

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

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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

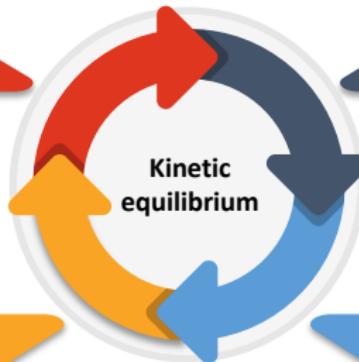
# Modelling of kinetic equilibria

## Total electromagnetic fields

- update given fields  $\mathbf{B}$ ,  $\mathbf{E}$

## Collisional guiding center orbits

- stochastic particle scattering
- massive calculation of orbits



## Contributions to fields

- Finite Element Method (Maxwell solver)
- change in vector potential  $\delta\mathbf{A}$
- change in electrostatic potential  $\delta\phi$

## Moments of distribution function

- box counting of test particles
- charge density  $\delta\rho$
- current density  $\delta\mathbf{j}$

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# 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,

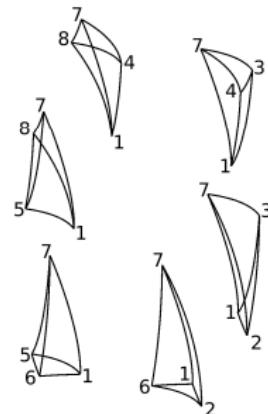
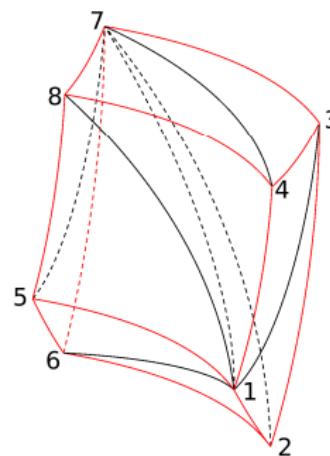
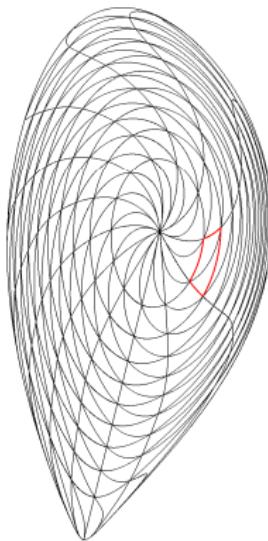
$$\dot{x}^i = \frac{v_{\parallel} \varepsilon^{ijk}}{\sqrt{g} B_{\parallel}^*} \frac{\partial A_k^*}{\partial x^j}, \quad A_k^* = A_k + \frac{v_{\parallel}}{\omega_c} B_k, \quad (1)$$

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

Approximate  $A_k$ ,  $B_k/\omega_c$ ,  $\omega_c$  and  $\Phi$  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

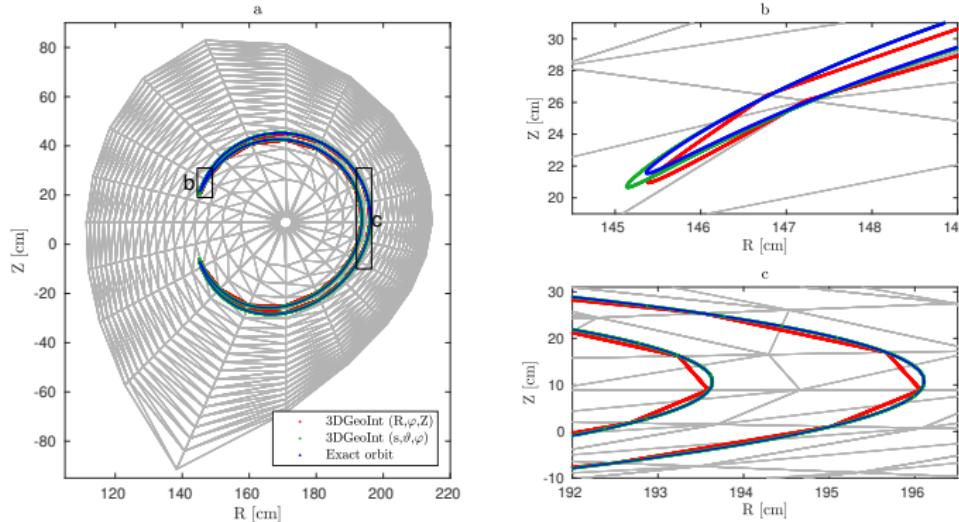
- The relative integration error of a single step between cell boundaries strongly **scales with the Larmor radius  $\rho$** .
- The error is in the order of

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

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

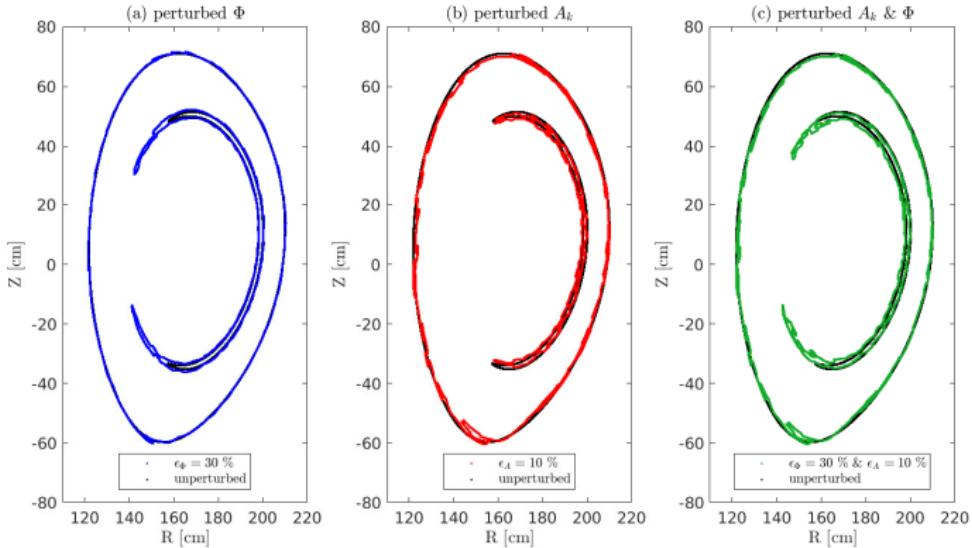
- The **error of the RK4 method** can be brought **below computer accuracy**.

# 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.

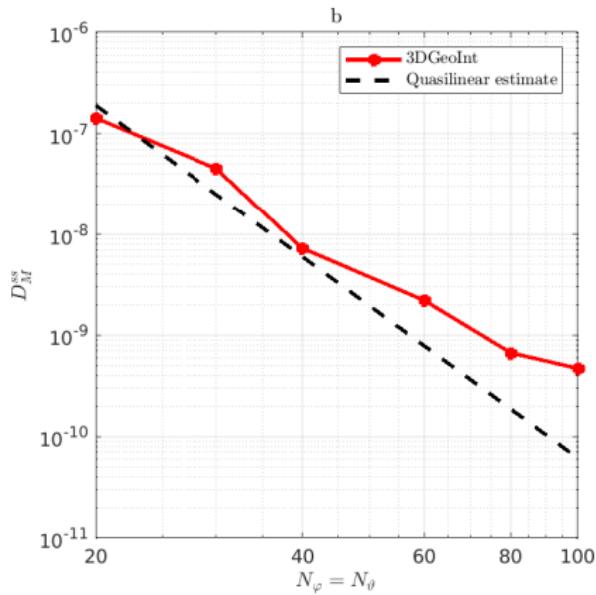
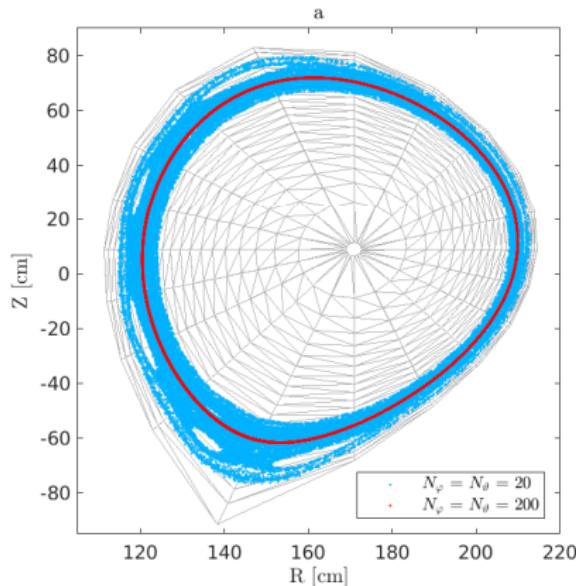
# Artifact: Numerical field line diffusion

- 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  $N_\vartheta$  and toroidal  $N_\varphi$  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  $(\vec{A}, \Phi)$  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.

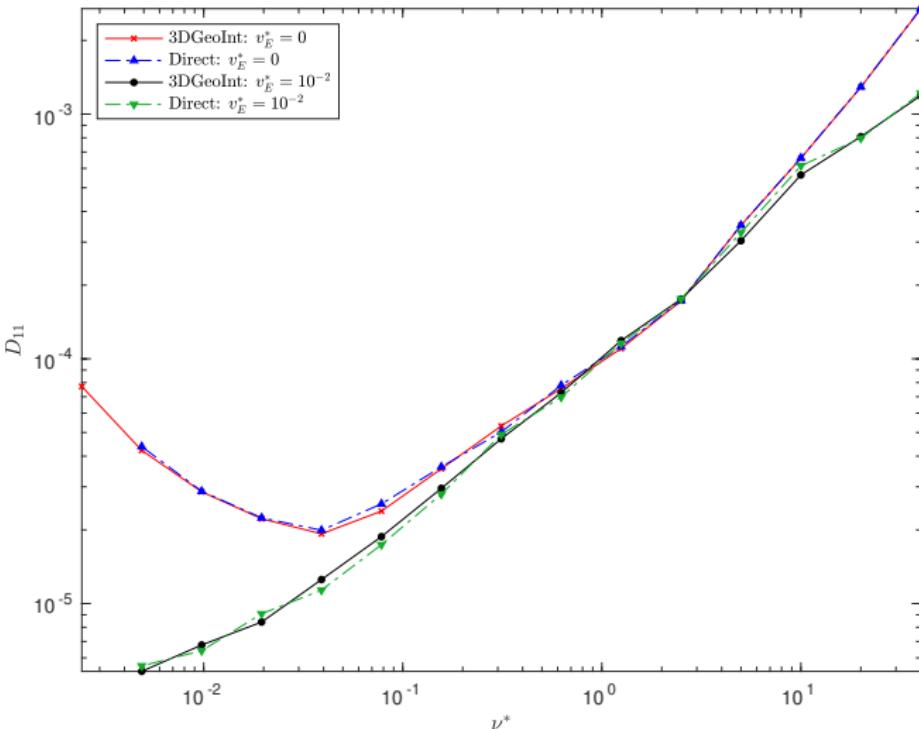
# Application: Mono-energetic radial transport coefficient

- 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).

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

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

# 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!