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

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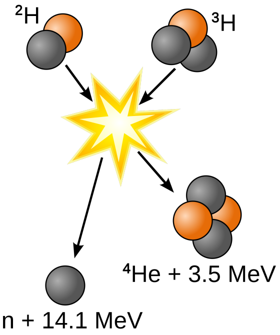
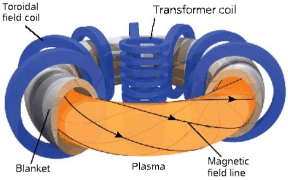
What is nuclear fusion?



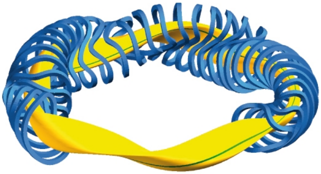
Deuterium + Tritium
$\rightarrow$ Helium + neutron

- Two or more atomic nuclei are combined to form one or more different atomic nuclei and subatomic particles
- 17.6 MeV are released as kinetic energy in the case for D+T fusion

What is the current approach to fusion?



Tokamak



Stellarator

- Heating of D-T plasma to $\sim 10^7$ K in toroidal magnetic configuration
- Self sustained reaction according to the Lawson Criterion for the triple product $n\tau T > C$
- Two main types of devices: Tokamaks and Stellarators

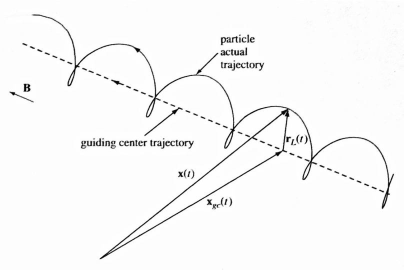
Theoretical descriptions of plasmas

- Magnetohydro-dynamics (MHD)
  - describes the plasma as an electrically conducting fluid
  - only valid at high particle collisionalities
    $\rightarrow$ velocity distributions are considered to be Maxwellian

- Kinetic Approach
  - description of plasma through discrete particle distribution functions $f(\vec{x}, \vec{v})$ of phase space
  - coupling Vlasov + Maxwells equations

- Gyro-kinetic Approach
  - averaging over gyrating motion around field lines
  - reduced distribution function $f(\vec{x}, v_{\|}, v_{\perp})$

Guiding center motion

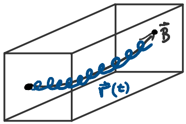


Guiding center motion

- particles gyrate around field lines
- $\rightarrow$ average over fast gyration
- corrections to motion in form of drifts
- for gyro-kinetic approach many particles need to be traced in boxes

Gorilla guiding center code

- **G**eometric **OR**bit **I**ntegration with **L**ocal **L**inearisation **A**pproach
- Integration of charged particle guiding center orbits in toroidal fusion devices



Target application - 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.
    $\rightarrow$ Global Monte Carlo modelling

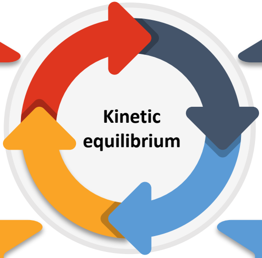
Modelling of kinetic equilibria

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 $\delta\mathbf{j}$

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,

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

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

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

$$\frac{\mathrm{d}z^i}{\mathrm{d}\tau} = a^i_k z^k + b^i. \tag{3}$$

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

$$\frac{\mathrm{d}z^i}{\mathrm{d}\tau} = \Lambda^{ij} \frac{\partial H}{\partial z^j}, \qquad \Lambda^{ij}(\mathbf{z}) = \left\{z^i, z^j\right\}_\tau , \qquad (4)$$

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.

Grid for **Gorilla**

- Grid necessary for calculations due to
  - linearization of field quantities
  - box counting scheme for distribution function

$\rightarrow$ guiding center orbits are computed between cell boundaries using a standard $RK4$-integrator

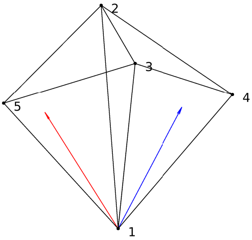
Grid must consist of tetrahedra due to linearization of field quantities

- linear system of equations for $\nabla f = \mathit{const}$.

$$f(\vec{x}_i) = f(\vec{x}_1) + (\vec{x}_i - \vec{x}_1) \cdot \nabla f,\ \ i \in \{1, 2, 3, 4\}$$

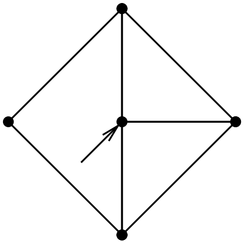
- this system is uniquely defined as the number of unknowns (=4) is equal to the number of values for f $\rightarrow$ no fitting for the case of tetrahedra

Linearization leads to continuous *f*



- influence of points $\{4{,}5\}$ vanishes on the plane spanned by $\{1{,}2{,}3\}$ $\rightarrow$ *f* is continuous at cell boundaries
- but: piece-wise constant gradients remain discontinuous at cell boundaries

No hanging nodes

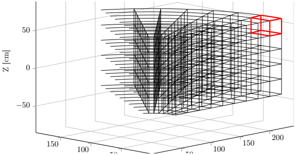


- adjacent tetrahedral faces must share three common vertices for linearized fields to be continuous
  $\rightarrow$ no hanging nodes!

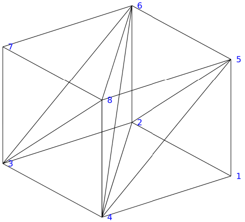
Further requirements

- whole domain must be unambiguously covered by tetrahedra $\rightarrow$ no holes or overlaps in grid
- tetrahedra must be uniquely indexed, also the corresponding neighboring tetrahedra and the faces through which they are connected
- periodic boundaries must be taken into account due to coordinate jump

Initial grid: cylindrical contour grid



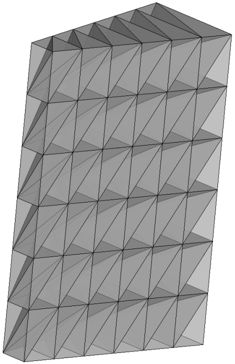
Hexahedra



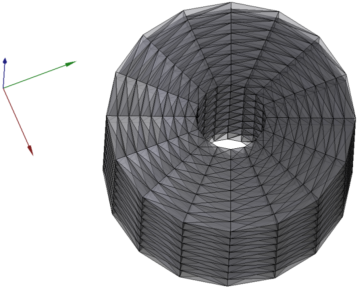
Tetrahedra

- vertices lie on contours of cylindrical coordinates (R, φ, Z)
- hexahedra are obtained by indexing vertices
- each hexahedron is cut into six tetrahedra
- neighboring tetrahedra need to be indexed for logics

Cylindrical contour grid

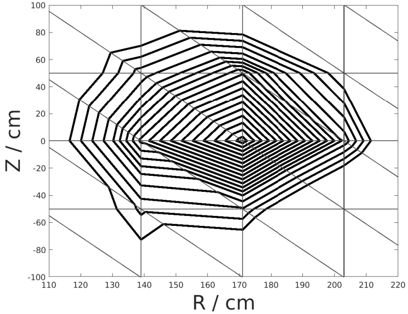


toroidal grid slice



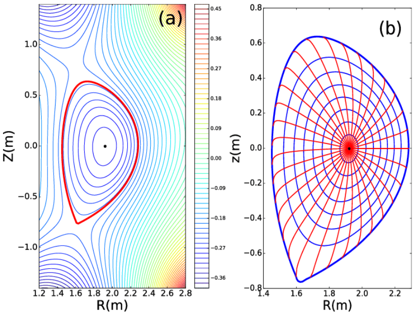
full cylindrical contour grid

Poincaré plots of guiding center orbits



- intersections of orbits with $\varphi = 0$ plane are marked with points
- points lie on well-defined contours
- polygonal shape due to linearization

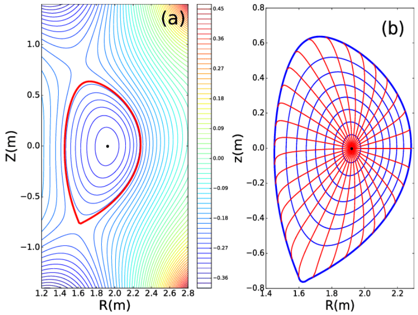
Idea: symmetry flux coordinates



Magnetic field topology

- coordinates (s, ϑ, φ)
  - $s \rightarrow$ minor-radial coordinate
  - $\vartheta \rightarrow$ poloidal coordinate
  - $\varphi \rightarrow$ toroidal coordinate
- field lines assume straight lines in SFC
- $\vec{A} \propto s \rightarrow$ no interpolation error due to linearization

Idea: symmetry flux coordinates



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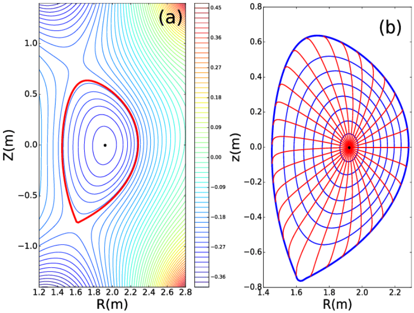
Problem with CCG: incompatible with SFC

Implementing a field aligned grid



Magnetic field topology

Computational method - efficiency

- Piecewise-constant coefficients of
$$\frac{\mathrm{d}z^i}{\mathrm{d}\tau} = a^i_k z^k + b^i$$
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.

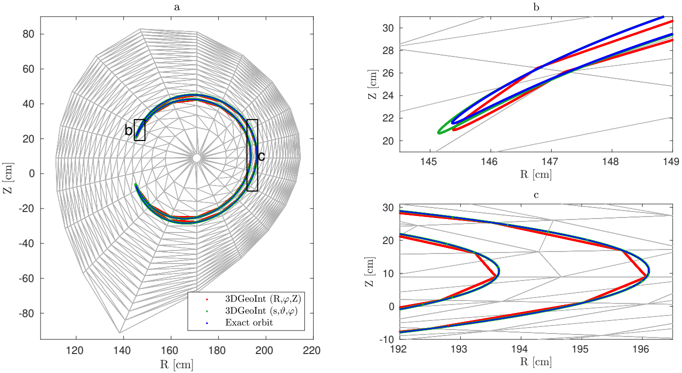
Error of the RK 4 method

- 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

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

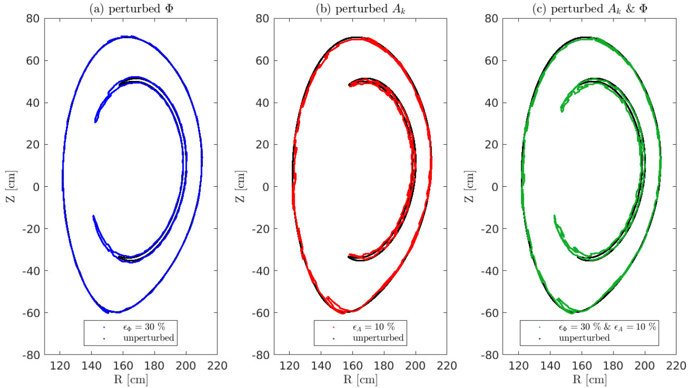
  with R, a, q and $\Delta\varphi$ denoting major radius, plasma radius, safety factor and toroidal cell length.
- The **error of the RK4 method** can be brought **below computer accuracy**.

Poincare plots of guiding center orbits



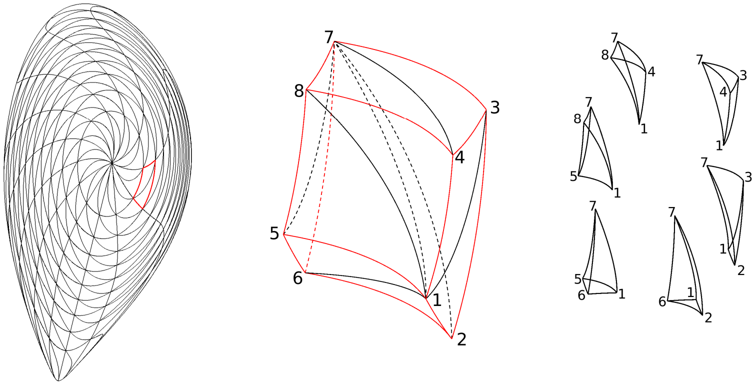
- Geometric integration: Not exact orbit shape.
- Axisymmetic (2D): Canonical toroidal angular momentum is preserved.

Axisymmetric noise of electrostatic and vector potential



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

3D field aligned grid: tetrahedral cells



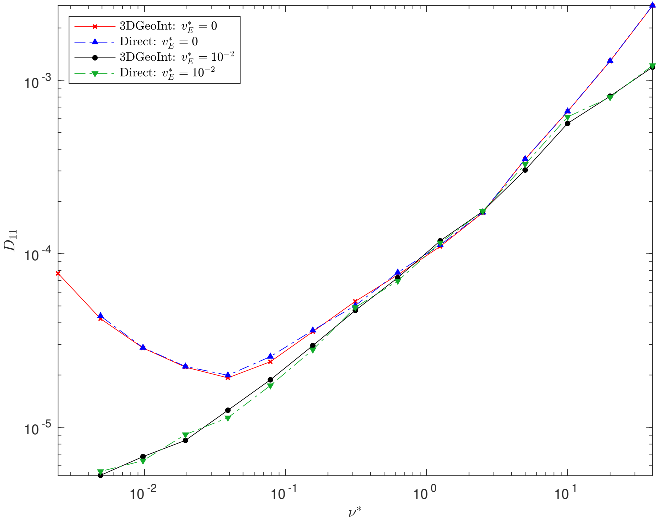
Application: Mono-energetic radial transport coefficient

- 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).

$$\frac{\partial f}{\partial t} = \frac{1}{s(\psi)} \frac{\partial}{\partial \psi} s D \frac{\partial f}{\partial \psi} \tag{6}$$

$$D = D(E, \psi) = \langle \frac{1}{2t} \left(\psi(t) - \psi(t_0)\right)^2 \rangle \tag{7}$$

Radial Transport in HYDRA (stellarator)



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

$$v_E^* = \frac{E_r}{v B_0}$$

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!