Field-aligned grid generation and enhancements of the guiding-center orbit code GORILLA

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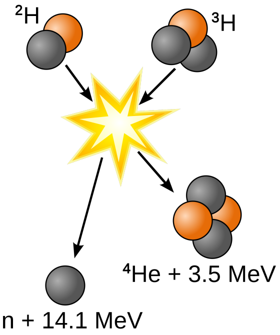
What is nuclear fusion?

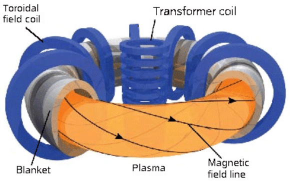


$$^{2}_{1}H^{+} + ^{3}_{1}H^{+} \rightarrow ^{4}_{2}He^{2+} + ^{1}_{0}n$$

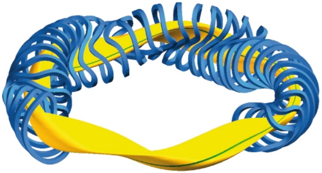
- Atomic nuclei are combined to form different atomic nuclei and subatomic particles
- 17.6 MeV are released as kinetic energy in fusion of Deuterium+Tritium

Figure taken from: https://de.wikipedia.org/wiki/Kernfusion#/media/Datei:Deuterium-tritium_fusion.svg

What is the current approach to fusion?



Tokamak[1]



Stellarator[2]

- Heating of D-T plasma to $\sim 10^8$ 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

[1] https://upload.wikimedia.org/wikipedia/commons/b/b3/W7X-Spulen_Plasma_blau_gelb.jpg

[2] https://www.researchgate.net/figure/Schematic-of-a-Tokamak-fusion-reactor\41719279

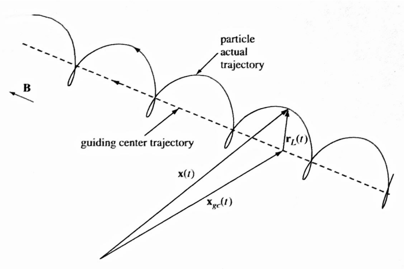
Theoretical descriptions of plasmas

- 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

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

Guiding center motion

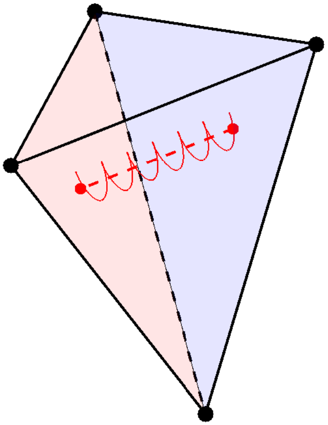


Guiding center motion

- 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

Figure taken from: http://www.thunderbolts.info/eg_draft/images/particle_trajectory_diagram_1126x844.jpg

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

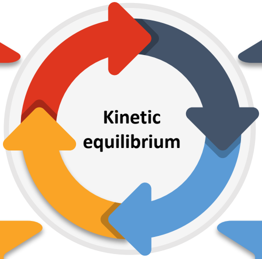
Target application: kinetic equilibria

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

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

Properties of 3D geometric integrator **Gorilla**

- **Physically correct long time orbit dynamics**
  - preserved total energy
  - preserved magnetic moment
  - preserved phase space volume
- **Low sensitivity to noise in fields**
- **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

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

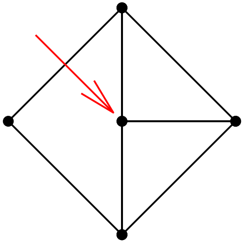
Spatial discretization: grid for **Gorilla**

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

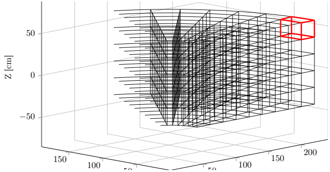
$\rightarrow$ guiding center orbits are computed between cell boundaries using a standard $RK4$-integrator

Requirements to grid

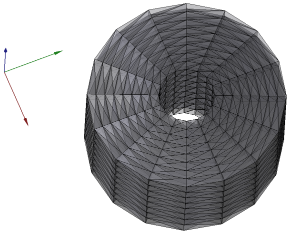
- linear scalar functions of space have **four** degrees of freedom $\rightarrow$ **tetrahedral** grid elements for uniquely determined function coefficients
- no holes or overlaps in grid
- continuous linearized field components
  $\rightarrow$ no hanging nodes



Previous grid in cylindrical coordinates

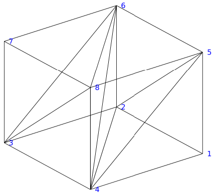


Hexahedra

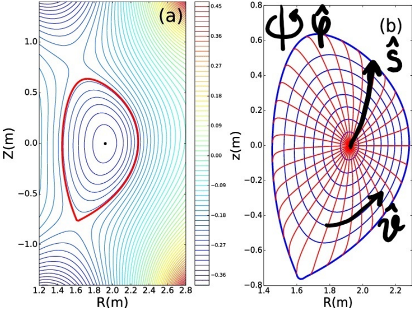


Cylindrical Contour Grid

- vertices lie on contours of cylindrical coordinates (R, φ, Z)
- hexahedra are obtained via indexing
- each hexahedron is cut into six tetrahedra:



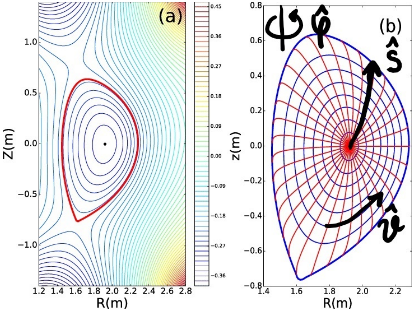
Next step: symmetry flux coordinates (SFC)



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
- $\vec{A} \propto s \cdot \hat{\varphi} \rightarrow$ no error due to linearization

Idea: symmetry flux coordinates



Magnetic field topology

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  - $s \rightarrow$ minor-radial coordinate
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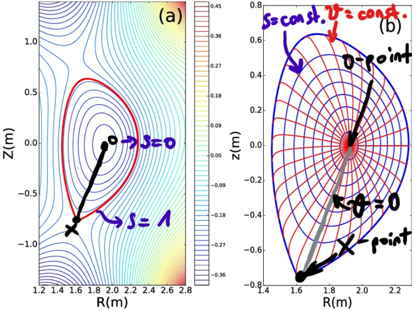
  - $\varphi \rightarrow$ toroidal coordinate
- field lines assume straight lines in SFC
- $\vec{A} \propto s \rightarrow$ no interpolation error due to linearization

Problem with CCG: incompatible with SFC

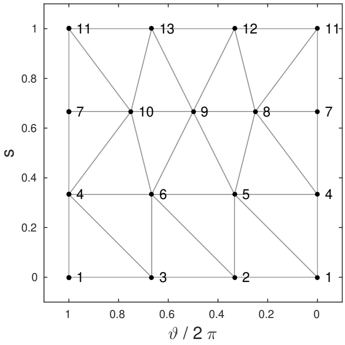
Implementing a field aligned grid



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 $\rightarrow$ extrude to 3D
- connect vertices to form tetrahedra

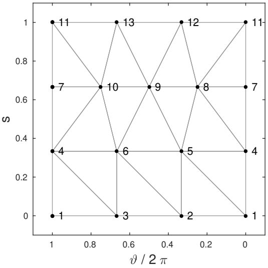
Generate grid vertices

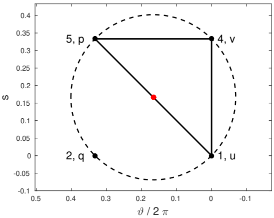


2D grid vertices

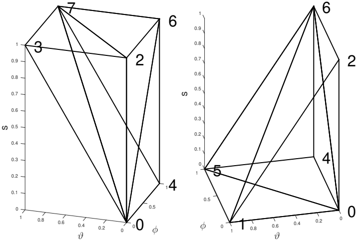
- Generate the vertex positions in poloidal plane
  - set number of points per ring
  - scale point distributions according to scaling functions for s, ϑ
- Extrude vertex coordinates toroidally $(s, \vartheta, \varphi = 0) \rightarrow (s, \vartheta, \varphi)$

Mesh tetrahedra using Delaunay condition



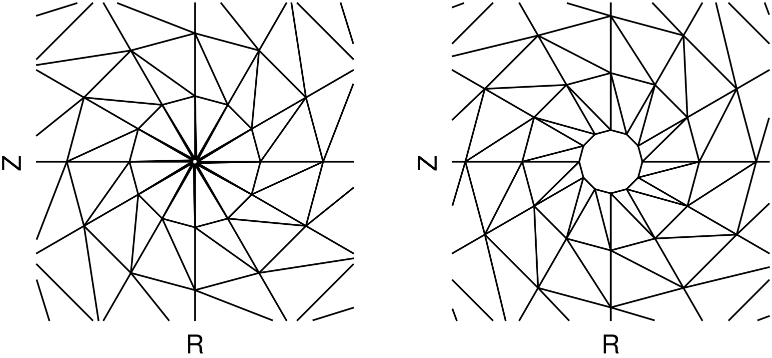


- index vertices to prism face of correct type → Delaunay condition



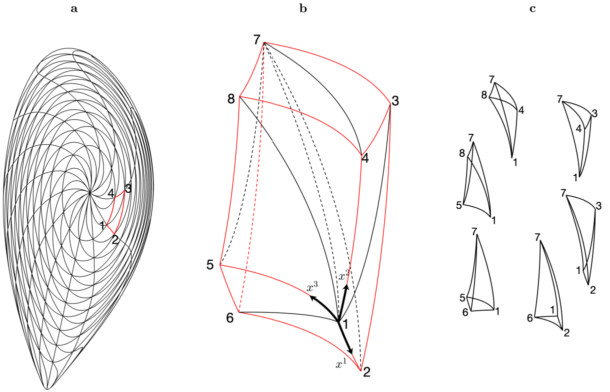
Prism types used for tetrahedra indexing

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

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

  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.

Analytical solution to ODE set

- get homogeneous solution
- get particular solution from variation of constants

$$\to x^i(\tau) = \psi^i_l \left(\bar{\psi}^l_k x^k_{(0)} e^{\lambda^l \tau} + \frac{\bar{\psi}^l_k D^k}{a-\lambda^l}(e^{a\tau} - e^{\lambda^l \tau}) + \right.$$

$$\left. \frac{\bar{\psi}^l_k F^k}{2a-\lambda^l}(e^{2a\tau} - e^{\lambda^l \tau}) - \frac{\bar{\psi}^l_k E^k}{\lambda^l}(1 - e^{\lambda^l \tau}) \right)$$

Analytical solution to ODE set

- get homogeneous solution
- get particular solution from variation of constants

$$\rightarrow x^i(\tau) = \psi^i_l \left(\bar{\psi}^l_k x^k_{(0)} e^{\lambda^l \tau} + \frac{\bar{\psi}^l_k D^k}{a-\lambda^l} (e^{a\tau} - e^{\lambda^l \tau}) + \frac{\bar{\psi}^l_k F^k}{2a-\lambda^l} (e^{2a\tau} - e^{\lambda^l \tau}) - \frac{\bar{\psi}^l_k E^k}{\lambda^l} (1 - e^{\lambda^l \tau}) \right)$$

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

New approach: Taylor expansion of solution

ODE set:

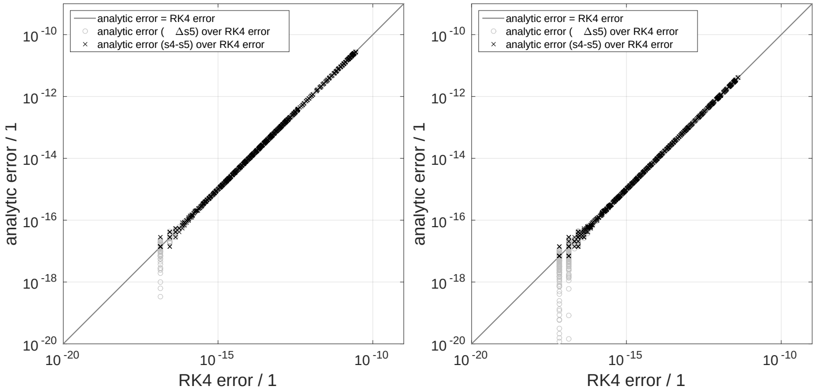
$$\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}\tau} = \hat{\mathbf{a}}\mathbf{z} + \mathbf{b}$$

Taylor series:

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

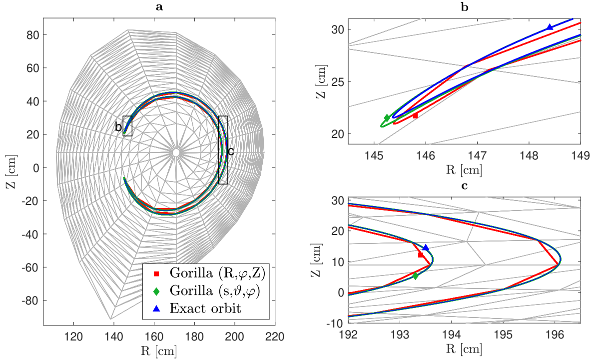
$\rightarrow$ $RK4$ corresponds to fourth order expansion, thus the fifth order estimates the $RK4$-error!

Evaluating the *RK*4 error



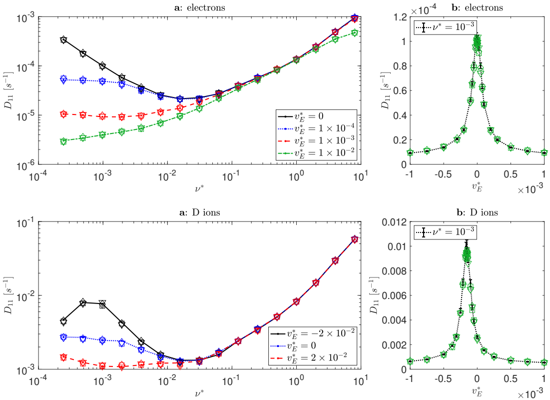
$(N_s, N_\vartheta, N_\varphi) = 5 \times 5 \times 5 \qquad (N_s, N_\vartheta, N_\varphi) = 12 \times 12 \times 12$

Poincare plots of guiding center orbits



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

Radial Transport in a stellarator using MC



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

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

Mono-energetic radial diffusion coefficient,
$E_{kin} = 3$ keV, $s_0 = 0.6$

Conclusion

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

Thank you for your attention!