EPFL

TSVV3 Bi-Weekly Meeting

Curvilinear Coordinates in GBS

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21st September 2022

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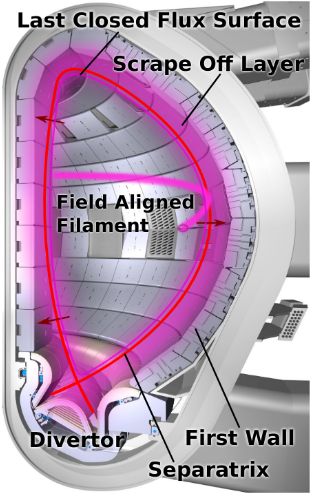
Outline

Motivation

The Shape of a Tokamak

- Magnetic shape: core, edge, scrape-off layer.
- Wall shape: curved main chamber, divertor



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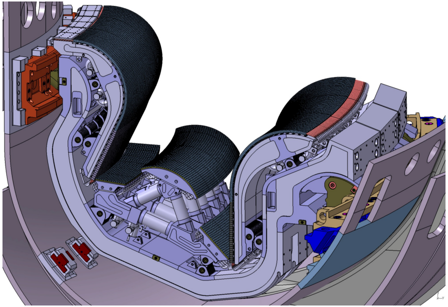
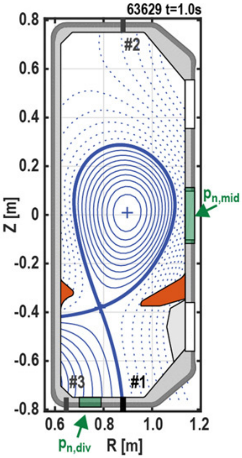


Wall Geometry Matters

Especially for Neutrals

- Baffled TCV discharges with increased neutral pressure (Reimerdes et al. 2021),
- SPARC's super-X "tunnel" divertor (Kuang et al. 2020),
- Existing simulations accounting for geometry



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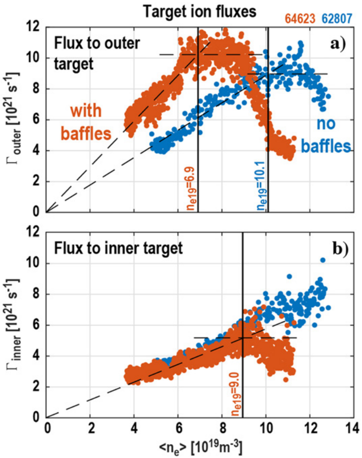

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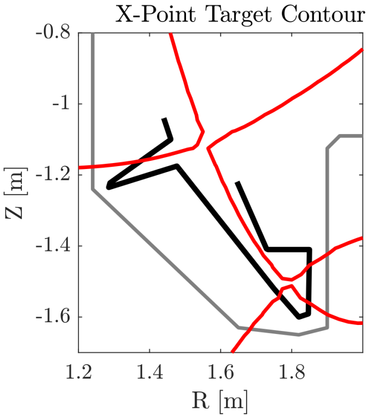

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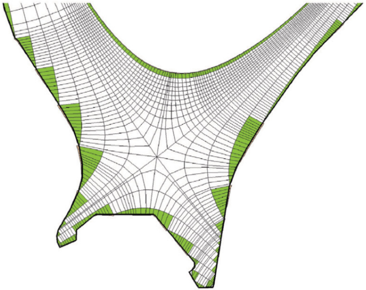

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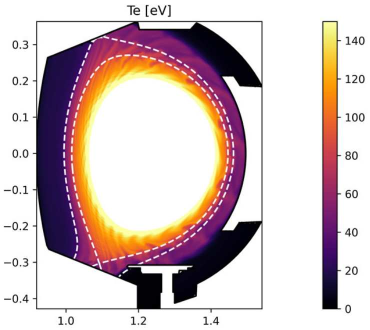

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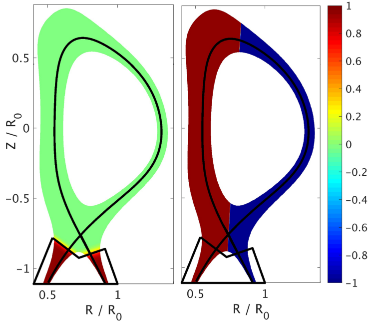
  - SOLEDGE suite (Bufferand et al. 2021)
  - GRILLIX (Stegmeir et al. 2019)
  - FELTOR
  - BOUT++



Edge and SOL Turbulence Simulation

With the GBS Code

Theory

- Two-fluid drift-reduced Braginskii
- Kinetic neutrals
- Improved BCs (Loizu et al. 2012)

Numerics

- 4^{th} order Runge-Kutta (time)
- 4^{th} order finite differences (space)
- Non-field aligned cartesian grid
- GMRES / MUMPS

$$\frac{\partial n}{\partial t} = -\frac{\rho_*^{-1}}{B}\{\phi, n\} + \frac{2}{B}[C(p_e) - nC(\phi)] - \nabla_\parallel(n v_{\parallel e}) + D_n \nabla_\perp^2 n + S_n + \nu_{iz} n_n - n_i \nu_{rec}$$

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Edge and SOL Turbulence Simulation

With the GBS Code

How to include wall geometry in GBS?

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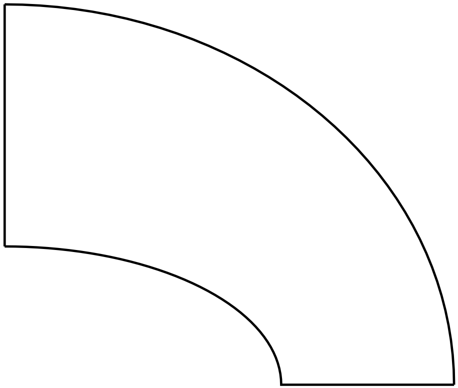
Towards Realistic Wall Geometry in GBS

Realistic Wall Geometry is not a “New” Problem

- Finite difference (FD) method on curvilinear grids,
- Finite element method or Galerkin method,
- Finite volume method or discontinuous Galerkin method,
- Penalization method or “immersed boundary” (IB) method,



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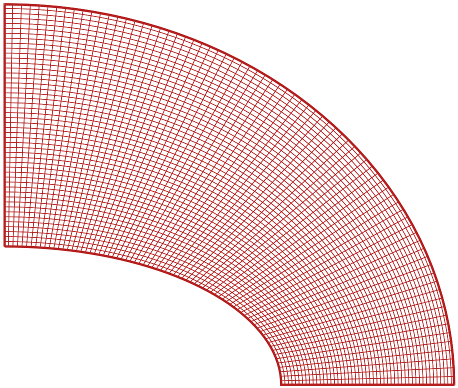

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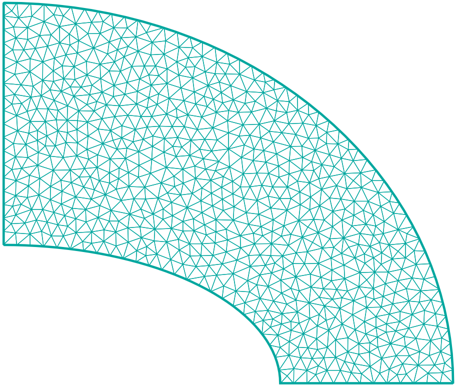

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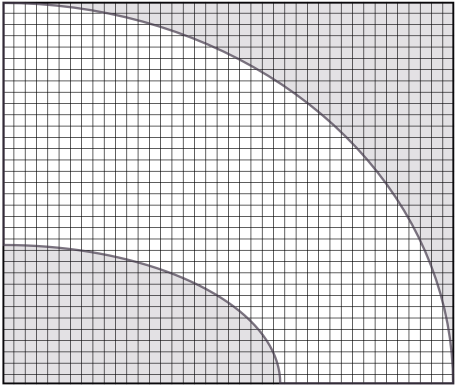


Curvilinear Grids

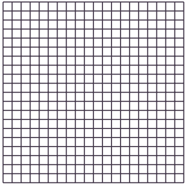
Consider “boundary-fitted” grids

- Computational variables $\{\xi^i\} \rightarrow (R, Z, \phi)$

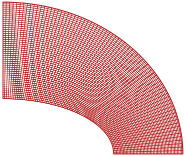
$$\frac{\partial n}{\partial R} = \frac{\partial \xi^i}{\partial R}\frac{\partial n}{\partial \xi^i}$$

- Retain finite difference convergence
- (Almost) No refactoring needed

Logical grid:

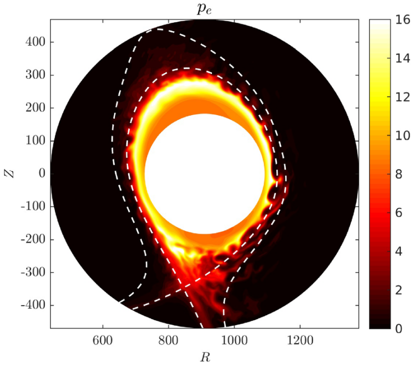


Physical grid:



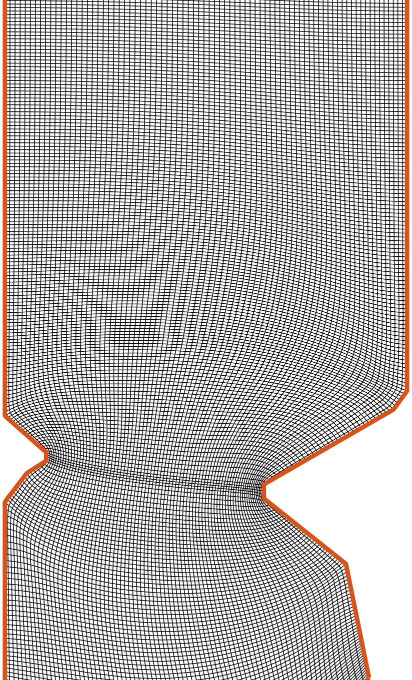
How to Generate a Grid?

- Analytically, e.g. toroidal coordinates
  $(R, Z) = ((R_0 + r)\cos(\theta), r\sin(\theta))$



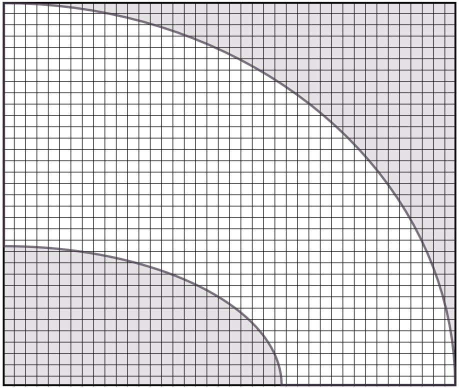
How to Generate a Grid?

- Analytically, e.g. toroidal coordinates $(R, Z) = ((R_0 + r)\cos(\theta), r\sin(\theta))$
- Numerically
  - Transfinite interpolation
  - Elliptic methods (EGG)
  - Spline-based EGG (IgA applications)



The Penalization Method

- Include the boundary in the simulation domain
- Add artificial "penalization" terms
- Transition layer



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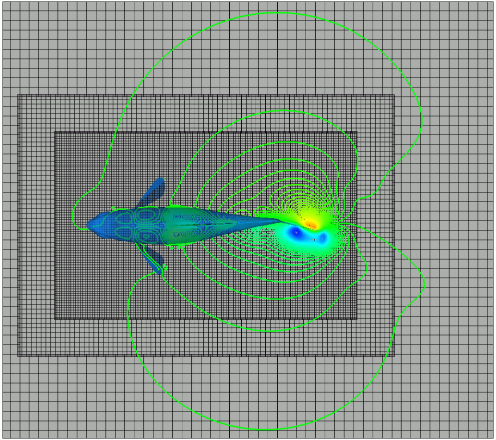

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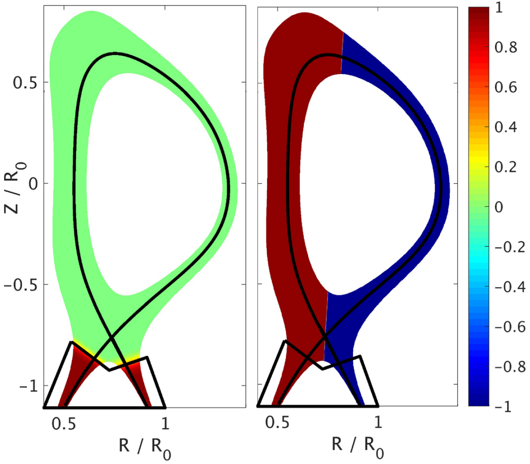

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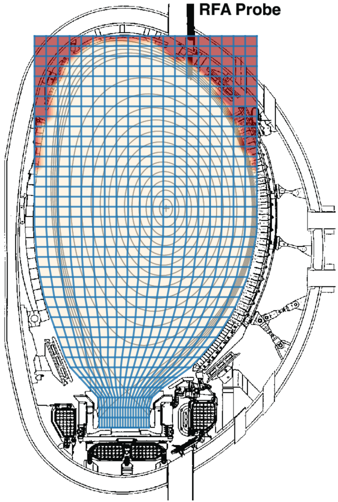


Progress Towards First Simulations

What needs to be changed in GBS?

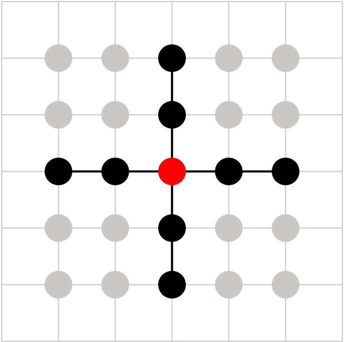
In particular, the FD stencils:

More

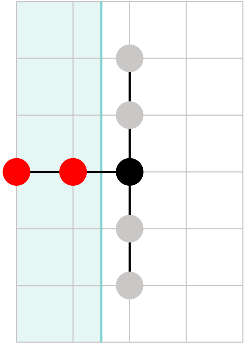
$$\nabla^2 f = g^{jk}\frac{\partial^2 f}{\partial\xi^j\partial\xi^k} - g^{ij}\Gamma^k_{ij}\frac{\partial f}{\partial\xi^k}$$

$$\frac{\partial f}{\partial\eta} = \sqrt{g_{22}}\left(\frac{\partial f}{\partial s} - \sqrt{g_{22}}g^{12}\frac{\partial f}{\partial\xi}\right)$$

$\nabla^2 f$

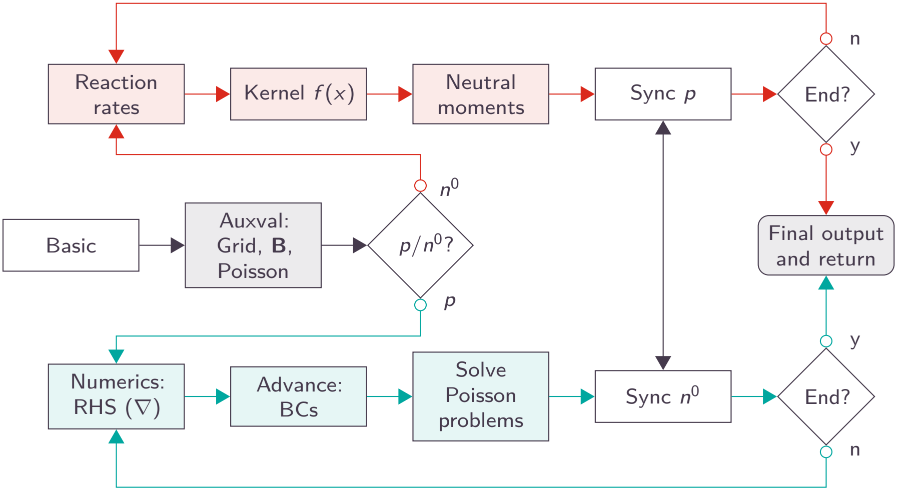


$\partial f/\partial s$

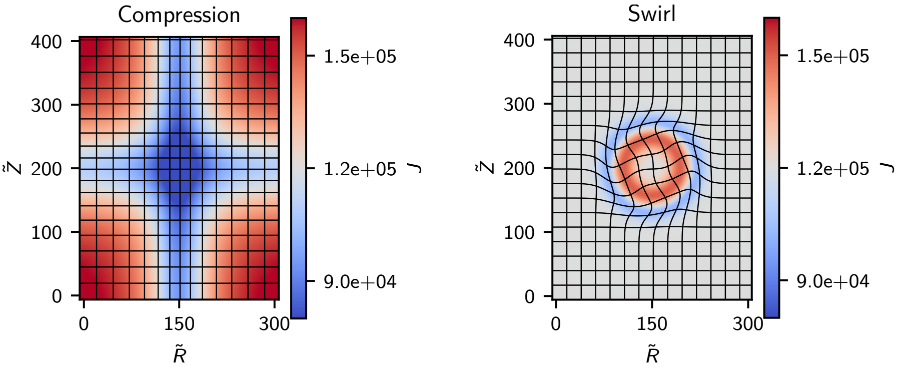


Where does the Code Change?

A Typical Run



Testing with GBS is Underway



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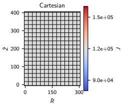

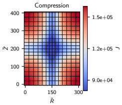

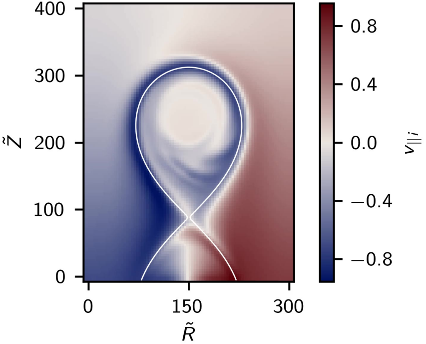

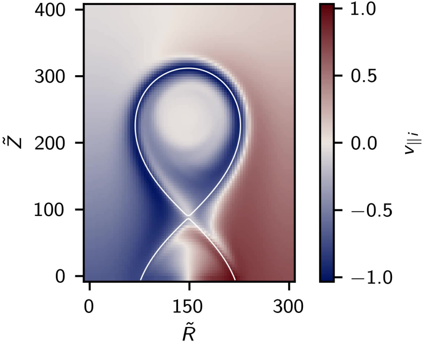

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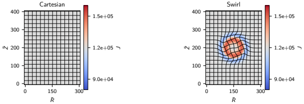
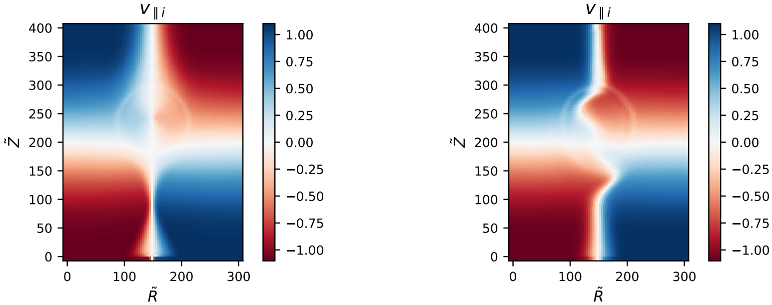


Current status: fixing initial and boundary conditions



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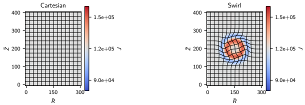

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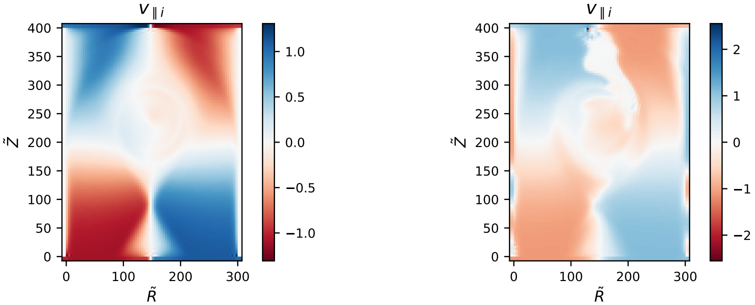

Outlook

Future Plan

- Timeline
  - Spring 2023: Working plasma module
  - Winter 2023: Working neutrals module
  - Mid 2024: Verified implementation, production
- Expected issues
  - Conflicting changes (additional staggering ▸ More, GPU porting, update of Poisson solvers, momentum-energy reformulation, merge of André's work on neutrals, refactoring)
  - Potential for numerical instabilities ▸ More

References I

- Bufferand, Hugo Georges et al. (2021). "Progress in Edge Plasma Turbulence Modelling Hierarchy of Models from 2D Transport Application to 3D Fluid Simulations in Realistic Tokamak Geometry". In: *Nuclear Fusion*. DOI: 10.1088/1741-4326/ac2873.
- Dekeyser, W. et al. (Apr. 9, 2021). "Plasma Edge Simulations Including Realistic Wall Geometry with SOLPS-ITER". In: *Nuclear Materials and Energy*, p. 100999. DOI: 10.1016/j.nme.2021.100999.
- Kuang, A. Q. et al. (Oct. 2020). "Divertor Heat Flux Challenge and Mitigation in SPARC". In: *Journal of Plasma Physics* 86.5. DOI: 10.1017/S002237782000117.
- Loizu, J. et al. (Dec. 1, 2012). "Boundary Conditions for Plasma Fluid Models at the Magnetic Presheath Entrance". In: *Physics of Plasmas* 19.12, p. 122307. DOI: 10.1063/1.4771573.

References II

- Reimerdes, H. et al. (Jan. 2021). "Initial TCV Operation with a Baffled Divertor". In: *Nuclear Fusion* 61.2, p. 024002. DOI: 10.1088/1741-4326/abd196.
- Stegmeir, A. et al. (May 1, 2019). "Global Turbulence Simulations of the Tokamak Edge Region with GRILLIX". In: *Physics of Plasmas* 26.5, p. 052517. DOI: 10.1063/1.5089864.

Finite Differences

and the Stencils

Go back

All references to "physical" space, all gradients (including Poisson and Ampère) solvers,

$$\frac{\partial f}{\partial x} = \frac{\partial \xi^i}{\partial x}\frac{\partial f}{\partial \xi^i}$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial \xi^i}{\partial x}\frac{\partial \xi^j}{\partial x}\frac{\partial^2 f}{\partial \xi^i \partial \xi^j} + \frac{\partial^2 \xi^j}{\partial x^2}\frac{\partial f}{\partial \xi^j}$$

All (Neumann) boundary conditions. Let s the direction normal to the wall,

$$\frac{\partial f}{\partial s} = \frac{\partial \xi^i}{\partial s}\frac{\partial f}{\partial \xi^i}$$

Expand $\partial_s = \sqrt{g_{22}}\boldsymbol{\nabla}\eta \cdot \boldsymbol{\nabla}$,

$$\frac{\partial f}{\partial \eta} = \sqrt{g_{22}}\left(\frac{\partial f}{\partial s} - \sqrt{g_{22}}g^{12}\frac{\partial f}{\partial \xi}\right)$$

Another form of the Laplacian

$$\nabla^2 f = \frac{1}{J}\frac{\partial}{\partial \xi^j}\left(J g^{mj}\frac{\partial f}{\partial \xi^m}\right)$$

Metric tensors

$$g^{ij} = \frac{\partial \xi^i}{\partial x^k}\frac{\partial \xi^j}{\partial x^k}$$

$$g_{ij} = \frac{\partial x^k}{\partial \xi^i}\frac{\partial x^k}{\partial \xi^j}$$

$$\Gamma^k_{ij} = \frac{\partial^2 x^m}{\partial \xi^i \partial \xi^j}\frac{\partial \xi^k}{\partial x^m}$$

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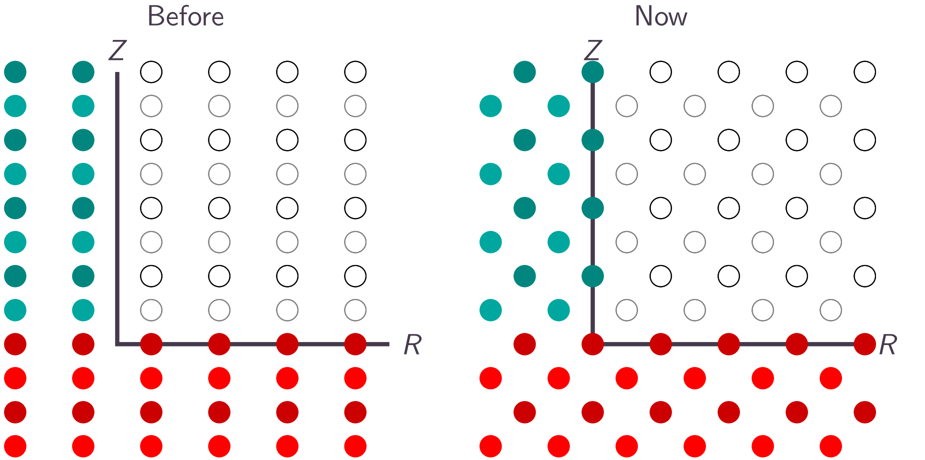
Additional Grid Staggering

Go back Velocity grid: Density grid:



Numerical Instabilities

Original Authors: Micol Bassini & Davide Mancini

Louis Stenger

Go back The RK4 method has a narrow *stability region* along the imaginary axis.

Original discretization of the parallel Laplacian $\nabla_{\parallel}^2 f = \mathbf{b}\cdot\nabla(\mathbf{b}\cdot\nabla f)$ has complex eigenvalues.

$$\begin{aligned}\nabla_{\parallel}^2 f = &\left(\partial_Z\Psi\partial^2_{RZ}\Psi - \partial_R\Psi\partial^2_{ZZ}\Psi\right)\partial_R f \\ &+\left(\partial_R\Psi\partial^2_{RZ}\Psi - \partial_Z\Psi\partial^2_{RR}\Psi\right)\partial_Z f + \Big[\\ &\quad (\partial_Z\Psi)^2\,\partial^2_{RR}f + (\partial_R\Psi)^2\,\partial^2_{ZZ}f \\ &\quad -2\partial_R\Psi\partial_Z\Psi\partial^2_{RZ}f \\ &\Big] + 2\partial_Z\Psi\partial^2_{R\varphi}f - 2\partial_R\Psi\partial^2_{Z\varphi}f + \partial^2_{\varphi\varphi}f \\ &+\mathcal{O}(\epsilon,\delta)\end{aligned}$$

Instead, prefer the following formulation,

$$\nabla_{\parallel}^2 f = \nabla\cdot(\mathbf{bb}\nabla f),$$

implemented at second order accuracy. Discretized operator is hermitian, therefore *real* eigenvalues.