Integration of the guiding-center equations in toroidal fields utilizing a local linearization approach

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Conventional methods for integrating the guiding-center equations [1] utilize high order interpolation of the electromagnetic field in space. In Ref. [2], a novel procedure for integration of 3D guiding-center orbits was introduced in which high order interpolation of the electromagnetic field is replaced by a local linearization approach. In particular, the electromagnetic field quantities A_k, B_k/ω_c, ω_c and Φ are independently approximated by continuous piecewise linear functions. These field quantities are respectively the covariant components of the vector potential and the normalized unit vector of the magnetic field, the cyclotron frequency and the electrostatic potential. The local linearization is achieved by splitting the space into tetrahedral cells. Specifically, each cell of a regular hexahedral grid in an arbitrary coordinate system is split into six tetrahedral cells as shown in Fig. 1. Upon linear interpolation of the field quantities, this specific splitting realization preserves the symmetry of the electromagnetic field over any of the coordinates if this coordinate corresponds to the symmetry direction. In particular, in the case of an axisymmetric field, the toroidal symmetry of the field is preserved, resulting in the preservation of the canonical (toroidal) angular momentum of the orbits.

As a result (details can be found in Ref. [2] and [3]), in each cell the guiding-center equations of motion [1] can be transformed into a set of four linear ODEs with constant coefficients

$$\frac{\mathrm{d}z^i}{\mathrm{d}\tau} = a^i_l z^l + b^i, \tag{1}$$

where $z^i = x^i$ (guiding-center position) for $i = 1,2,3$ and $z^4 = v_{||}$ (parallel velocity).

This local linearization approach retains the Hamiltonian structure of the guiding-center equations. For practical purposes this means that the total energy, the magnetic moment and the phase space volume are conserved. Furthermore, the approach reduces computational effort and sensitivity to noise in the electromagnetic field.

Since the coefficients of the linear ODE set are discontinuous at spatial cell boundaries, orbit intersections with those boundaries must be computed exactly when integrating particle trajectories. In Ref. [2], the linear ODE set is solved numerically by the Runge-Kutta (RK) method and intersections with cell boundaries are found by Newton's method. Alternatively and more effectively, an analytical solution of the ODE set in the form of a polynomial series can be used where the intersections are known analytically up to the 4^{th} polynomial order. This is facilitated by the fact that the field lines are straight within cells, and, in absence of the cross-field drift, the exact solution of Eq. (1) is a second order polynomial with respect to the orbit parameter τ. Consequently, the corrections introduced by the cross-field drift scale with powers of the Larmor radius. Hence, for electrons sufficient accuracy is achieved already with the second order series in the orbit parameter. An additional advantage of the series expansion is that various path integrals over dwell times in spatial cells used within Monte Carlo procedures for the evaluation of velocity space moments of the distribution function are known analytically.

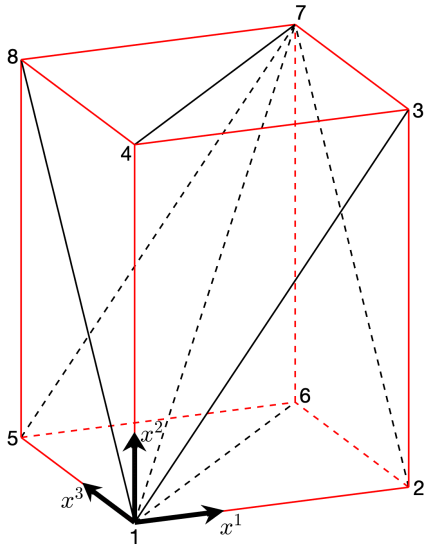

Figure 1: Splitting realization of a hexahedron in arbitrary curvilinear coordinate system (x^1, x^2, x^3). The hexahedron (red) is split into six tetrahedral cells. Spitting is invariant over 120° rotations around vertex 1.

The adverse consequence of above linearization is diffusive behaviour of orbits. In real space coordinates, this behaviour is already a property of the field lines. Consequently, the method in real space coordinates is only applicable to weakly perturbed toroidal fields such as tokamaks with external 3D perturbations where the artificial diffusion can be made negligibly small by moderate grid refinement. However, the artificial diffusion has been small even for essentially 3D fields when magnetic flux coordinates have been used in Ref. [3]. There, field-aligned symmetry flux coordinates have been used for a realistic stellarator configuration and non-aligned symmetry flux coordinates have been used for a tokamak with perturbed axial symmetry.

It should be noted that artificial chaos of the field lines is fully avoided in general toroidal fields if local magnetic coordinates are used [4, 5] in which the field lines are accurately described by the interpolated cell mapping using bi-cubic splines. Since two of these coordinates are magnetic, $\mathbf{B}\cdot\nabla x^1 = \mathbf{B}\cdot\nabla x^2 = 0$, the piecewise linearization does not introduce any change to the field line behaviour. However, the present orbit integration method cannot be applied as is because it

needs the continuity of the field quantities which is violated by the piecewise linear representation at the "periodic" boundary between neighbouring local coordinate systems, $x^3 = const$. This is caused by the fact that straight lines in one coordinate system are not straight in the other system due to the nonlinear coordinate mapping. Therefore, in the tetrahedra adjacent to the periodic boundary, the field quantities must be accurately interpolated over the "perpendicular" (x^1, x^2) coordinates, and the equations of motion do not form a linear set (1) anymore. In these cells, the original nonlinear guiding-center equations must be solved numerically.

The integration method has already been used in Ref. [3] for the application of collisionless guiding-center orbits in an axisymmetric tokamak and a realistic three-dimensional stellarator configuration. There, the method demonstrated stable long-term orbit dynamics conserving invariants. Further, in the same publication, the method was applied to the Monte Carlo evaluation of transport coefficients. There, the computational efficiency of the integration method was shown to be an order of magnitude higher than with a standard fourth order RK integrator.

Since publication of Ref. [3], the integration method has furthermore been also applied to the computation of fusion alpha particle losses in a realistic stellarator configuration. Fig. 2 shows the confined fraction f_c of 3.5 MeV fusion alpha particles as a function of the trace time. In Fig. 2 (a) 1000 particles are traced for 1 s, whereas in Fig. 2 (b) 10000 particles are traced for 0.01 s. All guiding-center orbits are started from $s = 0.6$ with a homogeneous distribution of the pitch parameter. The reference result is obtained by utilizing the "exact" guiding-center orbits which are computed with an adaptive RK 4/5 integrator with a relative tolerance of 10^{-9} in splined fields. The quasi-geometric integration method is performed with its *Polynomial 4* and *adaptive RK 4/5* options and in addition three different settings for the grid size are examined, namely $N_s = N_\vartheta = N_\varphi = 70$, $N_s = N_\vartheta = N_\varphi = 100$ and $N_s = N_\vartheta = N_\varphi = 200$.

It could been shown that the inherent artificial chaos of the method, which is induced by the linearization of the electromagnetic field, strongly scales with the particle's Larmor radius. Consequently, the quasi-geometric integration method is not suited to be used for tracing of high-energetic 3.5 MeV fusion alpha particles for the slowing-down time of 1 s. Nevertheless, for the trace time of 0.01 s the confined fraction results computed with the quasi-geometric integration method and an appropriate choice of the grid size lie within the 95 % confidence interval of the reference computation while showing a significant CPU speed-up. In particular, the fastest sufficiently accurate method is GORILLA with the solution in form of a polynomial series truncated at $K = 2$ and an angular grid size of $N_\vartheta \times N_\varphi = 100 \times 100$. This method is roughly 3 times faster than the fastest reference method, namely the adaptive RK4/5 integrator with a relative tolerance of 10^{-6}. The results for the confined fraction of this comparatively short trace time could be used for an early classification into regular and chaotic orbit types

within fusion alpha loss computations in a similar manner as in Ref. [6]

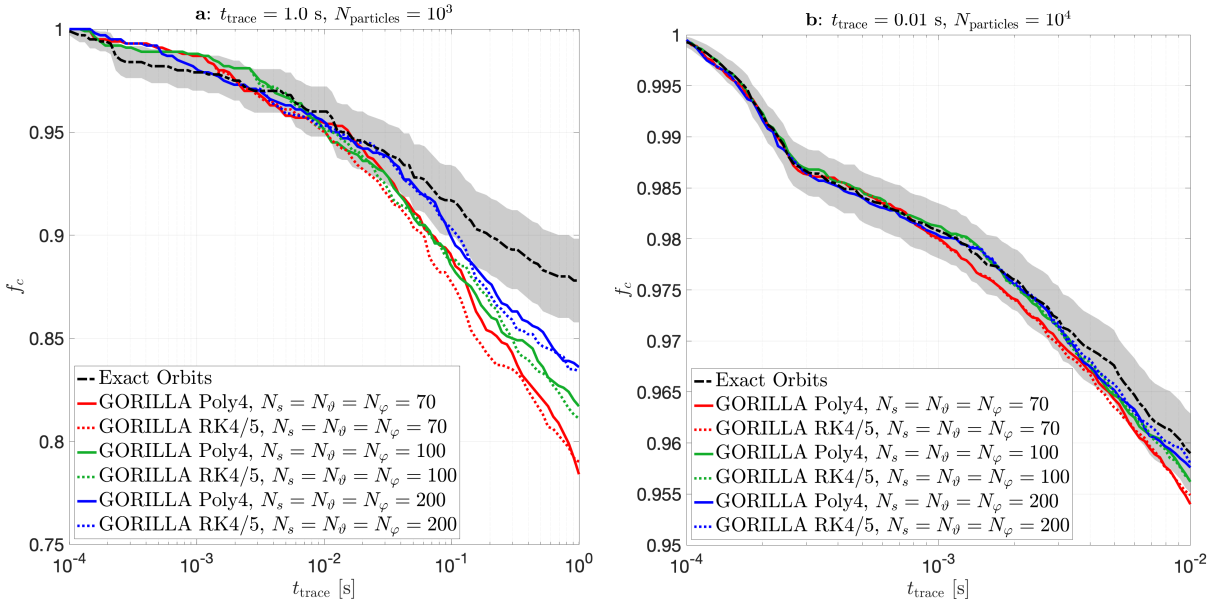

Figure 2: Confined fraction f_c of 3.5 MeV fusion alpha particles as a function of the trace time in 3D stellarator field configuration. (a) 1000 particles are traced for 1 s. (b) 10000 particles are traced for 0.01 s.
The guiding-center orbits are started from $s = 0.6$ with a homogeneous distribution of the pitch parameter. Orbits are evaluated by GORILLA and the results of f_c are compared to those obtained by exact guiding-center orbits from the reference guiding-center orbit computation. In the case of GORILLA, the method (*Polynomial* or *Runge-Kutta*) and the choice of the grid size are in accordance with the legend. Error bands at $\pm 1.96\sigma$ around the curve of f_c obtained with the exact guiding-center orbits describe the 95 % confidence interval due to the Monte Carlo error.

The numerical implementation of this method has been made publicly available on GitHub with the name **G**uiding-center **OR**bit **I**ntegration with **L**ocal **L**inearization **A**pproach (**GORILLA**); see Ref. [7].

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Zenodo: https://doi.org/10.5281/zenodo.4593661