

# Wall Geometry & Curvilinear Grids in GBS

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TSVV3 Annual Meeting

GBS and Wall Geometry

Dealing with Realistic Wall Geometry

Synthetic Test Case

Baffled TCV-like Case

- Quasi-neutrality
- Ordering of turbulence  $\tau \ll \Omega_{ci}^{-1}, \rho_s \ll L_{\perp}$
- Large aspect ratio
- Strong toroidal, axisymmetric magnetic field

$$\frac{\partial n}{\partial t} = \left[ -\frac{\rho_*^{-1}}{B} \{\phi, n\} + \frac{2}{B} [C(p_e) - nC(\phi)] \right] - \nabla_{\parallel} (n v_{\parallel e})$$

$$+ D_n \nabla_{\perp}^2 n \quad + S_n \quad + v_{iz} n_n - n_i v_{rec}$$

- Mono-atomic species,
- Short and long neutral mean free paths considered,
- Physical processes: ionization, charge exchange, recombination, recycling, reflection

At each timestep, need to compute and invert the “kernel matrix”,

$$\begin{bmatrix} n_n \\ \Gamma_{\text{out},n} \end{bmatrix} = \begin{bmatrix} v_{\text{cx}} K_{p \rightarrow p} & (1 - \alpha_{\text{refl}}) K_{b \rightarrow p} \\ v_{\text{cx}} K_{p \rightarrow b} & (1 - \alpha_{\text{refl}}) K_{b \rightarrow b} \end{bmatrix} \begin{bmatrix} n_n \\ \Gamma_{\text{out},n} \end{bmatrix} + \begin{bmatrix} n_{n[\text{rec}]} + n_{n[\text{out},i]} \\ \Gamma_{\text{out},n[\text{rec}]} + \Gamma_{\text{out},n[\text{out},i]} \end{bmatrix}$$

$n_n$ : neutral density,  $\Gamma_{\text{out}}$ : outflowing neutral flux,  $\alpha_{\text{refl}}$ : reflection coefficient,  $p$ : plasma,  $b$ : boundary,  $\text{cx}$ : charge exchange,  $\text{rec}$ : recombination,  $i$ : ionization

- Each element composed of direct and reflected paths, e.g.

$$K_{p \rightarrow p} = K_{p \rightarrow p}^{\text{dir}} + \alpha_{\text{refl}} K_{p \rightarrow p}^{\text{refl}}$$

- For each path, compute a path integral, e.g.

$$K_{p \rightarrow p}^{\text{dir}}(\mathbf{x}, \mathbf{x}') = \int_0^{+\infty} \frac{1}{r_{\perp}} \Phi_{\perp i}(\mathbf{v}_{\perp}) \exp\left[-\frac{1}{v_{\perp}} \int_0^{r_{\perp}} v_{\text{eff}}(\mathbf{x}'') dr''_{\perp}\right] dv_{\perp}.$$

Plasma:

- GBS evolves
  - 6 fields explicitly in time  $n, v_{\parallel e}, v_{\parallel i}, T_e, T_i, \omega$
  - 2 potentials  $\phi$  (electrostatic),  $\psi$  (electromagnetic)
- 4<sup>th</sup> order spatial finite differences
- Dual  $\varphi, Z$ -staggered Cartesian grid
- Runge-Kutta 4<sup>th</sup> order in time

Neutrals:

- Low-resolution Cartesian grid,
- Dense matrix inversion

Matrix systems solved with PETSc (GMRES).

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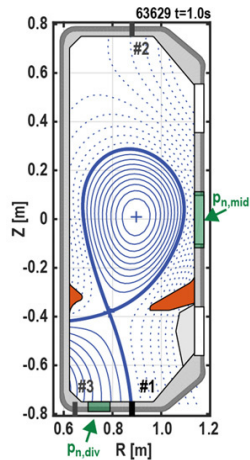
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# Wall Geometry Matters

## Especially for Neutrals

- Baffled TCV discharges with increased neutral pressure (Reimerdes et al. 2021),
- SPARC's super-X "tunnel" divertor (Kuang et al. 2020),
- TCV future tightly baffled divertor (Sun et al. 2023),

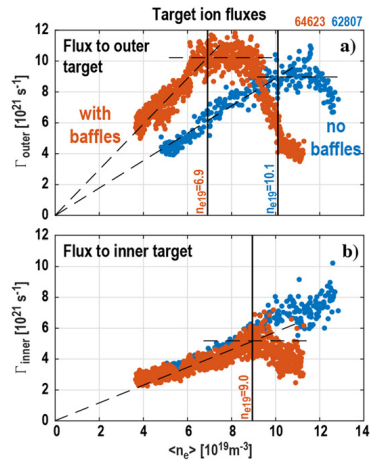




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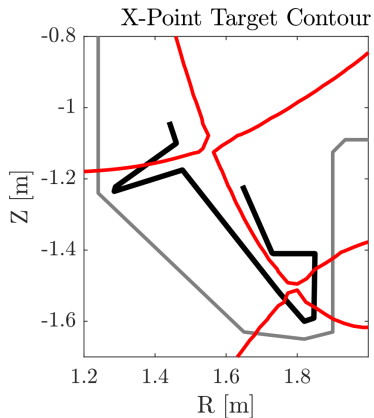
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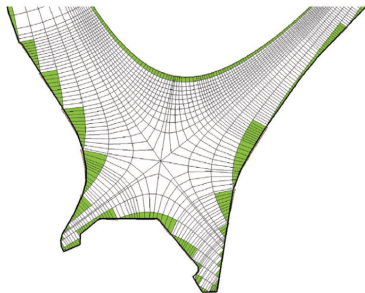
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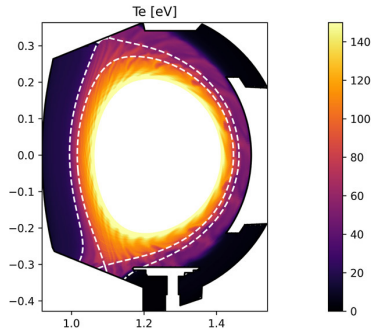
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- Simulation tools
  - SOLPS-ITER (Dekeyser et al. 2021)
  - BOUT++ (Dudson et al. 2021)
  - SOLEDGE3X-HDG (Bufferand et al. 2021)
  - SOLEDGE, GRILLIX (penalization) (Body et al. 2020)
  - FELTOR (FV-FCI) (Wiesenberger et al. 2017)



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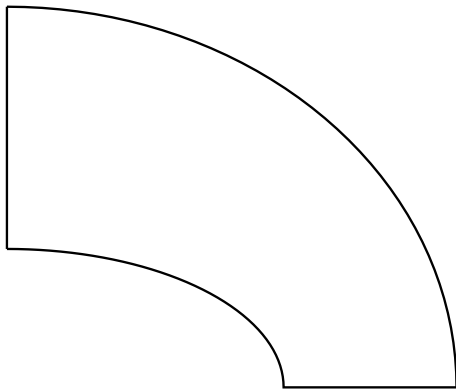
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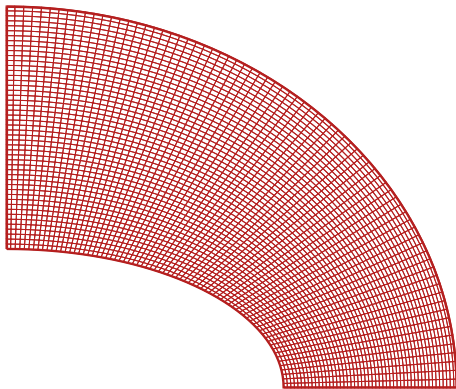
# Techniques to Include Wall Geometry Exist

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



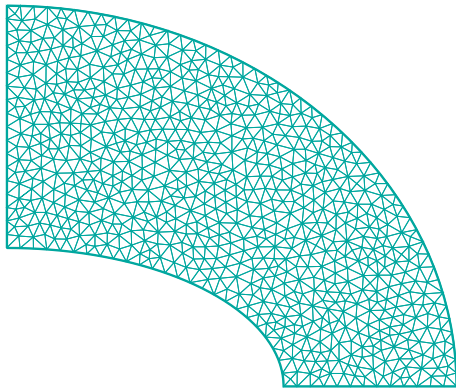
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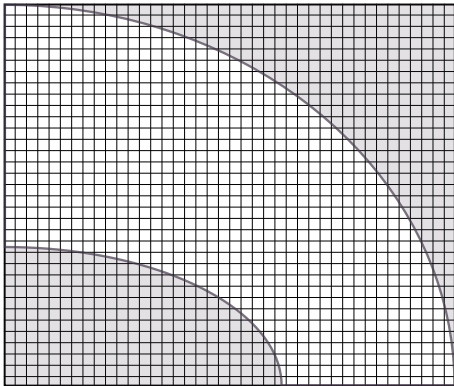


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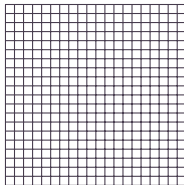
Consider “boundary-fitted” grids

- Coordinate transformation:  
Computational variables  $\{\xi^i\}_i \rightarrow (R, \varphi, Z)$

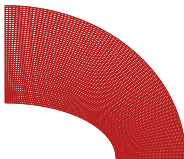
$$\frac{\partial n}{\partial R} = \frac{\partial \xi^i}{\partial R} \frac{\partial n}{\partial \xi^i}$$

- GBS is axisymmetric, transform only a single poloidal plane  $\xi^3 = \varphi$
- Retain finite difference convergence
- (Almost) No refactoring needed. User perspective: one new optional input to provide.

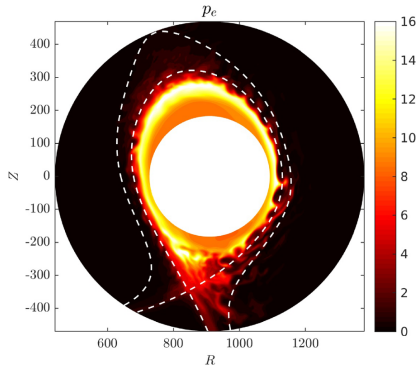
*Logical grid:*



*Physical grid:*

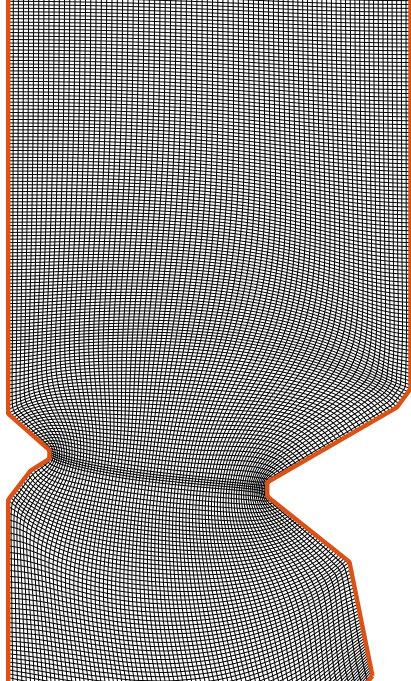


- Analytically, e.g. toroidal coordinates  
 $(R, Z) = ((R_0 + r) \cos(\theta), r \sin(\theta))$



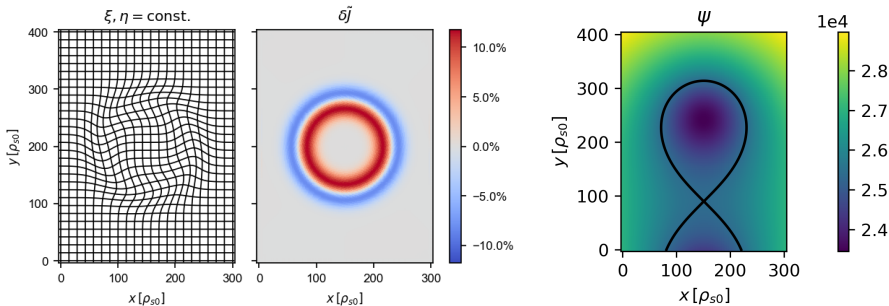
# How to Generate a Grid?

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

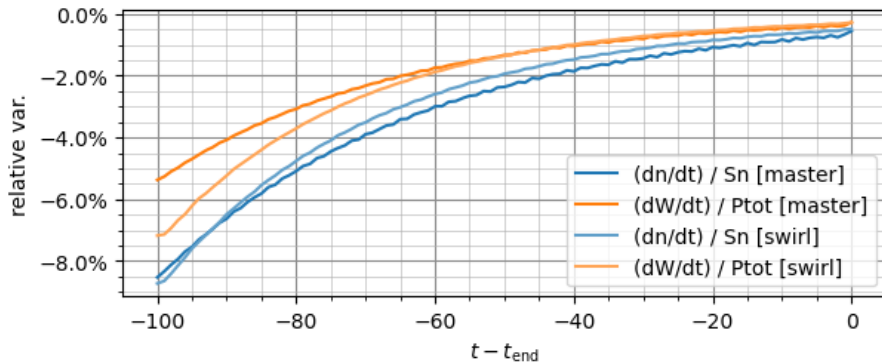


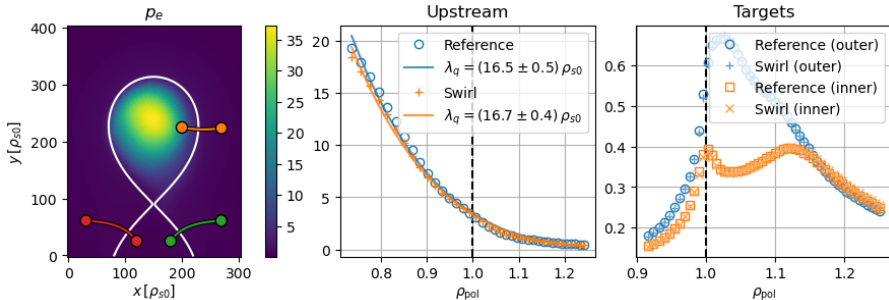
# A “Swirl” Case to Test the Inner Domain

Analytical definition. Keep the boundary conditions free from side effects. Activate all metric elements. Direct comparison to main version.

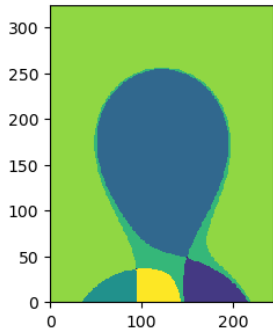
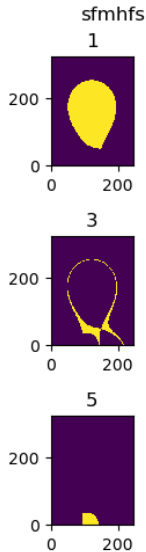


## Comparison of Rectilinear and Curvilinear Cases





- Orthogonal coordinates useful to split B-aligned and cross-field transport.
- $\mathbf{B} = B_\varphi \mathbf{e}_\varphi + \nabla\varphi \times \nabla\psi$
- Flux surfaces:  $\psi$ -isolines
- Orthogonal coordinate “ $\chi$ ”

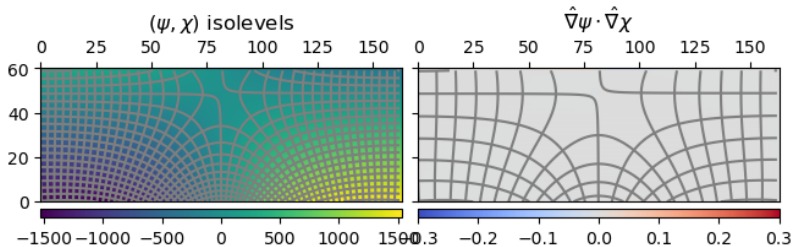


# Finding $\chi$ given $\psi$

The simplest system,  $\nabla\chi = \nabla\psi^T$  is overdetermined,

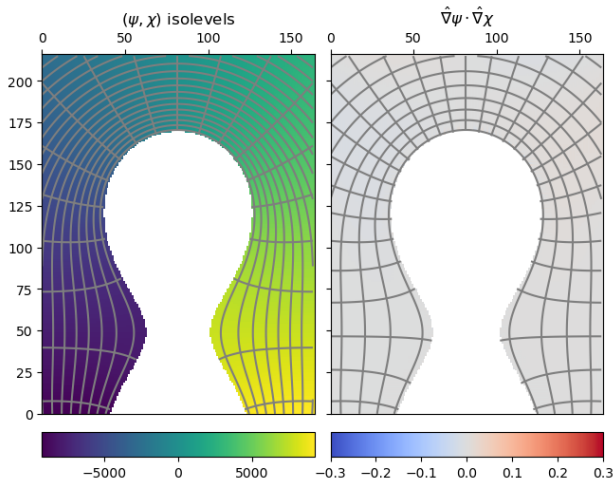
$$\mathbf{Ax} = \begin{bmatrix} D_x \\ D_y \end{bmatrix}_{2n \times n} [\chi]_n = \begin{bmatrix} D_y \\ -D_x \end{bmatrix}_{2n \times n} [\psi]_n = \mathbf{b}$$

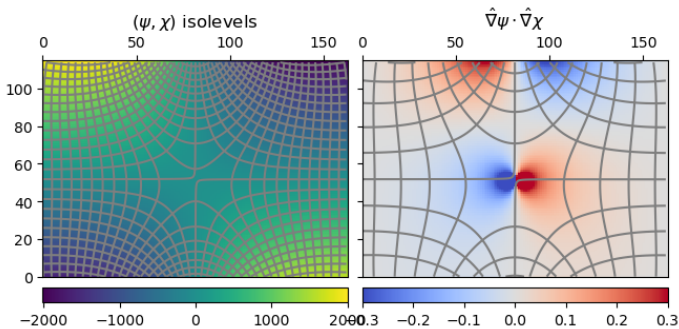
but a LSQR solver (minimize  $\|\mathbf{Ax} - \mathbf{b}\|$ ) converges





... also works for “sparse” domains ...





Why did it work so far? We have been solving the Cauchy-Riemann equations. If a solution exists, also imply  $\Delta\psi = \Delta\chi = 0$  and a corresponding conformal map is defined  $f = \psi + i\chi$ . But in our case,  $\nabla \times \mathbf{B}_{\text{pol}} = \Delta\psi = J \neq 0$ .

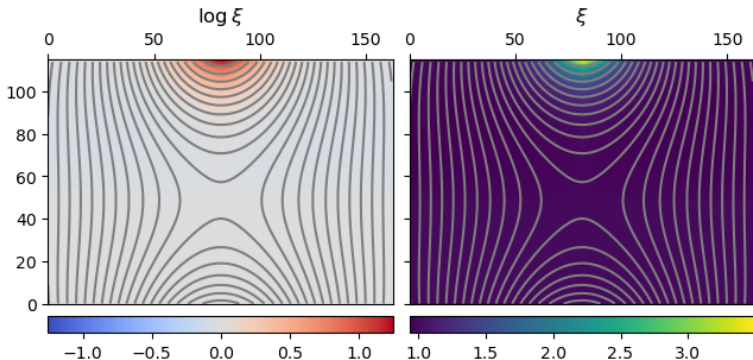
# Let's assume $\psi$ can be rescaled

Let  $\psi_h = h(\psi)\psi$ ,

$$\nabla\psi_h = (h + h'\psi)\nabla\psi = \xi\nabla\psi,$$

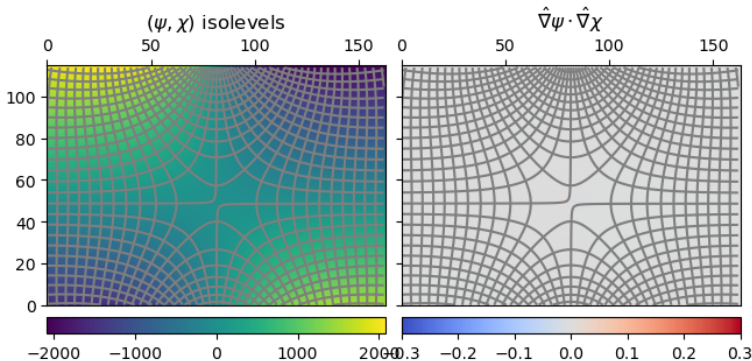
require  $\xi > 0$ . Require also  $\Delta\psi_h = 0 = \xi\Delta\psi + (\nabla\psi \cdot \nabla)\xi$ . Solve

$$(\nabla\psi \cdot \nabla)\log\xi = -\Delta\psi$$

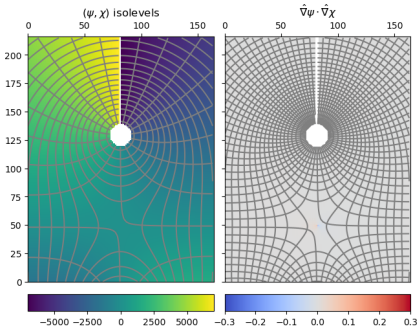


# Solve for $\chi$ using the rescaled $\psi$

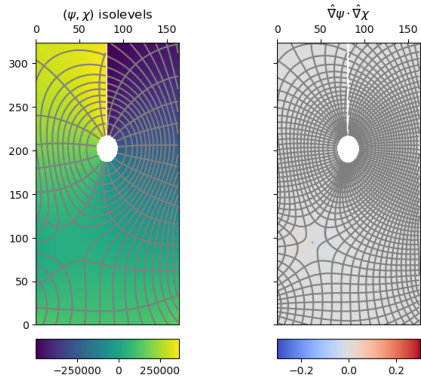
We're solving the over-determined system again, this time with  $\psi_h$  in place of  $\psi$ ,  $\nabla\chi = \nabla\psi_h^T$ .

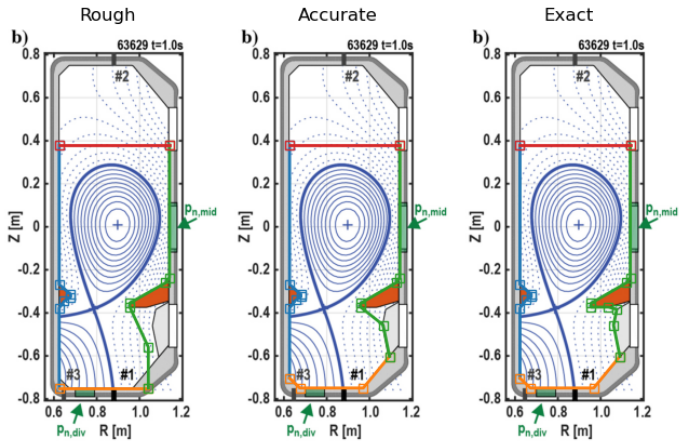


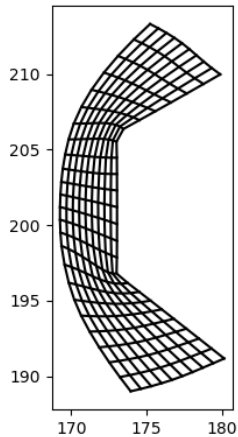
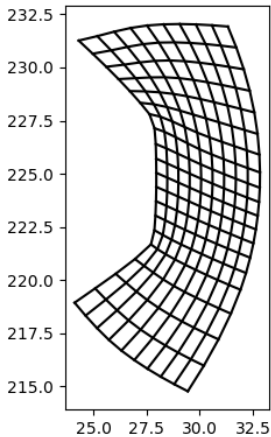
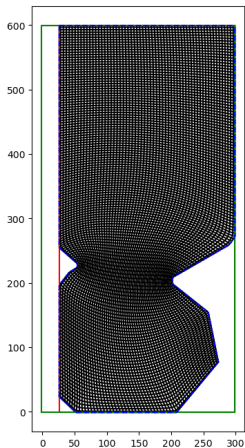
# Naive approach works outside closed field line regions

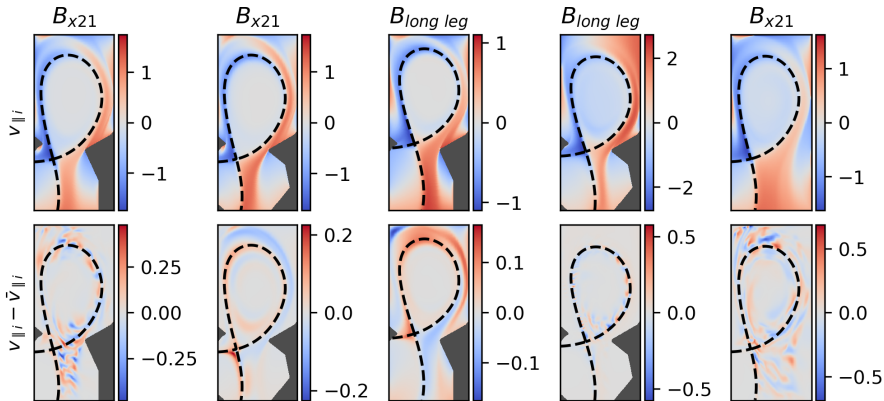


Actually “fixes” X21 defects



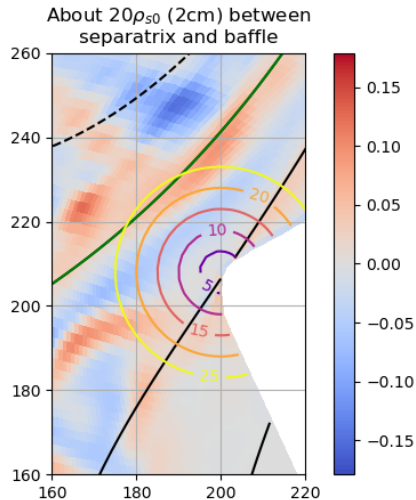








- Needs additional runtime before convergence
- Qualitative differences observed
  - Baffles enhance SOL parallel flows: very close to plasma (reduced domain, low-res  $\frac{1}{3}$ <sup>rd</sup> TCV)
  - Electrostatic potential (not shown): Stronger gradients due to baffle proximity, BC  $\phi = \lambda T_e$



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Updated from last year

- Run with a more realistic, larger, baffled TCV grid
- Refactor, cleanup, and merge back into currently developed GBS version
- Adapt the computation of neutrals

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# What Needs to be Done for the Neutrals?

For the inner domain, modifications *look* simple. The computation as it is done now,

1. Plasma fields are interpolated on the neutral grid
2. Point-to-point paths are constructed in  $R, \varphi, Z$  coordinates
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The hard part: Reflections, and in general, any computation involving wall's orientation.



-  **Body, Thomas et al. (2020).** “Treatment of Advanced Divertor Configurations in the Flux-Coordinate Independent Turbulence Code GRILLIX.” In: *Contributions to Plasma Physics 60.5-6*, e201900139. DOI: [10.1002/ctpp.201900139](https://doi.org/10.1002/ctpp.201900139).
-  **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](https://doi.org/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](https://doi.org/10.1016/j.nme.2021.100999).
-  **Dudson, Ben et al. (Aug. 6, 2021).** *BOUT++ v4.4.0*. Zenodo. DOI: [10.5281/zenodo.5167527](https://doi.org/10.5281/zenodo.5167527).

-  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/S0022377820001117](https://doi.org/10.1017/S0022377820001117).
-  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](https://doi.org/10.1088/1741-4326/abd196).
-  Sun, G. et al. (Apr. 20, 2023). *Performance Assessment of a Tightly Baffled, Long-Legged Divertor Configuration in TCV with SOLPS-ITER*. DOI: [10.48550/arXiv.2303.09195](https://doi.org/10.48550/arXiv.2303.09195). arXiv: [2303.09195](https://arxiv.org/abs/2303.09195) [physics]. preprint.
-  Wiesenberger, M., M. Held, and L. Einkemmer (July 2017). “Streamline Integration as a Method for Two-Dimensional Elliptic Grid Generation.” In: *Journal of Computational Physics* 340, pp. 435–450. DOI: [10.1016/j.jcp.2017.03.056](https://doi.org/10.1016/j.jcp.2017.03.056).