conservation of the invariants (1) is of primary importance for transport modelling in drift kinetic or drift fluid approximation while other accuracy requirements related to orbits can be significantly relaxed. Algorithms with such exact (up to computer accuracy) conservation of invariants are called *geometric integrators* (see, e.g., Ref. [8]). These integrators preserve the geometry of the exact phase space flow (in particular, orbits resulting from the integrator of this paper stay exactly closed in the poloidal plane $\varphi = const$ unless they cross the boundary of the computation domain), but the orbits do not necessarily satisfy Hamiltonian equations of motion with some (slightly modified) Hamiltonian as in the case of the symplectic integrators [9] being a sub-class of geometric integrators.

In the following sections we will introduce and study such an integrator suitable for transport modelling of axisymmetric fusion devices. In a comparison with commonly used general-purpose ODE integrators one can expect two advantages: First, in numerical

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efficiency; and second, such an algorithm should be less sensitive to the accuracy of the representation of the electromagnetic field allowing also for numerical inaccuracies resulting, in particular, from the statistical noise in the data.

2. Derivation of the integrator

In general magnetic field geometry, equations of guiding centre motion with invariants w and μ used as velocity space variables are [7]

$$\dot{\mathbf{r}} = \frac{v_\parallel \mathbf{B}^*}{B h_\parallel^*}, \qquad \mathbf{B}^* = \nabla \times \left(\mathbf{A} + \frac{mc v_\parallel}{eB}\mathbf{B}\right), \qquad h_\parallel^* = \frac{\mathbf{B}\cdot\mathbf{B}^*}{B^2}, \tag{2}$$

where $\mathbf{B}$ and $\mathbf{A}$ are magnetic field and vector potential, respectively, and $v_\parallel = v_\parallel(\mathbf{r}, w, \mu, \sigma)$ is determined by the first two Eqs. in (1) and parallel velocity sign $\sigma = \pm$. In axisymmetric geometry using cylindrical variables (R, φ, Z), equations of motion omitting the symmetry variable φ take the form

$$\dot{R} = -\frac{1}{R h_\parallel^*}\left(\frac{\partial A_\varphi}{\partial Z}\frac{1}{mB_\varphi}\left(p_\varphi - \frac{e}{c}A_\varphi\right) + \frac{mcB_\varphi}{2e}\frac{\partial}{\partial Z}\left(\frac{v_\parallel}{B}\right)^2\right),$$

$$\dot{Z} = \frac{1}{R h_\parallel^*}\left(\frac{\partial A_\varphi}{\partial R}\frac{1}{mB_\varphi}\left(p_\varphi - \frac{e}{c}A_\varphi\right) + \frac{mcB_\varphi}{2e}\frac{\partial}{\partial R}\left(\frac{v_\parallel}{B}\right)^2\right). \tag{3}$$

The varying part of $B_\varphi = B_\varphi(\psi)$ as a function of poloidal flux $\psi = -A_\varphi$ is of the order of plasma beta or of the square of the ratio of the poloidal and toroidal field strengths. In most tokamaks this variation is only a few percent and can be safely ignored. With this assumption, Eqs. (3) are rewritten as

$$\dot{R} = -\frac{1}{R h_\parallel^*}\frac{\partial}{\partial Z}\mathcal{H}, \qquad \dot{Z} = \frac{1}{R h_\parallel^*}\frac{\partial}{\partial R}\mathcal{H}, \tag{4}$$

where a Hamiltonian like function $\mathcal{H}$ is

$$\mathcal{H} = \frac{cB_\varphi}{e}\left(\frac{w}{B^2} - \frac{\mu}{B} - \frac{e\Phi}{B^2}\right) - \frac{e}{2mcB_\varphi}\left(A_\varphi - \frac{c}{e}p_\varphi\right)^2. \tag{5}$$

Particle orbits are then determined by the condition $\mathcal{H} = 0$. A numerically efficient low order approximation of these orbits can be obtained if one uses in (5) a linear interpolation for the following functions of coordinates $\mathbf{x} = (x^1, x^2) \equiv (R, Z)$,

$$f_A(\mathbf{x}) \equiv A_\varphi, \qquad f_B(\mathbf{x}) \equiv \frac{1}{B}, \qquad f_\Phi(\mathbf{x}) \equiv \frac{\Phi}{B^2}, \tag{6}$$

discretized on a triangular mesh required for the continuous piecewise linear interpolation. As a result, $\mathcal{H}$ (5) becomes a continuous piecewise quadratic function,

$$\mathcal{H} = \frac{1}{2}\sum_{i,j=1}^{2} a_{ij}(x^i - x_a^i)(x^j - x_a^j) - \frac{1}{2}\sum_{i,j=1}^{2} a_{ij}(x_0^i - x_a^i)(x_0^j - x_a^j), \tag{7}$$

where the coefficients a_{ij} are constant within a given triangle and are determined by initial values of the particle coordinates $\mathbf{x}_0$ and the velocity components $v_{\perp 0}$ and $v_{\parallel 0}$ in this triangle as follows,

$$a_{ij} = \frac{1}{\alpha}\left(v_{\perp 0}^2 + v_{\parallel 0}^2 + \frac{2ef_\Phi(\mathbf{x}_0)}{mf_B^2(\mathbf{x}_0)}\right)\frac{\partial f_B}{\partial x^i}\frac{\partial f_B}{\partial x^j} - \alpha\frac{\partial f_A}{\partial x^i}\frac{\partial f_A}{\partial x^j}. \tag{8}$$

Here, $\alpha = e\left(mcB_\varphi\right)^{-1}$, and the constants x_a^i are the solution to the following linear equation set,

$$\sum_{j=1}^{2} a_{ij}(x_0^j - x_a^j) = v_{\parallel 0} f_B(\mathbf{x}_0)\frac{\partial f_A}{\partial x^i} + \left(v_{\perp 0}^2 + 2v_{\parallel 0}^2 + \frac{4ef_\Phi(\mathbf{x}_0)}{mf_B^2(\mathbf{x}_0)}\right)\frac{f_B(\mathbf{x}_0)}{2\alpha}\frac{\partial f_B}{\partial x^i} - \frac{e}{m\alpha}\frac{\partial f_\Phi}{\partial x^i}. \tag{9}$$

The spatial particle trajectories, $\mathcal{H} = 0$, are then continuous piecewise second order curves. Note that vector potential and magnetic field module in (6) are treated as independent functions within the above linear interpolation, which does not hold the relation $B = |\nabla \times \mathbf{A}|$ anymore. Consequently, gradient-B drift is retained in the orbits while it would be absent if B would be computed from that relation. Due to continuous interpolation of all functions of the coordinates in Eq. (1), orbits are continuous also in the velocity space where preferable variables are $(v_\perp, v_\parallel)$. Those are more convenient for modelling of collisions and of anomalous transport, both required in transport simulations. A parametric (time-dependent) form of orbit segments is obtained from the equations of motion (4), which are further simplified by ignoring the Larmor radius correction, $h_\parallel^* \to 1$ and by replacing R with a constant $\bar{R}$ being the radial coordinate of the centre of mass of a given triangle,

$$\dot{x}^i = \frac{(-1)^i}{\bar{R}}\sum_{j=1}^{2} a_{3-i,j}\left(x^j - x_a^j\right). \tag{10}$$

This approximation does not affect the orbit shape. Namely, particles move along exactly the same orbits in the phase space but time dependence of phase space coordinates is slightly changed. Depending on the sign of the determinant $D = \det(a_{ij})$, orbits are either ellipses $(D > 0)$ or hyperbolas $D < 0$, respectively given by

$$x^i = x_a^i + x_c^i\cos(\omega\Delta t) + x_s^i\sin(\omega\Delta t), \qquad D > 0,$$

$$x^i = x_a^i + x_c^i\cosh(\omega\Delta t) + x_s^i\sinh(\omega\Delta t), \qquad D < 0, \tag{11}$$

where Δt is the integration time step,

$$\omega = \frac{|D|^{1/2}}{\bar{R}}, \qquad x_c^i = x_0^i - x_a^i, \qquad x_s^i = \frac{(-1)^i}{|D|^{1/2}}\sum_{j=1}^{2} a_{3-i,j}x_c^j. \tag{12}$$

The numerical implementation of this integrator is quite straightforward: One follows the test particle for the time step Δt (usually determined by collisions or anomalous transport) using Eqs. (11) and modifies its velocities $(v_\perp, v_\parallel)$ according to the conservation laws (1). If Δt exceeds the time to reach a boundary of the triangle, one stops the trajectory at this point of intersection. Its coordinates, $\mathbf{x}_b$, satisfy a quadratic equation, and the corresponding time can be found from (11) for $\mathbf{x} = \mathbf{x}_b$. Then one follows the particle in the next triangle using the point of intersection as a new starting point $\mathbf{x}_0$ and its local velocities as new $v_{\perp 0}$ and $v_{\parallel 0}$.

3. Benchmarking

We now compare the results obtained by the geometric integrator derived in the previous section and a conventional adaptive ODE integrator, *odeint* (Ref. [10]). The magnetic configuration we use is ITER-like (the same had been used in Ref. [4]) with zero electric field everywhere.

The triangular mesh required for the geometric integrator has been produced from a nearly orthogonal field-aligned quadrangular mesh used for fluid modelling by the B2 code [11]. The *odeint* [10] solver has been employed here for the full 3D system of guiding centre equations [7] in the covariant representation [12] for cylindrical coordinates. A very accurate divergence-free representation of the magnetic field based on 2D spline interpolation (5th order) of the poloidal flux function has been used for this integrator, which acts as a reference case.

As an example, a few collisionless trajectories calculated by the geometric integrator for trapped deuterium and iron ions are presented in Fig. 1 together with pertinent orbits from the reference case. In addition, the used triangular mesh is also shown. All orbits almost coincide in the overview figure (a), but the

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