TSVV3 status meeting, M. Wiesenberger, 21.9.22

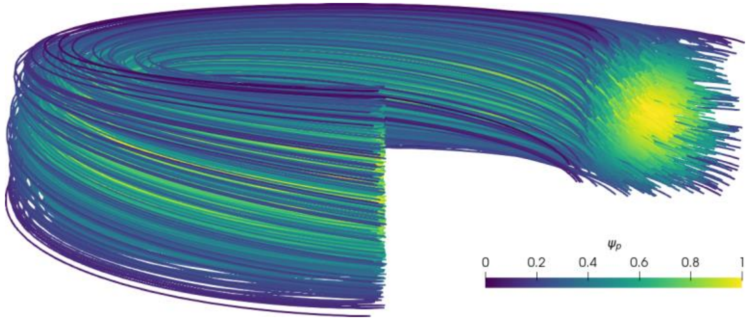
A finite volume FCI scheme

Outlook

1. Advantages and downsides of existing schemes
2. Finite volume **schemes in 1D**
3. The **FCI scheme** as a locally fieldaligned finite difference scheme
4. Putting it all together: **finite volume flux coordinate independent scheme** FVFCI – numerical tests
5. Conclusions and future work

To be published:
M. Wiesenberger and M. Held, A finite volume FCI scheme, Journal (2022)

Discretize Navier stokes along given magnetic field



$$\frac{\partial}{\partial t}n + \boldsymbol{\nabla} \cdot \left(nu\hat{\boldsymbol{b}}\right) = 0$$

$$\frac{\partial}{\partial t}(nu) + \boldsymbol{\nabla} \cdot \left(nu^2\hat{\boldsymbol{b}}\right) = -\nabla_{||}n + \nu_u\Delta_{||}u$$

$$\nabla_{||}f := \hat{\boldsymbol{b}} \cdot \boldsymbol{\nabla} f$$

$$\Delta_{||}u := \nabla \cdot (\hat{\boldsymbol{b}}\hat{\boldsymbol{b}} \cdot \nabla u)$$

Subset of both 3d drift- and gyro-fluid models if we **throw away all drifts and electro-magnetic fields** and only take ions

Features: **advection, Burger's term** (makes shocks)**, pressure gradient** and **parallel diffusion**

D. Michels, et al,, Comput. Phys. Commun. 264 (2021) 107986.
F. Hariri, et al, Plasma Phys. Control. Fusion 57 (5) (2015) 054001.
A. Stegmeir, et al, Plasma Phys. Control. Fusion 60 (3) (2018) 035005

Existing FCI schemes

Advantages (over non-aligned schemes)

+ Accurately **capture thin and fieldaligned character** of turbulence with **low numerical diffusion**
+ Enables simulations of medium to large scale tokamaks (without FCI **saving scales with R_0^3**, A. Stegmeir, T. Body and W. Zholobenko, submitted to CPC, 2022)

Downsides

- **Boundary conditions** remain a challenge (also in this work)
- **Finite differences** not well suited for advection equations. Better schemes available in **literature on advection schemes** in 1d (shock-capturing, stability, conservative properties)
- Sometimes Feltor **simulations crash** seemingly for no reason

Goal in this work

Combine FCI with 1d finite volume schemes

Existing literature for 1d advection equations

Godunov type schemes

+ conservative, shock capturing finite volume
- **Very unflexible** Riemann problem specific to set of equation needs to be solved to implement
- Diffusion term awkward to add

R. LeVeque, Finite Volume Methods for Hyperbolic Problems, 2002.

Staggered finite volume scheme

grid for velocity/momentum is shifted by ½

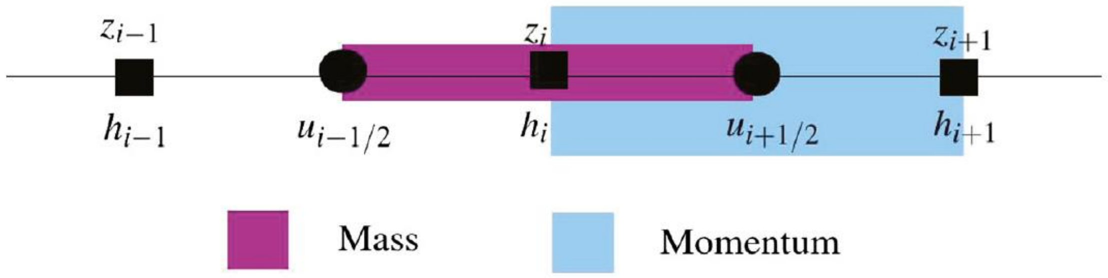
+ Flexible and easy to implement
- interpolation error when swapping from grid to staggered and back

R. Herbin, et al, ESAIM: M2AN 52 (3) (2018) 893–944.

Discontinuous Galerkin

+ high order, no need to stagger, shock-capturing
- high order may be overkill for a low resolution scheme
- Slope limiters hard to combine with non Osher type time integrators

J. S. Hesthaven and T. Warburton, Nodal Discontinuous Galerkin Methods 2008



Staggered finite volume in 1d

P. Gunawan, et al, Comput Geosci 19 (2015) 1197–1206.

Straight magnetic field

$$\frac{\partial}{\partial t} n = -\frac{\partial}{\partial x}(nu)$$

$$\frac{\partial}{\partial t} nu = -\frac{\partial}{\partial x}\left(nu^2 + n\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}t} n_k = -\frac{1}{\Delta x}(\hat{q}_{k+1/2} - \hat{q}_{k-1/2})$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(nu)_{k+1/2} = -\frac{1}{\Delta x}\left(\hat{f}_{k+1} - \hat{f}_k\right) - \frac{1}{\Delta x}[n_{k+1} - n_k]$$

$$\hat{q}_{k+1/2} := u_{k+1/2} \begin{cases} n_k + \frac{1}{2}\Lambda(\Delta n_{k+1/2}, \Delta n_{k-1/2}) & \text{if } u_{k+1/2} \geq 0 \\ n_{k+1} - \frac{1}{2}\Lambda(\Delta n_{k+3/2}, \Delta n_{k+1/2}) & \text{if } u_{k+1/2} < 0 \end{cases}$$

Fluxes are main ingredient in finite volume scheme

$$\hat{f}_k := q_k \begin{cases} u_{k-1/2} + \frac{1}{2}\Lambda(\Delta u_k, \Delta u_{k-1}) & \text{if } q_k \geq 0 \\ u_{k+1/2} - \frac{1}{2}\Lambda(\Delta u_{k+1}, \Delta u_k) & \text{if } q_k < 0 \end{cases}$$

Velocity staggered

$$\frac{\mathrm{d}}{\mathrm{d}t}n_k = -\frac{1}{\Delta x}(q_{k+1/2} - q_{k-1/2})$$

$$\frac{\mathrm{d}}{\mathrm{d}t}u_{k+1/2} = -\frac{1}{\Delta x}\left(\hat{f}_{k+1} - \hat{f}_k\right) - \frac{1}{\Delta x}\left[(n_{k+1} - n_k)\frac{1}{2}\left(\frac{1}{n_{k+1}} + \frac{1}{n_k}\right)\right] + \frac{\nu_u}{n_{k+1/2}(\Delta x)^2}(u_{k+3/2} - 2u_{k+1/2} + u_{k-1/2})$$

with

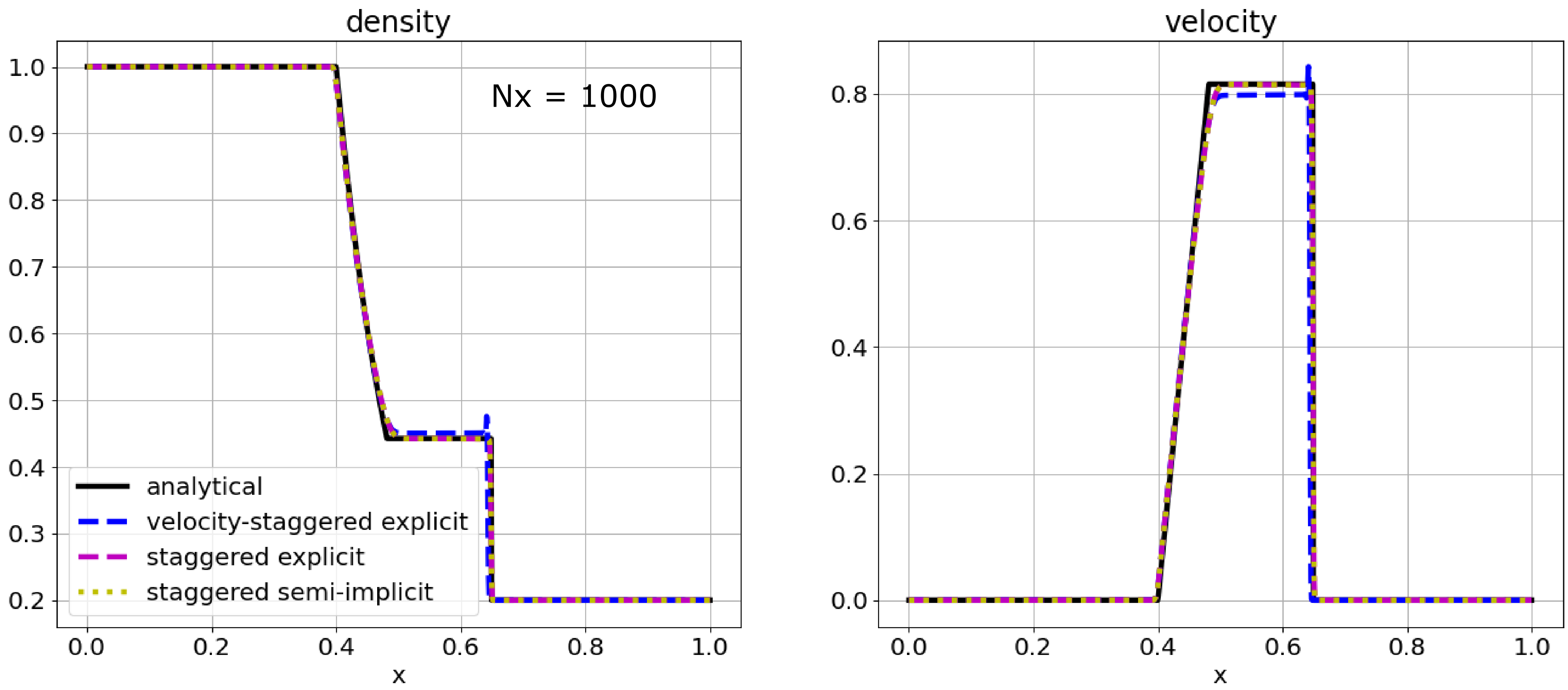
$$\hat{q}_{k+1/2} := u_{k+1/2}\begin{cases} n_k + \frac{1}{2}\Lambda(\Delta n_{k+1/2}, \Delta n_{k-1/2}) & \text{if } u_{k+1/2} \geq 0 \\ n_{k+1} - \frac{1}{2}\Lambda(\Delta n_{k+3/2}, \Delta n_{k+1/2}) & \text{if } u_{k+1/2} < 0 \end{cases}$$

$$\hat{f}_k := \frac{1}{2}u_k\begin{cases} u_{k-1/2} + \frac{1}{2}\Lambda(\Delta u_k, \Delta u_{k-1}) & \text{if } u_k \geq 0 \\ u_{k+1/2} - \frac{1}{2}\Lambda(\Delta u_{k+1}, \Delta u_k) & \text{if } u_k < 0 \end{cases}$$

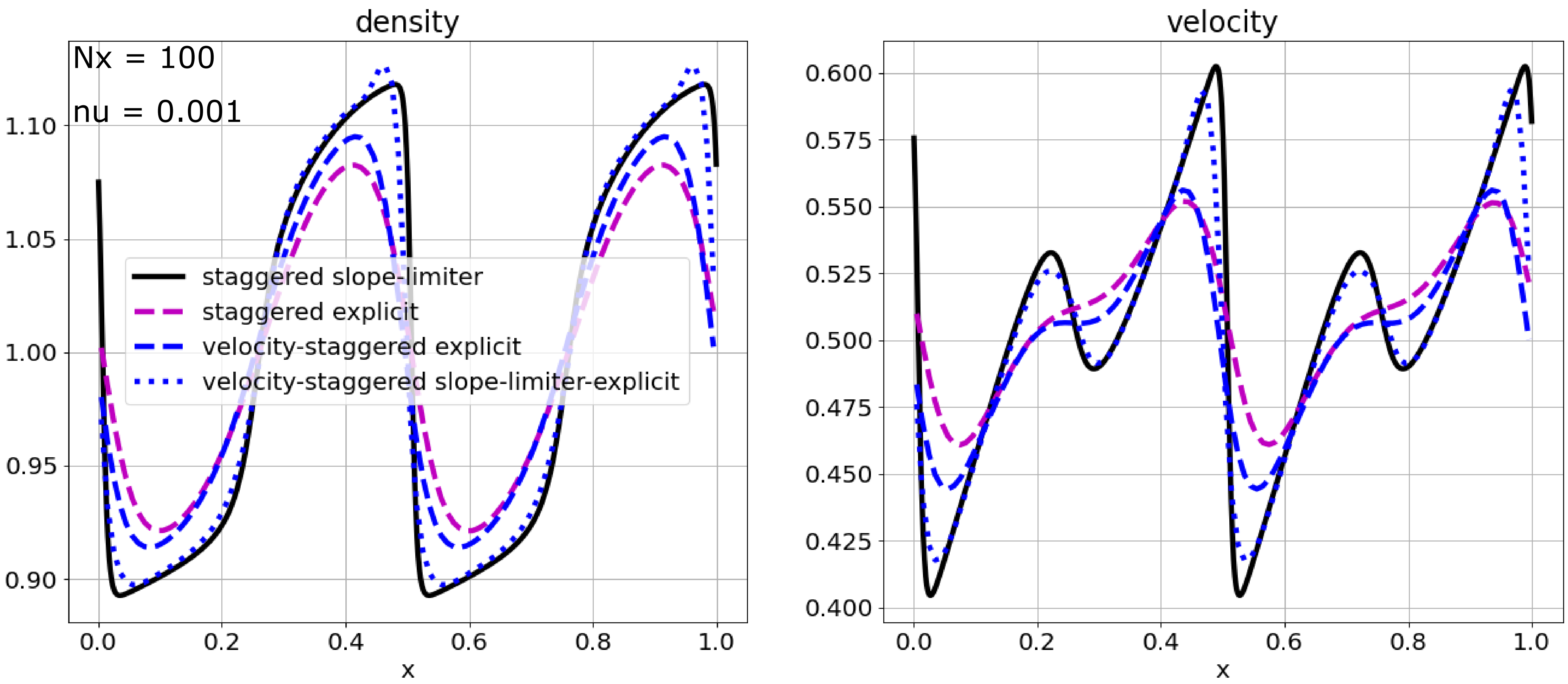
We could choose any scheme really …

Shock capturing

$$n_0(x) = \begin{cases} 1 \text{ if } x < 0.5 \\ 0.2 \text{ else} \end{cases} \qquad u_0(x) = 0$$



Advection schemes are diffusive (wave initial condition)



A fieldaligned coordinate system ρ, ζ, Φ

- Phi is fieldline label (we here choose Phi such that it **coincides with toroidal angle**) but other choices are possible
- Any **function can be pulled back** via

$$F(\rho,\zeta,\Phi) = f(R(\rho,\zeta,\Phi), Z(\rho,\zeta,\Phi), \varphi(\Phi))$$

- b only has **one non-zero component**

$$\nabla_{||} F(\rho,\zeta,\Phi) = b^\Phi \partial_\Phi F$$

$$\nabla \cdot (\hat{\boldsymbol{b}} F)(\rho,\zeta,\Phi) = \frac{1}{\sqrt{G}} \partial_\Phi \left(\sqrt{G} b^\Phi F \right)$$

$$\Delta_{||} F(\rho,\zeta,\Phi) = \frac{1}{\sqrt{G}} \partial_\Phi \left(\sqrt{G} b^\Phi b^\Phi \partial_\Phi F \right)$$

In ρ, ζ, Φ we can discretize using finite differences

$$\nabla_{\|}^{CC} F \rightarrow b_k^{\Phi} \frac{F_{k+1} - F_{k-1}}{2\Delta\Phi}$$

$$\nabla \cdot (\hat{\boldsymbol{b}} F)^{CC} \rightarrow \frac{\sqrt{G^{k+1}} b_{k+1}^{\Phi} F_{k+1} - \sqrt{G^{k-1}} b_{k-1}^{\Phi} F_{k-1}}{2\sqrt{G^k}\Delta\Phi}$$

$$\Delta_{\|}^{CC} F \rightarrow \frac{1}{\Delta\Phi^2}\left[\frac{\sqrt{G^{k+1/2}}}{\sqrt{G^k}} b_{k+1/2}^{\Phi} b_{k+1/2}^{\Phi}(F_{k+1} - F_k) - \frac{\sqrt{G^{k-1/2}}}{\sqrt{G^k}} b_{k-1/2}^{\Phi} b_{k-1/2}^{\Phi}(F_k - F_{k-1})\right]$$

Downsides

- Fieldlines do not close on themselves so **Phi boundary condition** “somewhat awkward”
- Fieldaligned coordinates **not possible with X-point**

Scott B., Phys. Plasmas 5, 2334 (1998)

FCI – only locally align

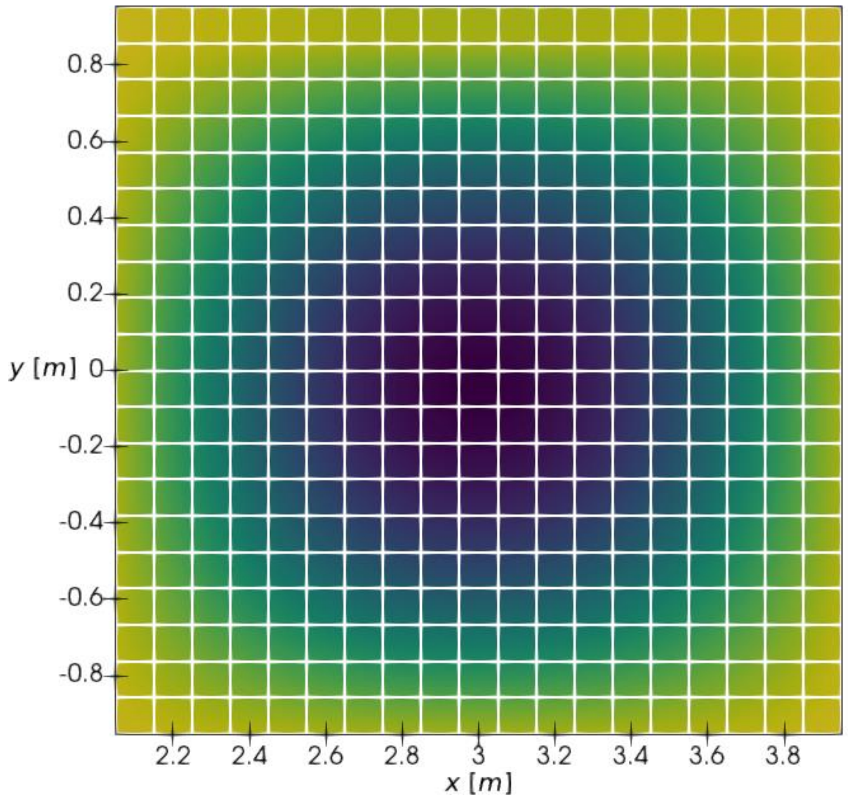
Two ingredients

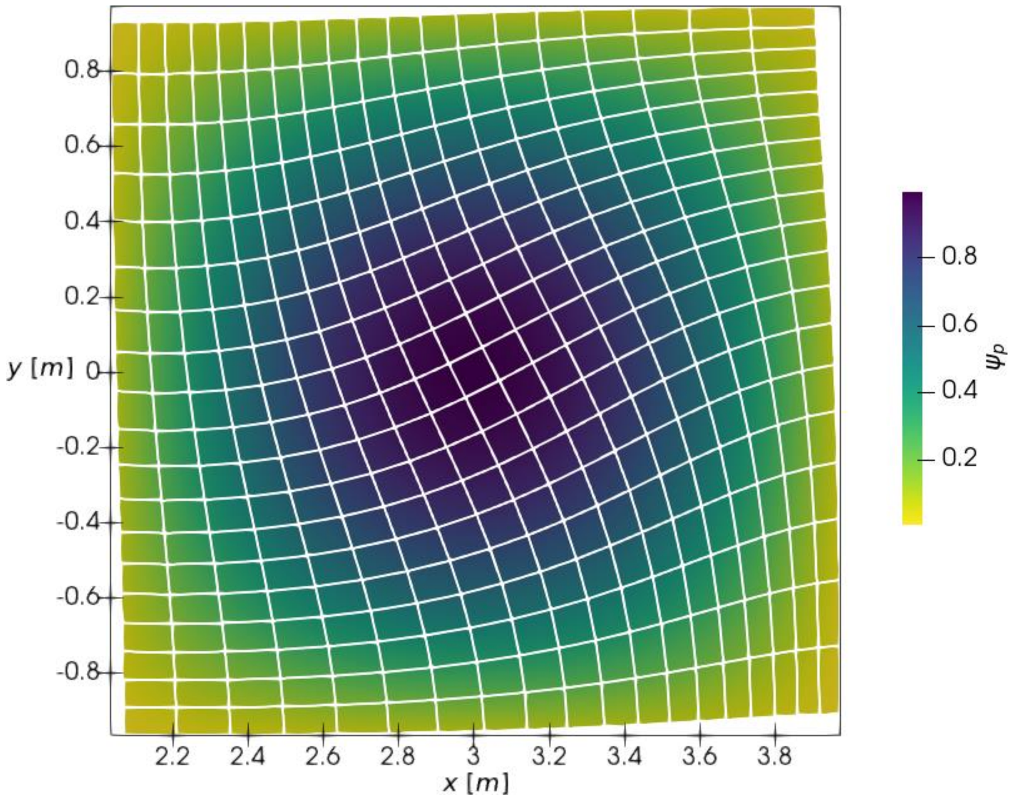
1. Atlas: construct **locally fieldaligned coordinate systems** at each toroidal plane. Each system originates at a toroidal plane.
2. Find **coordinate transformations** to pull back from cylindrical (non-aligned) to curvilinear (aligned) coordinate system

$$\begin{aligned} F_{k\pm1}(\rho,\zeta) :=& F(\rho,\zeta,\Phi_{k\pm1}) = f(R(\rho,\zeta,\Phi_{k\pm1}), Z(\rho,\zeta,\Phi_{k\pm1}), \varphi_{k\pm1}) \\ =:& (\mathcal{T}_{\pm\Delta\varphi} f_k)(\rho,\zeta) \end{aligned}$$

Fieldline (and volume) equations

$$\frac{\mathrm{d}R}{\mathrm{d}\varphi} = \frac{b^R}{b^\varphi},$$
$$\frac{\mathrm{d}Z}{\mathrm{d}\varphi} = \frac{b^Z}{b^\varphi},$$





$$\frac{\mathrm{d}\sqrt{G}}{\mathrm{d}\varphi} = \nabla \cdot \left(\frac{\hat{\boldsymbol{b}}}{b^\varphi}\right)\sqrt{G}$$

Volume must also be integrated for divergence

$$\nabla \cdot (\hat{\boldsymbol{b}}F)(\rho, \zeta, \Phi) = \frac{1}{\sqrt{G}}\partial_\Phi\left(\sqrt{G}b^\Phi F\right)$$

$$F(\rho, \zeta, \Phi_{k\pm1}) = f(R(\rho, \zeta, \Phi_{k\pm1}), Z(\rho, \zeta, \Phi_{k\pm1}), \varphi_{k\pm1})$$

Numerical coordinate transformation I
Simple interpolation (in 1d)

Discontinuous Galerkin expansion

$$f_h(x) = \sum_{n=1}^{N} \sum_{k=0}^{P-1} f_{nk} l^{nk}(x),$$

Any order

Finite Element expansion

$$f_h(x) = \sum_{n=1}^{N} f_n v^n(x)$$

Linear, cubic, ...

Insert coords

$$F_h(X^\pm) = F_{nk} l^{nk}(X^\pm) = f_h(x(X^\pm_{nk}))l^{nk}(X^\pm) = f_{mq} l^{mq}(x(X^\pm_{nk}))l^{nk}(X^\pm)$$

Define matrix

$$(I^\pm_{DG})_{nk}^{\ \ mq} := l^{mq}(x(X^\pm_{nk}))$$

$$(I^\pm_{FE})_n^{\ \ m} := v^m(x(X^\pm_n))$$

$$\boldsymbol{F}^\pm = I^\pm \boldsymbol{f}$$

$$\boldsymbol{F}^0 = \boldsymbol{f}$$

F. Hariri and M. Ottaviani, Comput. Phys. Commun., 184 (11) (2013) 2419–2429
A. Stegmeir, et al, Contrib. Plasma Phys. 54 (4-6) (2014) 549–554
M. Held, et al, Comput. Phys. Commun. 199 (2016) 29–39

Numerical coordinate transformation II
Projection (in 1d)

$$\bar{F}^{nk} := (S^{-1})^{ks} \int_{C_n} F_h(X^\pm) p_{ns}(X^\pm) \mathrm{d}X^\pm = (S^{-1})^{ks} \int_{C_n} f_h(x(X^\pm)) p_{ns}(X^\pm) \mathrm{d}X^\pm$$

"**Project onto base polynomial** in fieldaligned coordinate system (both dG and FE)"

Numerically integrate using K discretization points for each integral

$$\boldsymbol{F}^\pm = P_{DG} I^\pm_{DG,F} \boldsymbol{f}$$
$$\boldsymbol{F}^0 = P_{DG} Q_{DG} \boldsymbol{f} = \boldsymbol{f}$$

$$\boldsymbol{F}^\pm = S^{-1}_{FE} P_{FE} I^\pm_{FE,F} \boldsymbol{f}$$
$$\boldsymbol{F}^0 = S^{-1}_{FE} P_{FE} Q_{FE} \boldsymbol{f} = \boldsymbol{f}$$

We need to invert (tridiagonal) mass matrix

$$\boldsymbol{F}^\pm := P_{FE} I^\pm_{FE,F} \boldsymbol{f}$$
$$\boldsymbol{F}^0 := P_{FE} Q_{FE} \boldsymbol{f} = S_{FE} \boldsymbol{f}$$

A surprising alternative!!

S_FE is a **smoothing Kernel!**

A. Stegmeir, et al, Comput. Phys. Commun. 213 (2017) 111 – 121

N	N_φ	$\nabla_\parallel^{CC}$ Eq. (21c) error	order	$\nabla \cdot (\hat{\mathbf{b}} f)^{CC}$ Eq. (21f) error	order	$\Delta_\parallel^{CC}$ Eq. (22) error	order	$\int dV \nabla \cdot (\hat{\mathbf{b}} f)^{CC}$ error	order	$\int dV \Delta_\parallel^{CC} f$ error	order
10	**5**	8.01e-01	n/a	8.07e-01	n/a	4.95e-01	n/a	3.03e-07	n/a	8.86e-08	n/a
16	**10**	2.74e-01	1.55	2.79e-01	1.53	1.56e-01	1.67	5.10e-09	5.89	-4.57e-09	4.28
26	**20**	7.45e-02	1.88	7.59e-02	1.88	4.15e-02	1.91	-5.00e-10	3.35	1.48e-09	1.62
40	**40**	1.90e-02	1.97	1.94e-02	1.97	1.05e-02	1.98	-3.26e-10	0.62	-7.57e-10	0.97
64	**80**	4.78e-03	1.99	4.88e-03	1.99	2.64e-03	1.99	2.49e-09	-2.94	8.40e-10	-0.15

Table 2: Convergence Table for $K = 12$ and $N_R = N_Z = N$, using the dG interpolation Eq. (26).

N	N_φ	$\nabla_\parallel^{CC}$ Eq. (21c) error	order	$\nabla \cdot (\hat{\mathbf{b}} f)^{CC}$ Eq. (21f) error	order	$\Delta_\parallel^{CC}$ Eq. (22) error	order	$\int dV \nabla \cdot (\hat{\mathbf{b}} f)^{CC}$ error	order	$\int dV \Delta_\parallel^{CC} f$ error	order
8	**5**	8.01e-01	n/a	8.07e-01	n/a	4.96e-01	n/a	2.03e-05	n/a	-1.16e-05	n/a
15	**10**	2.74e-01	1.55	2.79e-01	1.53	1.56e-01	1.67	1.15e-06	4.14	-5.74e-07	4.34
30	**20**	7.45e-02	1.88	7.60e-02	1.88	4.15e-02	1.91	-3.99e-08	4.85	1.55e-06	-1.43
60	**40**	1.90e-02	1.97	1.94e-02	1.97	1.05e-02	1.98	1.99e-08	1.00	-1.76e-06	-0.19
120	**80**	4.78e-03	1.99	4.88e-03	1.99	2.65e-03	1.99	-3.57e-09	2.48	1.24e-06	0.50

Table 3: Convergence Table for $K = 12$, $N_R = N_Z = N$ and finite element projection method Eq. (50) .

A finite Volume flux coordinate Independent approach

Formulate 1d FV scheme in aligned coordinates

$$\frac{\mathrm{d}}{\mathrm{d}t} n_k = -\frac{\sqrt{\bar{G}^{k+1/2}}\bar{b}^{\varphi}_{k+1/2}\bar{q}_{k+1/2} - \sqrt{\bar{G}^{k-1/2}}\bar{b}^{\varphi}_{k-1/2}\bar{q}_{k-1/2}}{\Delta\varphi\sqrt{\bar{G}^k}}$$

Value centred

Origin at non-staggered plane

$$\bar{q}_{k+1/2} := \bar{u}_{k+1/2}\begin{cases}\bar{n}_k + \frac{1}{2}\Lambda(\Delta\bar{n}_{k+1}, \Delta\bar{n}_k) & \text{if } \bar{u}_{k+1/2} \geq 0\\ \bar{n}_{k+1} - \frac{1}{2}\Lambda(\Delta\bar{n}_{k+2}, \Delta\bar{n}_{k+1}) & \text{if } \bar{u}_{k+1/2} < 0\end{cases}$$

Flux centred

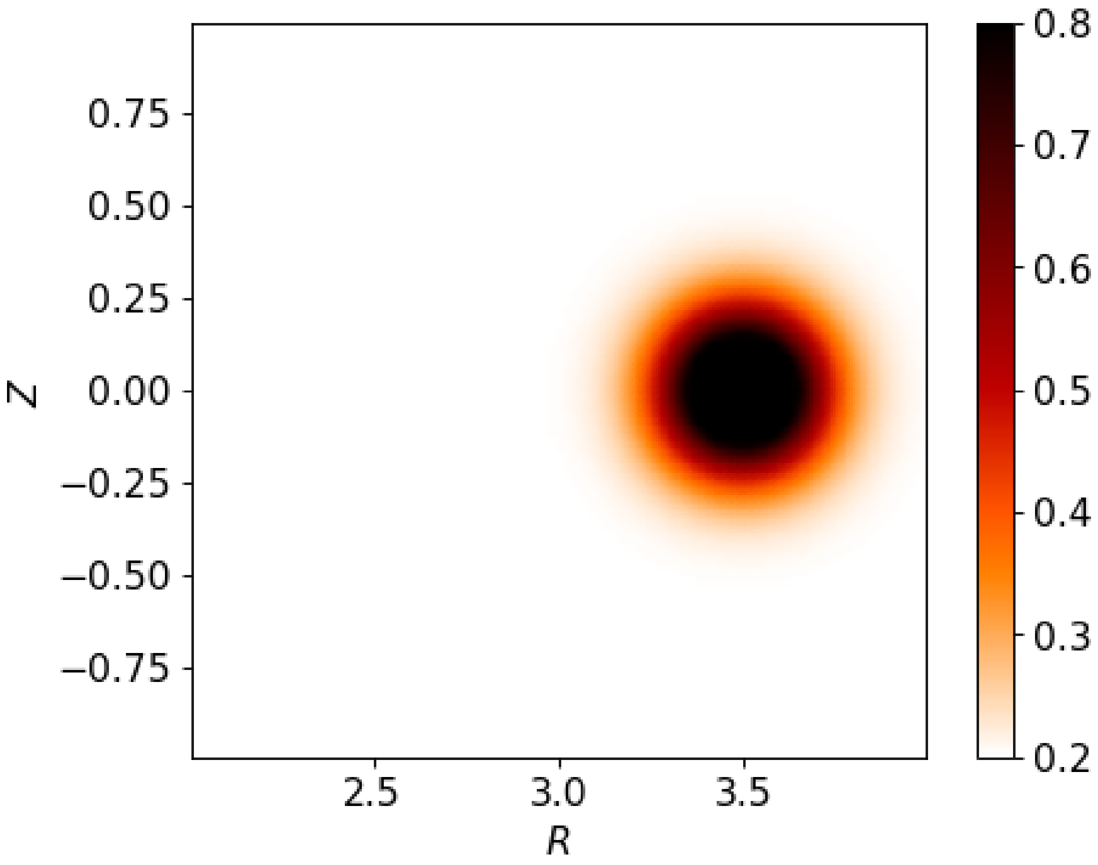
Origin at staggered plane

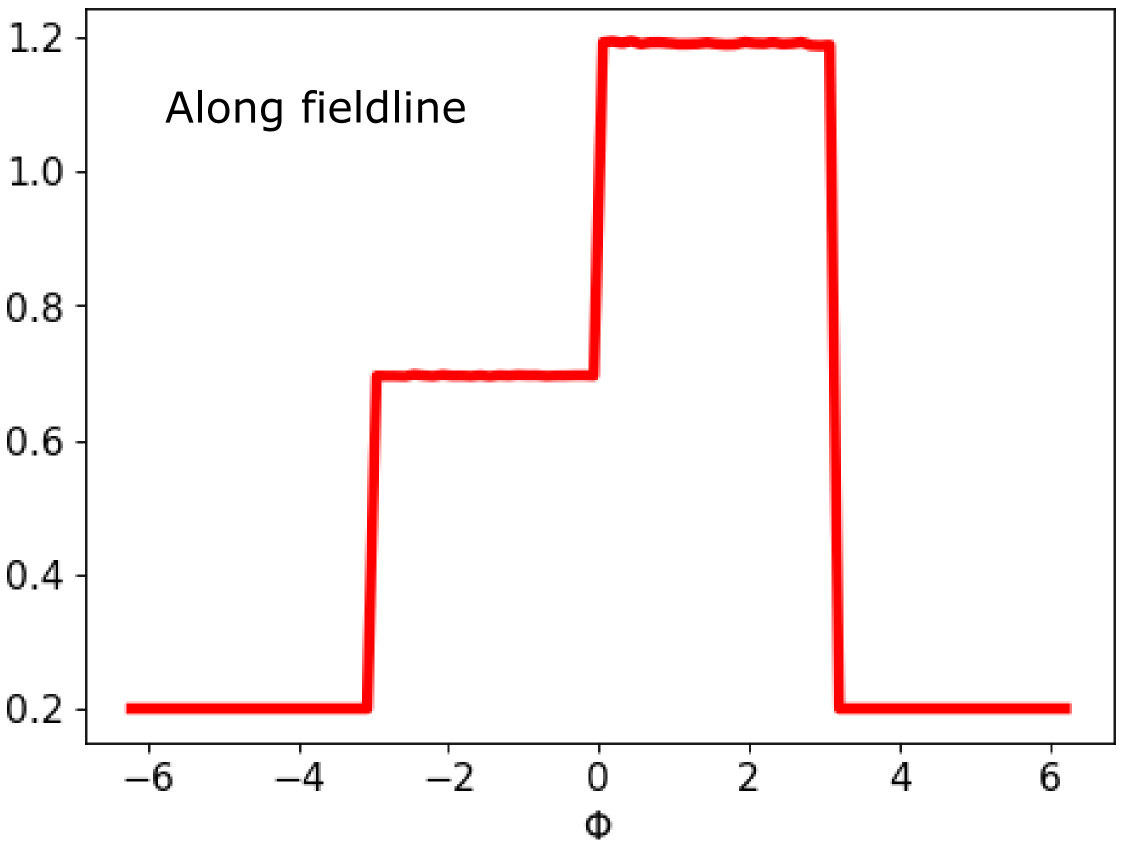
$$\bar{\bar{q}}_{k+1/2} := \bar{\bar{u}}_{k+1/2}\begin{cases}\bar{\bar{n}}_k + \frac{1}{2}\Lambda\left(\Delta\bar{\bar{n}}_{k+1}, \Delta\bar{\bar{n}}_k\right) & \text{if } \bar{\bar{u}}_{k+1/2} \geq 0\\ \bar{\bar{n}}_{k+1} - \frac{1}{2}\Lambda\left(\Delta\bar{\bar{n}}_{k+2}, \Delta\bar{\bar{n}}_{k+1}\right) & \text{if } \bar{\bar{u}}_{k+1/2} < 0\end{cases}$$

In a second step transform to non-staggered plane

$$\bar{q}_{k+1/2} := \mathcal{T}_{+\Delta\varphi/2}\bar{\bar{q}}_{k+1/2} \quad \bar{q}_{k-1/2} := \mathcal{T}_{-\Delta\varphi/2}\bar{\bar{q}}_{k-1/2}$$

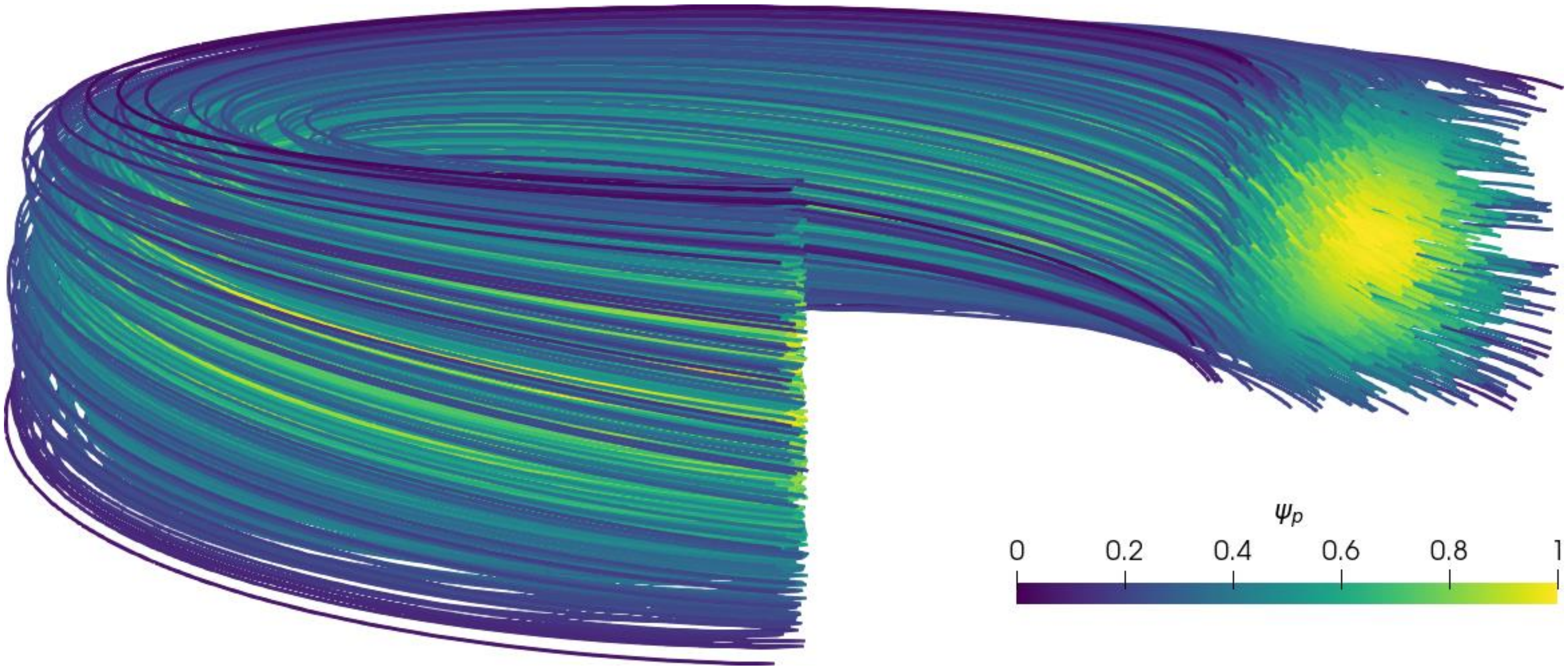
Fieldaligned initialization (zero velocity, zero viscosity)

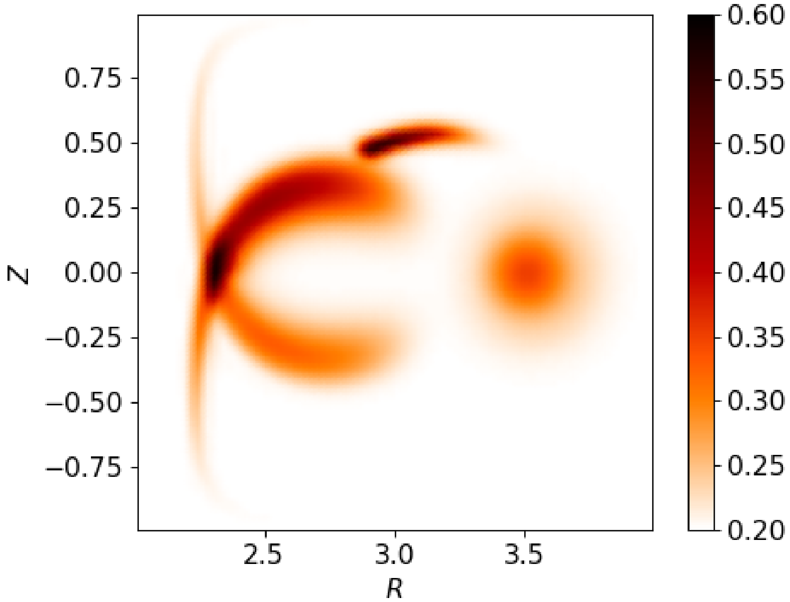


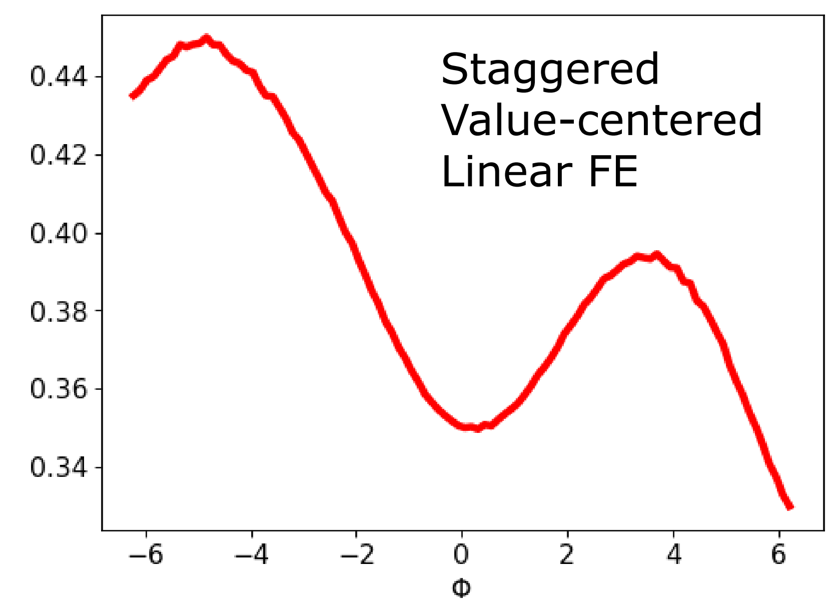


Pure interpolation always unstable => projection method for coordinate transformations

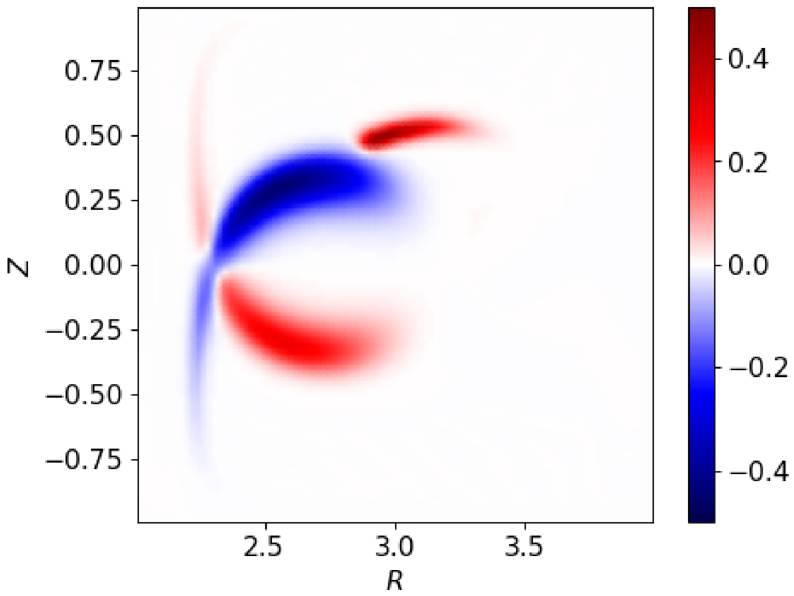
The magnetic field (aligned to boundary)

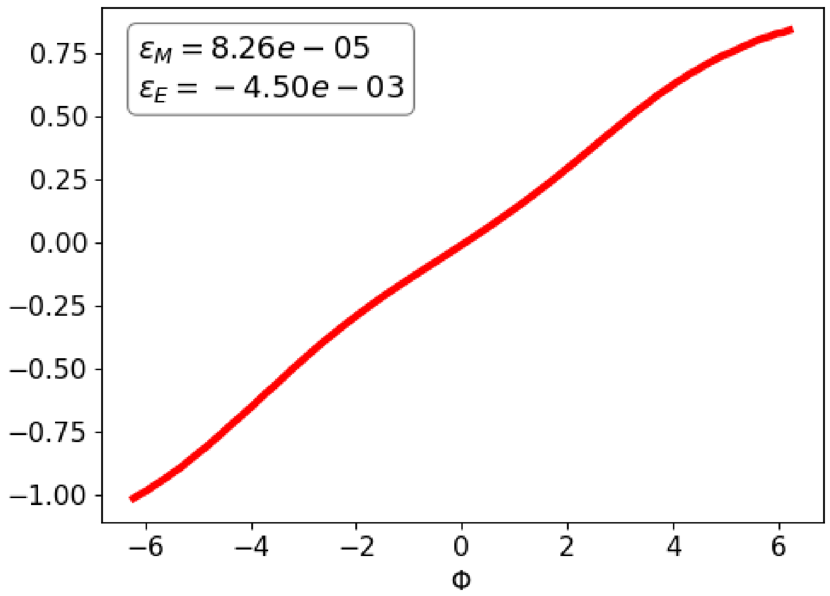






T = 20
96 x 96 x 50

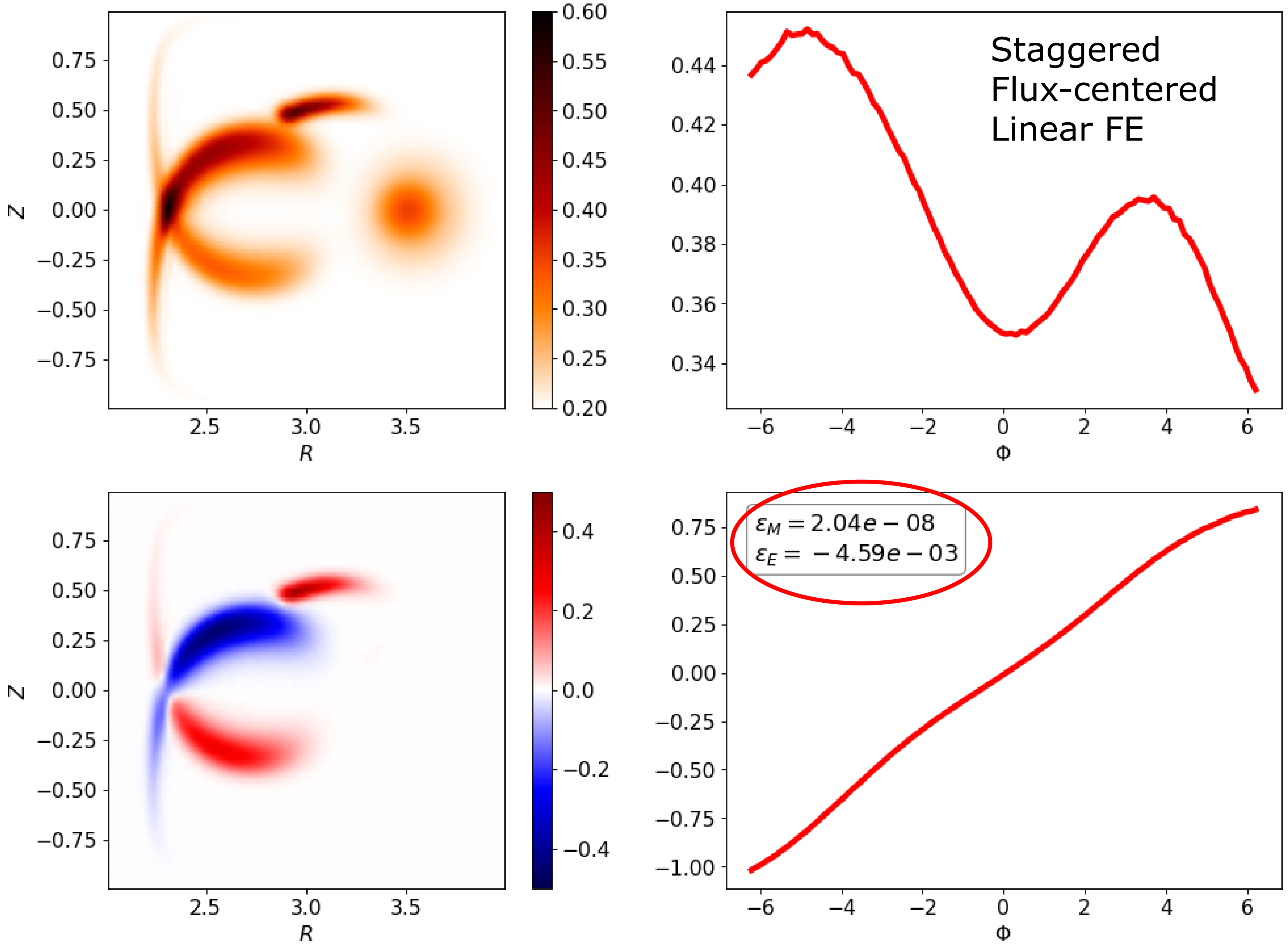




$$M(t) := \int n \mathrm{dV}$$

$$\cancel{P(t) := \int nu \mathrm{dV}}$$

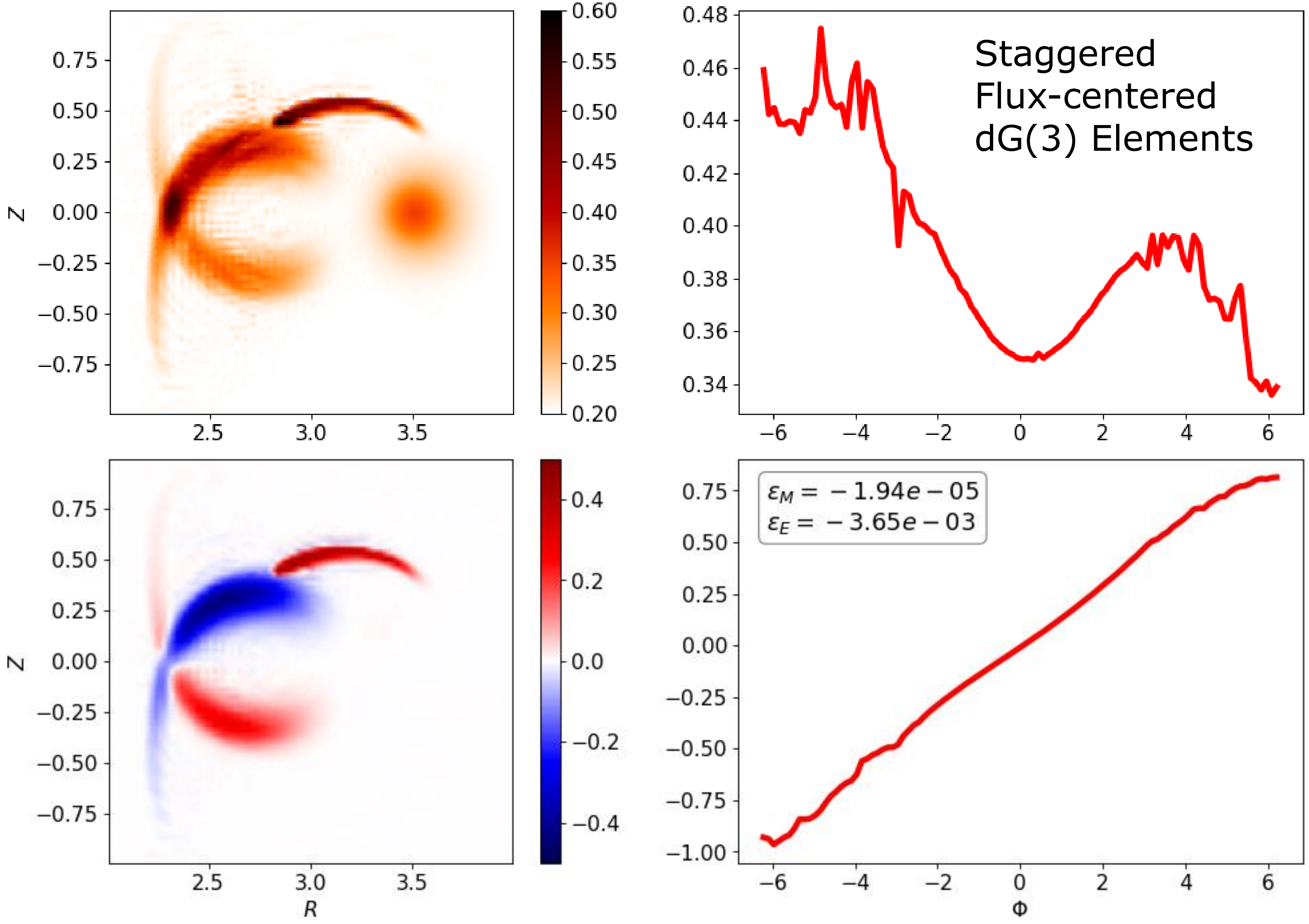
$$E(t) := \int n \ln n + \frac{1}{2} n u^2 \mathrm{dV}$$



T = 20

96 x 96 x 50

Without diffusion, dG scheme is unstable

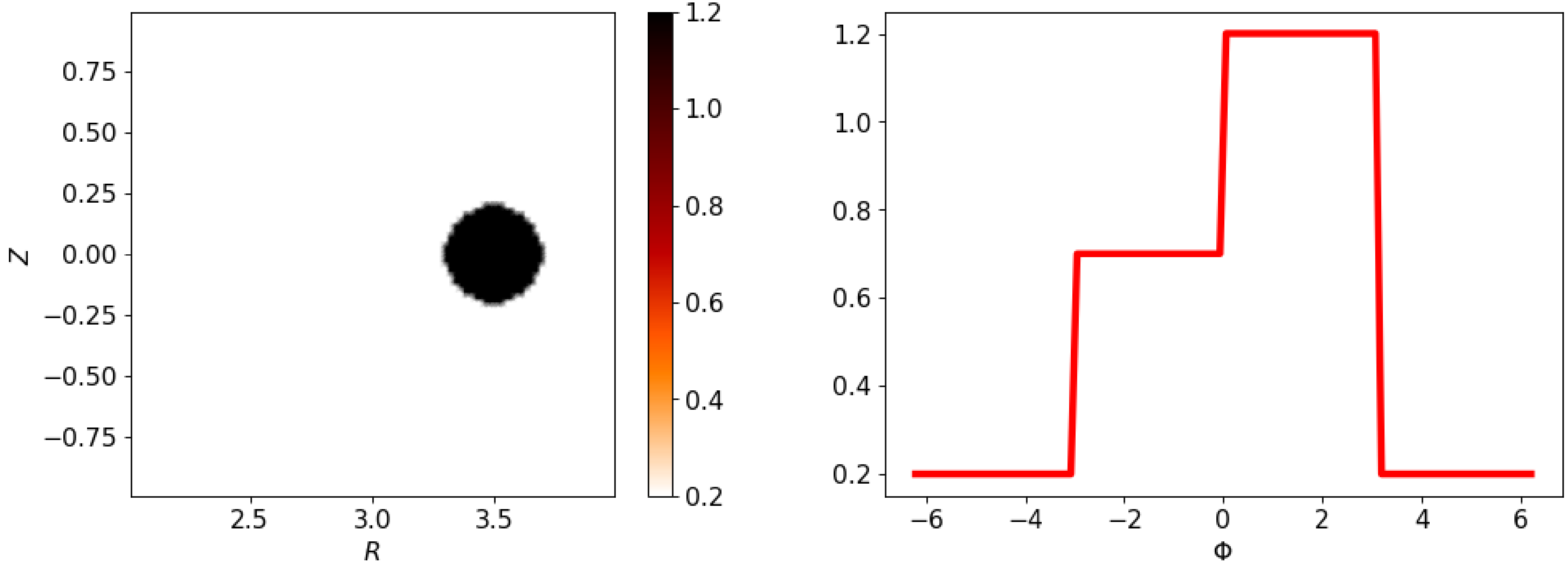


T = 20

96 x 96 x 50

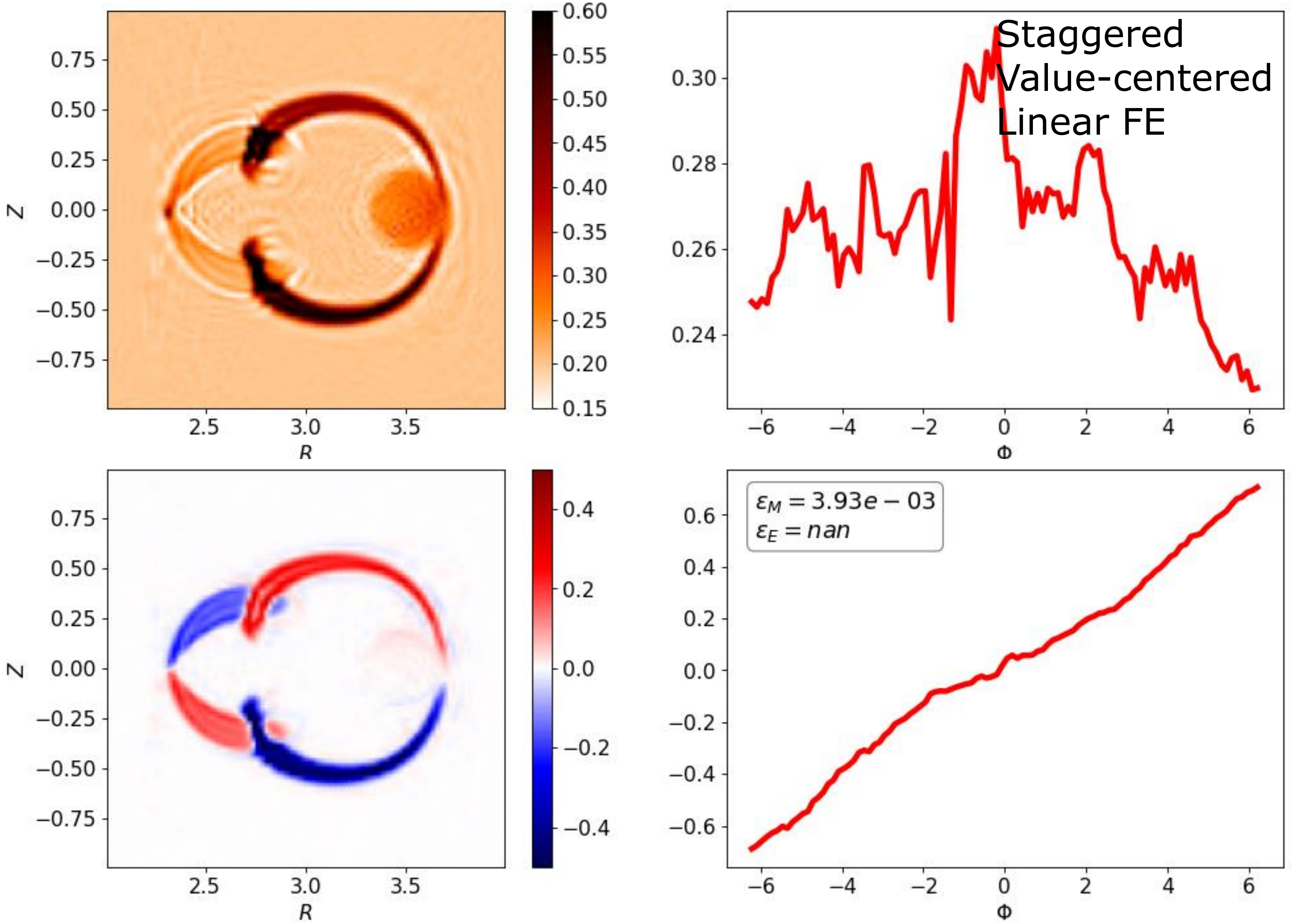
Simulation crashes shortly after, **missing smoothing kernel**

Shock in perpendicular plane (zero velocity, zero viscosity)



DTU

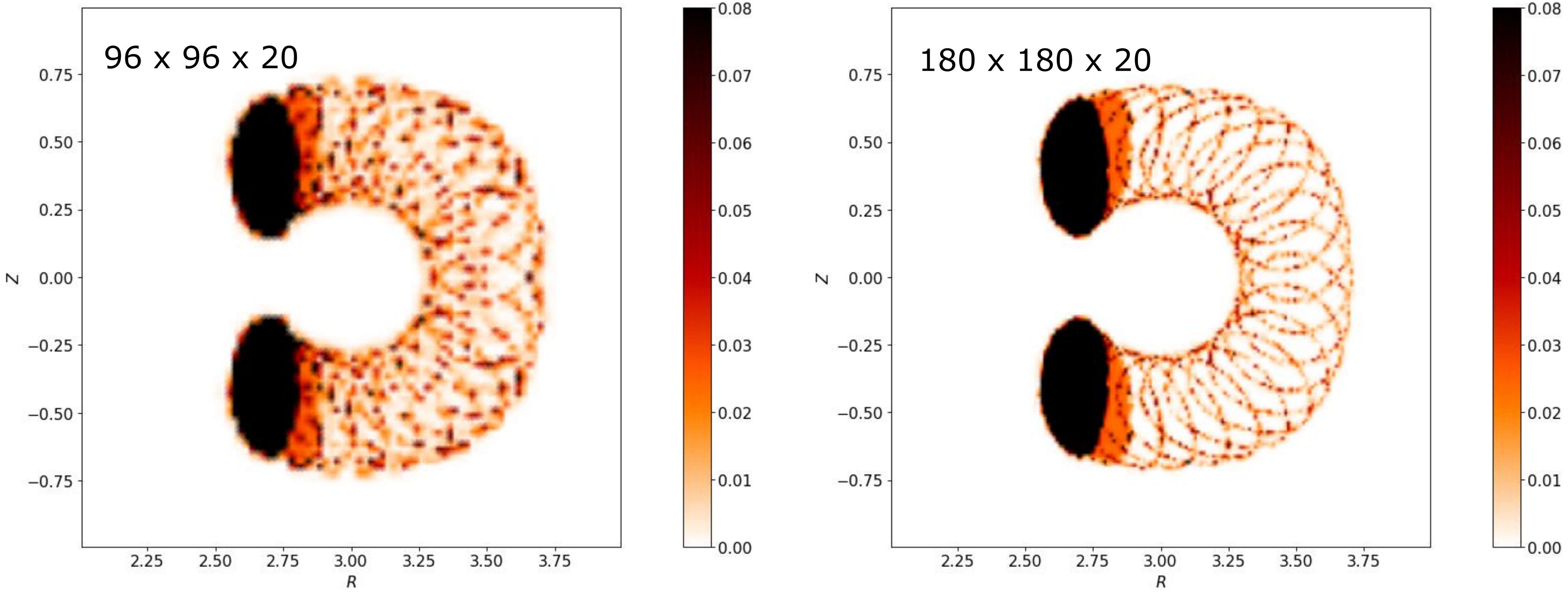
All schemes exhibit spurious oscillations (dG does not even start)



T = 30

96 x 96 x 50

Pressure gradient initial condition (should be zero)

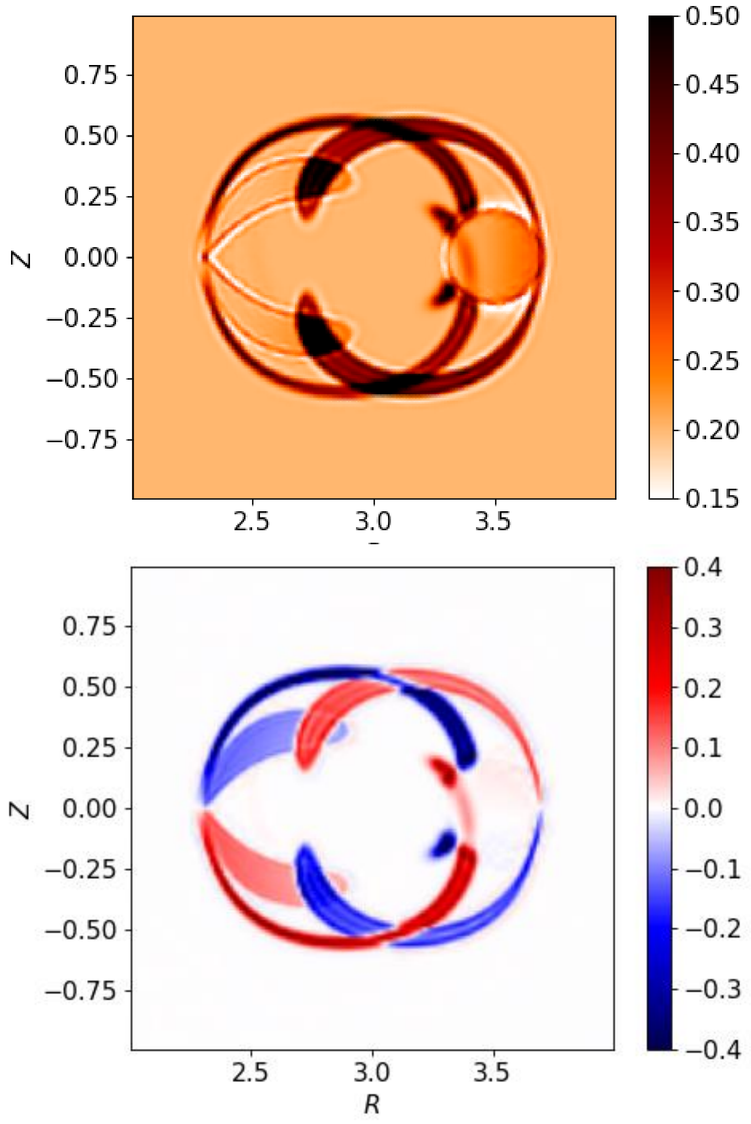


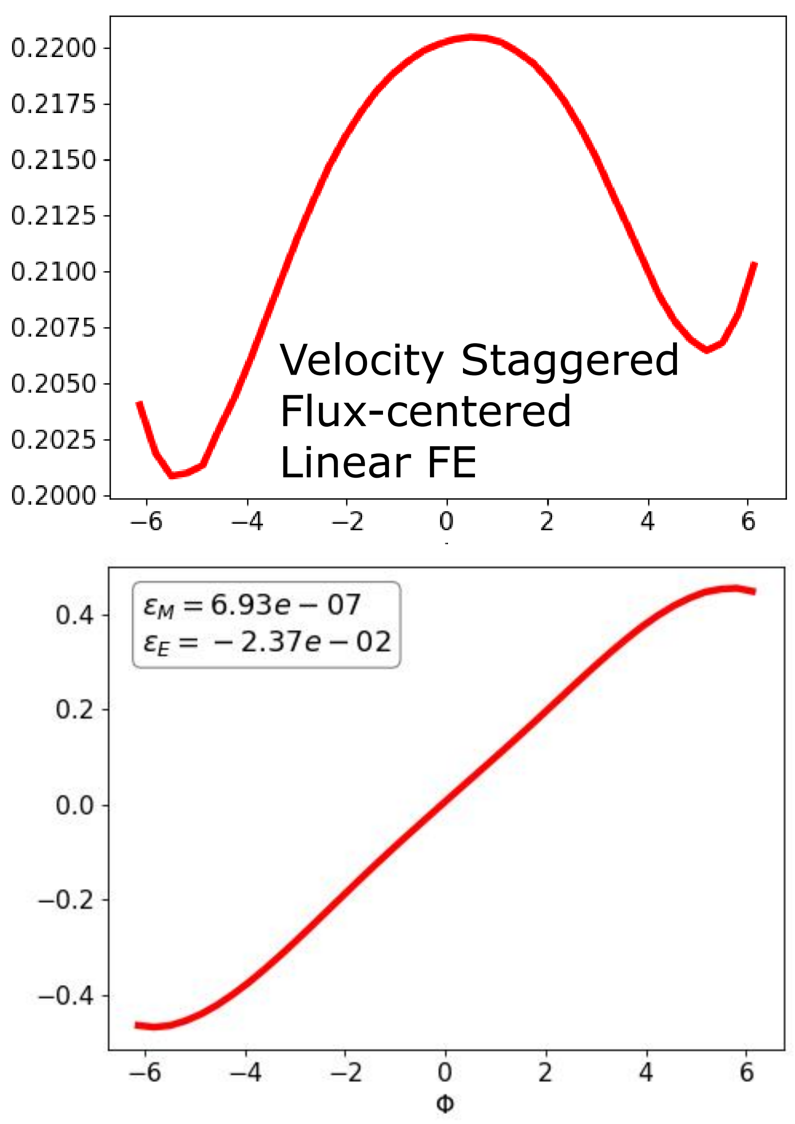
Coordinate transformation **introduces spurious oscillations** around steep gradients

Do not vanish for higher resolution

Parallel diffusion in **both density and velocity** equation needed

Perpendicular diffusion leads to **too restrictive CFL condition**





T = 40

96 x 96 x 50

nu_n = nu_u = 0.02

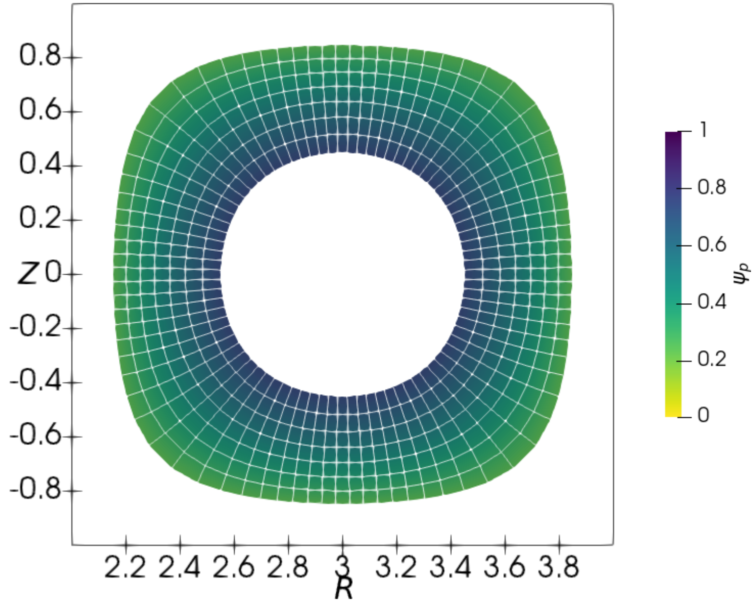
Conclusions

- **FV-FCI scheme** developed by **merging 1d finite volume scheme with FCI**
- For strong perpendicular gradients (parallel) **diffusion is necessary to stabilize** spurious oscillations caused by coordinate transformations
- Smoothing kernel in finite element interpolation seems to stabilize scheme
- **Flux-centred** approach seems to have best conservation properties

Future work

- Extension to **dG in parallel** direction seems straightforward
- Show that the **adjoint of pullback is a discretization of its inverse** (must translate to numerical expression).
- Leads to **exact conservation of mass** $$(\mathcal{T}_{+\Delta\varphi})^\dagger \equiv \mathcal{T}_{-\Delta\varphi}$$

FCI on curvilinear grid



		$\nabla_\parallel^{CC}$ Eq. (21c)		$\nabla\cdot(\hat{\mathbf{b}}f)^{CC}$ Eq. (21f)		$\Delta_\parallel^{CC}$ Eq. (22)		$\int dV \nabla\cdot(\hat{\mathbf{b}}f)^{CC}$		$\int dV \Delta_\parallel^{CC} f$	
N_η	N_φ	error	order	error	order	error	order	error	order	error	order
10	**5**	8.05e-01	n/a	8.10e-01	n/a	5.03e-01	n/a	-4.65e-03	n/a	8.65e-05	n/a
20	**10**	2.79e-01	1.53	2.84e-01	1.51	1.61e-01	1.64	-6.53e-04	2.83	9.41e-08	9.84
40	**20**	7.63e-02	1.87	7.79e-02	1.86	4.32e-02	1.90	-8.41e-05	2.96	1.39e-08	2.76
80	**40**	1.96e-02	1.96	2.01e-02	1.96	1.11e-02	1.96	-1.06e-05	2.99	1.43e-07	-3.36
160	**80**	5.15e-03	1.93	5.27e-03	1.93	3.12e-03	1.84	-1.29e-06	3.03	1.76e-07	-0.30

Table 4: Convergence Table for $K = 100$ and $N_\xi = 24$, using the linear projection method (50).

Compute all metric element in fieldaligned system

$$\begin{pmatrix} R_\rho & R_\zeta & R_\Phi \\ Z_\rho & Z_\zeta & Z_\Phi \\ \varphi_\rho & \varphi_\zeta & \varphi_\Phi \end{pmatrix} = \begin{pmatrix} \rho_R & \rho_Z & \rho_\varphi \\ \zeta_R & \zeta_Z & \zeta_\varphi \\ 0 & 0 & 1 \end{pmatrix}^{-1} = \begin{pmatrix} \zeta_Z & -\rho_Z & (\rho_Z\zeta_\varphi - \zeta_Z\rho_\varphi) \\ -\zeta_R & \rho_R & (\rho_\varphi\zeta_R - \zeta_\varphi\rho_R) \\ 0 & 0 & (\rho_R\zeta_Z - \zeta_R\rho_Z) \end{pmatrix} \frac{1}{(\rho_R\zeta_Z - \zeta_R\rho_Z)}$$

Nemov scheme

$$\frac{\mathrm{d}R}{\mathrm{d}\Phi} = \frac{b^R}{b^\varphi} \qquad \frac{\mathrm{d}Z}{\mathrm{d}\Phi} = \frac{b^Z}{b^\varphi}$$

$$\frac{\mathrm{d}\rho_R}{\mathrm{d}\Phi} = -\left(\frac{b^R}{b^\varphi}\right)_R \rho_R - \left(\frac{b^Z}{b^\varphi}\right)_R \rho_Z \qquad \frac{\mathrm{d}\rho_Z}{\mathrm{d}\Phi} = -\left(\frac{b^R}{b^\varphi}\right)_Z \rho_R - \left(\frac{b^Z}{b^\varphi}\right)_Z \rho_Z$$

$$\frac{\mathrm{d}\zeta_R}{\mathrm{d}\Phi} = -\left(\frac{b^R}{b^\varphi}\right)_R \zeta_R - \left(\frac{b^Z}{b^\varphi}\right)_R \zeta_Z \qquad \frac{\mathrm{d}\zeta_Z}{\mathrm{d}\Phi} = -\left(\frac{b^R}{b^\varphi}\right)_Z \zeta_R - \left(\frac{b^Z}{b^\varphi}\right)_Z \zeta_Z$$