

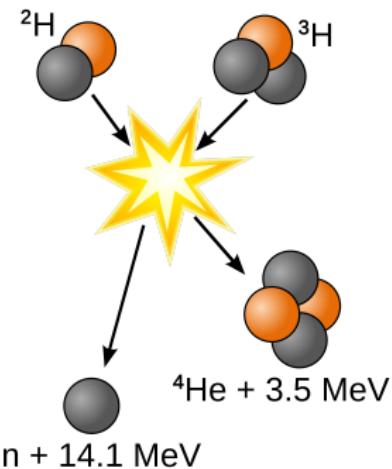
# Field-aligned grid generation and enhancements of the guiding-center orbit code GORILLA

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?

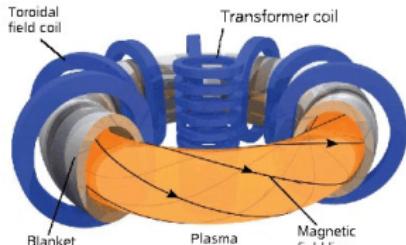


- Atomic nuclei are combined to form different atomic nuclei and subatomic particles
- 17.6 MeV are released as kinetic energy in fusion of Deuterium+Tritium

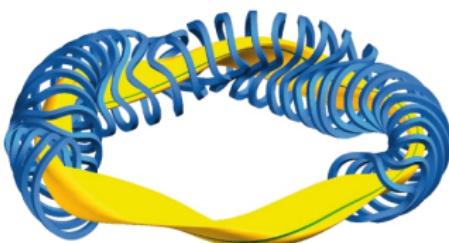


Figure taken from: [https://de.wikipedia.org/wiki/Kernfusion#/media/Datei:Deuterium-tritium\\_fusion.svg](https://de.wikipedia.org/wiki/Kernfusion#/media/Datei:Deuterium-tritium_fusion.svg)

# What is the current approach to fusion?



Tokamak<sup>[1]</sup>



Stellarator<sup>[2]</sup>

- 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

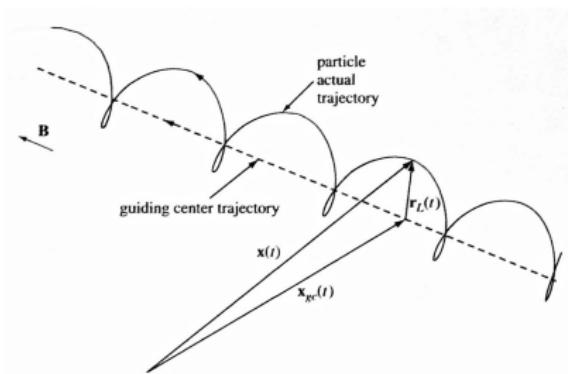
[1] [https://upload.wikimedia.org/wikipedia/commons/b/b3/W7X-Spulen\\_Plasma.blau.gelb.jpg](https://upload.wikimedia.org/wikipedia/commons/b/b3/W7X-Spulen_Plasma.blau.gelb.jpg)

[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
    - 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
- → 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](http://www.thunderbolts.info/eg_draft/images/particle_trajectory_diagram_1126x844.jpg)

# 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

Kinetic  
equilibrium

## 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.

# 3D geometric integrator **GORILLA**

(Geometric ORbit Integration with Local Linearisation Approach)

## Properties:

- **Physically correct long time orbit dynamics**
  - preserved total energy, magnetic moment and phase space volume
- **Low sensitivity to noise in fields**
- **Computationally efficient**
  - not exact orbit shape and time evolution

# Guiding-center equations for **GORILLA**

Hamiltonian form of guiding center equations in curvilinear coordinates:

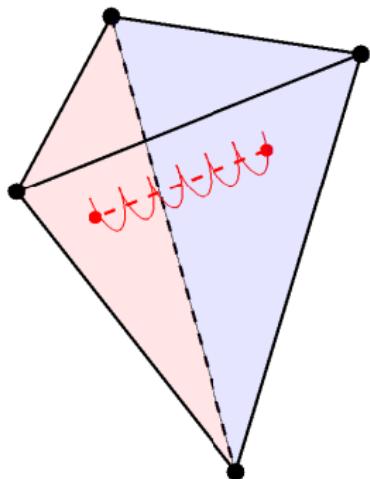
$$\dot{x}^i = \frac{v_{\parallel}\varepsilon^{ijk}}{\sqrt{g}B_{\parallel}^*} \frac{\partial A_k^*}{\partial x^j} \quad A_k^* = A_k + \frac{v_{\parallel}}{\omega_c} B_k \quad (1)$$

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

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

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

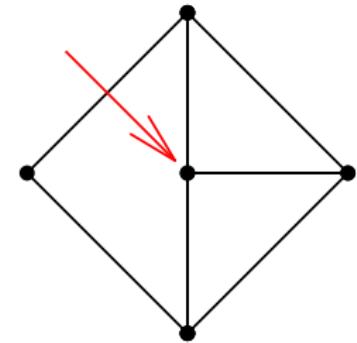
# Spatial discretization: grid for Gorilla



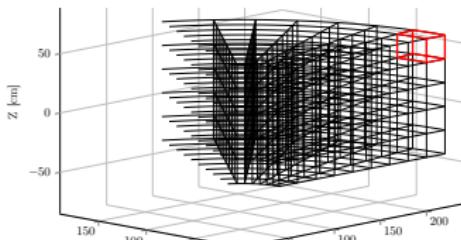
- Why do we need a grid?
  - linearization of field quantities
  - box counting scheme for distribution function
  
- What is the consequence?
  - guiding-center orbits need to be computed between cell boundaries

# Requirements to grid

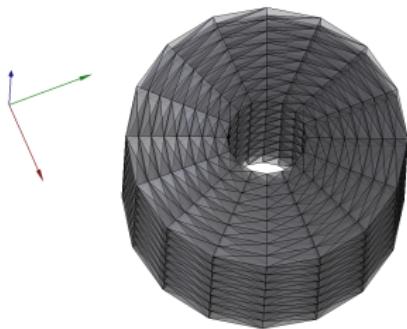
- linear scalar functions of space have **four** degrees of freedom → **tetrahedral** grid elements for uniquely determined function coefficients
- no holes or overlaps in grid
- continuous linearized field components  
→ no hanging nodes



# Previous grid in cylindrical coordinates

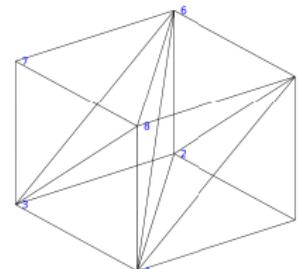


Hexahedra

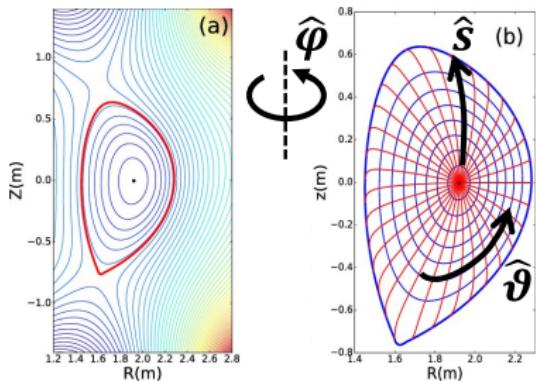


Cylindrical Contour Grid

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



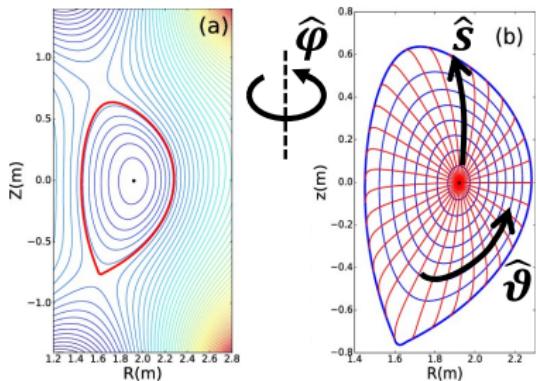
# Next step: symmetry flux coordinates (SFC)



Magnetic field topology

- coordinates  $(s, \vartheta, \varphi)$ 
  - $s \rightarrow$  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

# Next step: symmetry flux coordinates (SFC)

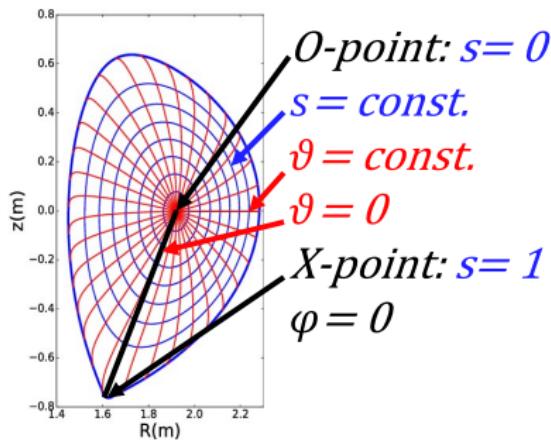


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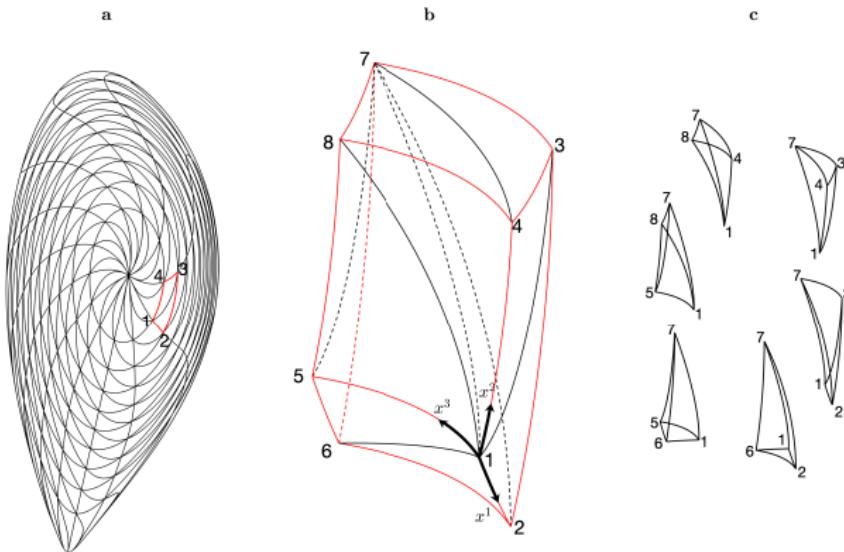
**Problem with CCG: incompatible with SFC!**

# Implementing a field aligned grid



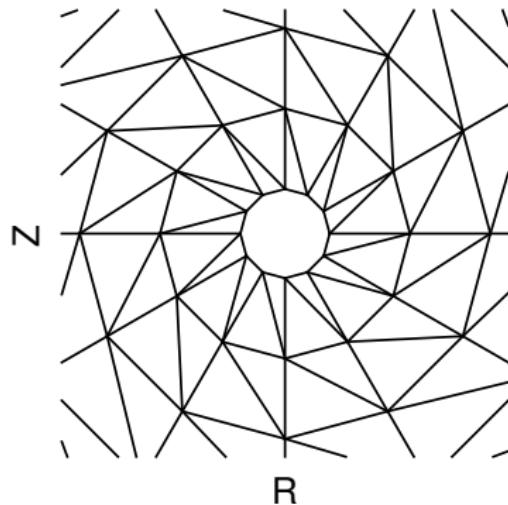
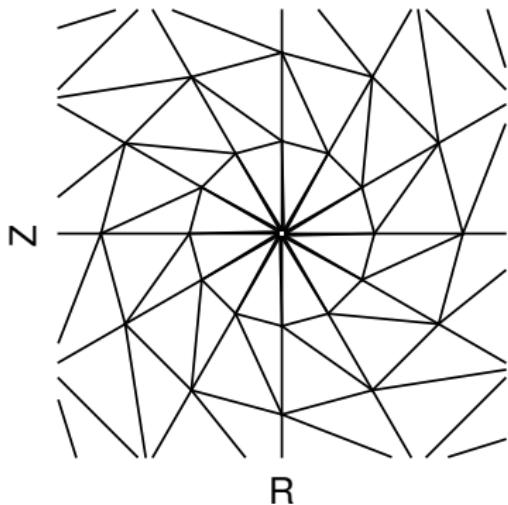
- find  $O$ -point and  $X$ -point
- field line integration for coordinate interpolation
- interpolation routine:  $(s, \vartheta, \varphi) \rightarrow (R, \varphi, Z)$  for evaluation of field quantities
- create 2D grid points  
→ extrude to 3D
- connect vertices to tetrahedra with Delaunay condition

# Field aligned grid



Poloidal cross-section and grid elements in real space

# One compromise: there is a hole



Center region of the grid with annulus

# Computational approach

- Piecewise-constant coefficients of

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

are discontinuous at cell boundaries:

→ orbit intersections must be computed accurately

- Eq. set (3) is numerically solved via **Runge-Kutta 4** in an iterative scheme using a **parabolic estimation** and **Newton's method**.

# Analytical solution to ODE set

- compute homogeneous solution
- find particular solution using 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:

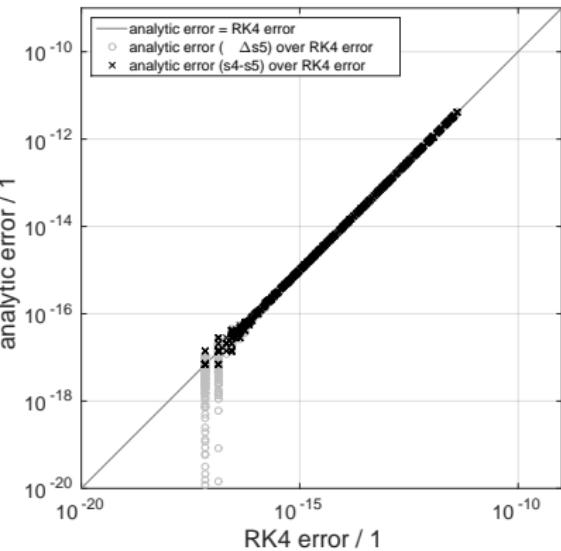
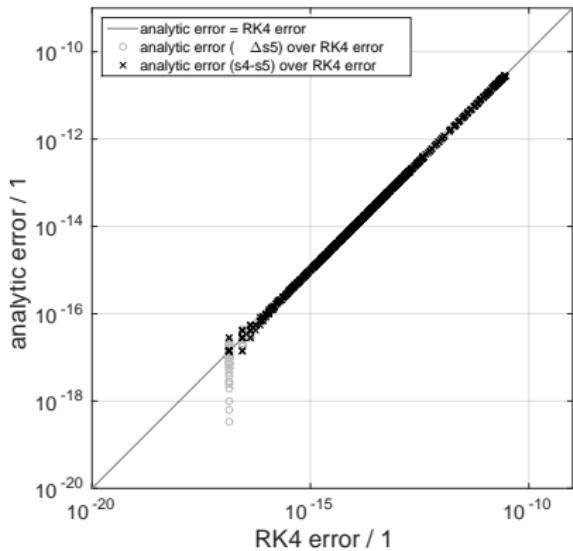
$$\frac{d\mathbf{z}}{d\tau} = \hat{\mathbf{a}}\mathbf{z} + \mathbf{b}$$

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!

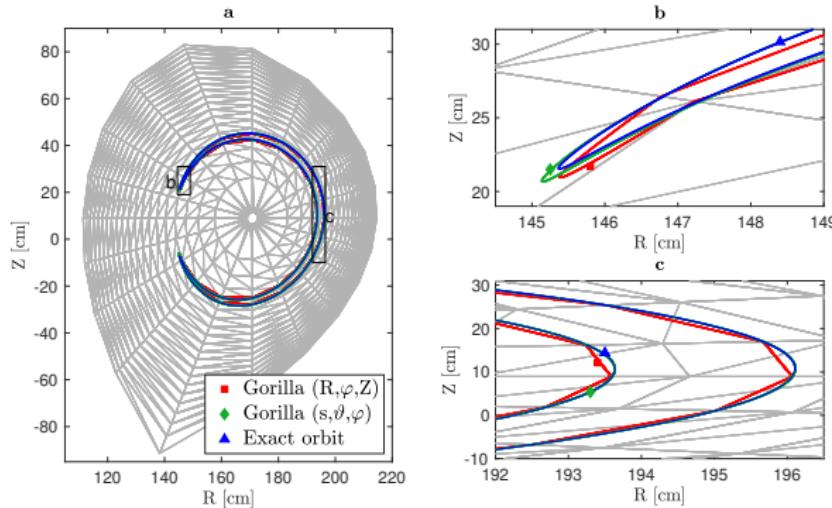
# Evaluating the *RK4* error



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

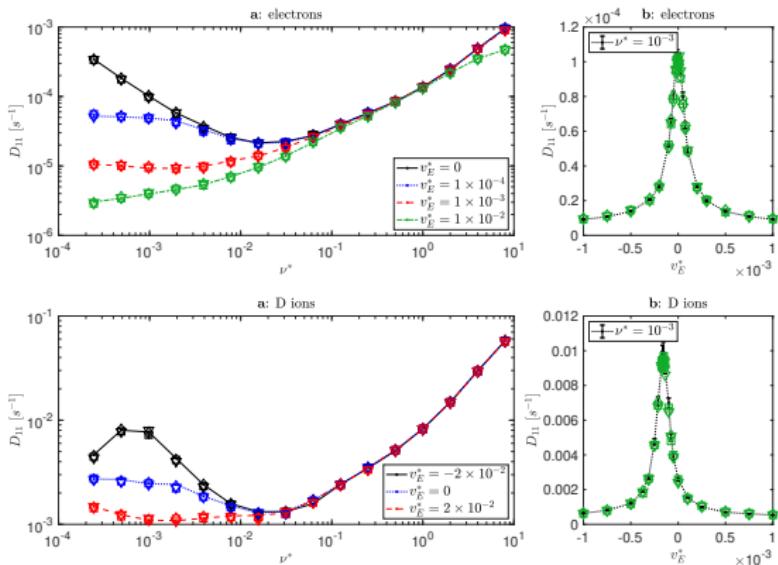
$$(N_s, N_\vartheta, N_\varphi) = 12 \times 12 \times 12$$

# 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 (Monte Carlo)



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

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

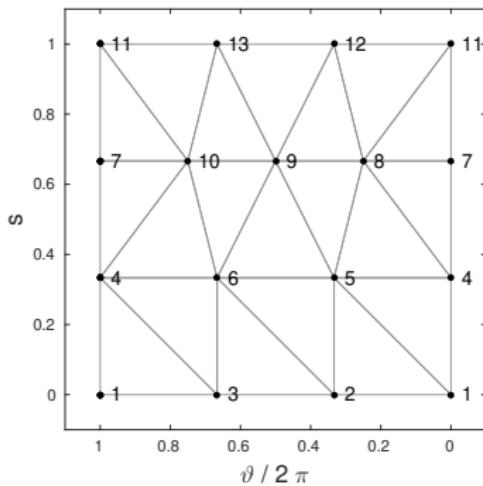
Mono-energetic radial diffusion coefficient,  
 $E_{kin} = 3 \text{ keV}, s_0 = 0.6$

# 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!

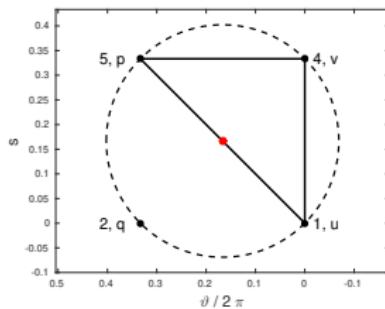
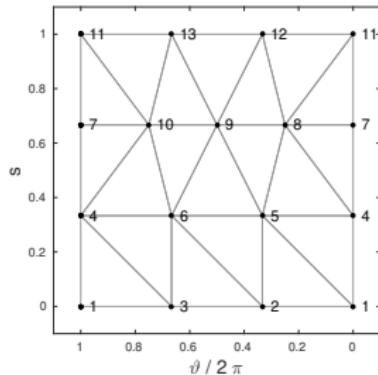
# Generate grid vertices



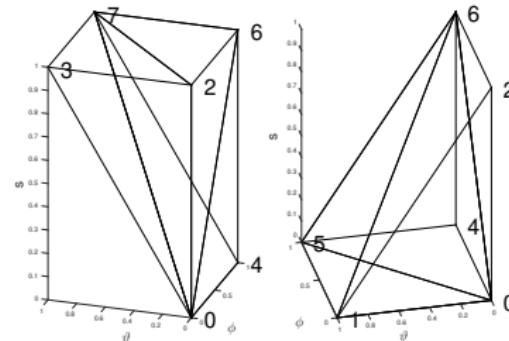
2D grid vertices

- 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