

Geometric Integration of Guiding Center Orbits in Magnetically Confined Plasmas and Applications

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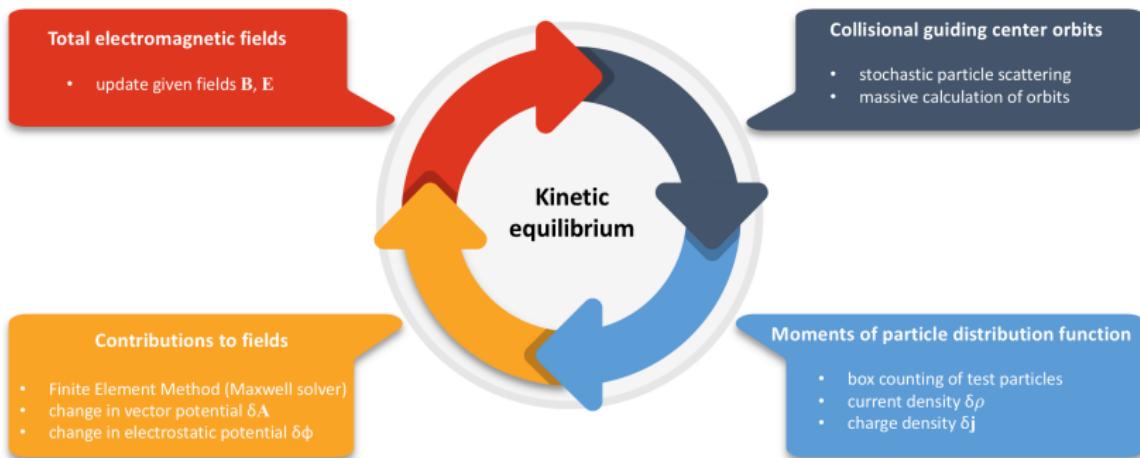
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Computation of kinetic equilibria

- Kinetic modelling of edge plasmas
- Quasi-steady plasma parameters in 3D toroidal fusion devices
 - Simple (cylindrical) modelling of perturbed tokamak equilibria shows that the problem of shielding of external perturbations is essentially kinetic.
 - 3D equilibria should be computed by using plasma response currents and charges in kinetic approximation.
→ Global Monte Carlo modelling

Modelling of kinetic equilibria



Requirements to orbit integrator

1. **Physically correct long time orbit dynamics**
2. **Low sensitivity to noise in fields:** Perturbation field from plasma response currents and charges is noisy due to stochasticity of particle collisions (Monte Carlo).
3. **Integrator efficiency:** Millions of orbits should be followed for few collision times at each iteration.
4. **Efficient box counting:** Orbit intersections with boundaries of grid cells should be traced efficiently.

3D geometric integrator properties

- **Physically correct long time orbit dynamics**
 - preserved total energy
 - preserved magnetic moment
 - preserved phase space volume
- **Computationally efficient:** Relaxed requirements to the accuracy of guiding center orbits
 - not exact orbit shape
 - not exact time evolution

Formulation of the geometric integrator

Use the Hamiltonian form of guiding center equations in curvilinear coordinates,

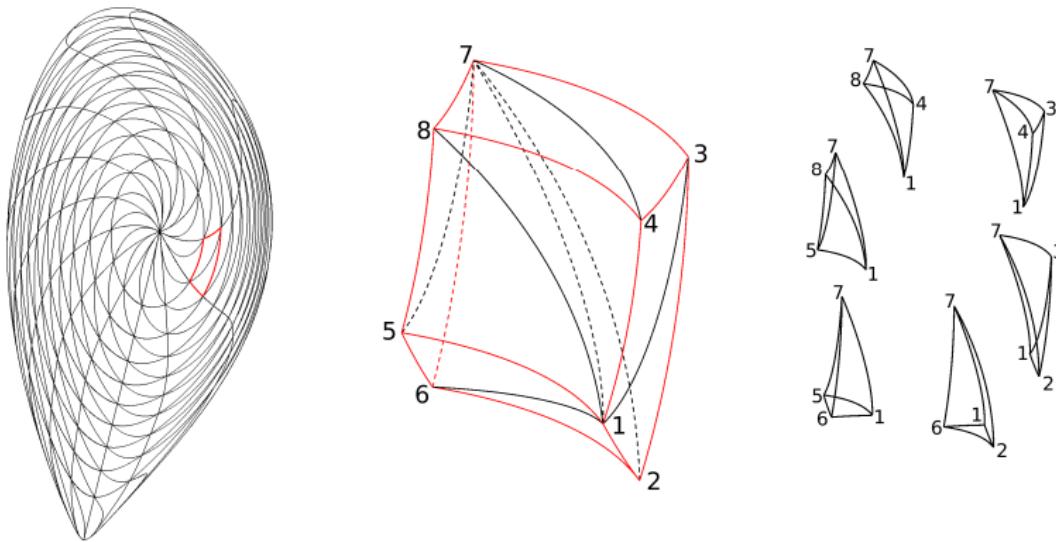
$$\dot{x}^i = \frac{v_{\parallel} \varepsilon^{ijk}}{\sqrt{g} B_{\parallel}^*} \frac{\partial A_k^*}{\partial x^j}, \quad A_k^* = A_k + \frac{v_{\parallel}}{\omega_c} B_k, \quad (1)$$

$$v_{\parallel} = \sigma \left(\frac{2}{m_{\alpha}} (w - J_{\perp} \omega_c - e_{\alpha} \Phi) \right)^{1/2}. \quad (2)$$

Approximate A_k , B_k/ω_c , ω_c and Φ by linear functions in spatial cells with equations of motion

$$\frac{dz^i}{d\tau} = a_k^i z^k + b^i. \quad (3)$$

3D field aligned grid: tetrahedral cells



Physically correct long time orbit dynamics

- Linear approximation of field quantities does **not** destroy the **Hamiltonian nature** of the original guiding center equations.
- Non-canonical Hamiltonian form of linear ODE set

$$\frac{dz^i}{d\tau} = \Lambda^{ij} \frac{\partial H}{\partial z^j}, \quad \Lambda^{ij}(\mathbf{z}) = \{z^i, z^j\}_\tau, \quad (4)$$

with Hamiltonian $H(\mathbf{z}) = v_{||}^2/2 - U(\mathbf{x})$ and antisymmetric Poisson matrix $\Lambda^{ij}(\mathbf{z})$.

- **Symplecticity:** Phase space volume is conserved.

Computational method - efficiency

- Piecewise-constant coefficients of

$$\frac{dz^i}{d\tau} = a_k^i z^k + b^i$$

are discontinuous at cell boundaries.

- Orbit intersections with tetrahedra faces must be computed exactly when integrating particle trajectories.
- The ODE set is numerically solved via **Runge-Kutta 4** in an iterative scheme.
- Iterative scheme uses **Newton's method** and a parabolic analytic estimation for the initial step length.

Error of the RK 4 method

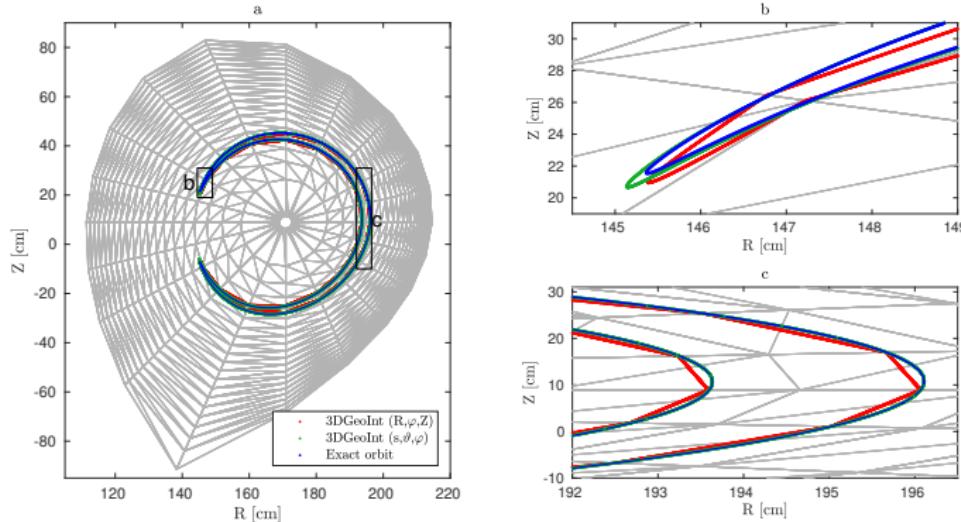
- The relative integration error of a single step between cell boundaries strongly **scales with the Larmor radius ρ** .
- The error is in the order of

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

with R , a , q and $\Delta\varphi$ denoting major radius, plasma radius, safety factor and toroidal cell length.

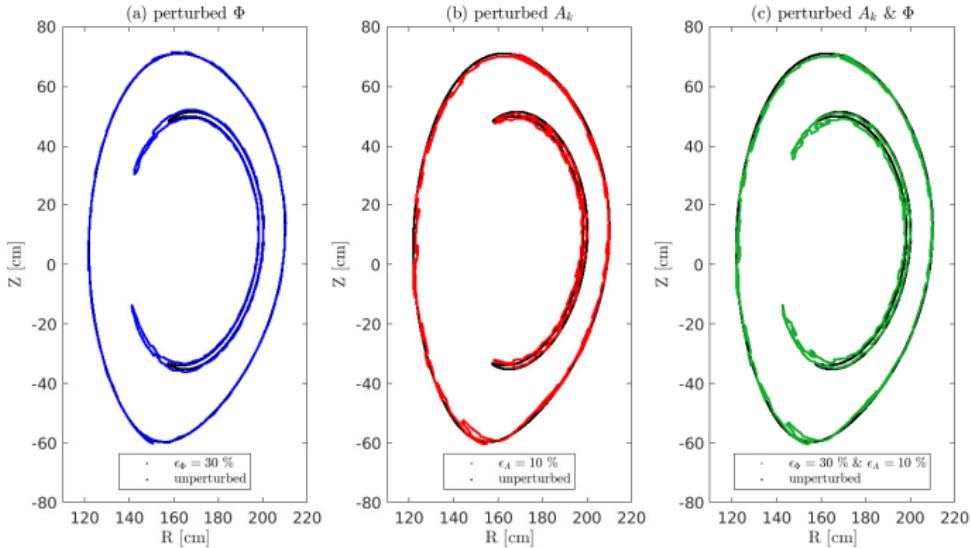
- The **error of the RK4 method** can be brought **below computer accuracy**.

Poincare plots of guiding center orbits



- Geometric integration: Not exact orbit shape.
- Axisymmetric (2D): Canonical toroidal angular momentum is preserved.

Axisymmetric noise of electrostatic and vector potential



- Similar orbit shape (compared to unperturbed orbit)
- Canonical toroidal angular momentum is preserved.

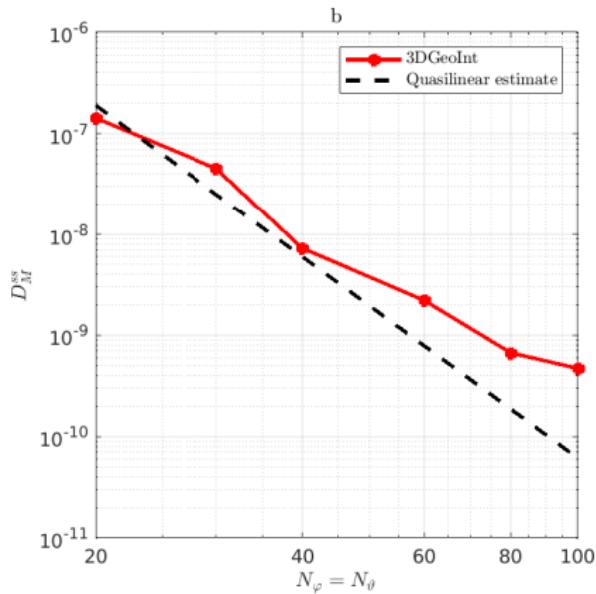
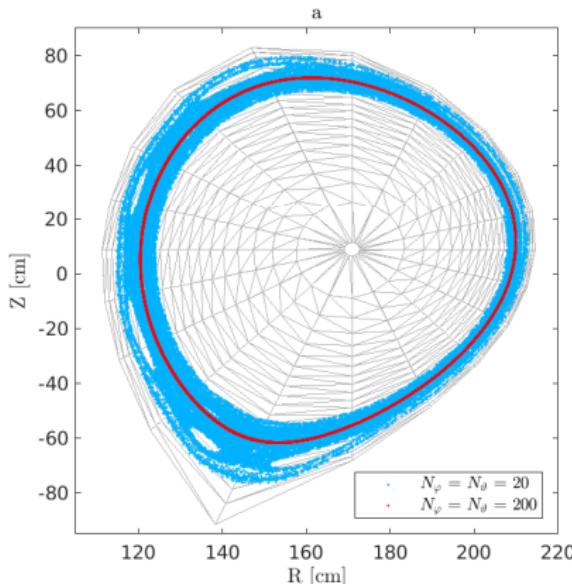
Artifact: Numerical field line diffusion

- Due to the linearization of fields for 3D configurations, **KAM surfaces do not exist anymore.**
→ **ergodic passing particle orbit**
- This behaviour is **diffusive** and its variance 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.
- **Strong inverse scaling** of D_M^{ss} with **poloidal N_ϑ and toroidal N_φ grid sizes**, which roughly agrees with

$$D_M^{ss} = \frac{2\pi^2}{3} \left(\frac{\psi_{\text{pol}} \epsilon_M}{\psi_{\text{tor}}^a} \right)^2 \frac{q^4 m_0^2 n_0^2 (m_0 N_\vartheta + n_0 N_\varphi)^2}{N_\vartheta^2 N_\varphi^2 (q N_\varphi - N_\vartheta)^2}. \quad (6)$$

(quasilinear theory)

Artifact: Numerical field line diffusion



Artifact: Numerical field line diffusion II

- Numerical diffusion can be put **below the level of classical electron diffusion** using a **mild grid refinement**.
- When tracing orbits in a **VMEC stellarator field** numerical diffusion is effectively **minimized by using symmetry flux coordinates**.
 - Numerical diffusion results only from the FLR effects which lead roughly to the same order of perturbations as in weakly perturbed tokamaks, $\varepsilon_M \sim \rho/a$.

Turning artifact into feature:

Numerical Diffusion for Anomalous Transport modelling:

- 3D noise in (\vec{A}, Φ) leads to artificial diffusion.
- Use this diffusion as an additional transport mechanism to model anomalous transport.
- The resulting orbits are physically consistent .
- Adjust amplitude of the noise to reproduce phenomenological transport coefficient.

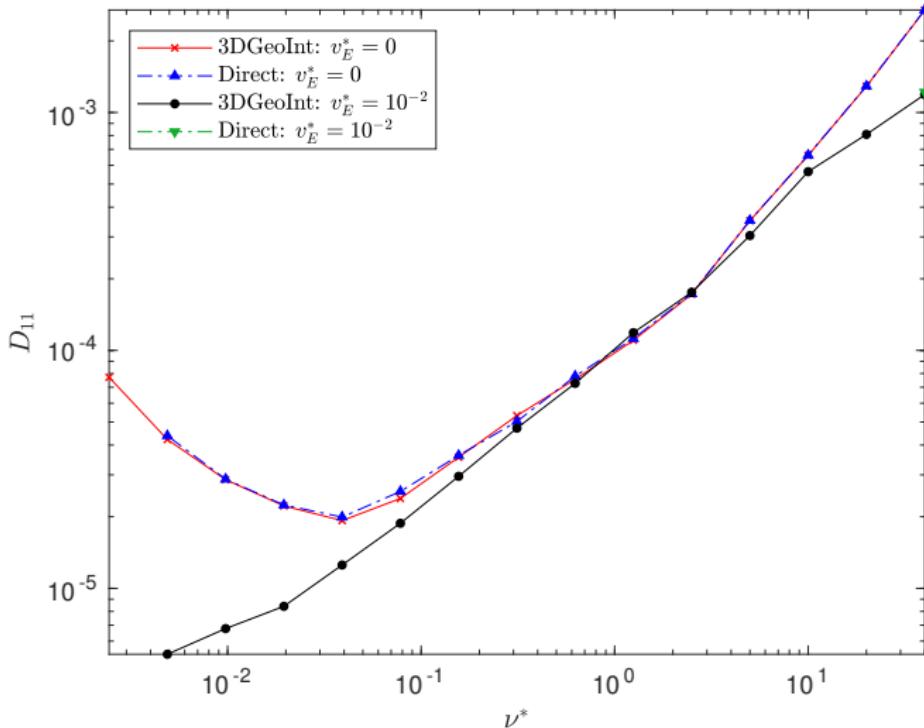
Application: Mono-energetic radial transport coefficient

- Mono-energetic radial transport coefficient as a function of collisionality is evaluated with the Monte Carlo method.
- Collisions are realized by pitch angle scattering (Lorentz scattering operator).

$$\frac{\partial f}{\partial t} = \frac{1}{s(\psi)} \frac{\partial}{\partial \psi} s D \frac{\partial f}{\partial \psi} \quad (7)$$

$$D = D(E, \psi) = \left\langle \frac{1}{2t} (\psi(t) - \psi(t_0))^2 \right\rangle \quad (8)$$

Radial Transport in HYDRA (stellarator)



$$\nu^* = \frac{R_0 \nu_c}{\iota V}$$

$$v_E^* = \frac{E_r}{vB_0}$$

Conclusion

Advantages:

- Physically correct long time orbit dynamics
- Particle coordinates and velocities are implicitly given at cell boundaries.
- Low sensitivity to noise in electromagnetic fields
- Computational efficiency

Limitations:

- Artificial numerical diffusion is induced by piecewise linear field quantities.

Thank you for your attention!