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

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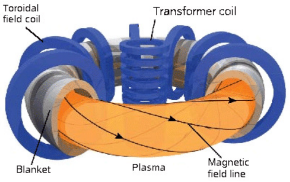
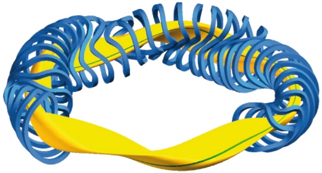
# What is the current approach to fusion?




Tokamak[1]



Stellarator[2]

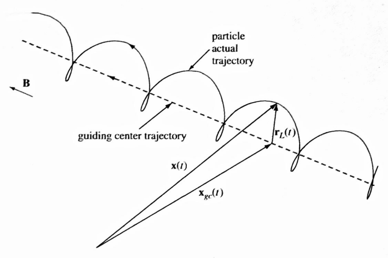
- Heating of D-T plasma to $\sim 10^8$ K in toroidal magnetic configuration
- Two main types of devices:
  - Tokamaks
  - Stellarators

[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)
  - conducting fluid
  - high particle collisionalities
- Kinetic Approach
  - distribution function $f(\vec{x}, \vec{v})$
- Gyro-kinetic Approach
  - averaging over gyro-motion
  - $f(\vec{x}, v_{||}, v_{\perp})$




Guiding center motion[3]

[3] http://www.thunderbolts.info/eg_draft/images/particle_trajectory_diagram_548x389.jpg

# 3D geometric integrator **GORILLA**

(**G**eometric **OR**bit **I**ntegration with **L**ocal **L**inearisation **A**pproach)

## Properties:

- **Physically correct long time orbit dynamics**
  - preserved total energy, magnetic moment and phase space volume
- **Insensitive to noise in fields**
- **Computationally efficient**
  - relaxed requirement to orbit shape and time evolution

# Guiding-center equations for **GORILLA**

Hamiltonian form of guiding center equations in curvilinear coordinates:

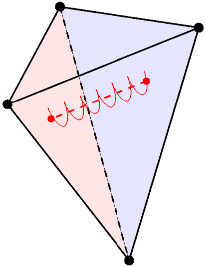
$$\dot{x}^i = \frac{v_\parallel \varepsilon^{ijk}}{\sqrt{g} B_\parallel^*} \frac{\partial A_k^*}{\partial x^j} \qquad A_k^* = A_k + \frac{v_\parallel}{\omega_c} B_k \tag{1}$$

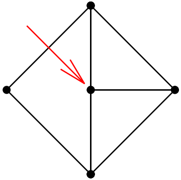
$$v_\parallel = \sigma \left( \frac{2}{m_\alpha} \left( w - J_\perp \omega_c - e_\alpha \Phi \right) \right)^{1/2} \tag{2}$$

Linearization of $A_k, B_k/\omega_c$, $\omega_c$ and $\Phi$ in spatial cells $\rightarrow$ equations of motion:

$$\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}\tau} = \hat{\mathbf{a}}\mathbf{z} + \mathbf{b} \tag{3}$$

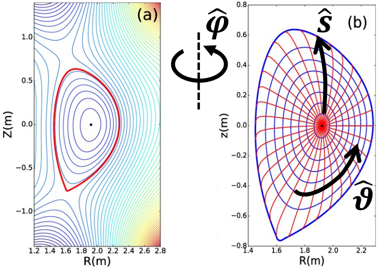
# Spatial discretization: grid for **Gorilla**





- Why do we need a grid?
  - linearization of field quantities
  - box counting scheme for distribution function
- Requirements to grid:
  - tetrahedral grid elements
  - no holes or overlaps
  - no hanging nodes

# Field-aligned grid in symmetry flux coordinates

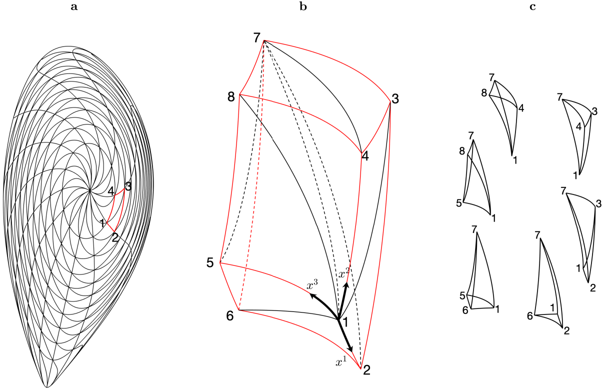



Magnetic field topology[4]

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

[4] https://www.researchgate.net/profile/Yawei_Hou/publication/335218824/figure/fig1

# Field-aligned grid




Poloidal cross-section and grid elements in real space

# Computational approach

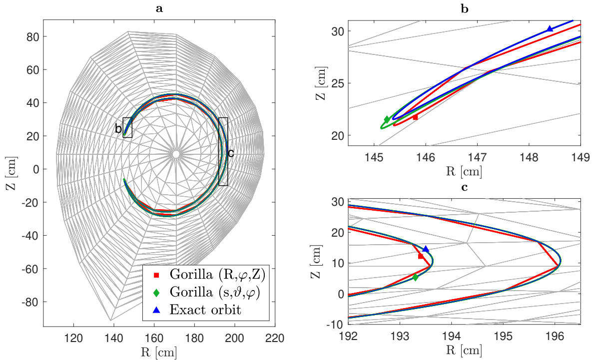
- Piecewise-constant coefficients of

$$\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}\tau} = \hat{\mathbf{a}}\mathbf{z} + \mathbf{b} \tag{3}$$

  are discontinuous at cell boundaries:
  $\rightarrow$ orbit intersections must be computed accurately

- **Runge-Kutta 4** in iterative scheme using a **parabolic estimation** and **Newton's method**

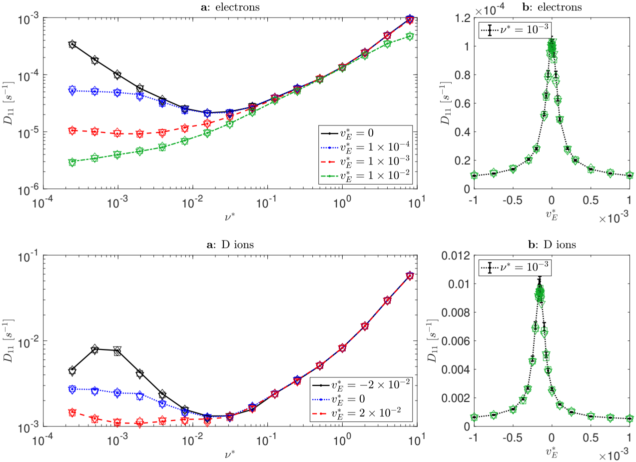
# Poincaré plots of guiding center orbits




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

# Radial Transport in a Stellarator (Monte Carlo)

## Mono-energetic radial diffusion coefficient $D_{11}$




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

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

**Init. cond.:**

$E = 3$ keV

$s_0 = 0.6$

# Conclusion and Outlook

- 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
- Computation of quasi-steady plasma parameters and kinetic equilibria

# Thank you for your attention!

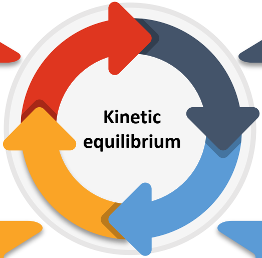
# Target application: kinetic equilibria

**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 integrator:

**1.** physically correct long time orbit dynamics

**2.** low sensitivity to noise in fields

**3.** high computational efficiency

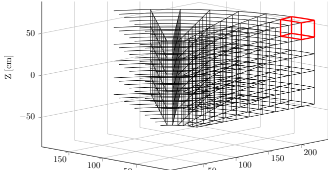
# Physically correct long time orbit dynamics

- 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

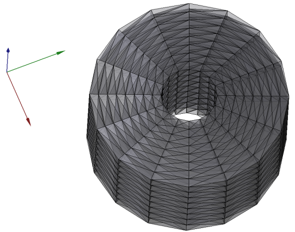
$$\frac{\mathrm{d}z^i}{\mathrm{d}\tau} = \Lambda^{ij}\frac{\partial H}{\partial z^j}, \qquad \Lambda^{ij}(\mathbf{z}) = \left\{z^i, z^j\right\}_\tau, \tag{4}$$

  with Hamiltonian $H(\mathbf{z}) = v_\parallel^2/2 - U(\mathbf{x})$ and antisymmetric Poisson matrix $\Lambda^{ij}(\mathbf{z})$.
- **Symplecticity:** Phase space volume is conserved.

# Previous grid in cylindrical coordinates

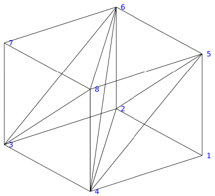



Hexahedra

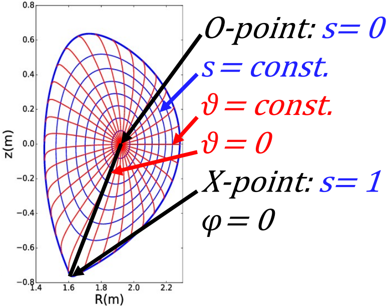


Cylindrical Contour Grid

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

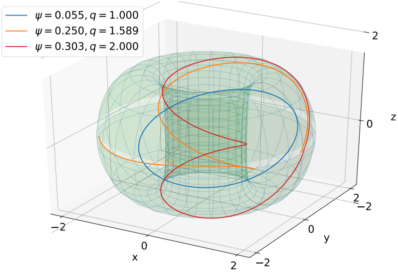


# Implementing the field-aligned grid




- 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 tetrahedra with Delaunay condition

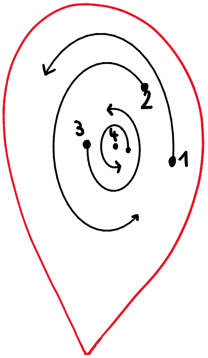
# Field-line integration




Selected field lines in torus

- Field line equations:
  $$\frac{\mathrm{d}R}{\mathrm{d}\varphi} = \frac{B^R}{B^\varphi}, \ \frac{\mathrm{d}Z}{\mathrm{d}\varphi} = \frac{B^Z}{B^\varphi}$$
- Safety factor:
  $$q = \frac{B^\varphi}{B^\vartheta}, \ \mathrm{d}\varphi = q\mathrm{d}\vartheta$$
  - if $q$ is irrational, the field line forms a flux surface

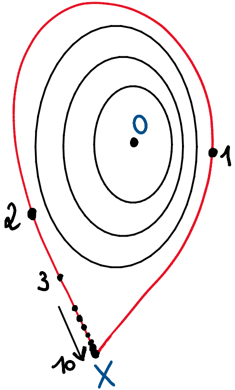
# Finding the $O$-point




Iterative scheme for finding the $O-point$

- start at point 1, follow $\vec{B}$ for 10 toroidal turns in $(R, \varphi, Z)$
- 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



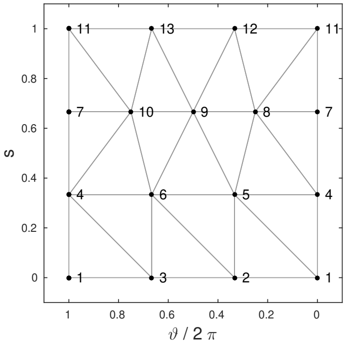

Iterative scheme for finding the $X - point$

- 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

# Construct conversion routine from field line data

- parametrize line segment from $O$-point to $X$-point
- integrate field lines in equidistant steps for one poloidal turn
- save $(R, Z)$ data $\rightarrow$ $s$ is constant, $\vartheta$ is equidistant
- interpolate data for coordinate conversion
  - periodic splines in $\vartheta$
  - lagrange polynomials in $s$

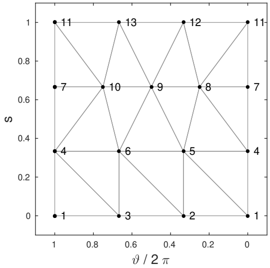
# Generate grid vertices

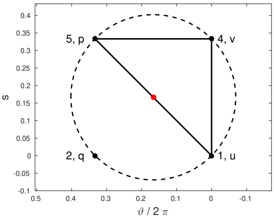



2D grid vertices

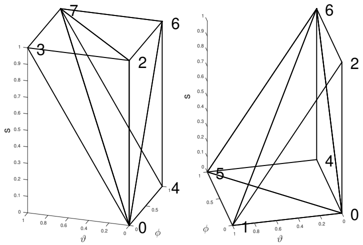
- Generate the vertex positions in poloidal plane
  - set number of points per ring
  - scale point distributions according to scaling functions for $s$, $\vartheta$
- Extrude vertex coordinates toroidally $(s, \vartheta, \varphi = 0) \rightarrow (s, \vartheta, \varphi)$

# Mesh tetrahedra using Delaunay condition



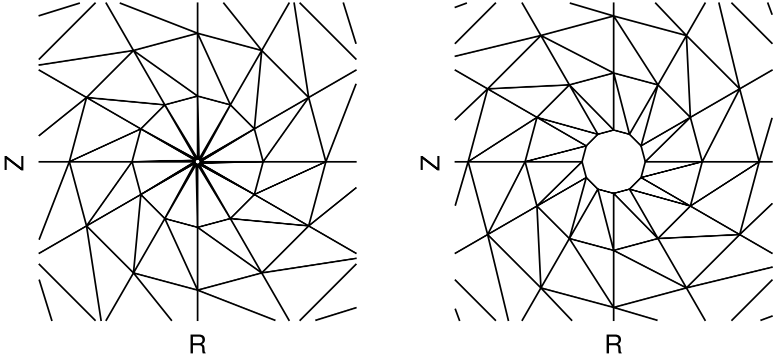




- index vertices to prism face of correct type → Delaunay condition



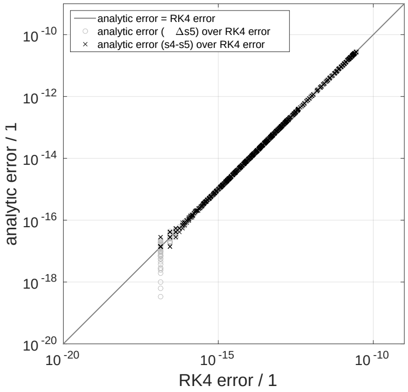

Prism types used for tetrahedra indexing

# One compromise: there is a hole

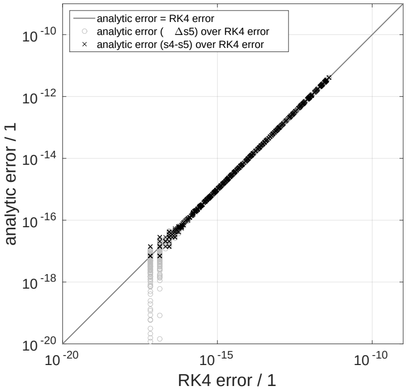



Center region of the grid with annulus

# Evaluating the *RK*4 error

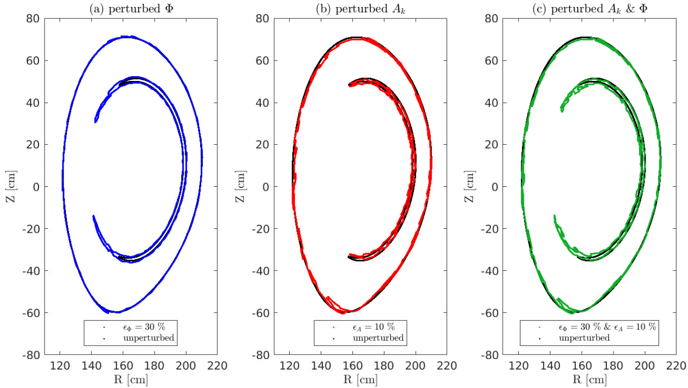



$$(N_s, N_\vartheta, N_\varphi) = 5 \times 5 \times 5$$




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

# Axisymmetric noise of electrostatic and vector potential




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