

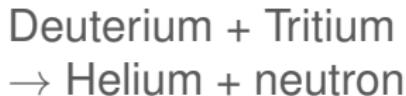
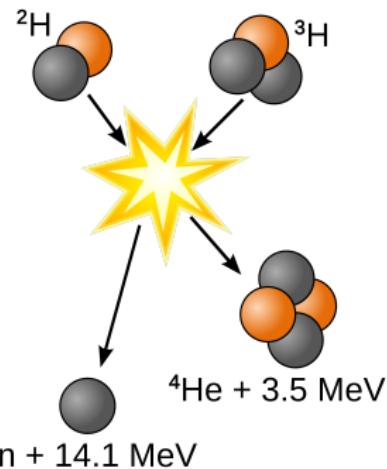
Geometric Integration of Guiding Center Orbits in Magnetically Confined Plasmas and Applications

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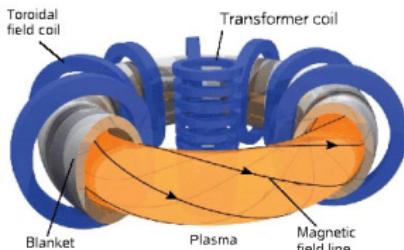
10. July 2020, Seminar Presentation, Graz

What is nuclear fusion?

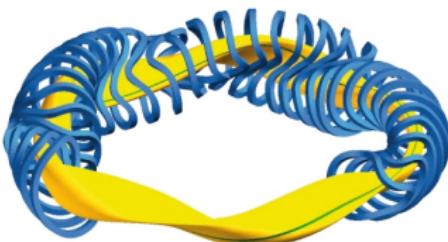


- Two or more atomic nuclei are combined to form one or more different atomic nuclei and subatomic particles
- 17.6 MeV are released as kinetic energy in the case for D+T fusion

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

■ Magnetohydrodynamics (MHD)

- describes the plasma as an electrically conducting fluid
- only valid at high particle collisionalities
→ velocity distributions are considered to be Maxwellian

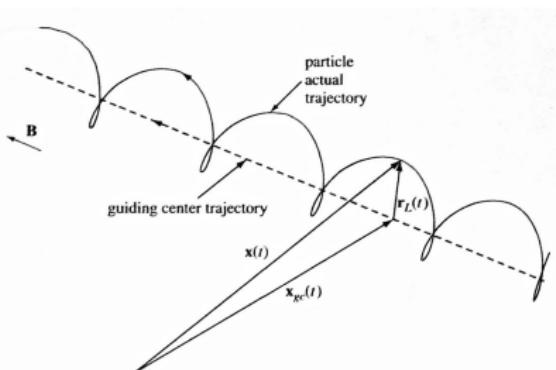
■ Kinetic Approach

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

■ Gyro-kinetic Approach

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

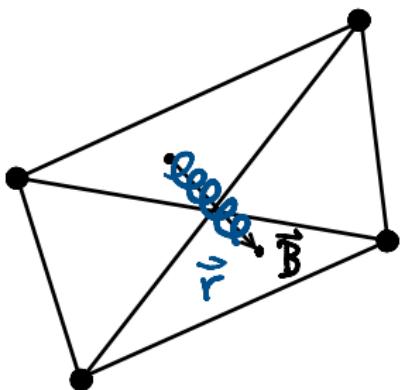
Guiding center motion



Guiding center motion

- particles gyrate around field lines
- → 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



- Geometric ORbit Integration with Local Linearisation Approach
- 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.
→ Global Monte Carlo modelling

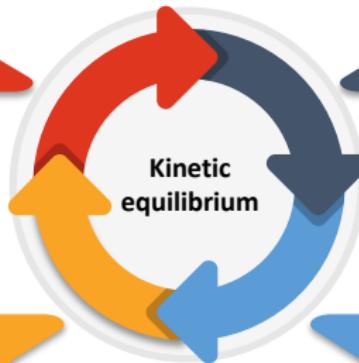
Modelling of kinetic equilibria

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,

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

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

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

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

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.

Grid for Gorilla

- Grid necessary for calculations due to
 - linearization of field quantities
 - box counting scheme for distribution function
- guiding center orbits are computed between cell boundaries using a standard *RK4*-integrator

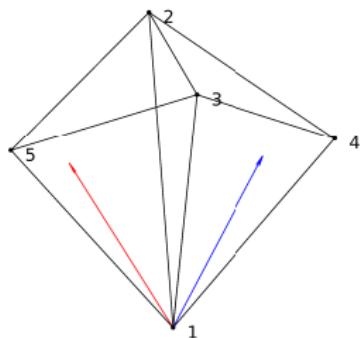
Grid must consist of tetrahedra due to linearization of field quantities

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

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

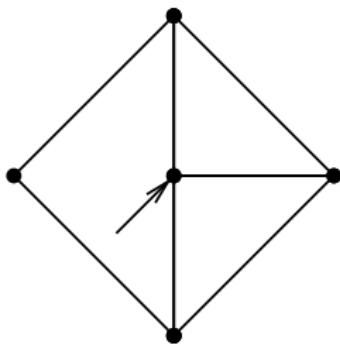
- this system is uniquely defined as the number of unknowns (=4) is equal to the number of values for f
 \rightarrow no fitting for the case of tetrahedra

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

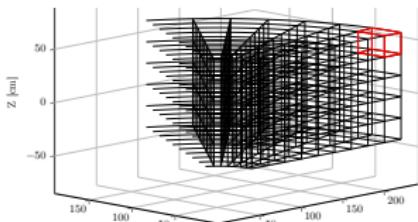


- adjacent tetrahedral faces must share three common vertices for linearized fields to be continuous
→ no hanging nodes!

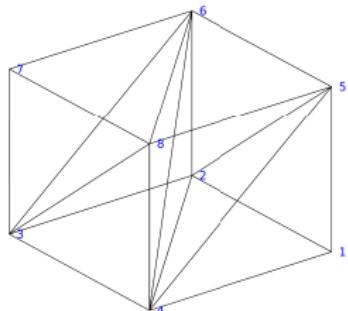
Further requirements

- whole domain must be unambiguously covered by tetrahedra → 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



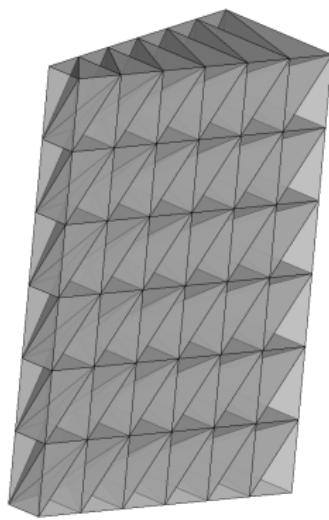
Hexahedra



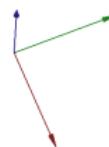
Tetrahedra

- 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

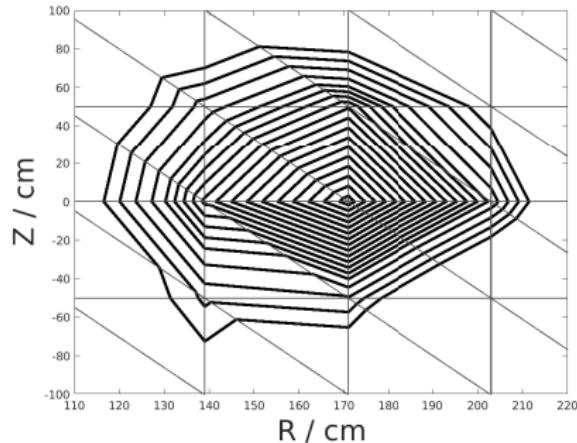


toroidal grid slice



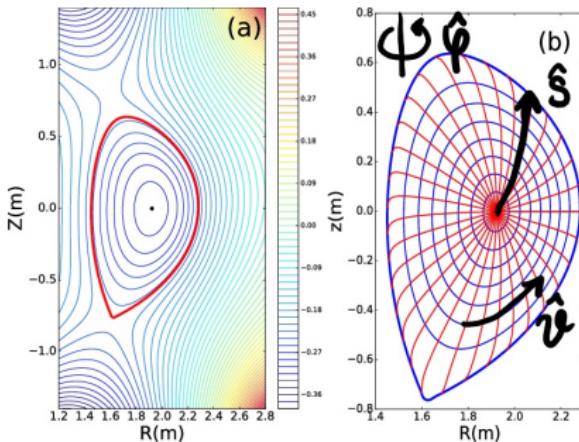
full cylindrical contour grid

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

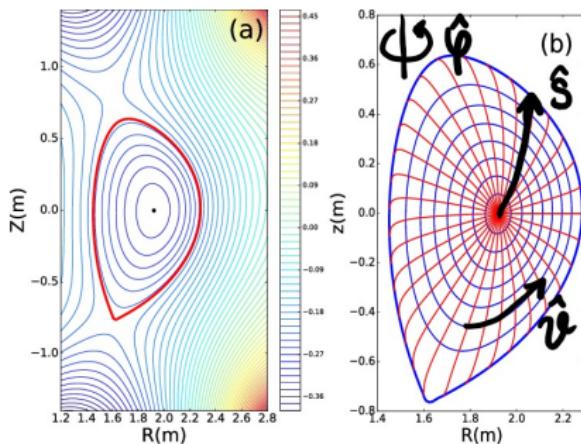
Idea: symmetry flux coordinates



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

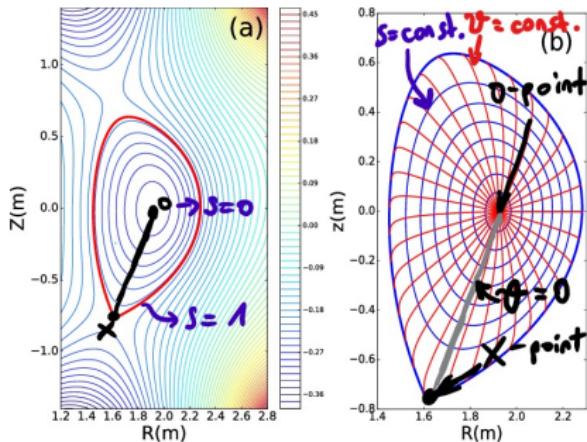


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Problem with CCG: incompatible with SFC

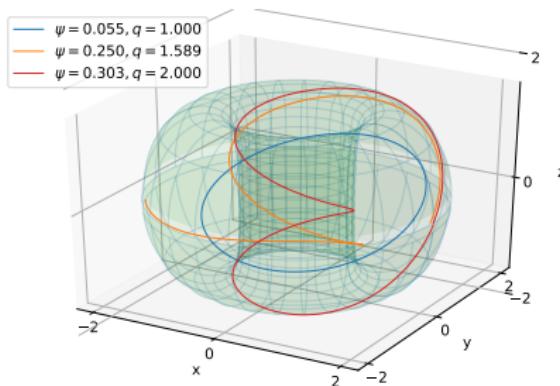
Implementing a field aligned grid



Magnetic field topology

- find O -point and X -point
- field line integration for coordinate interpolation
- interpolation routine: $(s, \vartheta, \varphi) \rightarrow (R, \varphi, Z)$ for evaluation of field quantities
- create 2D grid points
→ extrude to 3D
- connect vertices to form tetrahedra

Field-line integration



Selected field lines in torus

- Field line equations:

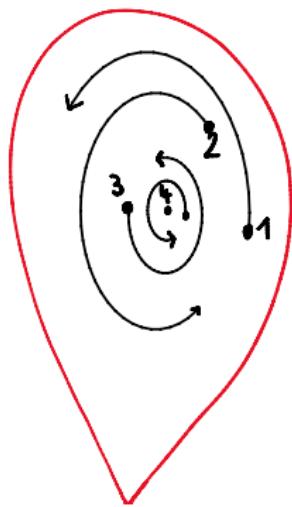
$$\frac{dR}{d\varphi} = \frac{B^R}{B^\varphi}, \quad \frac{dZ}{d\varphi} = \frac{B^Z}{B^\varphi}$$

- Safety factor:

$$q_s = \frac{B^\varphi}{B^\theta}, \quad d\varphi = q_s d\theta$$

- if q_s is irrational, the field line forms a flux surface

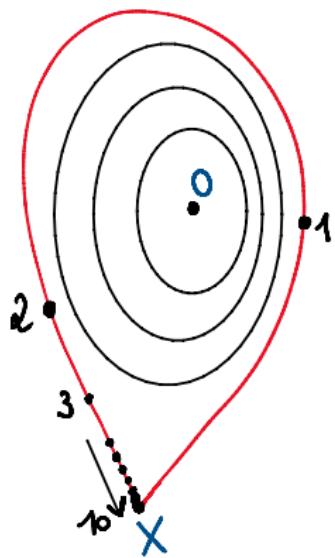
Finding the O -point



Iterative scheme for finding
the O – point

- start at point 1, follow \vec{B} for 10 toroidal turns in (R, φ, Z)
- compute average of $(R, Z) \rightarrow$ new starting point for the next iteration
- perform 20 iterations for satisfying accuracy of the magnetic axis

Finding the X-point



Iterative scheme for finding the *X – point*

- start inside and integrate field line for one poloidal turn
- increase distance to mag. axis and repeat until the field line does not cross → Separatrix
- perform iterative integrations with $\Delta\varphi = 2\pi/10 \rightarrow$ convergence, since $B^{pol} = 0$ at *X*-point

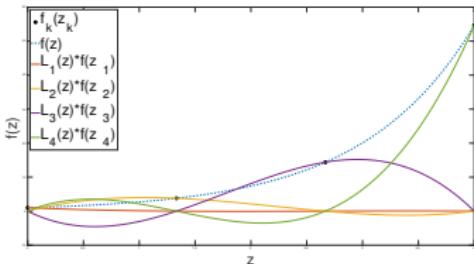
Massive computation of field lines

- parametrize line segment from O -point to X -point with 500 equidistant starting points $\rightarrow \vartheta = 0$ -contour
- integrate each line for one poloidal turn \rightarrow compute q_s
- integrate each line for one poloidal turn over 500 equidistant steps \rightarrow save (R, Z) together with poloidal and normalized toroidal flux s and poloidal angle $\vartheta = i/500$ with current step i
- due to axisymmetry φ is equal to the cyl. coordinates toroidal angle

Interpolation of (R, Z) from (s, ϑ)

- compute periodic spline coefficients in ϑ for each saved field line, $s = \text{const.}$ along a field line
- for a given value of ϑ , evaluate interpolated values of R, Z for field lines which are adjacent to s
- use Lagrange polynomial interpolation to compute $R(s, \vartheta), Z(s, \vartheta)$

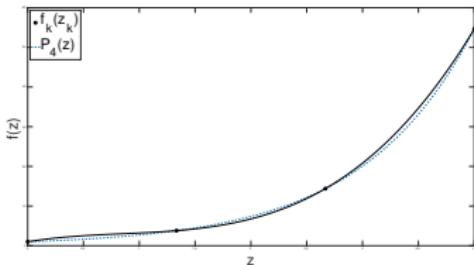
Lagrange polynomial interpolation



Depiction of $L_k(z)$

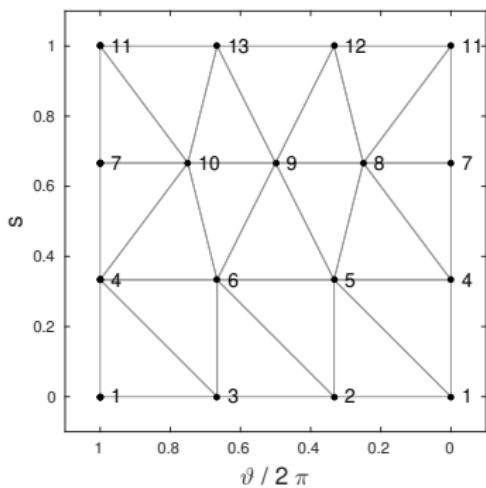
- $P_n(z) = \sum_{k=0}^n L_k(z)f_k$

- $L_k(z) = \prod_{j=0, j \neq k}^n \frac{z - z_j}{z_k - z_j}$



Depiction of $P_4(z)$

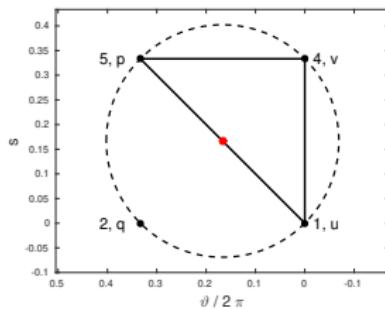
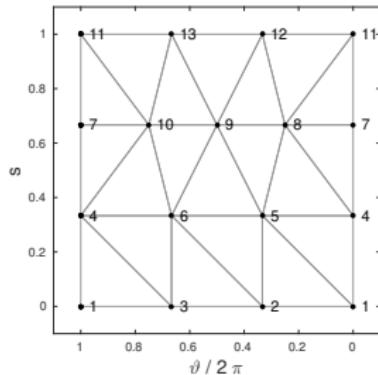
Generate grid vertices



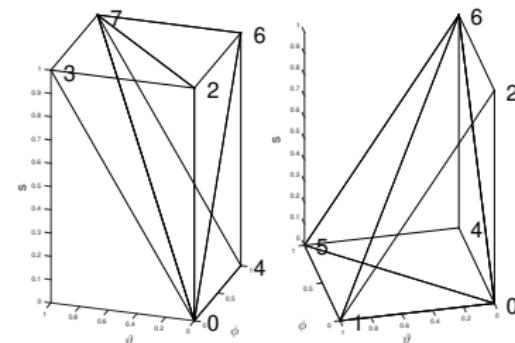
2D grid vertices

- Generate the vertex positions in poloidal plane
 - set number of points per ring
 - scale point distributions according to scaling functions for s, ϑ
- Extrude vertex coordinates toroidally $(s, \vartheta, \varphi = 0) \rightarrow (s, \vartheta, \varphi)$

Mesh tetrahedra using Delaunay condition

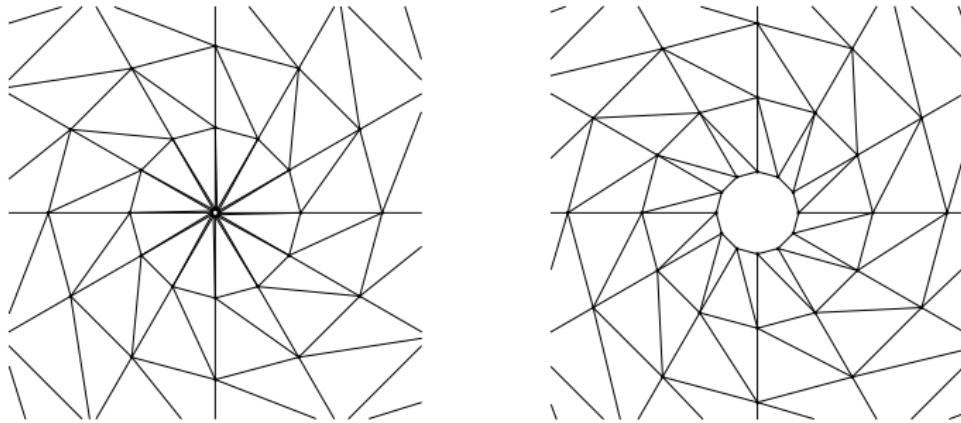


- index vertices to prism face of correct type
→ Delaunay condition



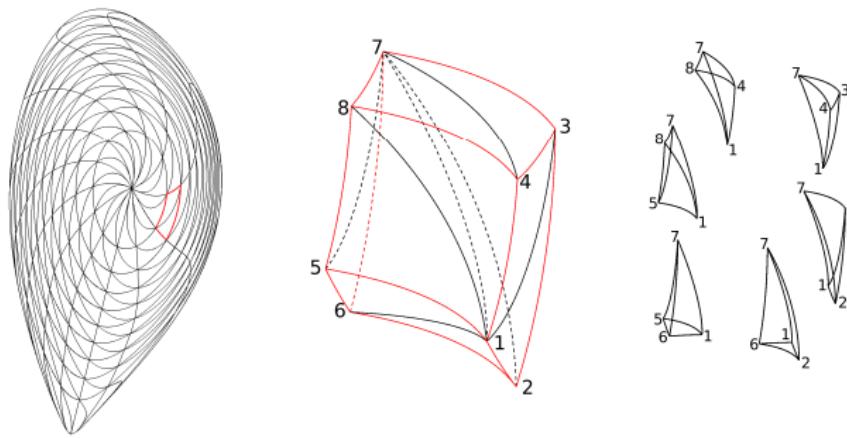
Prism types used for tetrahedra indexing

One compromise: there is a hole



Center region of the grid with annulus

Field aligned grid



Poloidal cross-section and grid elements of field aligned grid in real space

Computational approach

- 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.

Analytical solution to ODE set

$$x^i(\tau) = \psi_I^i \left(\bar{\psi}_k^I x_{(0)}^k e^{\lambda'^I \tau} + \frac{\bar{\psi}_k^I D^k}{a - \lambda'^I} (e^{a\tau} - e^{\lambda'^I \tau}) + \right. \\ \left. \frac{\bar{\psi}_k^I F^k}{2a - \lambda'^I} (e^{2a\tau} - e^{\lambda'^I \tau}) - \frac{\bar{\psi}_k^I E^k}{\lambda'^I} (1 - e^{\lambda'^I \tau}) \right)$$

Analytical solution to ODE set

$$\begin{aligned}x^i(\tau) = & \psi_I^i \left(\bar{\psi}_k^I x_{(0)}^k e^{\lambda' \tau} + \frac{\bar{\psi}_k^I D^k}{a - \lambda'} (e^{a\tau} - e^{\lambda' \tau}) + \right. \\& \left. \frac{\bar{\psi}_k^I F^k}{2a - \lambda'} (e^{2a\tau} - e^{\lambda' \tau}) - \frac{\bar{\psi}_k^I E^k}{\lambda'} (1 - e^{\lambda' \tau}) \right)\end{aligned}$$

Unfortunately, due to numerical inaccuracies and high computational cost, this is not useful!

New approach: Taylor expansion of solution

ODE set:

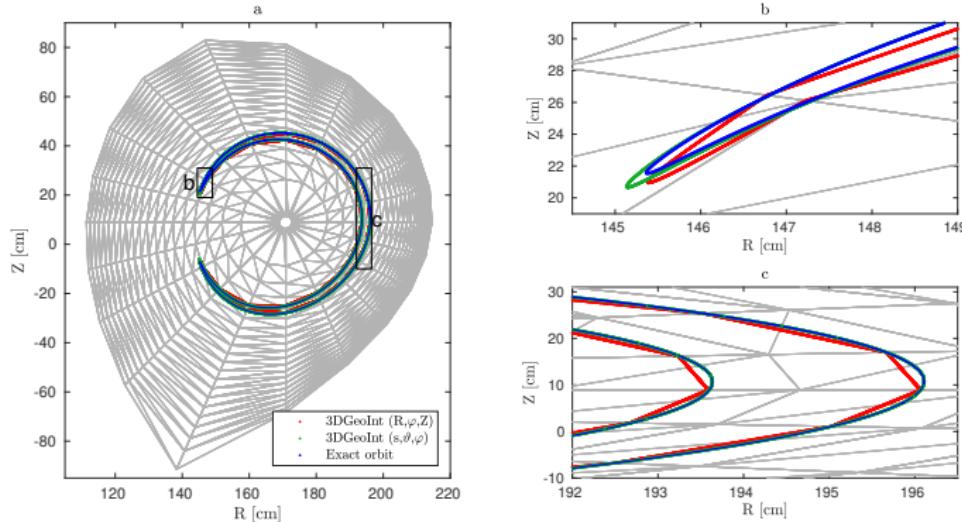
$$\frac{d\mathbf{z}}{d\tau} = \hat{\mathbf{a}}\mathbf{z} + \mathbf{b}$$

Taylor series:

$$\mathbf{z} = \mathbf{z}_0 + \sum_{k=1}^{\infty} \frac{\tau^k}{k!} \hat{\mathbf{a}}^{k-1} \cdot (\mathbf{b} + \hat{\mathbf{a}} \cdot \mathbf{z}_0)$$

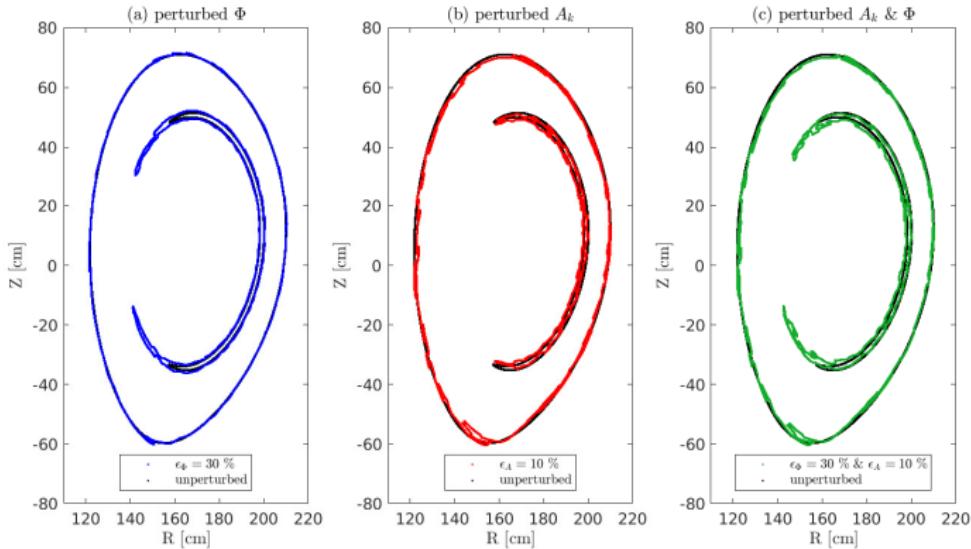
→ RK4 corresponds to fourth order expansion, thus the fifth order estimates the RK4-error!

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.

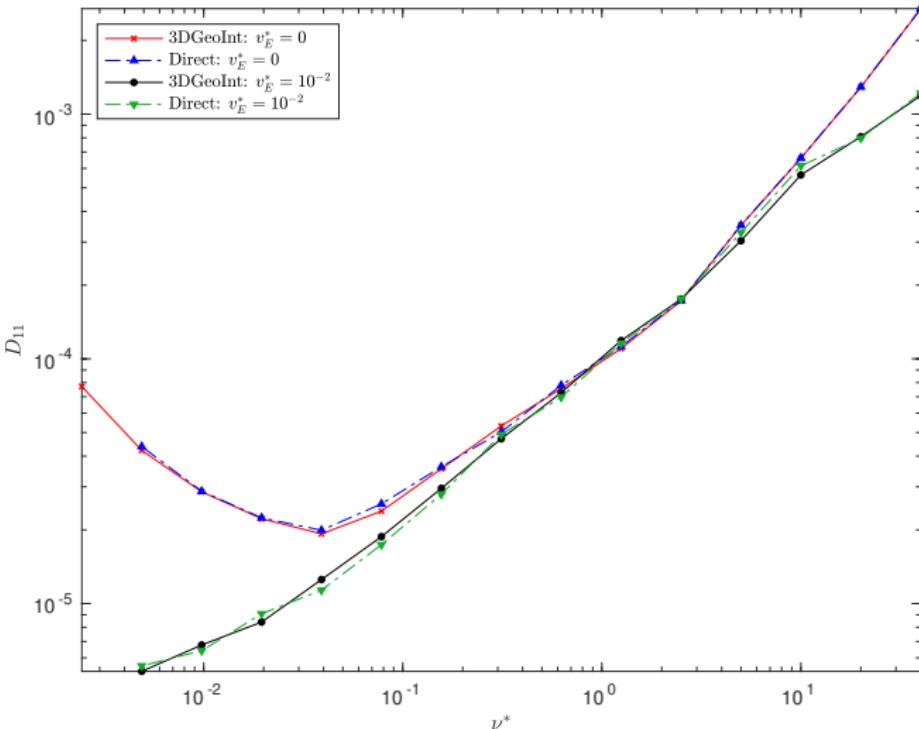
Application: Mono-energetic radial transport coefficient

- 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).

$$\frac{\partial f}{\partial t} = \frac{1}{s(\psi)} \frac{\partial}{\partial \psi} s D \frac{\partial f}{\partial \psi} \quad (5)$$

$$D = D(E, \psi) = \langle \frac{1}{2t} (\psi(t) - \psi(t_0))^2 \rangle \quad (6)$$

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!