Geometric integration of guiding-center orbits in piecewise linear toroidal fields

Lukas Bauer
Institute of Theoretical and Computational Physics - Plasma Physics
Group of Prof. W. Kernbichler (Graz University of Technology)

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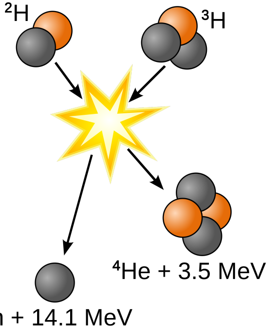
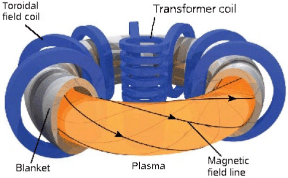
What is nuclear fusion?



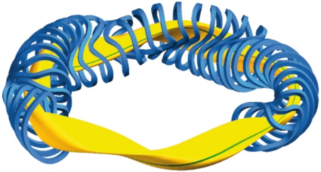
Deuterium + Tritium
$\rightarrow$ Helium + neutron

- 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 $\sim 10^8$ 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

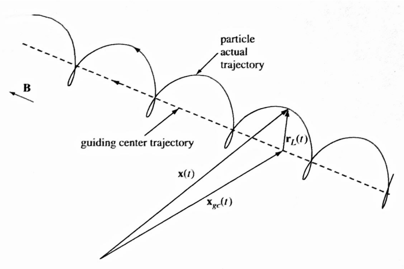
Theoretical descriptions of plasmas

- 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 $f(\vec{x}, v_{||}, v_{\perp})$

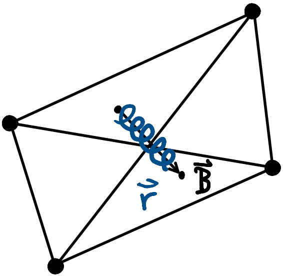
Guiding center motion



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

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

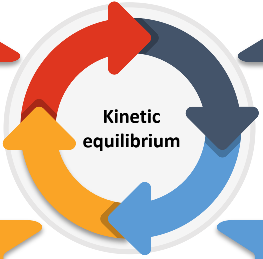
Modelling of kinetic equilibria

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.

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,

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

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

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

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

  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.

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

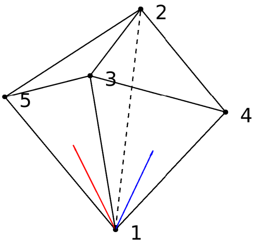
Requirements to grid: Tetrahedral cells

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

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

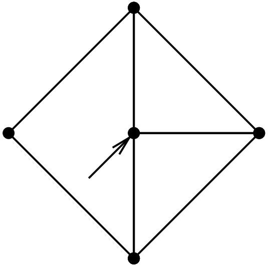
- this system is uniquely defined as the number of unknowns (=4) is equal to the number of values for f $\rightarrow$ no fitting for the case of tetrahedra

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

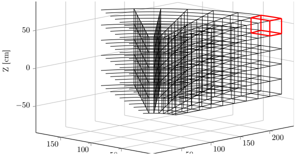


- adjacent tetrahedral faces must share three common vertices for linearized fields to be continuous
  $\rightarrow$ no hanging nodes!

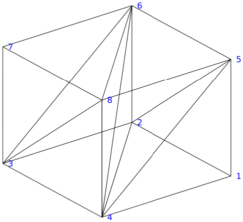
Further requirements

- 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



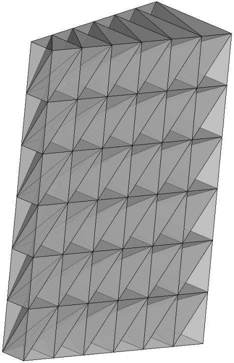
Hexahedra



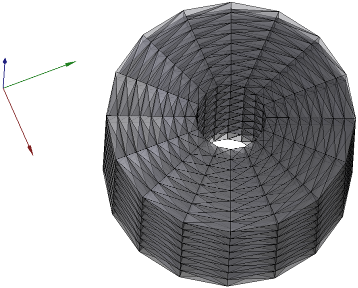
Tetrahedra

- 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

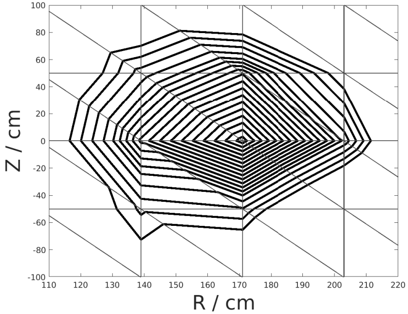


toroidal grid slice



full cylindrical contour grid

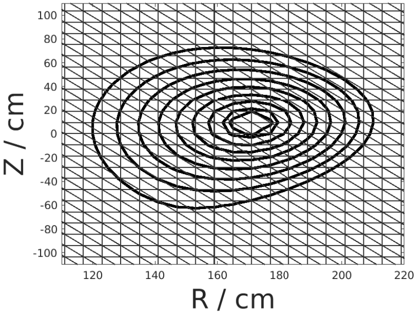
Poincaré plots of guiding center orbits



Passing orbit in coarse CCG

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

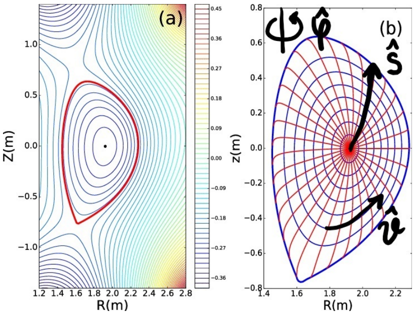
Poincaré plots of guiding center orbits



Passing orbit in finer CCG

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

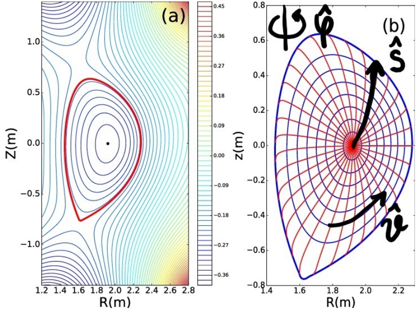
Idea: symmetry flux coordinates



Magnetic field topology

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

Idea: symmetry flux coordinates



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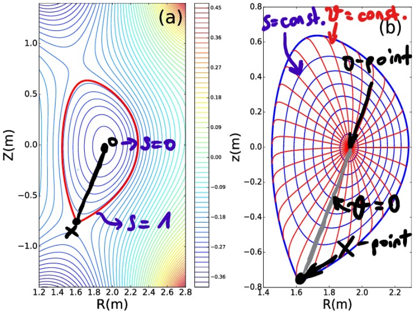
Problem with CCG: incompatible with SFC

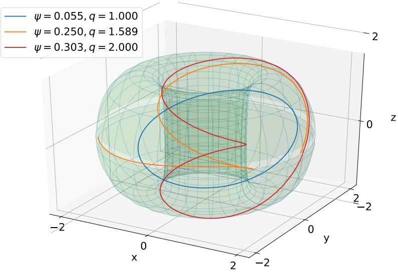
Implementing a field aligned grid



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

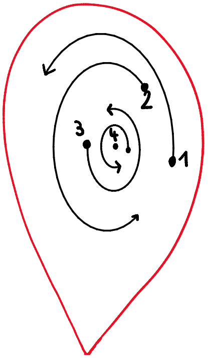
Field-line integration



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

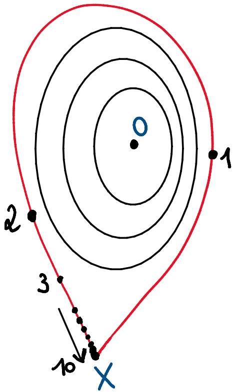
Finding the O-point



Iterative scheme for finding the $O - point$

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



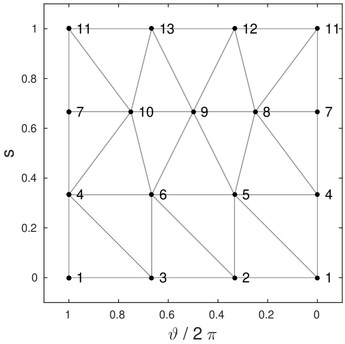
Iterative scheme for finding the $X - point$

- start inside and integrate field line for one poloidal turn
- increase distance to mag. axis and repeat until the field line does not cross $\rightarrow$ 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, ϑ is equidistant
- interpolate data for coordinate conversion
  - periodic splines in ϑ
  - lagrange polynomials in s

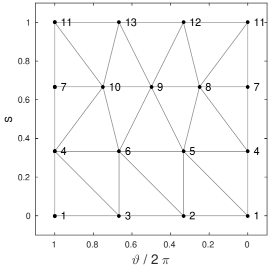
Generate grid vertices

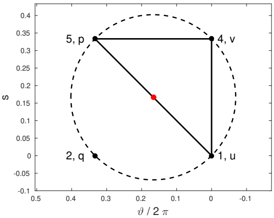


2D grid vertices

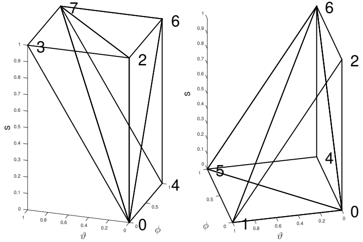
- Generate the vertex positions in poloidal plane
  - set number of points per ring
  - scale point distributions according to scaling functions for s, ϑ
- Extrude vertex coordinates toroidally $(s, \vartheta, \varphi = 0) \rightarrow (s, \vartheta, \varphi)$

Mesh tetrahedra using Delaunay condition



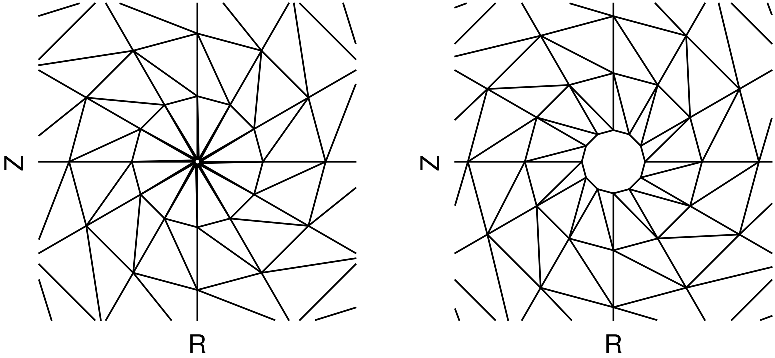


- index vertices to prism face of correct type $\rightarrow$ Delaunay condition



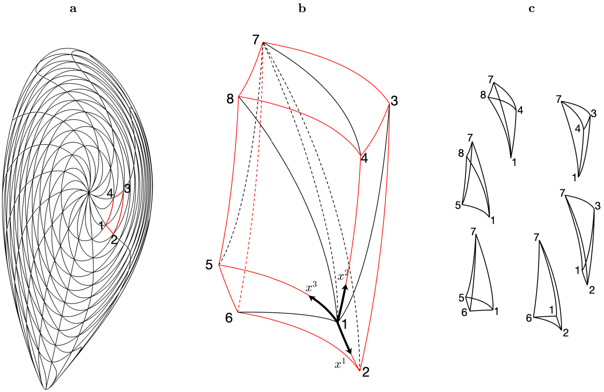
Prism types used for tetrahedra indexing

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

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

Analytical solution to ODE set

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- get particular solution from variation of constants

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

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

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

New approach: Taylor expansion of solution

ODE set:

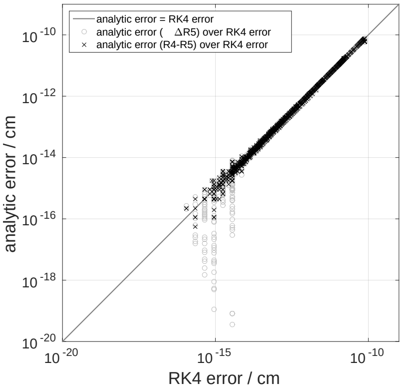
$$\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}\tau} = \hat{\mathbf{a}}\mathbf{z} + \mathbf{b}$$

Taylor series:

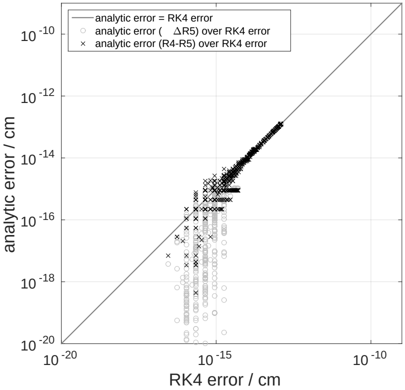
$$\mathbf{z} = \mathbf{z}_0 + \sum_{k=1}^{\infty} \frac{\tau^k}{k!} \hat{\mathbf{a}}^{k-1} \cdot (\mathbf{b} + \hat{\mathbf{a}} \cdot \mathbf{z}_0)$$

$\rightarrow$ *RK*4 corresponds to fourth order expansion, thus the fifth order estimates the *RK*4-error!

Evaluating the *RK*4 error - CCG

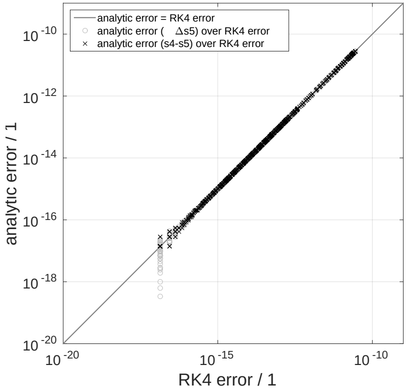


$(N_R, N_\varphi, N_Z) = 5 \times 5 \times 5$

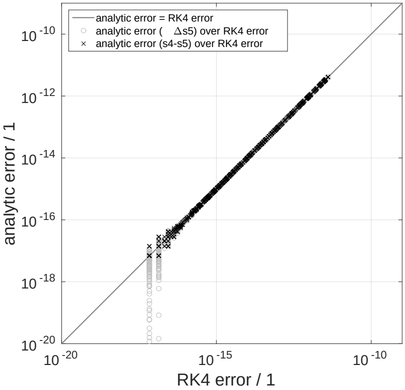


$(N_R, N_\varphi, N_Z) = 12 \times 12 \times 12$

Evaluating the $RK4$ error - FAG



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



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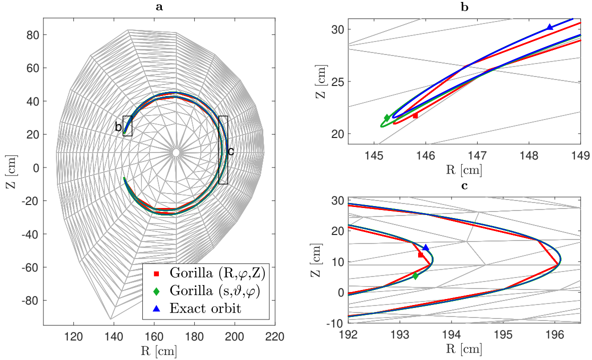
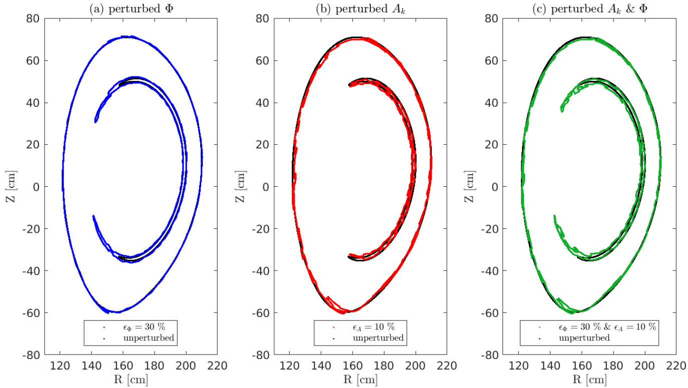
Poincare plots of guiding center orbits



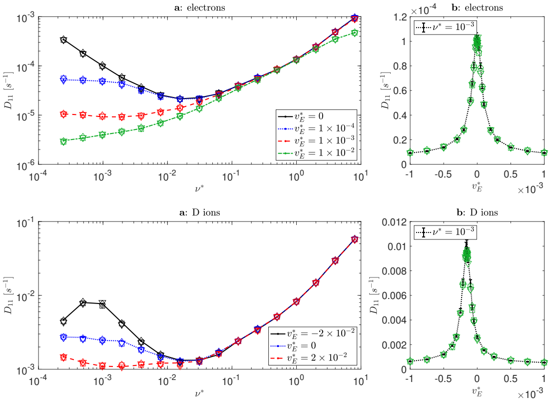
- Geometric integration: Not exact orbit shape.
- Axisymmetic (2D): Canonical toroidal angular momentum is conserved.

Axisymmetric noise of electrostatic and vector potential



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

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!