

## Three-dimensional geometric integrator for charged particle orbits in toroidal fusion devices

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Global kinetic computations of quasi-steady plasma parameters in 3D toroidal fusion devices with help of test particle methods such as kinetic modelling of 3D plasma equilibria [1] or kinetic modelling of edge plasmas put specific requirements on guiding center orbit integration methods. Namely, they should be computationally efficient, tolerant to statistical noise in the electromagnetic field and efficient in scoring statistical data from the orbits. Geometric integrators address these targets by releasing the requirement to the accuracy of guiding center orbits while preserving physically correct long time orbit dynamics. Such a 3D integrator preserving total energy, magnetic moment and phase space volume is presented here.

As a starting point, equations of guiding center motion in general curvilinear coordinates  $x^i$  are considered with invariants of motion  $w = m_\alpha v^2/2 + e_\alpha \Phi$  and  $J_\perp = m_\alpha v_\perp^2/(2\omega_c)$  being total energy and perpendicular adiabatic invariant, respectively, used as independent phase space variables,

$$\dot{x}^i = \frac{v_\parallel \epsilon^{ijk}}{\sqrt{g} B_\parallel^*} \frac{\partial A_k^*}{\partial x^j}, \quad A_k^* = A_k + \frac{v_\parallel}{\omega_c} B_k. \quad (1)$$

Here,  $e_\alpha$ ,  $m_\alpha$ ,  $A_k$ ,  $B_k$ ,  $\omega_c$ ,  $\Phi$  and  $\sqrt{g}$  are  $\alpha$ -species charge and mass, covariant components of vector potential and magnetic field, electrostatic potential, cyclotron frequency and metric determinant, respectively, and  $\sqrt{g} B_\parallel^* = \epsilon^{ijk} (B_i/B) \partial A_k^* / \partial x^j$ . The parallel velocity  $v_\parallel$  in (1) is not an independent variable but a known function of coordinates,

$$v_\parallel^2 = 2U, \quad U = U(\mathbf{x}) = \frac{1}{m} (w - J_\perp \omega_c(\mathbf{x}) - e_\alpha \Phi(\mathbf{x})). \quad (2)$$

Treating now  $v_\parallel$  as an independent variable, i.e. replacing the first expression of (2) with the differential equation  $\dot{v}_\parallel = (x^i \partial U / \partial x^i) / v_\parallel$ , the set (1) turns into

$$\begin{aligned} B_\parallel^* \sqrt{g} \dot{x}^i &= \frac{dx^i}{d\tau} = \epsilon^{ijk} \left( v_\parallel \frac{\partial A_k}{\partial x^j} + 2U \frac{\partial}{\partial x^j} \frac{B_k}{\omega_c} + \frac{B_k}{\omega_c} \frac{\partial U}{\partial x^j} \right), \\ B_\parallel^* \sqrt{g} \dot{v}_\parallel &= \frac{dv_\parallel}{d\tau} = \epsilon^{ijk} \frac{\partial U}{\partial x^i} \left( \frac{\partial A_k}{\partial x^j} + v_\parallel \frac{\partial}{\partial x^j} \frac{B_k}{\omega_c} \right). \end{aligned} \quad (3)$$

Note that no invariant of motion has been completely replaced by  $v_\parallel$  in (3) because  $U$ , being a function of coordinates, is still defined by the second expression of (2). Besides that, the time

variable is replaced by an orbit parameter  $\tau$  related to time by  $dt = B_{\parallel}^* \sqrt{g} d\tau$ . If needed, the time evolution can be obtained implicitly from the integral  $t(\tau)$  of the equation above.

The special form (3) allows to reduce computational effort and noise sensitivity by independently approximating field quantities  $A_k, B_k/\omega_c, \omega_c$  and  $\Phi$  by continuous piecewise linear functions. This is achieved by splitting the space into tetrahedral cells. As a result, in each cell, equations of motion (3) turn into a set of four linear ODEs with constant coefficients

$$\frac{dz^i}{d\tau} = a_l^i z^l + b^i, \quad (4)$$

where  $z^i = x^i$  for  $i = 1, 2, 3$  and  $z^4 = v_{\parallel}$ . Since piecewise-constant coefficients of set (4) are discontinuous at the cell boundaries, orbit intersections with tetrahedra faces must be computed exactly when integrating particle trajectories. For this, equation set (4) is numerically solved within each cell using the Runge-Kutta 4 method in an iterative scheme, where Newton's method is used to obtain the integration step  $\Delta\tau$  required to reach the cell boundary.

In fact, a linear approximation of field quantities which locally breaks the physical connection between them does not destroy the Hamiltonian nature of the original set (1). Indeed, despite the approximation made, equation set (3) can still be cast to the non-canonical Hamiltonian form

$$\frac{dz^i}{d\tau} = \Lambda^{ij} \frac{\partial H}{\partial z^j}, \quad \Lambda^{ij}(\mathbf{z}) = \{z^i, z^j\}_{\tau}, \quad (5)$$

where the Hamiltonian function is  $H(\mathbf{z}) = v_{\parallel}^2/2 - U(\mathbf{x})$  and  $\Lambda^{ij}(\mathbf{z})$  is an antisymmetric Poisson matrix. The latter is linked to Poisson brackets that are slightly re-defined from those in Ref. [3] due to a different orbit parameter,

$$\{f, g\}_{\tau} = b_*^i \left( \frac{\partial f}{\partial x^i} \frac{\partial g}{\partial v_{\parallel}} - \frac{\partial g}{\partial x^i} \frac{\partial f}{\partial v_{\parallel}} \right) + \varepsilon^{ijk} \frac{\partial g}{\partial x^i} \frac{\partial f}{\partial x^j} \frac{B_k}{\omega_c}, \quad b_*^i = \varepsilon^{ijk} \left( \frac{\partial A_k}{\partial x^j} + v_{\parallel} \frac{\partial}{\partial x^j} \frac{B_k}{\omega_c} \right). \quad (6)$$

To get set (3), one occurrence of  $v_{\parallel}^2$  is replaced by  $2U(\mathbf{x})$ . A geometric Poisson integrator with conservative features of symplectic integrators follows since first of (2) is accurately preserved during integration.

The iterative scheme converges after roughly two Newton steps, due to an analytic estimation for the necessary initial step length using a parabolic solution of the simplified ODE set (4), where  $a_l^i = 0$  for  $1 \leq i, j \leq 3$  and  $a_4^4 v_{\parallel}(\tau) = a_4^4 v_{\parallel,0}$ . This initial guess in fact ignores terms linear in Larmor radius. Furthermore, for similar reasons the error of the RK4 method can be brought below computer accuracy, since the relative integration error of a single step between cell boundaries strongly scales with the Larmor radius  $\rho$  and is of the order of

$$\frac{\delta R(\Delta\tau)}{a} \sim \frac{\rho^3}{q^4 R^3} \Delta\varphi^5, \quad (7)$$

with  $R, a, q$  and  $\Delta\varphi$  denoting major radius, plasma radius, safety factor and toroidal cell length. By properly orienting the tetrahedra with respect to the symmetry direction, axisymmetry in

case of 2D fields is exactly preserved upon linearization. Consequently, the canonical toroidal angular momentum  $p_\phi = mv_\parallel B_\phi/B + A_\phi e/c$  remains invariant. Fig. 1 depicts Poincaré plots of  $10^7$  toroidal turns for equivalent starting parameters in cylindrical and symmetry flux coordinates, compared to an exact orbit for the full non-linearized 3D system. It can be seen that even for the coarse grid in Fig. 1, leading to differences in orbits obtained in different coordinate systems, the effect of the integration error (7) is negligible.

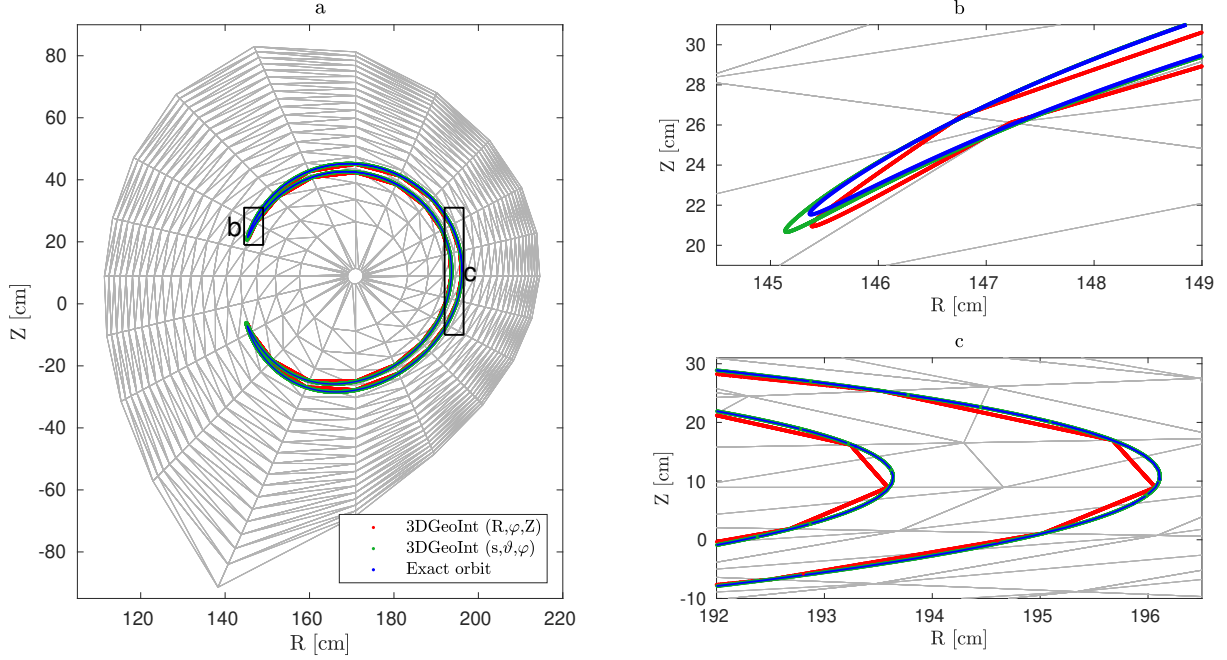


Figure 1: (a) Poincaré plot with  $10^7$  toroidal turns of a 1.5 keV D ion in axisymmetric ASDEX Upgrade configuration with a tetrahedral grid size of  $20 \times 20 \times 20$ . 3D Geometric Integrator: red (cylindrical coordinates), green (symmetry flux coordinates) - Exact orbit: blue. (b) and (c) are magnifications of the pertinent zones in (a).

In case of 3D magnetic fields the consequence of linearization of field quantities is that KAM surfaces do not exist anymore. This is demonstrated in Fig. 2 where a small harmonic perturbation has been added in unperturbed flux coordinates  $(s, \vartheta, \phi)$  to the axisymmetric vector potential  $A_\phi = \psi_{\text{pol}}(s)(1 + \epsilon_M \cos(m_0 \vartheta + n_0 \phi))$  with  $\epsilon_M = 0.01$ ,  $m_0 = n_0 = 2$  leading to a visibly ergodic passing particle orbit at coarse grid resolution. This behaviour is diffusive and its variance, computed in the normalized toroidal flux  $s$  for the ensemble of test particles starting from the same perturbed flux surface, can be described by a field line diffusion coefficient  $D_M^{ss}$  as  $\langle \delta s^2 \rangle = 2D_M^{ss}N$  where  $N$  is the number of toroidal orbit turns. Nevertheless, due to a strong inverse scaling of  $D_M^{ss}$  with poloidal  $N_\vartheta$  and toroidal  $N_\phi$  grid sizes, which roughly agrees with

$$D_M^{ss} = \frac{2\pi^2}{3} \left( \frac{\psi_{\text{pol}} \epsilon_M}{\psi_{\text{tor}}^a} \right)^2 \frac{q^4 m_0^2 n_0^2 (m_0 N_\vartheta + n_0 N_\phi)^2}{N_\vartheta^2 N_\phi^2 (q N_\phi - N_\vartheta)^2} \quad (8)$$

estimated from the quasilinear theory ( $\psi_a$  is toroidal flux at the edge) this numerical diffusion can be put below the level of classical electron diffusion using a mild grid refinement.

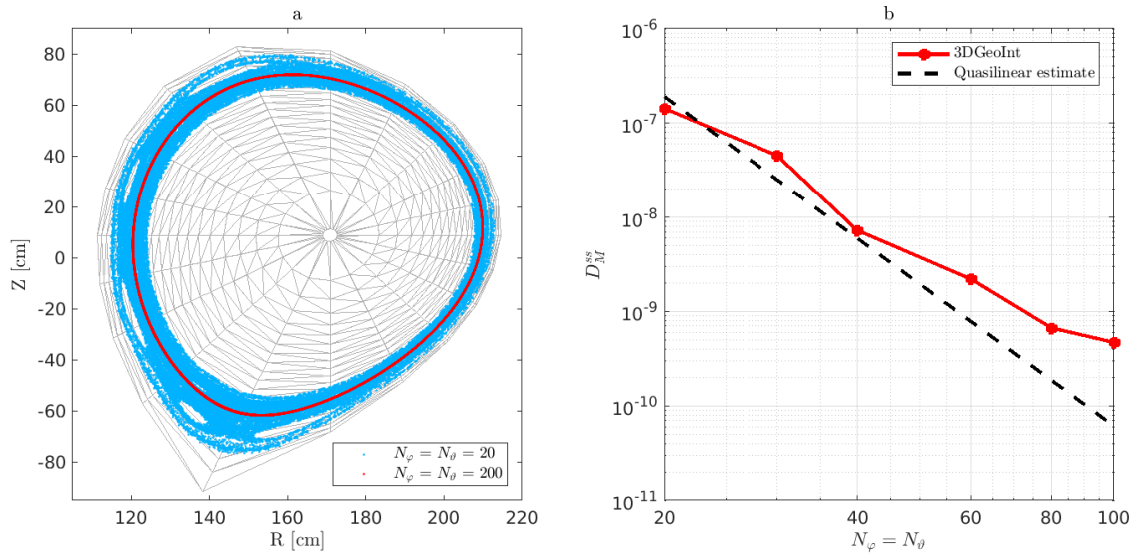


Figure 2: (a) Poincaré plot with 77 000 toroidal turns of two low energy particles with negligible FLR effects in ASDEX Upgrade configuration with typical non-axisymmetric 0.1 % relative helical perturbation of vector potential  $A_\phi$  and different grid sizes. (b) Magnetic field line diffusion coefficient with respect to grid size of the 3D Geometric Integrator compared to quasilinear estimate.

When applied to a stellarator field in symmetry flux coordinates computed by the VMEC code numerical diffusion in the solver is also effectively minimized by grid refinement because it results only from the FLR effects which lead roughly to the same order of perturbations as in weakly perturbed tokamaks,  $\epsilon_M \sim \rho/a$ .

Similar to the 2D geometric integrator of Ref. [2], the 3D geometric integrator is less sensitive to noise in field data than methods relying upon high order polynomial interpolation and automatically computes dwell times within spatial grid cells without extra effort. The later quantities are required for statistical scoring of orbits in Monte Carlo computations of macroscopic parameters, such as plasma response currents and charges caused by external non-axisymmetric perturbations in tokamaks or parameters of the edge plasma in devices with 3D field geometry.

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