On symplectic integration of the guiding-center equations in general 3D toroidal fields using GORILLA

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In Ref. [1], a method for quasi-geometric integration of the guiding-center equations in general 3D toroidal fields was introduced. Realized in the GORILLA code [2], this method reduces the set of guiding-center equations to a linear ODE set with piece-wise constant coefficients by approximating the guiding-center Lagrangian $\mathcal{L}$ with a continuous piecewise linear function of the coordinates,

$$\mathcal{L}^{(L)} = \frac{e_\alpha}{c} A_i^{*(L)} \dot{x}^i - J_\perp \dot{\phi} - H^{(L)} \qquad \text{with} \tag{1}$$

$$A_i^{*(L)} = A_i^{(L)} + v_\parallel \left(\frac{B_i}{\omega_c} \right)^{(L)} \qquad \text{and} \qquad H^{(L)} = \omega_c^{(L)} J_\perp + \frac{m_\alpha v_\parallel^2}{2} + e_\alpha \Phi^{(L)}. \tag{2}$$

Here, x^i, $v_\parallel$, $J_\perp$ and ϕ are the independent phase-space variables which are, respectively, the guiding-center position, the parallel velocity, the perpendicular adiabatic invariant and the gyrophase. Further, A_i, B_i, ω_c and Φ are the covariant components of the vector potential and the magnetic field, the cyclotron frequency and the electrostatic potential. Charge e_α and mass m_α of the considered species α enter $\omega_c = e_\alpha B/(m_\alpha c)$ together with the magnetic field modulus $B = \sqrt{B_i B^i}$ and the speed of light c. Superscripts (L) are used for quantities being piecewise linear functions of the coordinates. In GORILLA, this special representation of the electromagnetic field is achieved by performing a 3D linear interpolation within tetrahedral cells which can be built on the basis of the spatial discretization of edge plasma codes, in particular, of the kinetic neutral code EIRENE. Thus, direct data exchange with these codes is facilitated. Since this method is not limited by field topology, its primary target is to model edge plasmas of toroidal devices with a general 3D geometry.

Since publication of Ref. [1], where the computation domain for guiding-center orbits was limited to the plasma core, GORILLA's field linearization approach has been extended to the scrape-off layer (SOL). In the particular case of SOLEDGE3X-EIRENE [3], a 2D triangular mesh is provided and the given triangles are extruded in the toroidal direction to create slices of triangular prisms. Subsequently, each prism is split in a special manner into three tetrahedra. Specifically, the poloidal magnetic flux is used as as a key orientation quantity for the splitting mechanism to obtain a 3D tetrahedral grid that is consistent with GORILLA's logics and the utilized piecewise linear representation of the electro-magnetic field. Fig. 1 shows 3 keV D ion guiding-center orbits being projected to the poloidal $\varphi = 0$ plane in the axisymmetric WEST configuration. The guiding-center orbits are started from several poloidal flux surfaces (starting positions are indicated with points) with a pitch parameter $v_{\|}/v = 0.9$ and are, further, evaluated by GORILLA in 3D utilizing the 2D triangular discretization of SOLEDGE3X-EIRENE. The figure clearly shows orbits starting in the plasma core and being confined to drift-surfaces (green), orbits starting in the SOL and being lost to the wall or to the divertor (blue) and a transient orbit starting in the plasma core, further drifting to the SOL, and subsequently being lost (red).

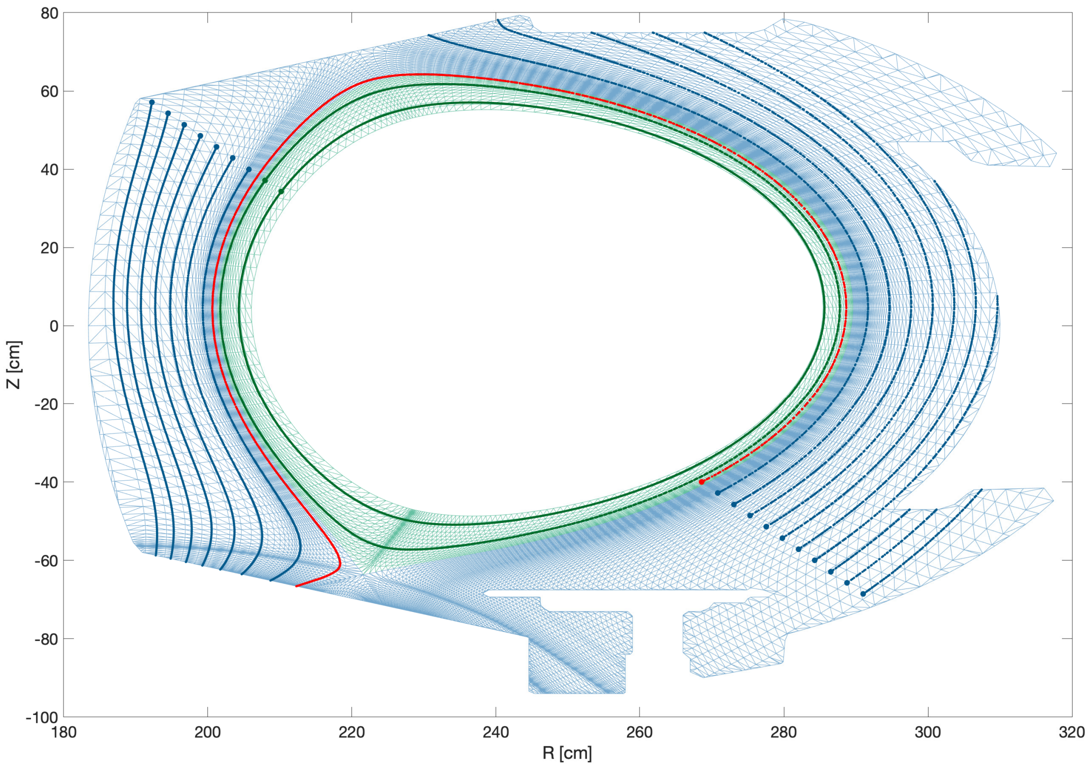

Figure 1: Poloidal projection ($\varphi = 0$) of guiding-center orbits of 3 keV D ions in the axisymmetric WEST tokamak configuration. The guiding-center orbits are evaluated in 3D with GORILLA utilizing the 2D triangular mesh of SOLEDGE3X-EIRENE. The orbit starting positions are indicated with points.

In GORILLA, guiding-center orbits are traced using a time-like orbit parameter τ. Originally, the integration method has been realized for the approximate, lowest order time dynamics such that the shape of the orbits in the phase-space was corresponding to a Hamiltonian system but the evolution in time could lead to minor artifacts in dwell time averages which are required for the computation of the spatial distribution of macroscopic parameters (density, plasma flows, pressure tensor). In this present work, the accurate time dynamics outlined in Ref. [1],

$$\frac{\mathrm{d}t}{\mathrm{d}\tau} = \frac{e_\alpha}{m_\alpha c}\varepsilon^{ijk}\left(\frac{B_i}{\omega_c}\right)^{(L)}\frac{\partial A_k^{*(L)}}{\partial x^j}, \tag{3}$$

has been realized in GORILLA resulting in orbits fulfilling the Hamiltonian properties in the whole extended phase-space. The correctness of the novel time dynamics is implicitly verified by computing the 1$^{\text{st}}$ Poincaré invariant J in the extended phase-space, which is given by

$$J = \frac{1}{2\pi}\oint \Lambda_\nu \, \mathrm{d}z^\nu, \tag{4}$$

where $z^\nu = z^\nu(\tau) = \left(x^i, v_\parallel, \phi, J_\perp, t\right)$ is the set of coordinates in the extended phase-space and $\Lambda_\nu = \Lambda_\nu(\mathbf{z}(\tau)) = \left(e_\alpha c^{-1}A_i^{*(L)}, 0, J_\perp, 0, -H^{(L)}\right)$ is the extended symplectic co-vector of the related piecewise linear guiding-center Lagrangian of Eq. 1, $\mathcal{L}^{(L)} = \Lambda_\nu \dot{z}^\nu$.

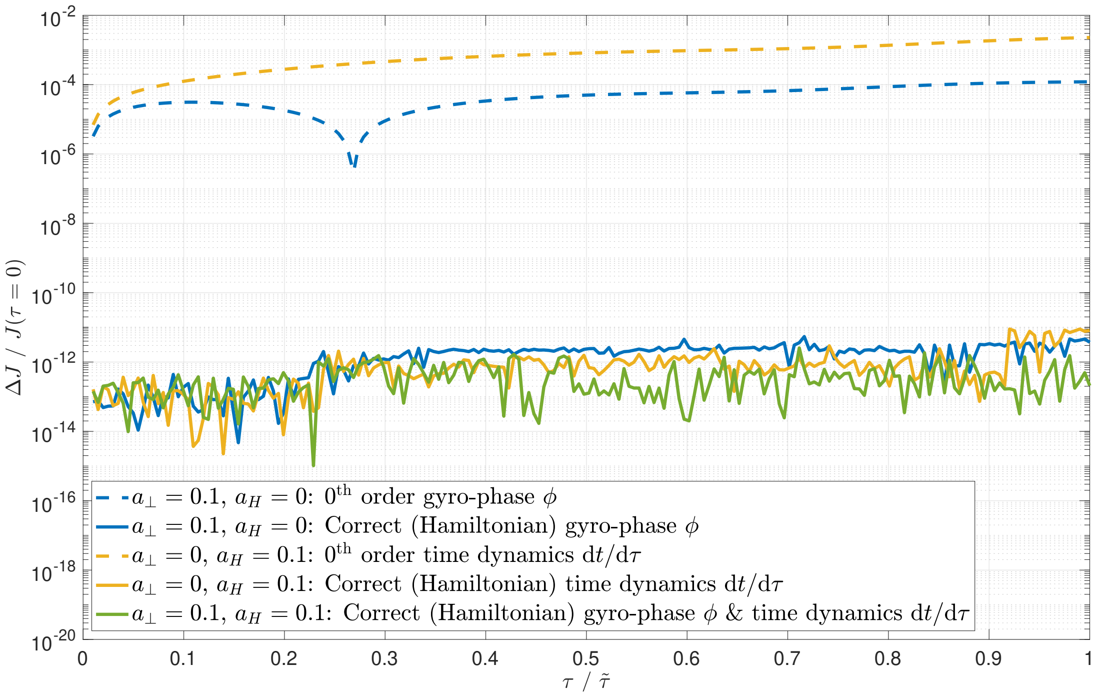

Figure 2: Relative error of the 1$^{\text{st}}$ Poincaré invariant as a function of the normalized orbit parameter $\tau/\tilde{\tau}$.

In Fig. 2 the relative error of the 1$^{\text{st}}$ Poincaré invariant is depicted as a function of the normalized orbit parameter $\tau/\tilde{\tau}$, where $\tilde{\tau}$ corresponds to the elapsed (time-like) value in which a strongly passing particle is traced for one toroidal field period. The 1$^{\text{st}}$ Poincaré invariant is computed by following a closed phase-space contour which is parameterized by $\xi \in [0, 2\pi]$ and which is initially located in the poloidal plane $\varphi = 0$ of the coordinate space. The initial values of the remaining extended phase-space coordinates are $t(\tau = 0) = 0$, $\phi(\tau = 0) = 0$, $J_\perp(\tau = 0) = \bar{J}_\perp(1 + a_\perp \cos\xi)$ and $H(\tau = 0) = \bar{H}(1 + a_H \sin\xi)$. The cases of $a_\perp = 0$ and/or $a_H = 0$ correspond to constant $J_\perp$ and/or constant H hyper-surfaces. In the zeroth order time dynamics J is preserved in the usual phase-space on constant H hyper-surfaces. In contrast,

for non-constant H in the extended phase-space, J is only poorly conserved in the zeroth order time dynamics. However, J is strongly conserved when using the recently implemented correct (Hamiltonian) time dynamics. The same conservation behavior of J is true also for the conjugated pair ϕ and $J_\perp$. In Fig. 3 a closed contour of starting positions of the guiding-center orbits $x^i(\tau = 0)$, which is utilized for the evaluation of 1^{st} Poincaré invariant, as well as the time evolution of this contour can be seen.
The conservation of the 1^{st} Poincaré invariant in the extended phase-space is not only a prerequisite for an artifact-free computation of distribution function moments which is needed specifically for the computation of particle and flow densities, but furthermore a strong numerical evidence that the integration method itself is symplectic, in fact.

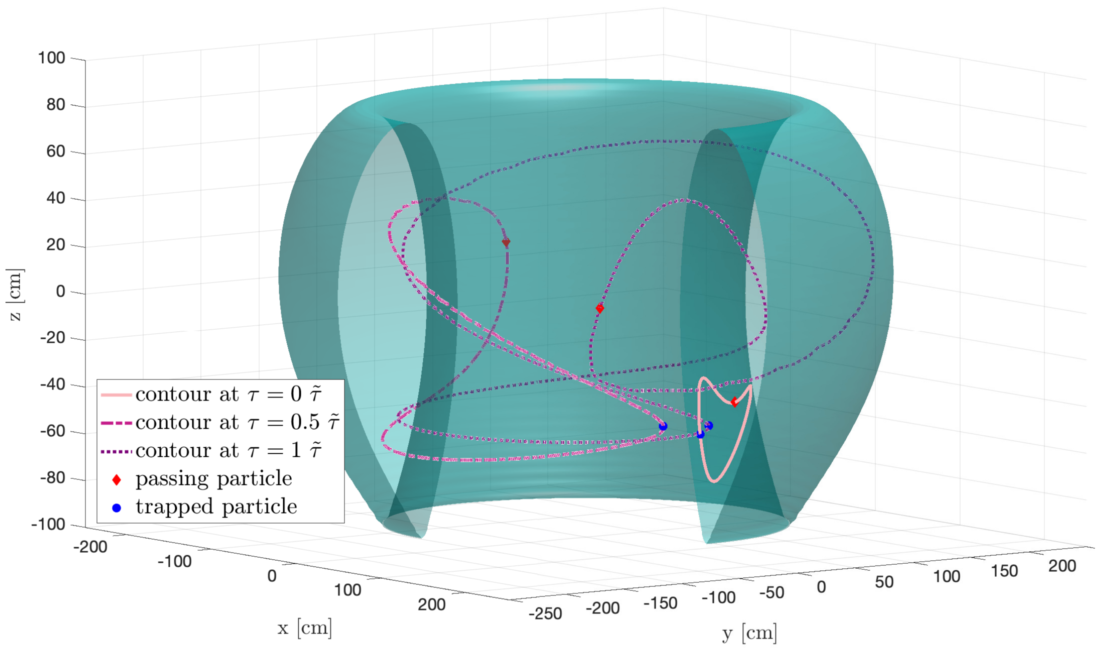

Figure 3: Time evolution of a contour of guiding-center positions utilized for the evaluation of the 1^{st} Poincaré invariant.

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