

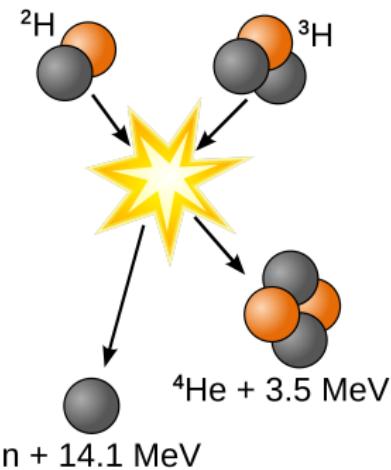
Field-aligned grid generation and enhancements of the guiding-center orbit code GORILLA

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What is nuclear fusion?

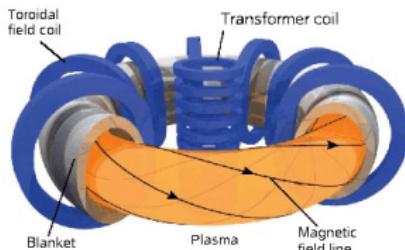


- Atomic nuclei are combined to form different atomic nuclei and subatomic particles
- 17.6 MeV are released as kinetic energy in fusion of Deuterium+Tritium

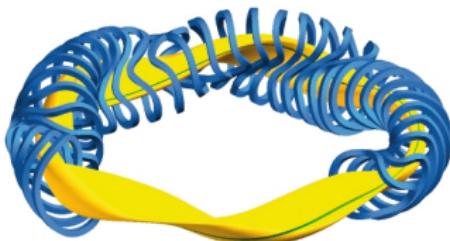


Figure taken from: https://de.wikipedia.org/wiki/Kernfusion#/media/Datei:Deuterium-tritium_fusion.svg

What is the current approach to fusion?



Tokamak



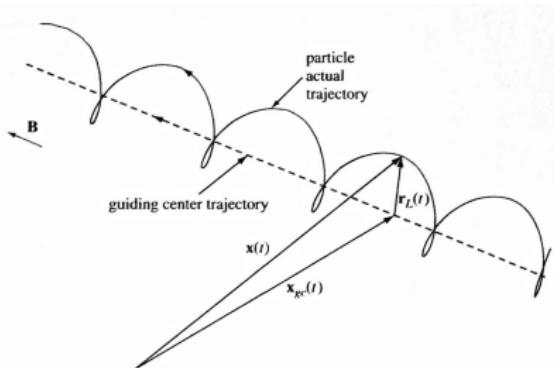
Stellarator

- 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

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

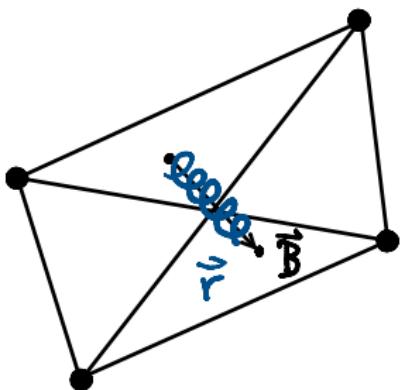
Guiding center motion



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

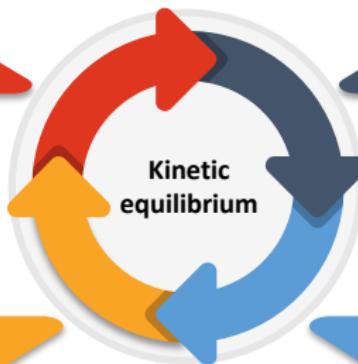
Modelling of kinetic equilibria

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.

Gorilla 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

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

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

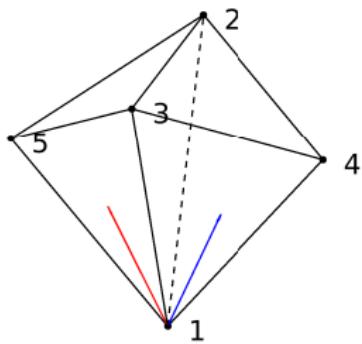
Requirements to grid: Tetrahedral cells

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

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

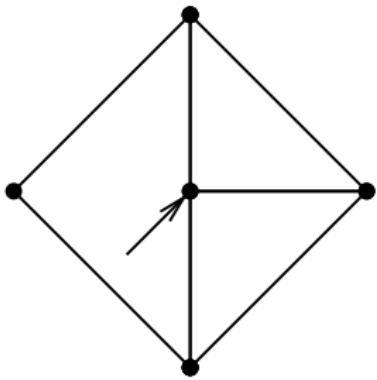
- this system is uniquely defined as the number of unknowns (=4) is equal to the number of values for f
 \rightarrow no fitting for the case of tetrahedra

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

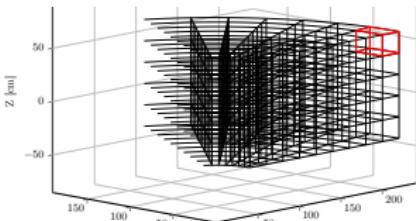


- adjacent tetrahedral faces must share three common vertices for linearized fields to be continuous
→ no hanging nodes!

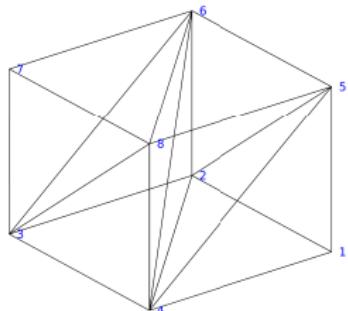
Further requirements

- 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



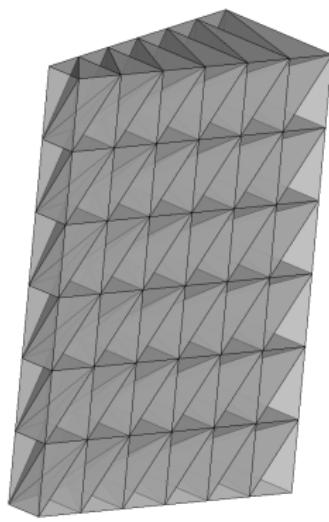
Hexahedra



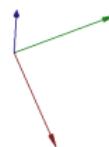
Tetrahedra

- 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

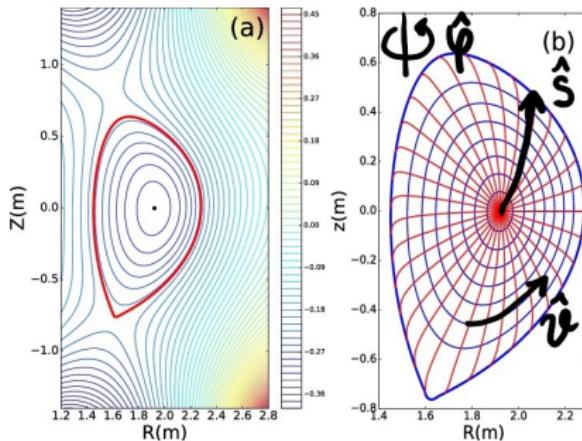


toroidal grid slice



full cylindrical contour grid

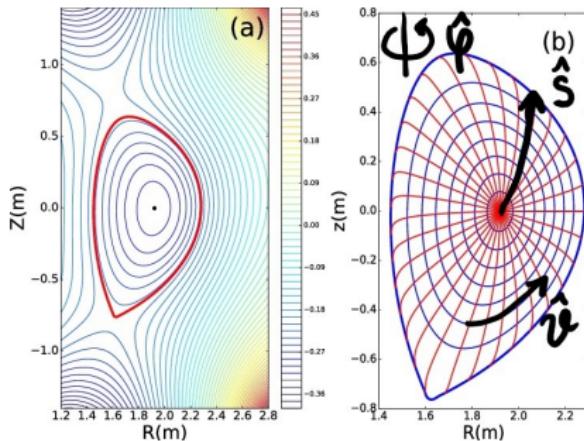
Idea: symmetry flux coordinates



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

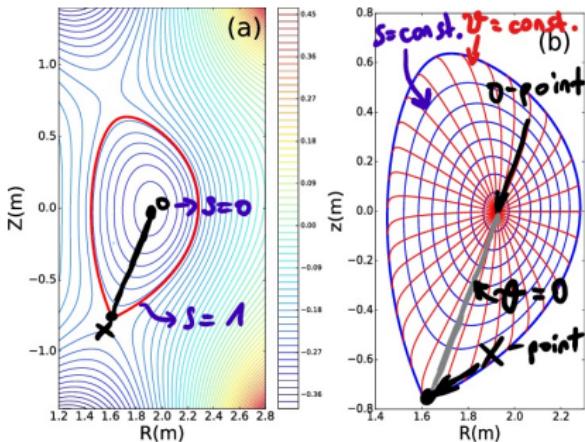


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Problem with CCG: incompatible with SFC

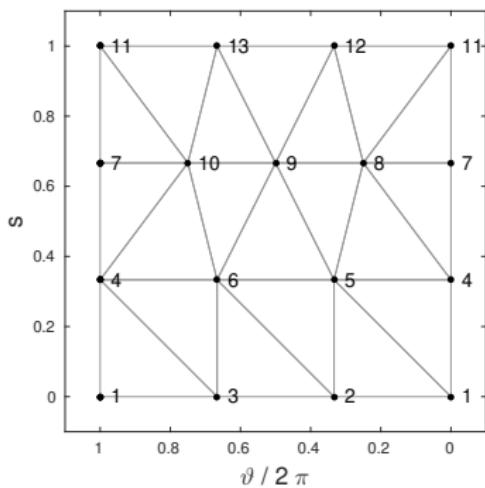
Implementing a field aligned grid



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

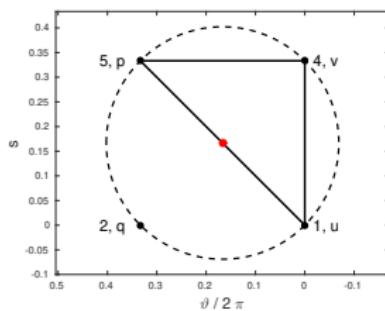
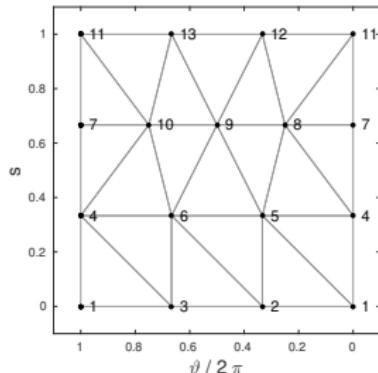
Generate grid vertices



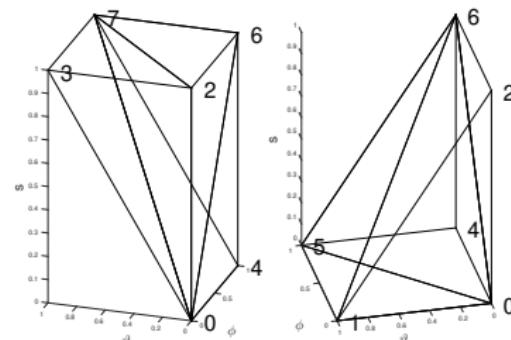
2D grid vertices

- 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

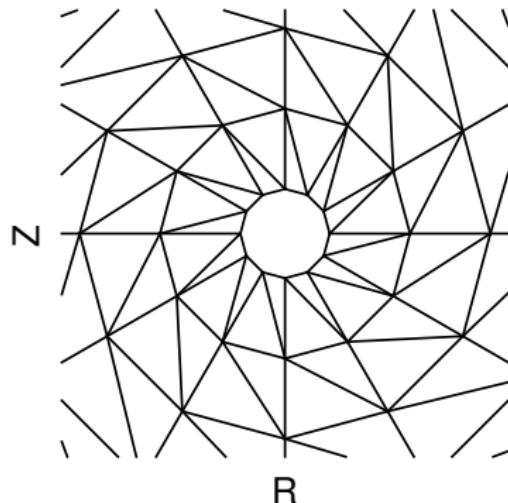
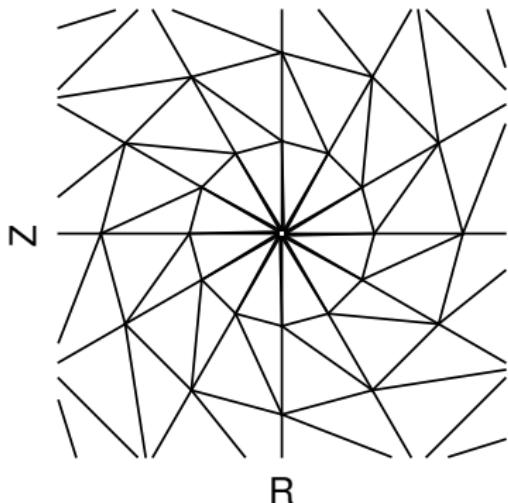


- index vertices to prism face of correct type
→ Delaunay condition



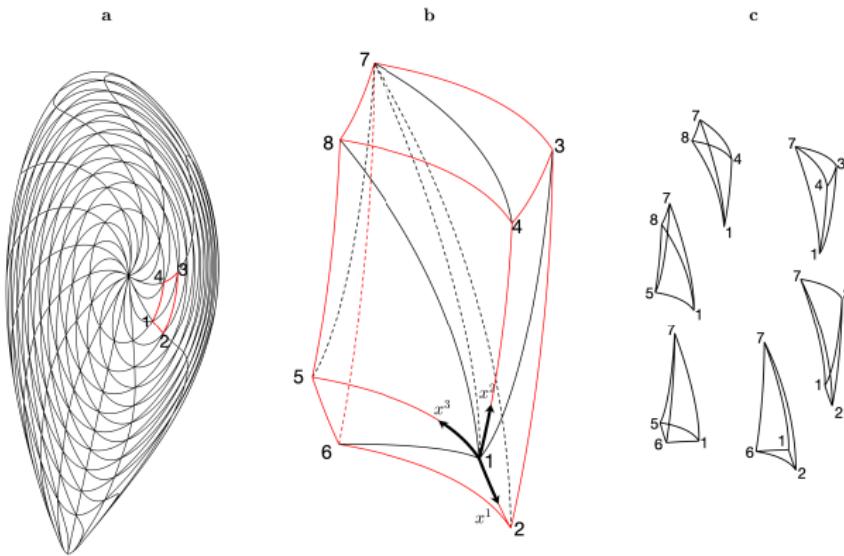
Prism types used for tetrahedra indexing

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

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

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

Analytical solution to ODE set

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

New approach: Taylor expansion of solution

ODE set:

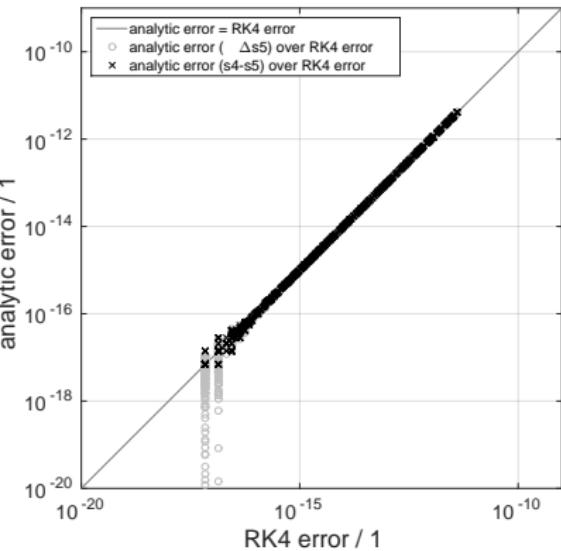
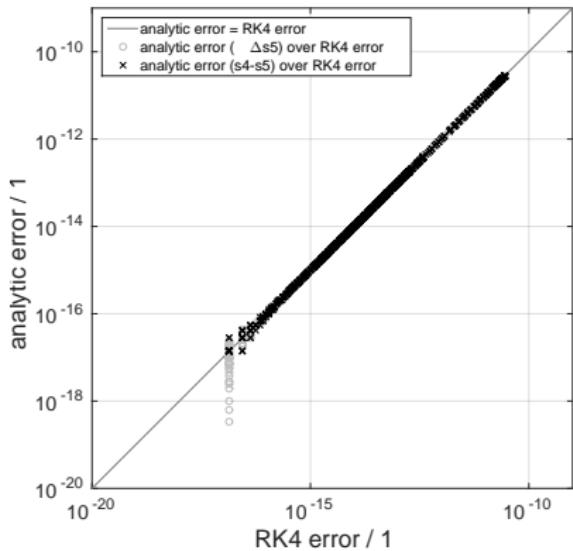
$$\frac{d\mathbf{z}}{d\tau} = \hat{\mathbf{a}}\mathbf{z} + \mathbf{b}$$

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!

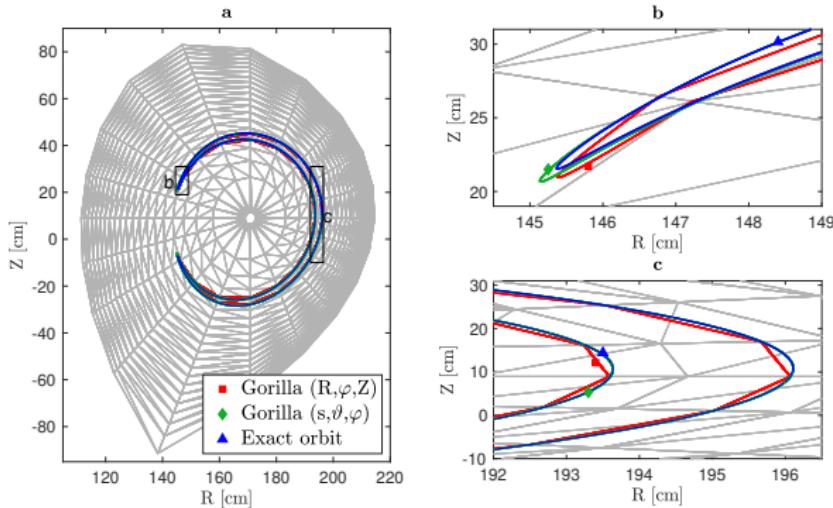
Evaluating the *RK4* error



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

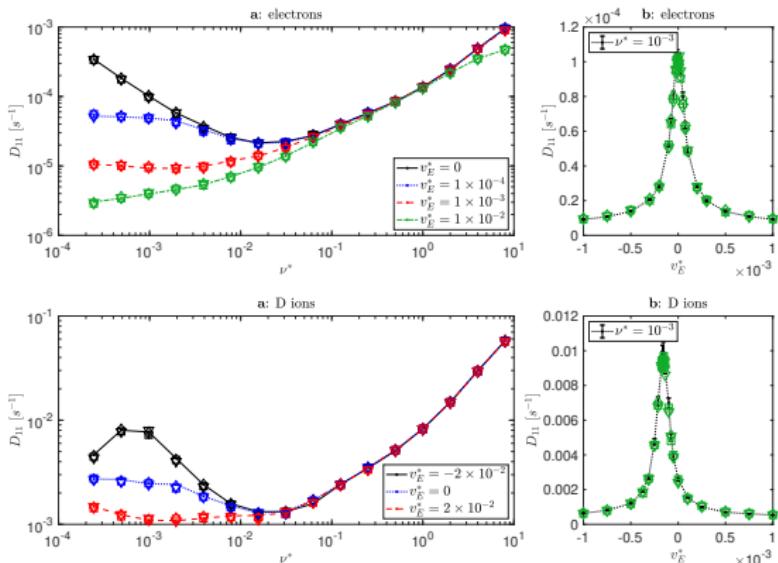
$$(N_s, N_\vartheta, N_\varphi) = 12 \times 12 \times 12$$

Poincare plots of guiding center orbits



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

Radial Transport in a stellarator using MC



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

$$v_E^* = \frac{E_r}{vB_0}$$

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

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!