EUROfusion

European boundary plasma modelling towards reactor relevant simulations

P. Tamain

for the ETASC-TSVV3 team

IRFM

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

Thanks to contributions of

L. Anton, W. Arter, T. Baelmans, T. Body, H. Bufferand, N. Carlevaro, S. Carli, G. Ciraolo, A. Coroado, D. Coster, W. Dekeyser, B. Dudson, N. Fedorczak, G. Fourestey, B. Frei, P. Ghendrih, G. Giorgiani, M. Groth, D. Harting, M. Held, G. Huijsmans, P. Innocente, O. Maj, Y. Marandet, F. Militello, G. Montani, D. Moulton, V. Naulin, A. Nielsen, J. Olsen, J. Omotani, J. Parker, F. Parra, J. Rasmussen, P. Ricci, C. Ridgers, F. Riva, F. Schwander, E. Serre, A. Stegmeir, F. Subba, P. Tamain, A. Thrysøe, D. Tskhakaya, N. Varini, M. Wiesenberger, R. Zagorski, W. Zholobenko

cea

Aix*Marseille université
Initiative d'excellence

KU LEUVEN

EPFL
ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE
SWISS PLASMA CENTER

CHALMERS

Aalto University

Technical University of Denmark
DTU

CCFE
CULHAM CENTRE FOR FUSION ENERGY

YORK
UNIVERSITÉ
UNIVERSITY

IPP
Max-Planck-Institut für Plasmaphysik

IPP
INSTITUTE OF PLASMA PHYSICS
OF THE CZECH ACADEMY OF SCIENCES

IFPiLM

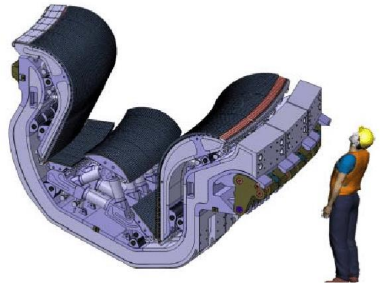
POLITECNICO DI TORINO

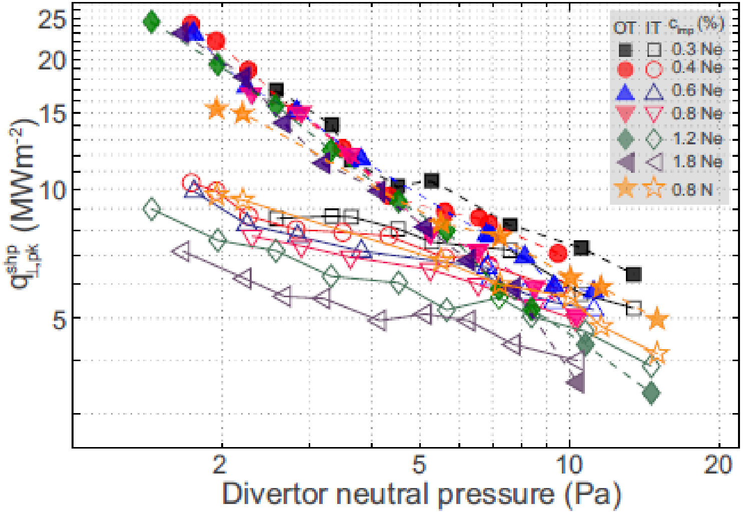
CONSORZIO RFX
Ricerca Formazione Innovazione

ENEA

Edge fluid modelling = key tool for exhaust issues

- **Edge plasma modelling fluid codes** = key tools for **design** and definition of **operational space**
    - Heat exhaust (target fluxes, erosion…)
    - Particle exhaust (pumping capabilities)
    - Stability and performances (impurities and radiation distribution)





- E.g., **ITER divertor physics basis** based on **SOLPS** (-4.3 & -ITER) simulations

[Pitts et al., NME 2019]

Why a boundary code for reactors?

- DEMO pushes the **power exhaust challenge** further
  - Strong constraints on operational space **margins**
  - **Reliability** of predictions critical
- Current **limits of existing tools**
  - **Missing physics** hidden in free parameters (λ_q, S, flux limits…)
  - **Not enough computationally efficient** on modern HPC

    (e.g., MST case ~days, DEMO case ~months)

	AUG	JET	ITER (Q=10)	DEMO
R_{geo} (m)	1.65	2.9	6.2	**8.8**
B_T (T)	2.5	2.6	5.3	**5.8**
I_P (MA)	1.2	2.5	15	**20.3**
n_{GW} (10^{20}m^{-3})	1.4	1.0	1.2	**0.8**
P_{heat} (MW)	26	25	150	**300**
$f_{rad,core}$	0.25	0.4	0.33	**0.5**
P_{sep} (MW)	20	16	100	**150**
$P_{sep}/P_{L\text{-}H}$	4.5	1.8	1.4	**1.1**
P_{sep}/R (MW/m)	12	5.2	17	**17**
$P_{sep}B_0/R$ (MW·T/m)	30	13	88	**99**
P_{sep}/B_p (MW/T)	58	39	96	**138**

$q_{||} \propto$

$c_z \propto$

[Reimerdes, 4th IAEA DEMO Prog. Workshop]

Context: ETASC-TSVV3 project

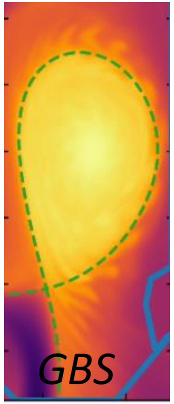
- Effort in the frame of **EUROfusion** Theory and Advanced Simulation Coordination (**E-TASC**), with 2 complementary arms:
  - **TSVV** tasks (Theory, Simulation, Validation and Verification): develop state-of-the-art codes
  - **ACHs** (Advanced Computing Hubs): support TSVVs in code development

- Staged deployment of strategy:
  - **5 pilot TSVV tasks** in June 2019 – Dec. 2020
  - **14 full TSVV tasks** launched in April 2021 for 5 years

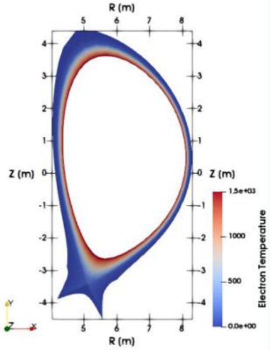
    [https://www.euro-fusion.org/news/2021/march/eurofusion-e-tasc/]

- One task (pilot and full) dedicated to **development of next generation boundary plasma fluid code for reactor relevant applications**

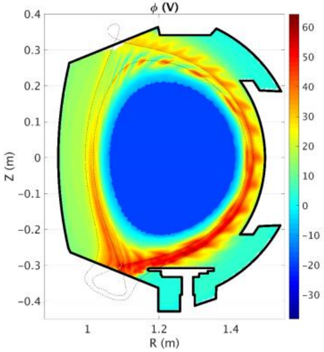
Consortium gathering European expertise


GBS

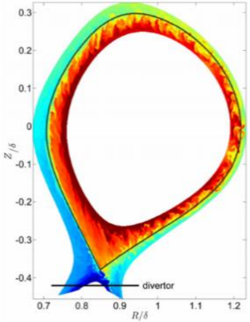

FELTOR



SOLPS-ITER



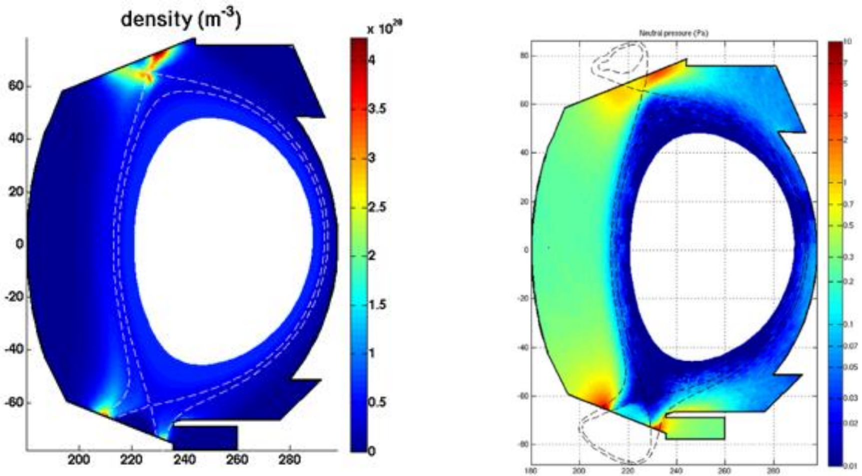
SOLEDGE3X



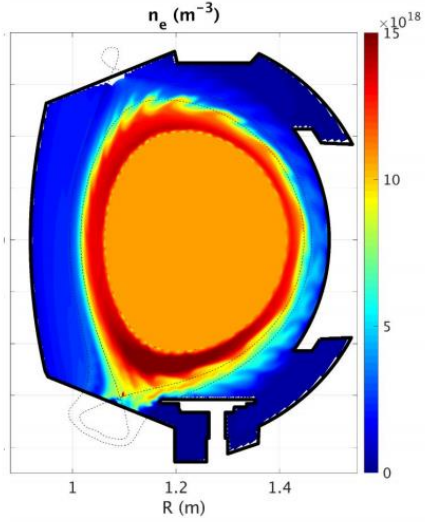
GRILLIX

Going beyond the state-of-the-art

- State-of-the-art schematically composed of 2 legs:
  1. **2D mean-field** fluid modelling (SOLPS, EDGE2D, SOLEDGE…) including PWI, neutrals and impurities physics
  2. **3D turbulence** modelling (TOKAM3X, GBS, BOUT++, GRILLIX, FELTOR…) without considering other boundary plasma physics



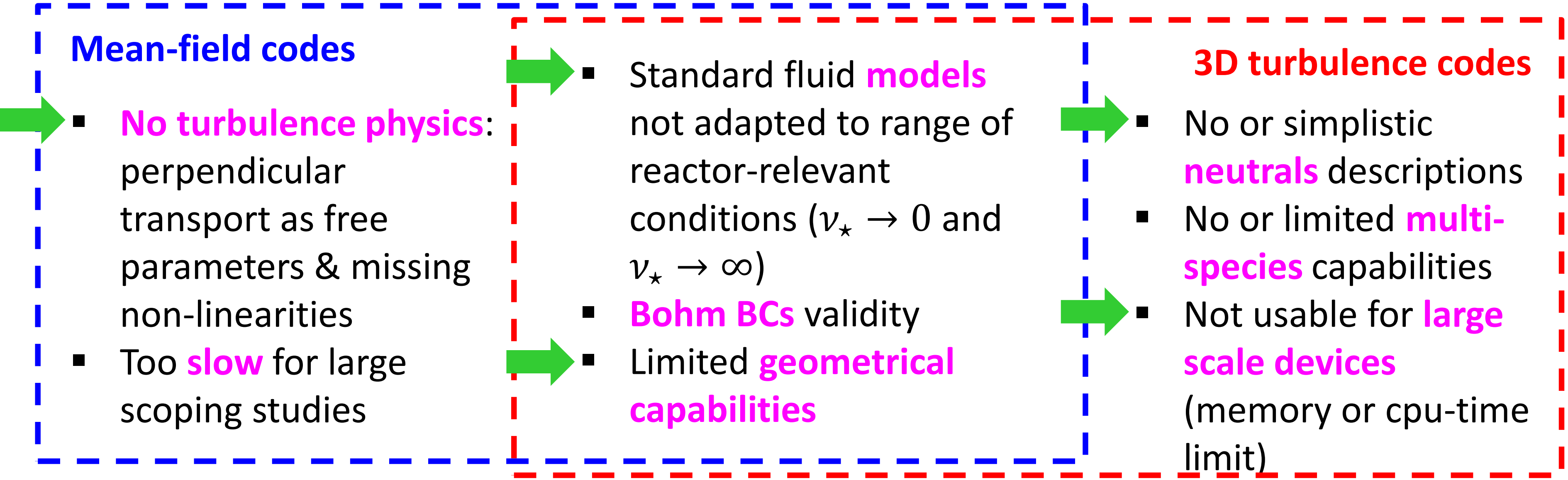
WEST 2D mean-field simulation



WEST 3D turbulence simulation

Going beyond the state-of-the-art

- State-of-the-art schematically composed of 2 legs:
  1. **2D mean-field** fluid modelling (SOLPS, EDGE2D, SOLEDGE…) including PWI, neutrals and impurities physics
  2. **3D turbulence** modelling (TOKAM3X, GBS, BOUT++, GRILLIX, FELTOR…) without considering other boundary plasma physics



Mean-field codes

- **No turbulence physics**: perpendicular transport as free parameters & missing non-linearities
- Too **slow** for large scoping studies

- Standard fluid **models** not adapted to range of reactor-relevant conditions ($\nu_\star \to 0$ and $\nu_\star \to \infty$)
- **Bohm BCs** validity
- Limited **geometrical capabilities**

3D turbulence codes

- No or simplistic **neutrals** descriptions
- No or limited **multi-species** capabilities
- Not usable for **large scale devices** (memory or cpu-time limit)

Towards full-f gyro-fluid models

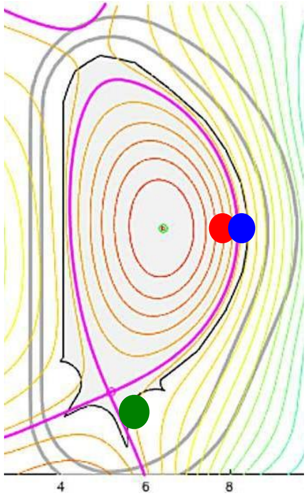
- ❖ **Drift-fluid models** = current work-horse of edge plasma modelling
  - Based on **collisional Braginskii or Zhdanov closure**
  - But DEMO's **extreme collisionality range** questions validity

Pedestal
$n_e \sim 10^{20}\ m^{-3}$
$T_e \sim 10keV$

Upstream SOL
$n_e \sim 3.10^{19}\ m^{-3}$
$T_e \sim 500eV$

Target plates
$n_e \sim 10^{21}\ m^{-3}$
$T_e \sim 3eV$

6 orders of magnitude in ν_e!

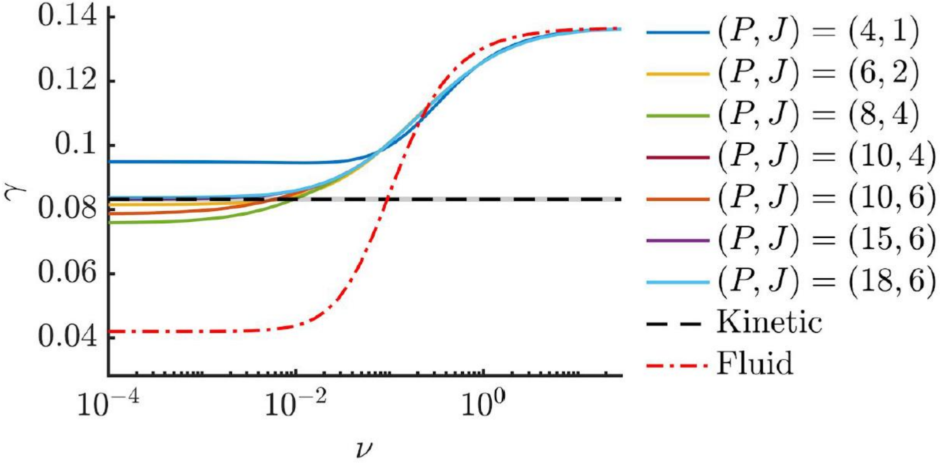


- ❖ Long term target of project: **full-f gyro-fluid models**
  - 👍 Capture **key kinetic effects even at low ν_*** + natural diamagnetic cancellation
  - 👍 Equations structure similar to drift-fluid
  - 👎 **Closures and boundary-conditions to be developed** and tested

N-moments gyro-fluid approach

- **N-moments gyro-fluid** model
  - Projection of gyrokinetic equation on **arbitrary number of fluid moments** using Hermite-Laguerre polynomials
  - Expansion of full **non-linear gyrokinetic Coulomb collision** operator

- Numerical implementation of linearized version
  - **ITG fluid and collisionless limits can be retreived** with finite number of moments



[Frei et al., JPP 2020; Jorge et al., JPP 2019]

Modelling turbulence without DNS (1)

- Heuristic **k-epsilon model** inspired from RANS models in CFD

  [Baschetti et al., *submitted to NF, preprint: https://hal.archives-ouvertes.fr/hal-03081473]*

Turbulence energy κ: $\partial_t \kappa + \boldsymbol{\nabla}_{\parallel}(\kappa u_{\parallel} \boldsymbol{b}) - \boldsymbol{\nabla}_{\perp} \cdot (D_\kappa \boldsymbol{\nabla} \kappa) = \gamma_\kappa \kappa - \frac{1}{D_\omega}\kappa^2 - \varepsilon$

Dissipation rate ϵ: $\partial_t \varepsilon + \boldsymbol{\nabla}_{\parallel} \cdot (\varepsilon u_{\parallel} \boldsymbol{b}) - \boldsymbol{\nabla}_{\perp} \cdot (D_\varepsilon \boldsymbol{\nabla} \varepsilon) = \gamma_\varepsilon \varepsilon - \frac{V}{\kappa^{3/2}}\varepsilon^2$

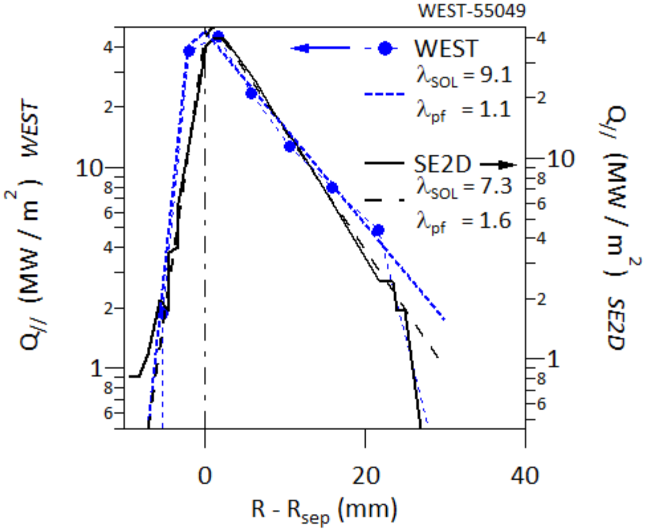
$$\boxed{D_n = C_\nu \frac{\kappa^2}{\epsilon}}$$

- Closure relying on:
  1. Theoretical considerations on leading instabilities (interchange here) and dissipation (Kolmogorov cascade here)
  2. Experimental scaling laws for λ_q

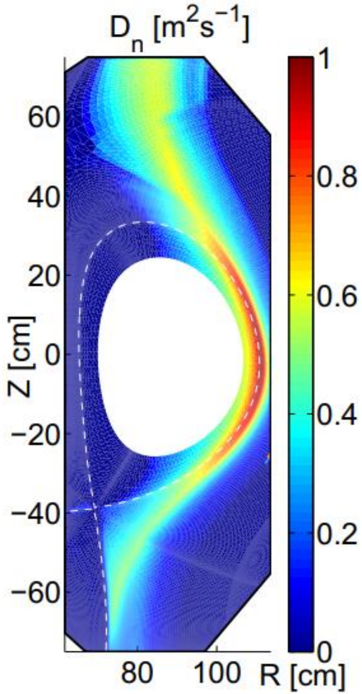
  ⇒ **Single free parameter** (C_ν) for self-consistent determination of transport at every point in space at **negligible extra computing cost**

Modelling turbulence without DNS (2)

- Model results **confronted to experiments** on **TCV** and **WEST**
  - **Remarkable agreement** in both machines in several configuration once C_ν tuned (once and for all)
  - Recovers spatial distribution (ballooning) of turbulent transport



[Baschetti et al., *submitted to NF*]



[Baschetti et al., *Journal of Physics: Conference Series, 2018]*

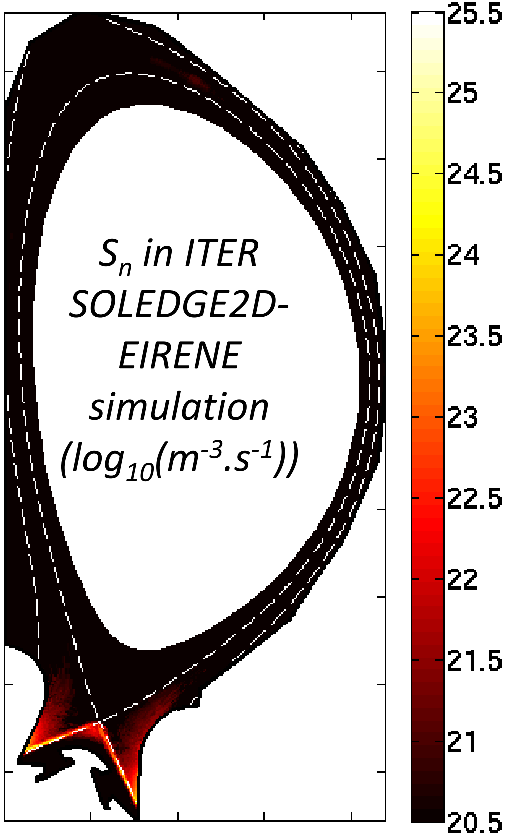
Neutrals, the elephant in the room of turbulence codes

- Neutrals essentially ignored up to recently in turbulence codes

- But **neutrals mandatory for reactor relevant studies**:
  1. in large devices (e.g. ITER): $S_N^{recycl} > 100 \times S_N^{fuel}$ *[Kukushkin, JNM2011]*
  2. Numerous experimental indications of **impact of neutrals on turbulence** and/or confinement *[Carralero, NF 2014; Tamain, JNM 2015]*
  3. Impact of **turbulence on A&M physics**: recycling, detachment… *[Marandet, NF 2011; Havlickova, JNM 2011]*

- Proof of principle **coupling between turbulence code and neutrals** already performed in idealistic conditions:
  - 2D or limited geometry
  - Attached conditions
  - Incomplete neutral terms in plasma model

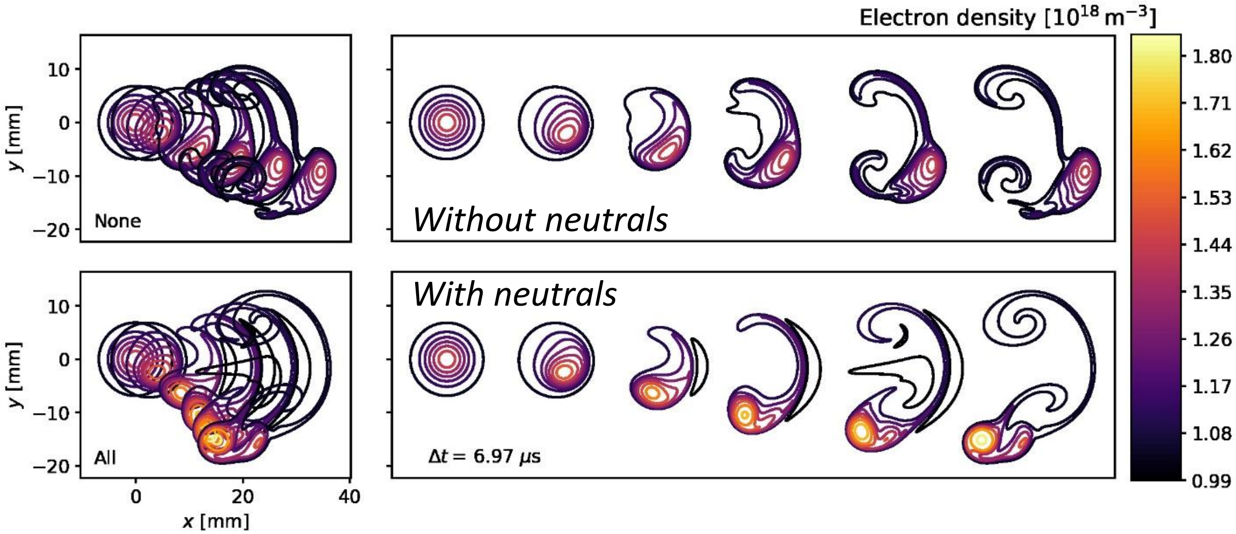
  [Fan, NME 2019; Tamain, PSI 2018; Wersal, NF 2015]



S_n in ITER SOLEDGE2D-EIRENE simulation ($\log_{10}(m^{-3}.s^{-1})$)

An advanced fluid neutrals model

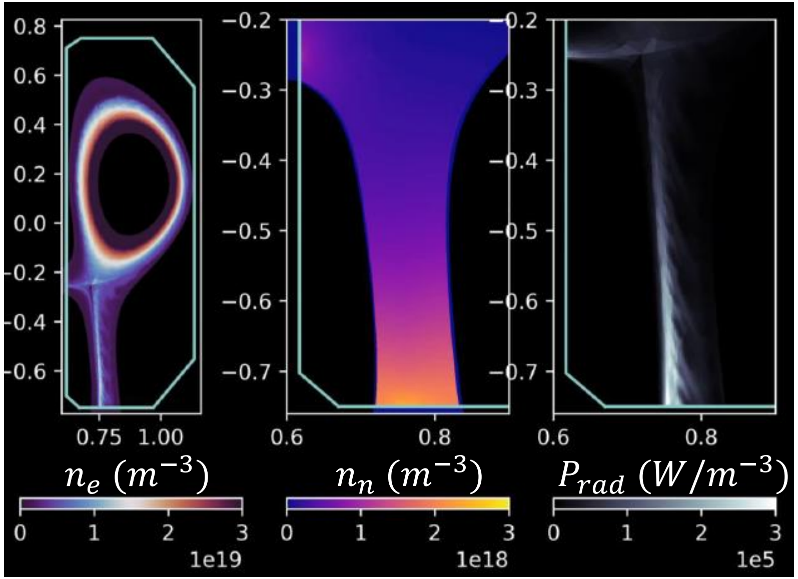
- Advanced **fluid neutrals model** developed and implemented in nHESEL code
  - **separate isothermal neutral species** with characteristic temperatures corresponding to neutrals origin (recycling, Franck-Condon, charge-exchange)
- Simulations show **strong impact on filamentary dynamics**
  - Specific **importance of neutrals terms in vorticity** (perp. momentum) balance



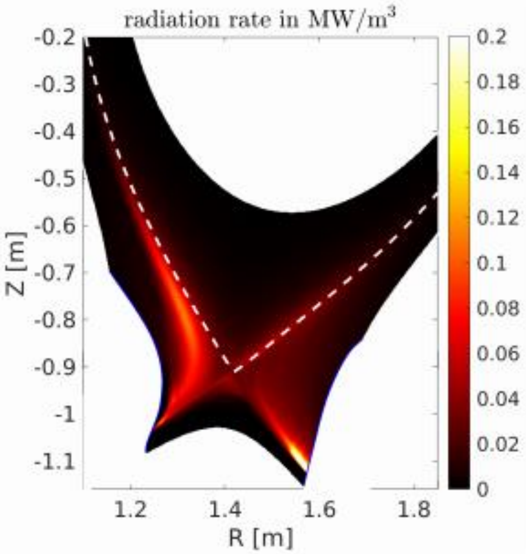
[Thrysøe, PoP 2020]

Fluid neutrals and turbulence in realistic geometry

- **Fluid neutrals models** have been implemented in the **GRILLIX** and **SOLEDGE3X** **3D turbulence codes** *[Zholobenko, IAEA FEC 2020; Bufferand, IAEA FEC 2020]*
  - Strong impact (**better match**) compared with simulation w/o neutrals
  - Neutrals recycling strongly **increase simulation equilibration time** $\propto \frac{1}{1-R_{eff}}$ => costly!



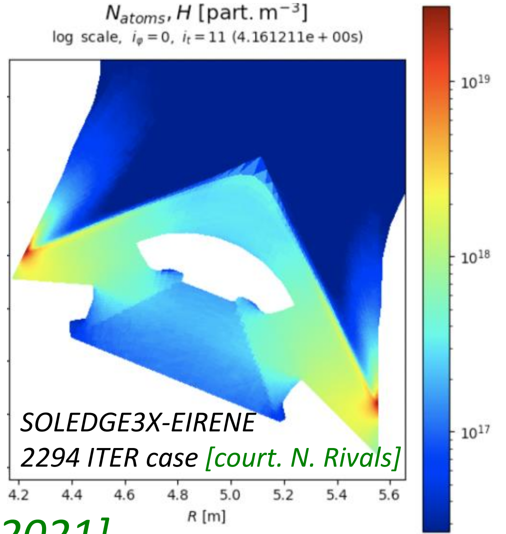
SOLEDGE3X / TCV



GRILLIX / ASDEX

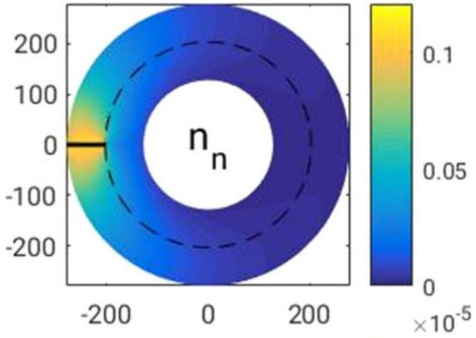
Two parallel paths for inclusion of kinetic neutrals

1. Rely on **EIRENE** Monte-Carlo kinetic neutrals code
   - **SOLEDGE3X coupled with EIRENE** with first application to 2D mean-field ITER simulations
   - Search of time-dependent fluctuating solution raises **questions on coupling scheme**: can we avoid calling EIRENE at each time step? How to increase the time-order of the coupling to EIRENE?...



SOLEDGE3X-EIRENE
2294 ITER case [court. N. Rivals]

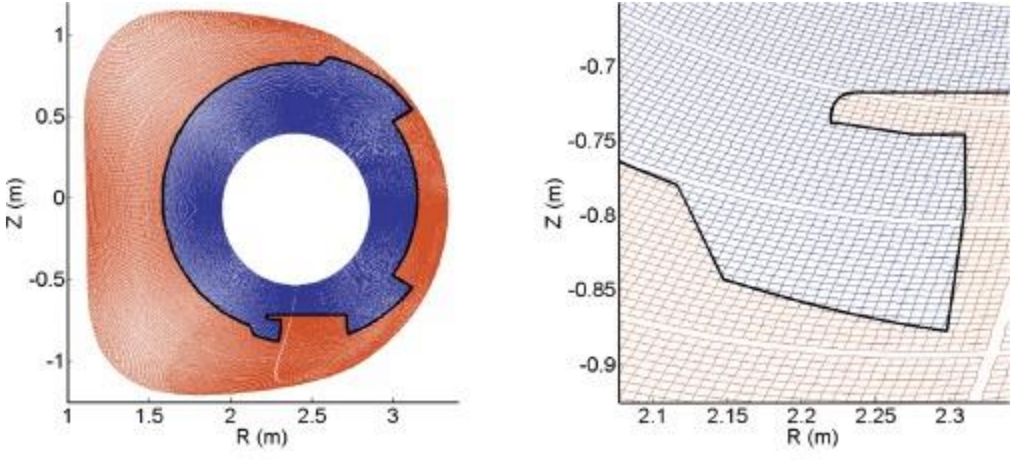
2. Development of **method of characteristics** *[Coroado, PoP 2021]*
   - 👍 No Monte-Carlo noise, can be generalized to treat ionized species such as D_2^+ molecules (tested in GBS)
   - ? A&M model to be complexified and open question on **manageability of numerical cost** for large simulations (large implicit system to invert)



Self-consistent wall and magnetic geometries?

- Issue: **magnetic and wall geometry non conformal**
  - mandatory to treat self-consistently for PWI issues
  - Numerical difficulty even in 2D mean-field codes

  [Tamain et al., NME 2021]



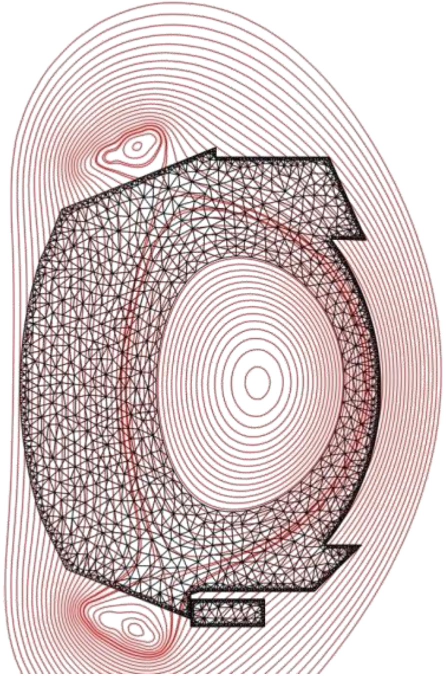
(a) (b)

- **3 parallel options** explored:
  1. Use of **penalization techniques** (immersed boundary conditions)
  2. **Specific discretization scheme** at the boundary
  3. **Finite Elements** discretization => HDG method

Development of a HDG boundary plasma solver

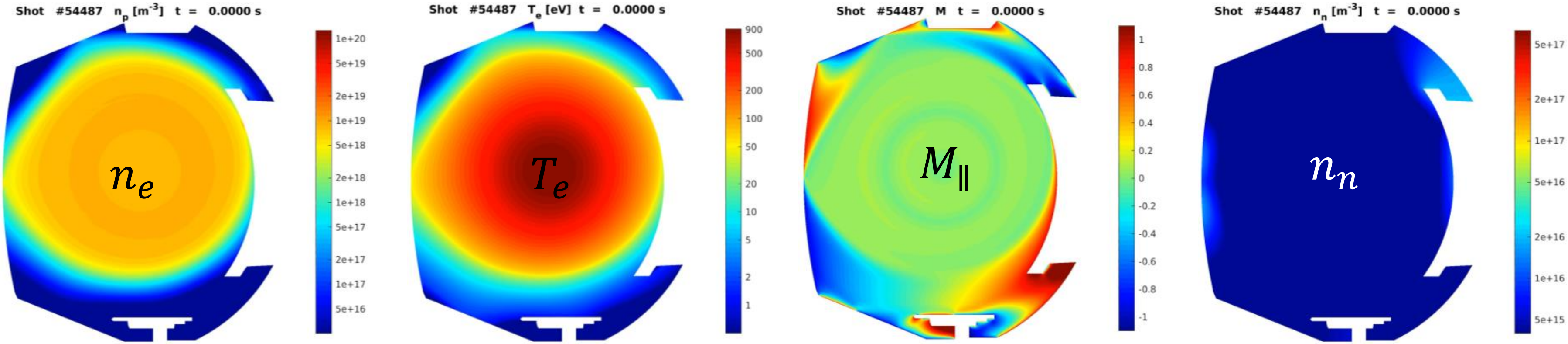
- **FE methods** offer the flexibility to treat magnetic + wall geometry self-consistently
- Choice = **(Hybrid) Discontinuous Galerkin**
  - **Pros:** highly **parallelizable**, easy **adaptivity** (h and p), **robust**, already tested with reduced models

    [Giorgiani, JCP 374 (2018); Wiesenberger, CPC 238 (2019)]
  - **Cons:** **complex** to implement, little experience for edge plasma modelling, especially with turbulence
- Development of **new h/p-adaptative European HDG solver** (“EBC”)
  - test of model implementation in existing **SOLEDGE-HDG** solver in support



Equilibrium independent HDG boundary plasma solver

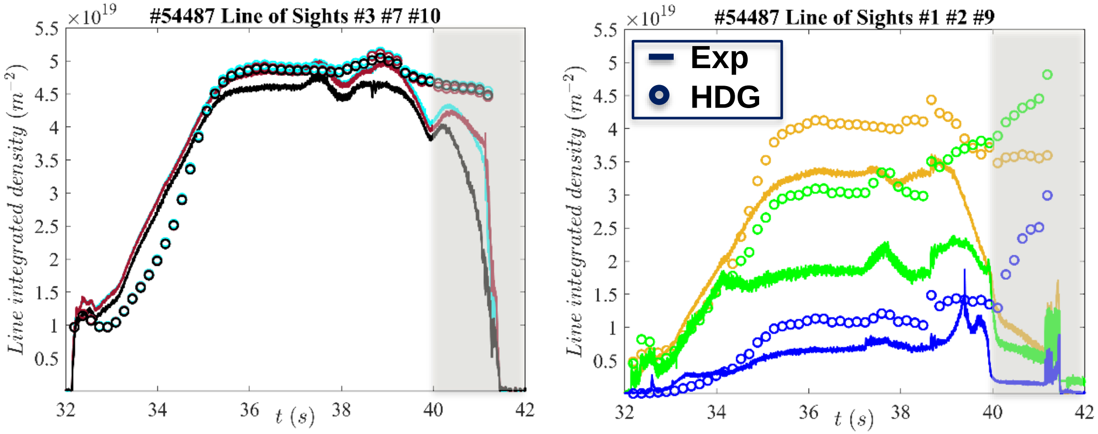
- **2D mean-field model** implemented with **fluid neutrals** in **HDG** solver
  - Allows **dynamic equilibrium** simulations **from plasma center to first-wall** in full geometry
- Application to simulation of WEST pulse from break-down to termination



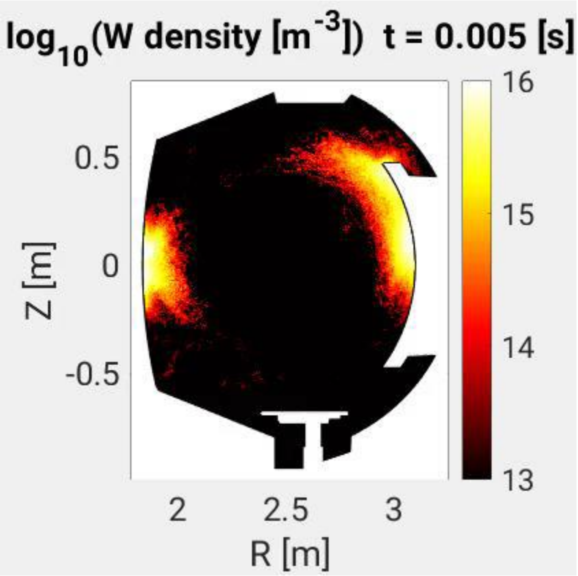
[M. Scotto et al., in prep]

Equilibrium independent HDG boundary plasma solver

- **2D mean-field model** implemented with **fluid neutrals** in **HDG** solver
  - Allows **dynamic equilibrium** simulations **from plasma center to first-wall** in full geometry
- Application to simulation of WEST pulse from break-down to flat-top
  - W content strongly driven by plasma initial phase

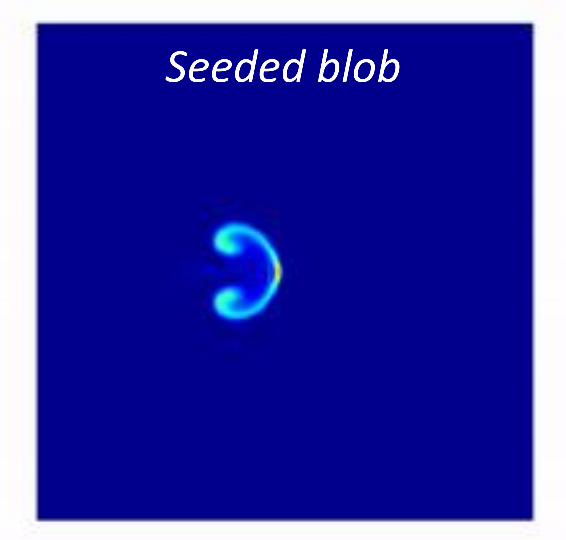


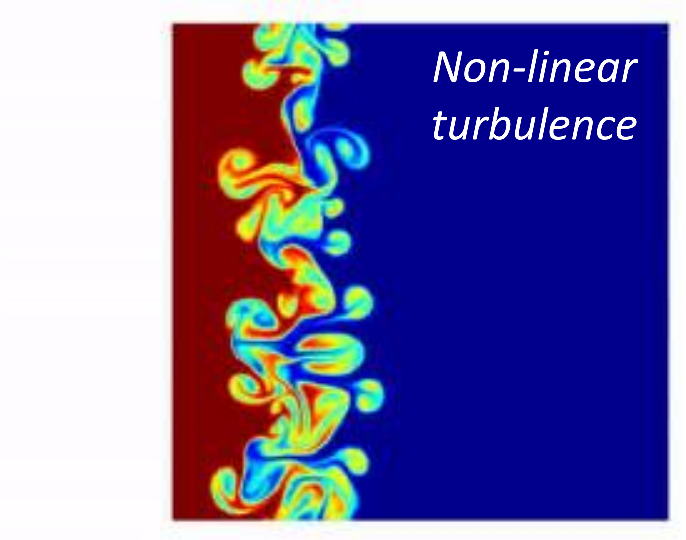
[M. Scotto et al., in prep]



HDG modelling of 2D turbulence interchange

- **2D isothermal interchange turbulence** implemented in **HDG** solver
- Very first test demonstrates **capability to treat physical instabilities and turbulence** from linear growth to non-linear saturation

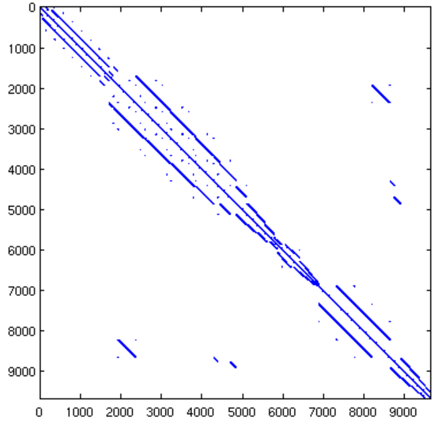




[courtesy G. Giorgiani]

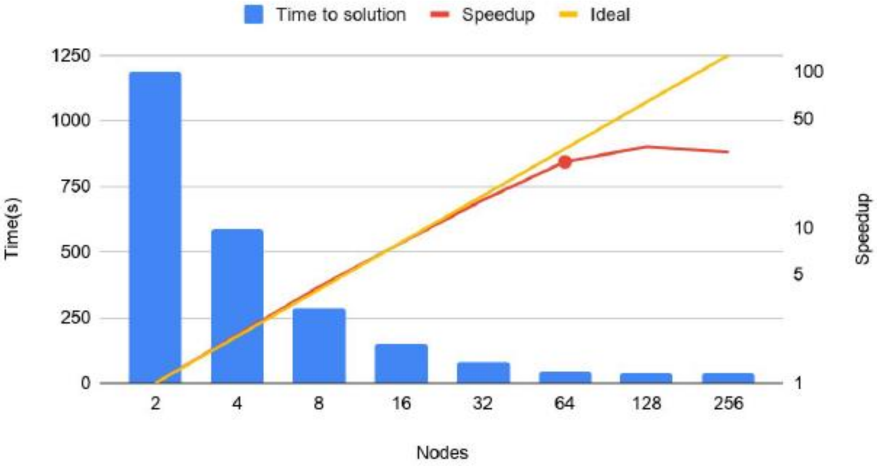
Breaking fluid codes’ bottleneck

- **Elliptic solvers** are central to all drift-fluid / gyro-fluid models
  - Needed to link plasma quantities (W / $J_{//}$) to EM potentials (ϕ / $\tilde{\psi}$)
  - Known to be the **main bottleneck** of all existing edge codes



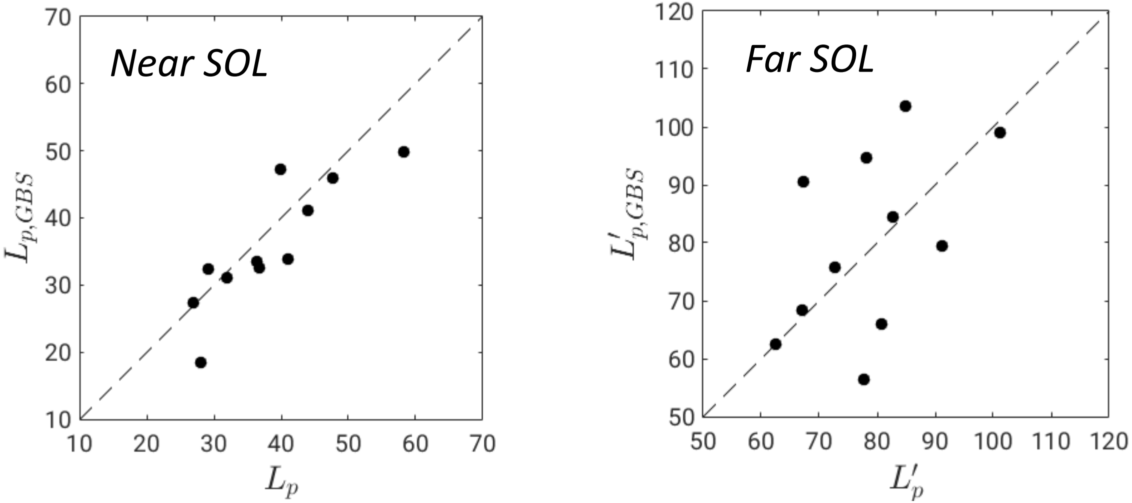
Matrix structure from ES potential solver in SOLEDGE3X diverted case

- **Performance analysis** of available linear solvers started at EPFL
  - Use of AMG solver (Hypre) as preconditioner for Krylov subspace method (GMRES) promising
  - gain of factor of 20 in parallel efficiency vs direct solver (MUMPS) on 64 nodes
  - move to **GPU** under investigation



How the project used JFRS-1 time in 2020?

- Exploitation of **GBS** 3D turbulence code to analyze dependency of SOL width with collisionality and heating power in **full-scale TCV simulations**
  - **theory-based scaling law for near and far SOL decay length** derived and compared to simulations
  - First step of **step-ladder towards ITER** simulations



[Giacomin, submitted to NF]

Some feedback on JFRS-1 usage

- Overall **very positive experience** with the machine and the support team
  - **Initial difficulties** with installation and execution of code, especially pour performances
  - **Close interaction with help-desk** allowed to solve the issue, running with performances significantly better than on Marconi HPC

Conclusion and prospects

- European boundary plasma modelling project = joint effort for **development of next generation boundary plasma fluid codes** for reactor relevant applications

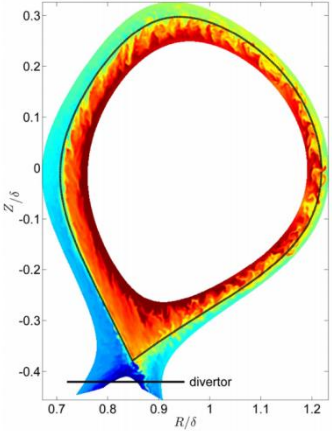
- 2-stage approach:
  1. Multifrontal approach of upstream issues: develop and test solutions capitalizing on existing codes and their specificities
  2. Convergence of effort on reduced set of tools integrating best approaches planned from 2024

- Significant **progress after pilot phase** of project:
  - Development of hierarchy of models: from **full-f gyro-fluid** to RANS-like **reduced turbulence models**
  - Successful initial implementation of **neutrals and multi-species physics in 3D turbulence codes**
  - Progress on **numerical treatment**, either in terms of geometrical discretization (HDG solver), or numerical methods (linear solvers)

Additional slides

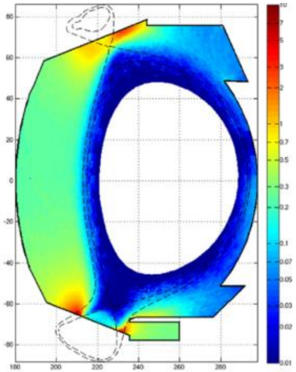
Physics requirements

- Physics of interest:
  - **Inter-ELM** conditions (no ELM in DEMO!)
  - Self-consistent **electromagnetic turbulent transport** mandatory for high fidelity side of model hierarchy
  - **Neutrals and impurities** for dissipation, including kinetic regimes
  - **Several main ion** species for D, T (& He)



[GRILLIX, courtesy A. Stegmeir]

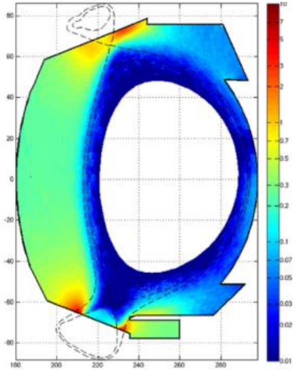
- Geometry:
  - from **first wall to pedestal top** => strong constraint on ν* range, but lower fidelity acceptable for pedestal physics (dedicated TSVV)
  - accurate discretization in **flexible magnetic geometry**, should allow RMPs, full 3D wished but not a priority
  - **wall conformity** mandatory even for complex wall shape



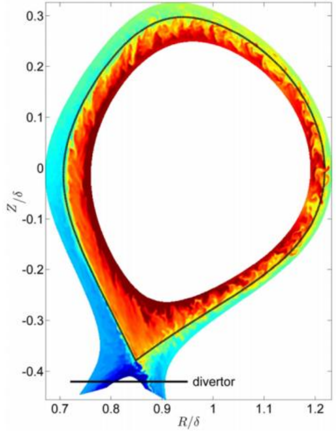
[SOLEDGE2D, courtesy WEST team]

Edge modelling at a crossroads

- Towards the **convergence of the 2 facets of edge plasma modelling**
  - **2D mean-field** fluid modelling at maturity (SOLPS, EDGE2D, SOLEDGE…)
  - **3D turbulence** modelling now reaching maturity (TOKAM3X, GBS, BOUT++, GRILLIX, FELTOR…)
- But also possible need of **additional physics**
  - e.g.: kinetic effects, collisional sheath conditions…
- Very ambitious but **in-line with on-going local efforts**
  - See for ex., neutrals integration in turbulence codes
  - **Constructive interaction** with local efforts



[SOLEDGE2D, courtesy WEST team]



[GRILLIX, courtesy A. Stegmeir]

A challenging task

- Rough estimate of computing power needs:

$R \approx 10m,\ a \approx 3m,\ \Delta r \approx 10cm$

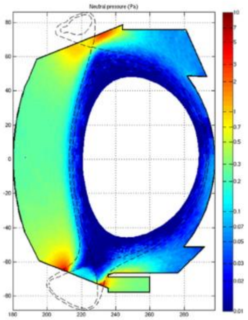
$\rho_L \approx 0.05 - 0.7\ mm\ (5eV - 1keV)$

$[3\ \times\ (>\ 20)\ ionized\ species] > 60\ fields$

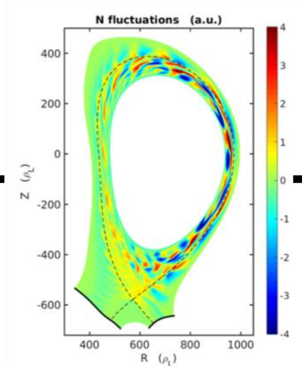
$> 2B\ dof$ per poloidal plane

$> 200B\ dof$ for 3D domain

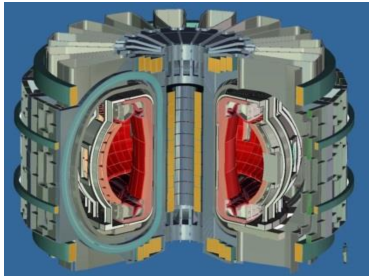
- Several orders of magnitude **larger than current record CFD simulation**



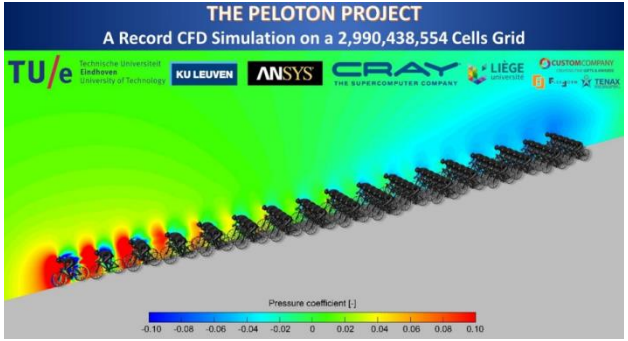
+



+

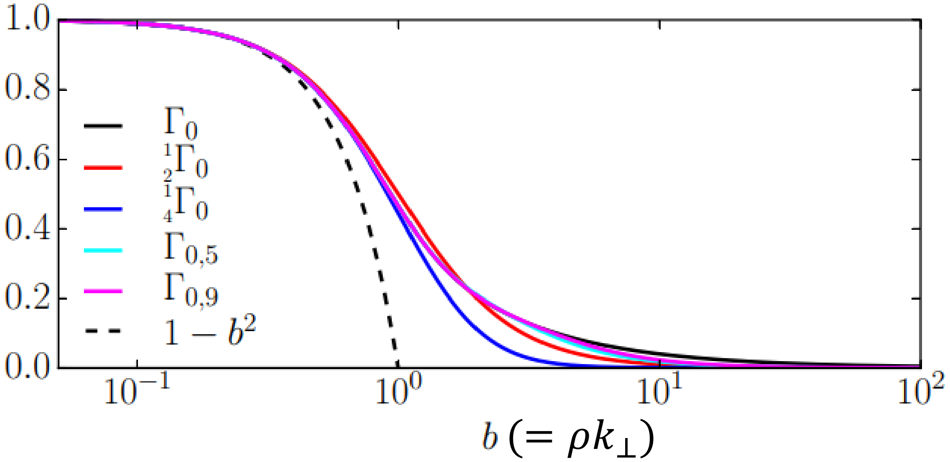


$\gg$



Closures in full-f gyro-fluid models

- Complementary development of **closures for full-f gyro-fluid models**
  - Closure based on **Padé-approximation** of FLR and polarization operators
  - Generalizes widely used δF Padé-model to full-f case
  - **Numerical implementation** under test in FELTOR code



[Held et al., NF 2020]

Review of BCs for fluid codes

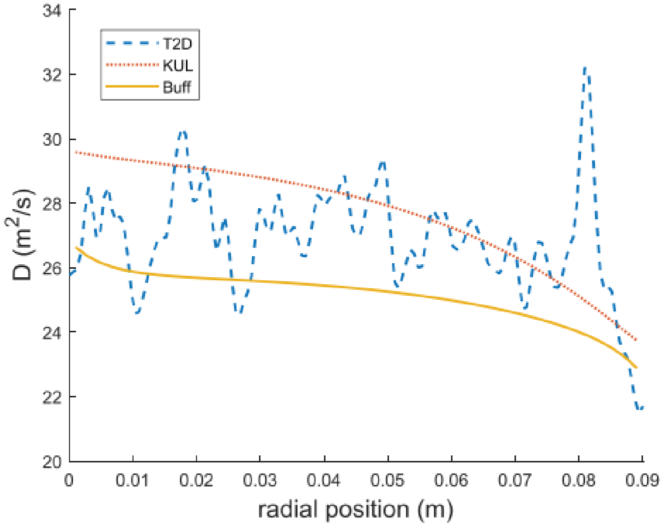
- Standard boundary conditions used in current fluid codes **not relevant for large range of reactor conditions**
  - low **collisionality** SOL, collisional sheath, **grazing** incidence, **multi-species** sheath…

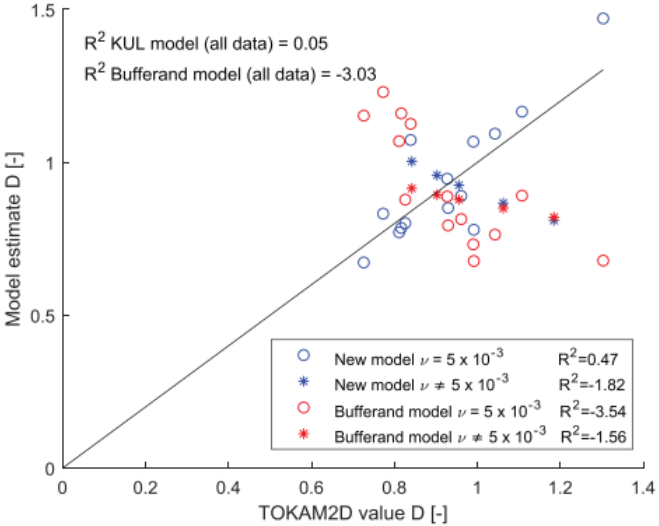
- **Review of literature** performed and compiled in internal report
  - Reports boundary conditions used in most current edge plasma codes
  - Identifies main weaknesses and margin for progress => **priorities for PIC code studies**
  - Proposes **first recommendations** for immediate improvement of BCs

$$V_{\parallel,i}^{SE} = C_{s,i} = \sqrt{\left(T_i^{SE} + Z_i T_e^{SE}\right)/m_i} \Rightarrow V_{\parallel,i}^{SE} = \sqrt{\left(T_i^{SE} + Z_i \frac{\partial \ln n_e}{\partial \ln n_i} T_e^{SE}\right)/m_i}$$

Modelling turbulence without DNS (3)

- **Analytical derivation of k-epsilon model** from fluid equation in 2D interchange turbulence model
  - Sets **theoretical foundations for heuristic model** developed at CEA
- Resulting 1D k-epsilon model able to capture radial transport in 2D slab interchange turbulence simulations





[Coosemans et al., PoP 2021]

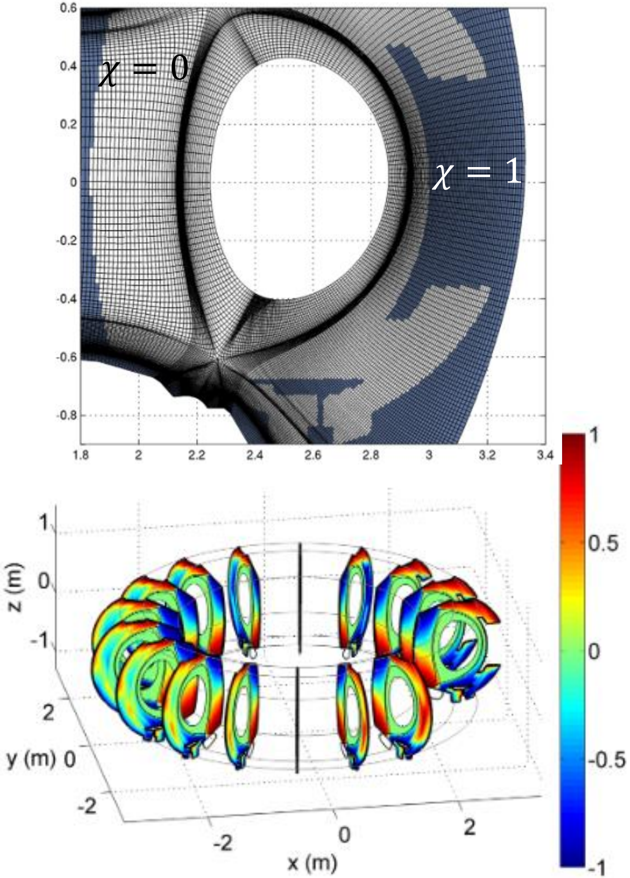
Development of immersed boundary conditions

- Inspired from CFD modelling, Bohm boundary conditions forced by **penalization method**
  - **Mask function χ** defines cells in the wall
  - Additional term forces wanted boundary conditions

$$\partial_t n_e + \vec{\nabla} \cdot (n_e \vec{u}) = S_n - \frac{\chi}{\eta_n} n_e$$

  - Successfully demonstrated in mean-field simulation, even 3D *[Bufferand et al., NME 2019]*
  - Open the way to use of cartesian structured mesh

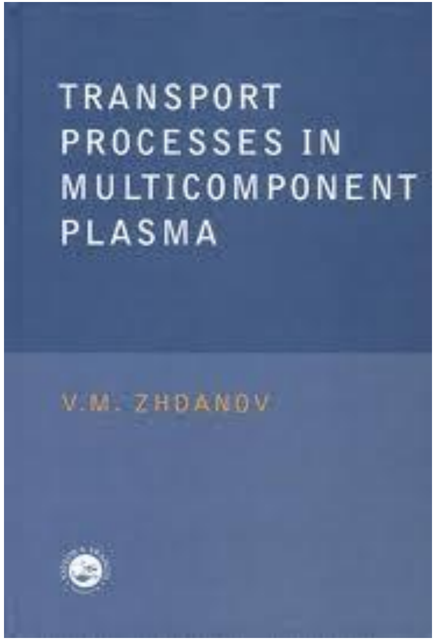
- **Open questions** remain on:
  - Generalization to vorticity equation (boundary condition on electrostatic potential)
  - Impact of having non smooth wall shape (stair-case): neutrals, numerical stability…



Multi-species treatment

- 3 distinct types of species:
  1. **Main ions**: D, T, possibly He => (gyro-)fluid model
  2. **Light impurities** => (gyro-)fluid model
  3. **Heavy impurities** => might require kinetic treatment

- For fluid approach, most advanced model = **Zdhanov**
  - generalization of Braginskii (no assumption on concentration or mass)
  - Use as **first milestone** but need to **test numerical implementation** in turbulence code before
  - In parallel, assess **possibility of moving full kinetic** for heavy impurities (could be fast on GPUs)



TRANSPORT PROCESSES IN MULTICOMPONENT PLASMA

V.M. ZHDANOV

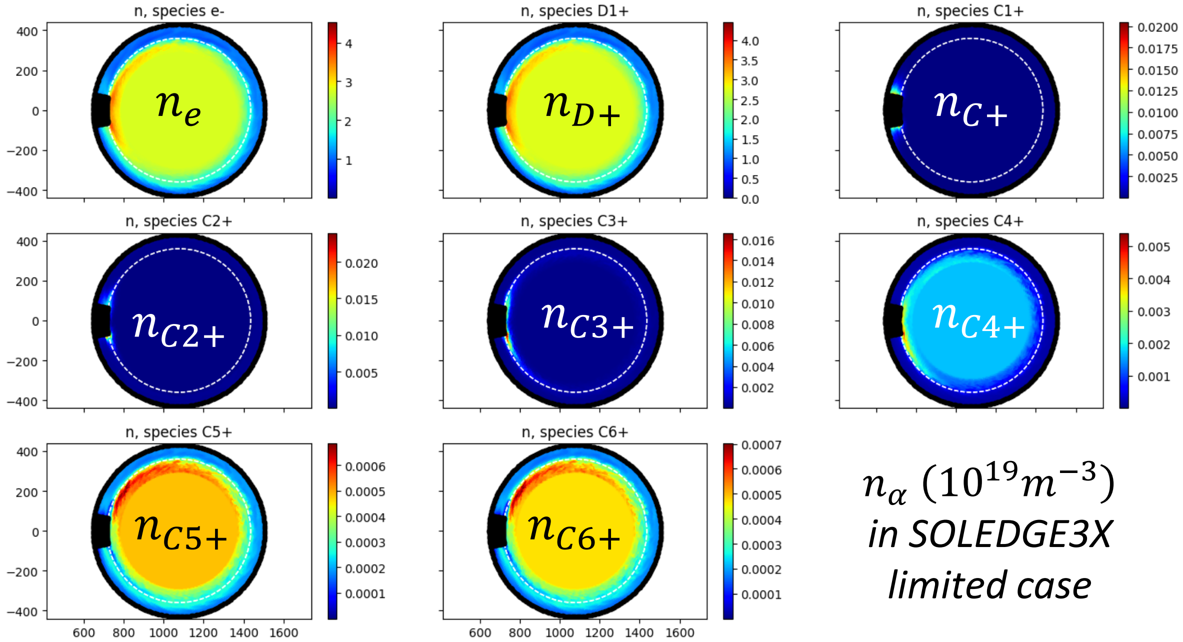
[Zdhanov, CRC Press (2002)]

Physics of impurities (1/2)

- Progress along 2 axes:
  1) Test of implementation of **Zhdanov closure** in 3D fluid turbulence code
  2) Investigation of implementation of self-consistent **2D turbulence multi-fluid model**

- Zhdanov closure **implemented in SOLEDGE3X-EIRENE**
  - Requires local solve of small dense linear system
  - Costly (as much as other explicit terms) but **no major difficulty**

[H. Bufferand et al., in prep.]



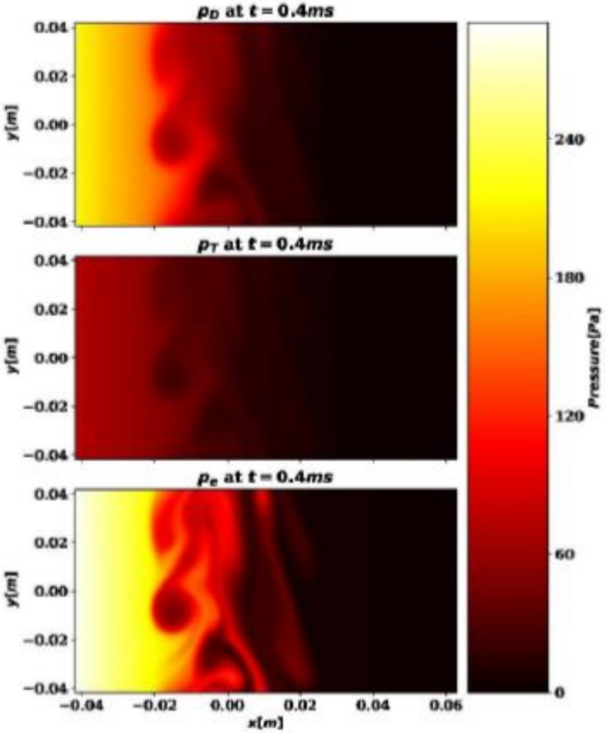
$n_\alpha\ (10^{19} m^{-3})$
in SOLEDGE3X
limited case

Physics of impurities (2/2)

- **Multi-species turbulent model** implemented and running in miHESEL
  - Self-consistent conservation of particle and energy balance requires inversion of **non-linear mass-matrix coupling all fields**!

$$\begin{pmatrix} -\Sigma_\alpha a_\alpha \mu_\alpha \nabla^2 & -\frac{\mu_1}{Z_1}\nabla^2 & -\frac{\mu_2}{Z_2}\nabla^2 & \cdots \\ -\frac{\mu_1}{Z_1}\nabla^2 & \frac{3}{2}\frac{1}{p_1} - \frac{\mu_1}{Z_1^2 a_1}\nabla^2 & 0 & \\ -\frac{\mu_2}{Z_2}\nabla^2 & 0 & \frac{3}{2}\frac{1}{p_2} - \frac{\mu_2}{Z_2^2 a_2}\nabla^2 & \\ \vdots & & & \ddots \end{pmatrix} \cdot \begin{pmatrix} \partial_t \phi \\ \partial_t p_1 \\ \partial_t p_2 \\ \vdots \end{pmatrix} = \cdots$$

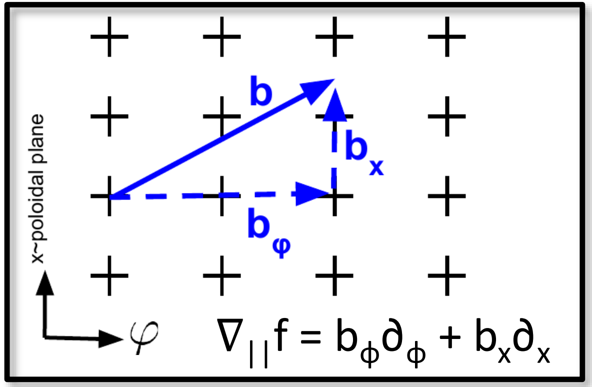
  - Very cumbersome to code and might be a show-stopper in terms of performances
  - Need to **investigate alternative methods**

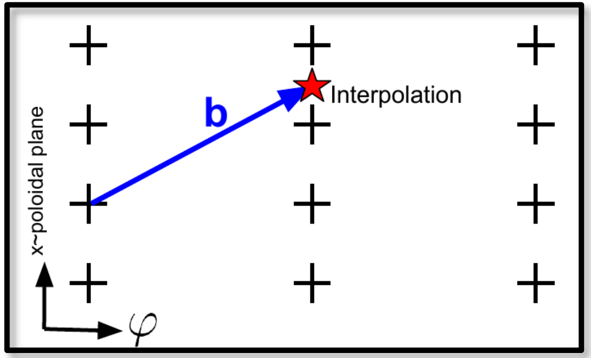


Parallel discretization (1/2)

- **2 options** on the table for **2 apparently contradictory demands**

	Description of field aligned structures (filaments)	Description of wall geometry and non-aligned structures (e.g., recycling)
FCI (projection-interpolation) method	+	**Discretization of BCs? Cost?**
High-order **non-aligned** schemes	**Cost?**	+

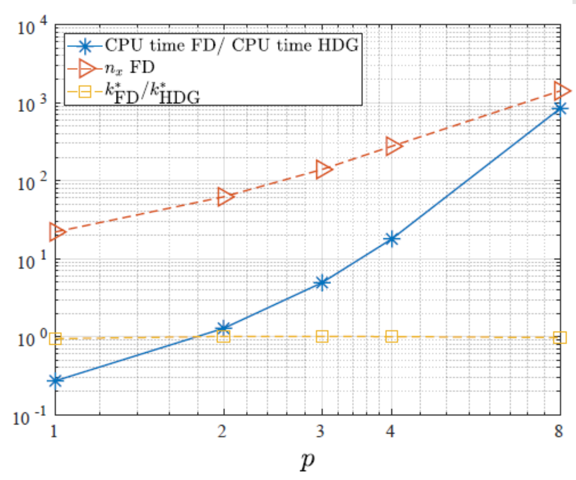




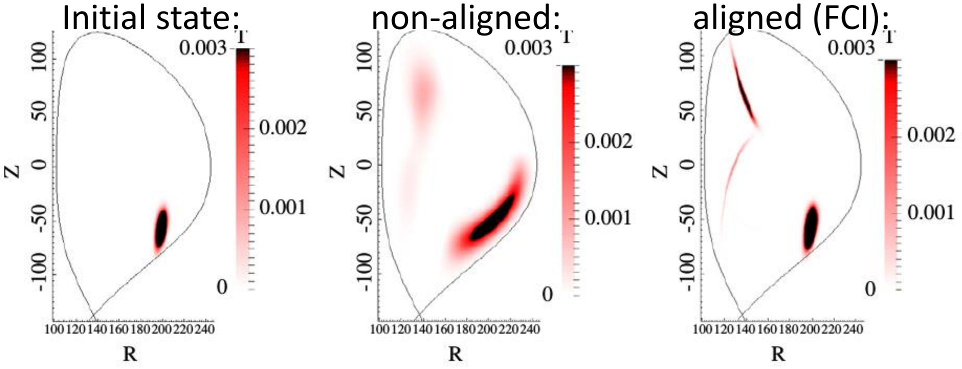
Parallel discretization (2/2)

- 2 actions on-going:
  1) **Evaluate both schemes** for aligned and non-aligned structures (“benchmark”)
  2) **Develop method** to treat boundary conditions with FCI in arbitrary wall geometry

- **Evaluation performed** in individual codes
  - **High-order (p=8) allows to recover precision** while keeping cpu time reasonnable



[G. Giorgiani et al., CPC 2020]



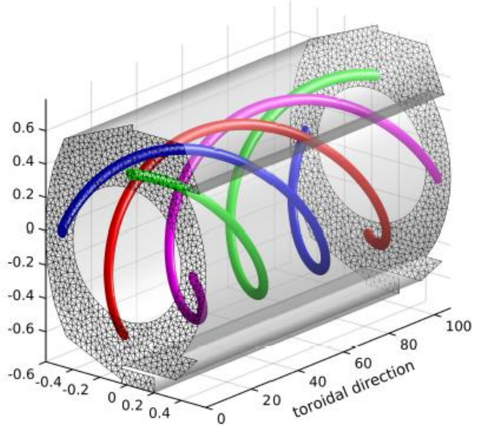
[FELTOR]

Parallel discretization (2/2)

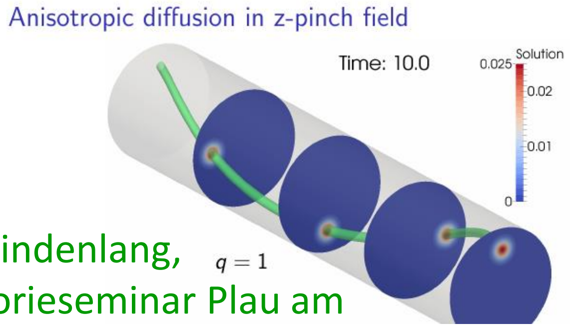
- 2 actions on-going:
  1) **Evaluate both schemes** for aligned and non-aligned structures (“benchmark”)
  2) **Develop method** to treat boundary conditions with FCI in arbitrary wall geometry

- **Evaluation performed** in individual codes
  - **High-order (p=8) allows to recover precision** while keeping cpu time reasonnable

- Benchmark started for **cross-code comparison**
  - Tools used: GRILLIX, FELTOR, SOLEDGE-HDG
  - Anisotropic diffusion in periodic Z-pinch → assess numerical diffusion vs cpu cost / stiffness



[G. Giorgiani et al., submitted to CPC]



[F. Hindenlang, Theorieseminar Plau am See, 2015]