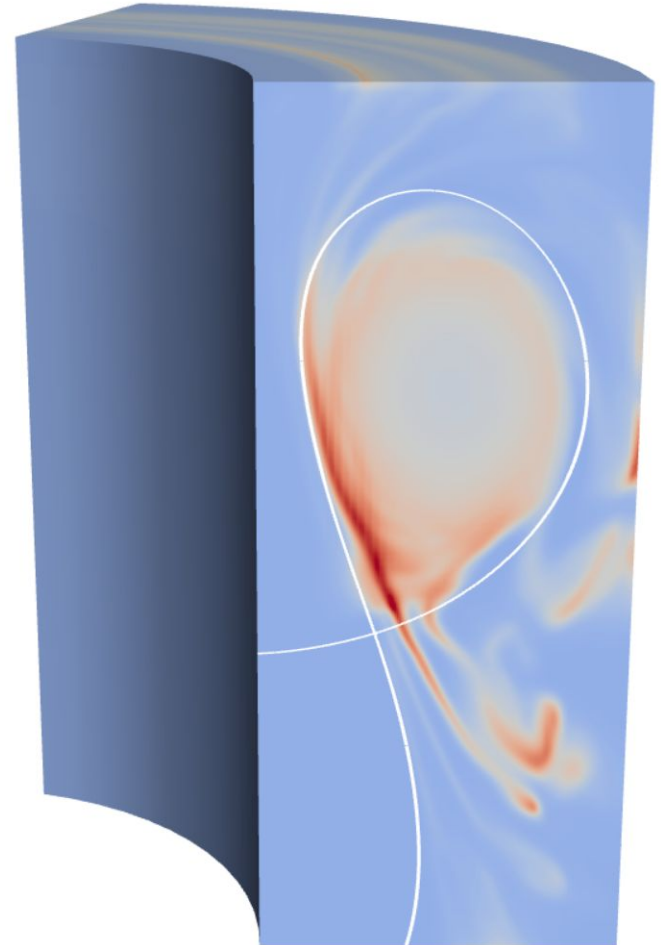


KINetic Deterministic NEutral Solver (KINDNES) - Library status and first benchmark vs EIRENE

D. Mancini, B. de Lucca, G. Drago, E. Lanti, P. Ricci
and the GBS team



Plasma simulations need a self-consistent fast neutral model

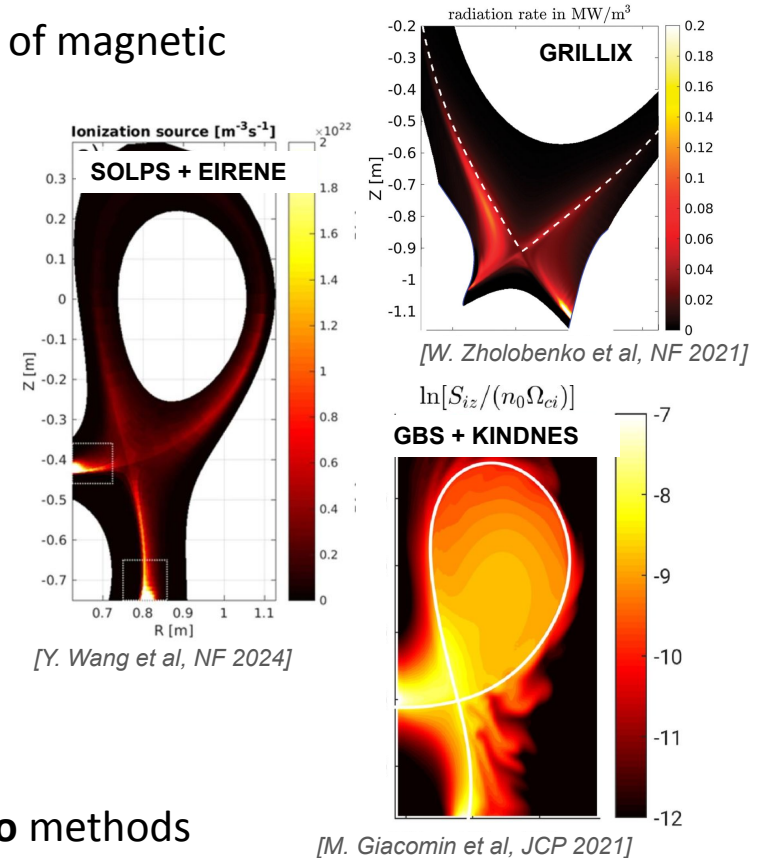
Accurate description of neutral dynamics at the boundary of magnetic confinement devices is fundamental to understand:

- Plasma recycling at the wall and heat exhaust
- Dissipative regimes like detachment [D. Mancini et al, NF 2024] or XPR [K. Eder et al, ArXiv 2025]
- Interplay between neutrals and **plasma turbulence** [C. Wersal et al, NF 2017]

Neutral codes are typically divided between:

- Fluid models (Hermes, nHesel, SolEdge2D, Grillix)
- Kinetic Monte Carlo models (Eirene, Degas2)

KINDNES allows a **kinetic** description **without Monte Carlo** methods

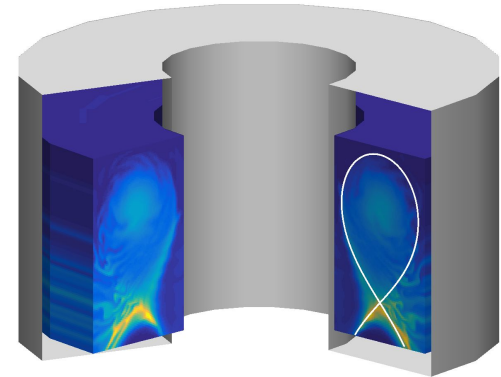
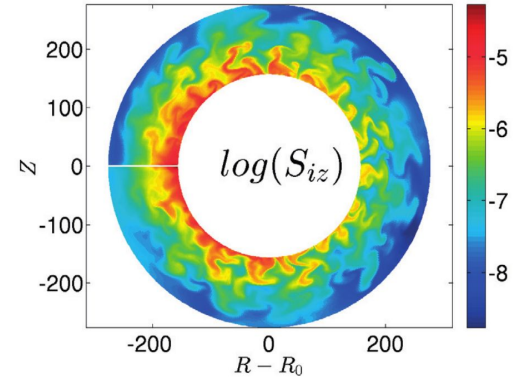


KINDNES born inside GBS, now a standalone library

Model born as an easy neutral solver inside GBS:

- First version thought on cartesian grid (same as GBS) and tested in limited scenario [C. Wersal et al, NF 2015]
- Used for **realistic sources** in turbulence simulations and **GPI synthetic diagnostic** [C. Wersal et al, NF 2017]
- Extended to diverted scenarios [D. Mancini et al, NF 2021] and multiple neutral species [A. Corrado et al, NF 2022]
- Qualitative agreement of density shoulder formation, detachment and turbulence diagnostics results [D. Mancini et al, PPCF 2026]

Now **KINDNES** is developed as a **standalone library** and quantitatively compared to EIRENE



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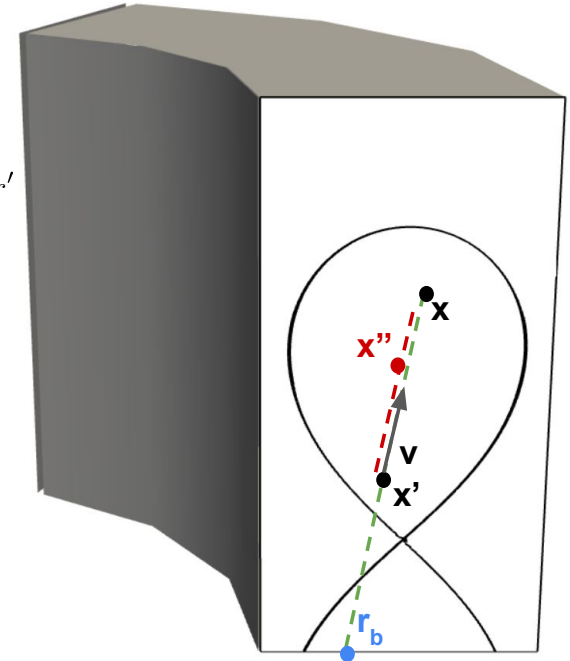
- **The basic elements of the model:**
 - Method of characteristics for kinetic neutrals
 - Solving on discrete grid
- The benchmark against EIRENE:
 - Status of KINDNES library
 - Comparison with EIRENE solution

Solution based on deterministic algorithm avoiding statistical noise of Monte Carlo methods

$$\frac{\partial f_D}{\partial t} + \mathbf{v} \cdot \frac{\partial f_D}{\partial \mathbf{x}} = -\nu_{iz} f_D - \nu_{cx} \left(f_D - \frac{n_D}{n_{D^+}} f_{D^+} \right) + \nu_{rec} f_{D^+}$$

Formal solution with method of characteristics
(neutrals move on straight paths):

$$f_D(\mathbf{x}, \mathbf{v}, t) = \int_0^{r_b} \left[\frac{S_D(\mathbf{x}', \mathbf{v}, t)}{v} + \delta(r' - r'_b) f_D(\mathbf{x}'_b, \mathbf{v}, t'_b) \right] \exp \left(-\frac{1}{v} \int_0^{r'} \nu_{\text{eff}, D}(\mathbf{x}'', t'') dr'' \right) dr'$$



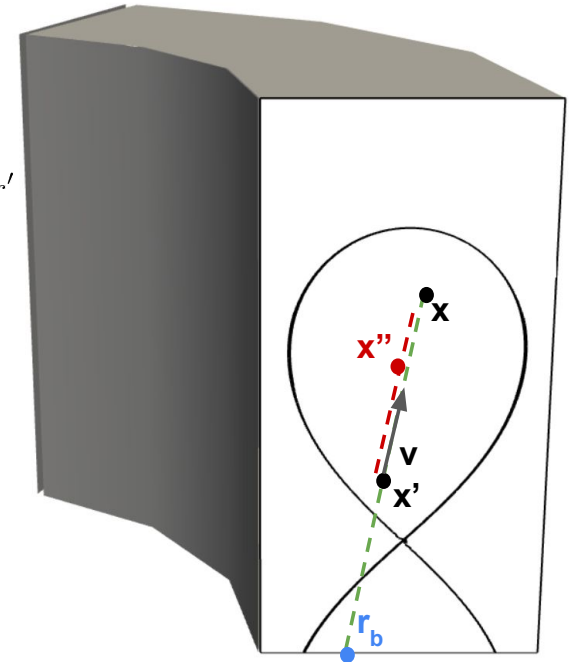
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- Volumetric source $S_D = \nu_{cx} n_D \frac{f_{D^+}}{n_{D^+}} + \nu_{rec} f_{D^+}$
- Boundary condition
- Decay rate $\nu_{\text{eff}, D} = \nu_{iz} + \nu_{cx}$



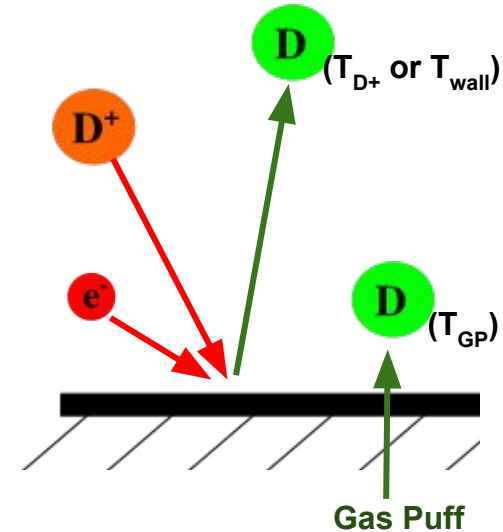
Boundary conditions describe emission, reflection and puffing

For the points on the boundary $\mathbf{x}_b$:

$$f_D(\mathbf{x}_b, \mathbf{v}) = (1 - \alpha_{\text{refl}}) \Gamma_{\text{out}} \chi_{\text{in}}(\mathbf{x}_b, \mathbf{v}) \\ + \alpha_{\text{refl}} [f_D(\mathbf{x}_b, \mathbf{v} - 2\mathbf{v}_\perp) + f_{D^+}(\mathbf{x}_b, \mathbf{v} - 2\mathbf{v}_\perp)] \\ + \Gamma_{\text{GP}, D} \chi_{\text{GP}}(\mathbf{x}_b, \mathbf{v})$$

Boundary condition at the wall describes:

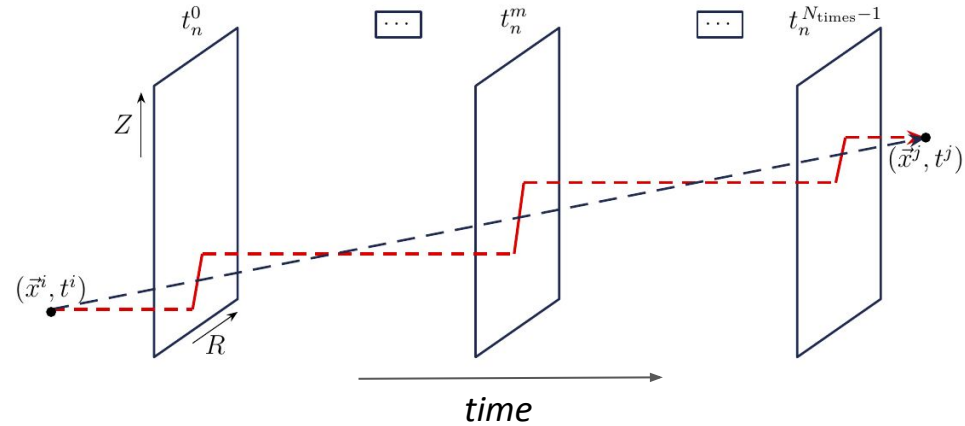
- Neutral recycling due to **ion** and **neutral** flux to the wall $\Gamma_{\text{out}} = \Gamma_{\text{out}, D} + \Gamma_{\text{out}, D^+}$
- Reflection (ion temperature) and re-emission (χ_{in})
- Additional sources like gas puff (χ_{GP})



Solution of the model recently extended for the general case

The formal solution of KINDNES model can be written without approximations:

- Neutral dynamics in 3D
[G. Drago, EPFL master thesis, 2025]
- Plasma evolves together with the neutrals [M. Szony, EPFL master thesis, 2026]
- First KINDNES paper with complete model in preparation by G. Drago



Typical KINDNES run exploits :

- Neutral adiabatic regime $1/\nu_{\text{eff}} < \tau_{\text{turb}} \longrightarrow \partial_t f_D = 0$
- Turbulence anisotropy $\lambda_{\text{mfp},D} \ll 1/k_{\parallel} \longrightarrow$ System solved plane by plane

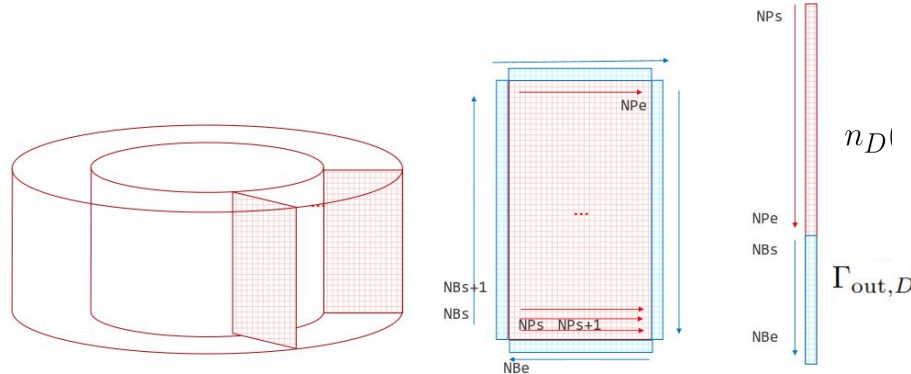
Model solved plane by plane on discrete grid

$$n_D(\mathbf{x}) = \int_{\Sigma} n_D(\mathbf{x}') \nu_{cx}(\mathbf{x}') K_{p \rightarrow p}(\mathbf{x}, \mathbf{x}') d\Sigma + \int_{\partial\Sigma} \Gamma_{\text{out},D}(\mathbf{x}'_b) K_{b \rightarrow p}(\mathbf{x}, \mathbf{x}'_b) d\sigma_b + n_{D,\text{rec}}(\mathbf{x}) + n_{D,\text{GP}}(\mathbf{x})$$

$$\Gamma_{\text{out},D}(\mathbf{x}_b) = \int_{\Sigma} n_D(\mathbf{x}') \nu_{cx}(\mathbf{x}') K_{p \rightarrow b}(\mathbf{x}_b, \mathbf{x}') d\Sigma + \int_{\partial\Sigma} \Gamma_{\text{out},D}(\mathbf{x}'_b) K_{b \rightarrow b}(\mathbf{x}_b, \mathbf{x}'_b) d\sigma_b + \Gamma_{\text{out},\text{rec}}(\mathbf{x}_b) + \Gamma_{\text{out},D+}(\mathbf{x}_b) + \Gamma_{\text{out},\text{GP}}(\mathbf{x}_b)$$

Discretized as a system on a linearized grid:

$$\begin{bmatrix} n_D \\ \Gamma_{\text{out},D} \end{bmatrix} = \begin{bmatrix} \nu_{cx} K_{pp} & K_{bp} \\ \nu_{cx} K_{pb} & K_{bb} \end{bmatrix} \begin{bmatrix} n_D \\ \Gamma_{\text{out},D} \end{bmatrix} + \begin{bmatrix} n_{D,\text{rec}} + n_{D,\text{GP}} \\ \Gamma_{\text{out},\text{rec}} + \Gamma_{\text{out},D+} + \Gamma_{\text{out},\text{GP}} \end{bmatrix}$$



Model solved plane by plane on discrete grid

Discretized as a system on a linearized grid:

$$\underbrace{\begin{bmatrix} n_D \\ \Gamma_{\text{out},D} \end{bmatrix}}_{\mathbf{x}} = \underbrace{\begin{bmatrix} \nu_{cx} K_{pp} & K_{bp} \\ \nu_{cx} K_{pb} & K_{bb} \end{bmatrix}}_K \underbrace{\begin{bmatrix} n_D \\ \Gamma_{\text{out},D} \end{bmatrix}}_{\mathbf{x}} + \underbrace{\begin{bmatrix} n_{D,\text{rec}} + n_{D,\text{GP}} \\ \Gamma_{\text{out},\text{rec}} + \Gamma_{\text{out},D+} + \Gamma_{\text{out},\text{GP}} \end{bmatrix}}_{\mathbf{b}}$$

- Neutral density from linear system inversion for each plane: $(\mathbb{1} - K) \mathbf{x} = \mathbf{b}$
- Integrating the previous equation for other moments yields $\mathbf{\Gamma}_{D,\perp}, \mathbf{\Gamma}_{D,\parallel}, T_D$

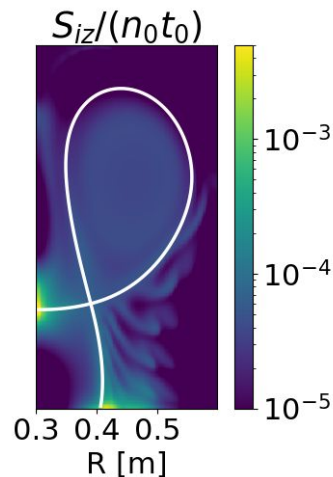
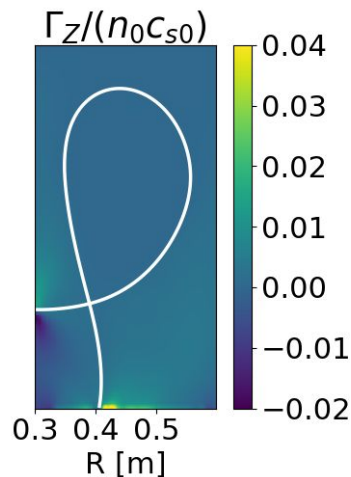
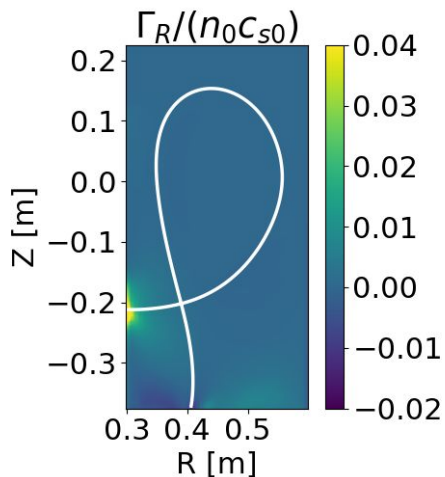
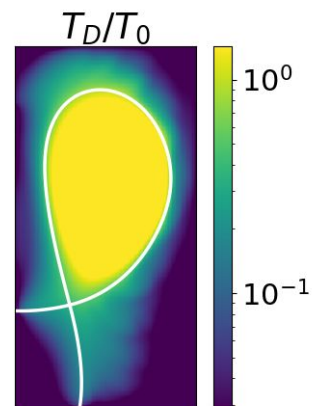
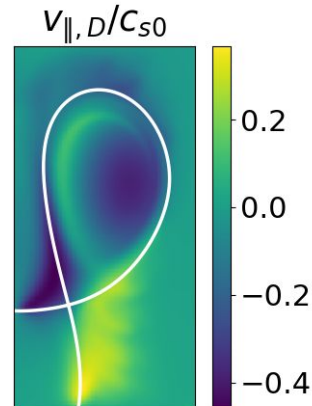
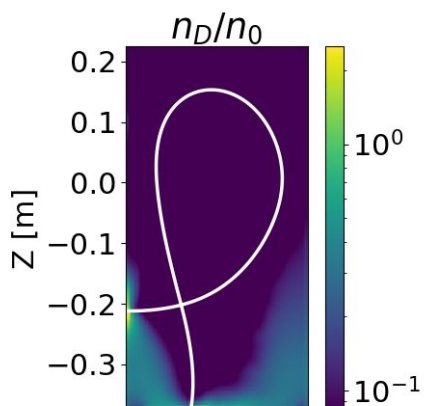
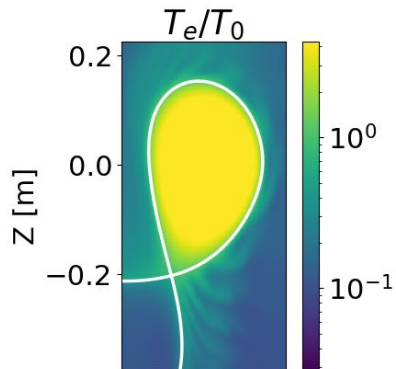
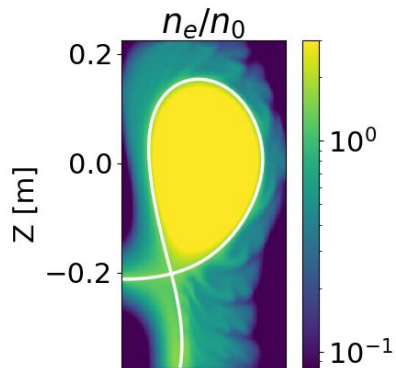
Implementation:

- Easy iterative solver with Petsc libraries → Advanced solver with HM method
- Highly parallelizable

[M. Guido et al, JCP 2026]

Neutral density solution reflects plasma fluctuations

Background plasma:



Index

- The basic elements of the model:
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- **The benchmark against EIRENE:**
 - Status of KINDNES library
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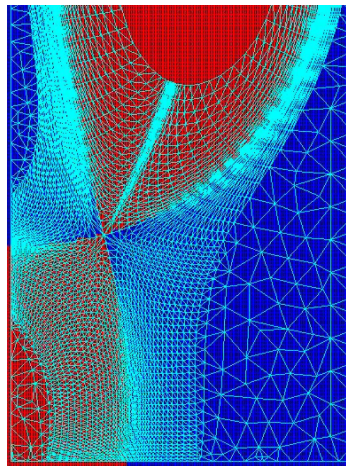
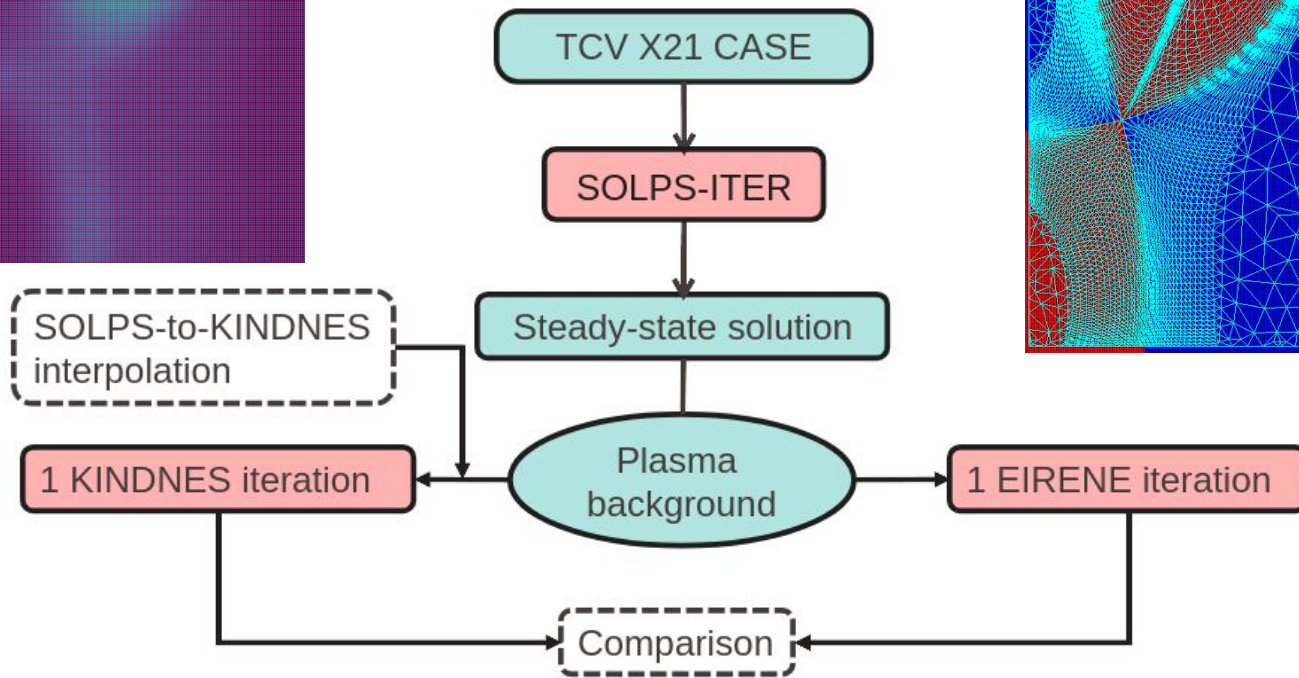
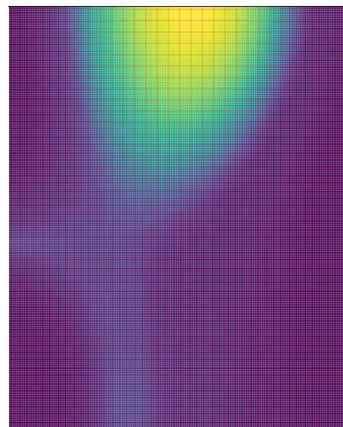
EIRENE limited to KINDNES physics implemented in the library

Some KINDNES features still moving from GBS to the new library:

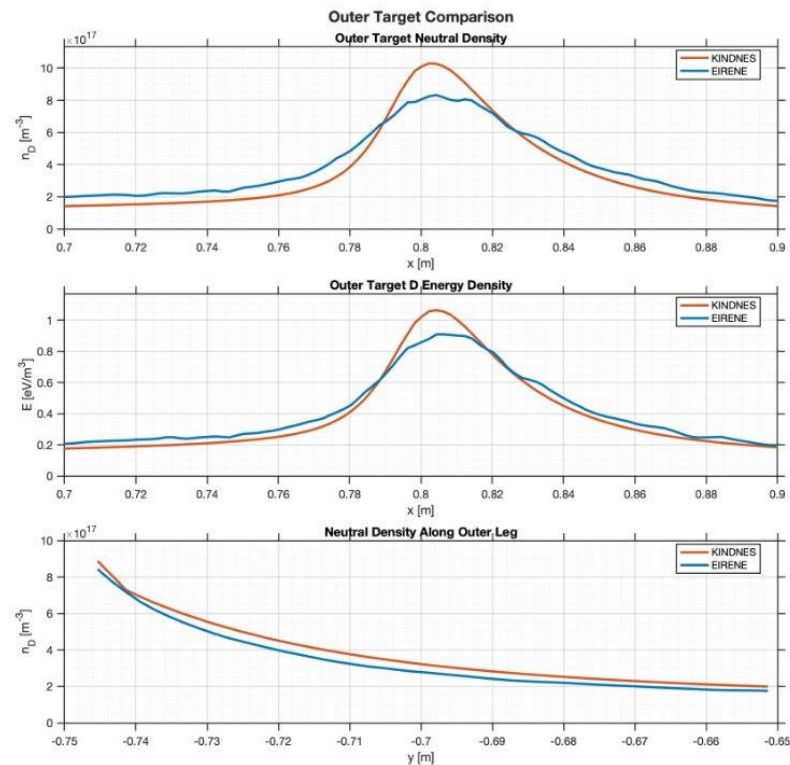
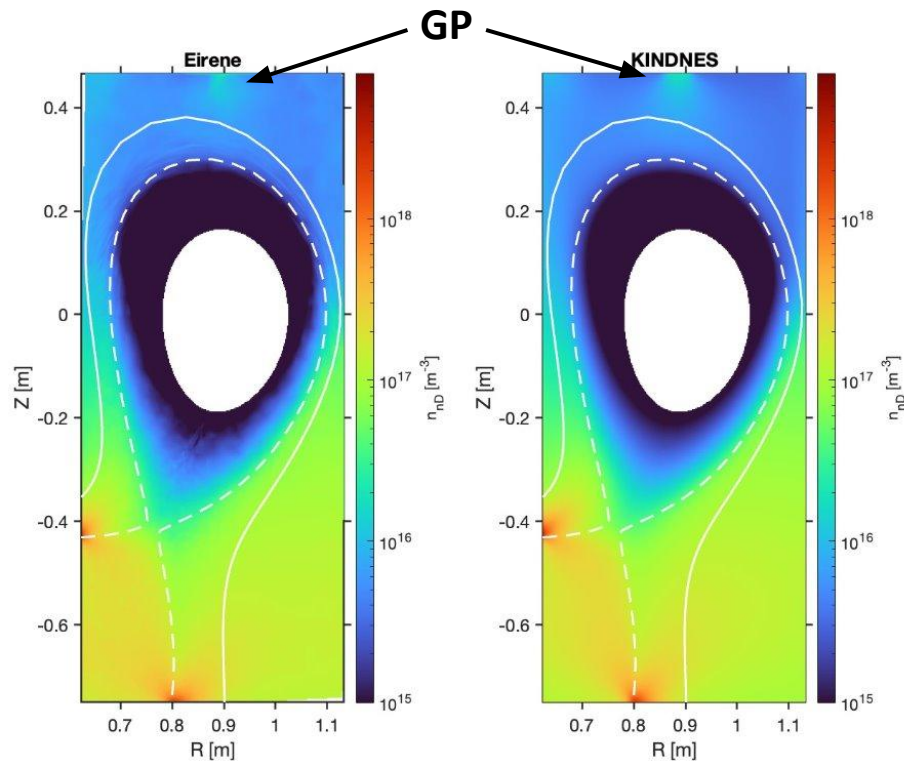
	Species	Fast reflections	Wall geometry	Reactions	Recycling
EIRENE	Multiple	Sheath acc. + TRIM	Flexible	AMJUEL/ HYDHEL	End of plasma mesh
GBS	D, D ₂	Specular reflection	Flexible	AMJUEL/ HYDHEL	On the wall
KINDNES (library)	D	Specular reflection (testing)	Rectangular wall	AMJUEL/ HYDHEL	On the wall

Benchmark uses only one species, without fast reflections, with rectangular wall

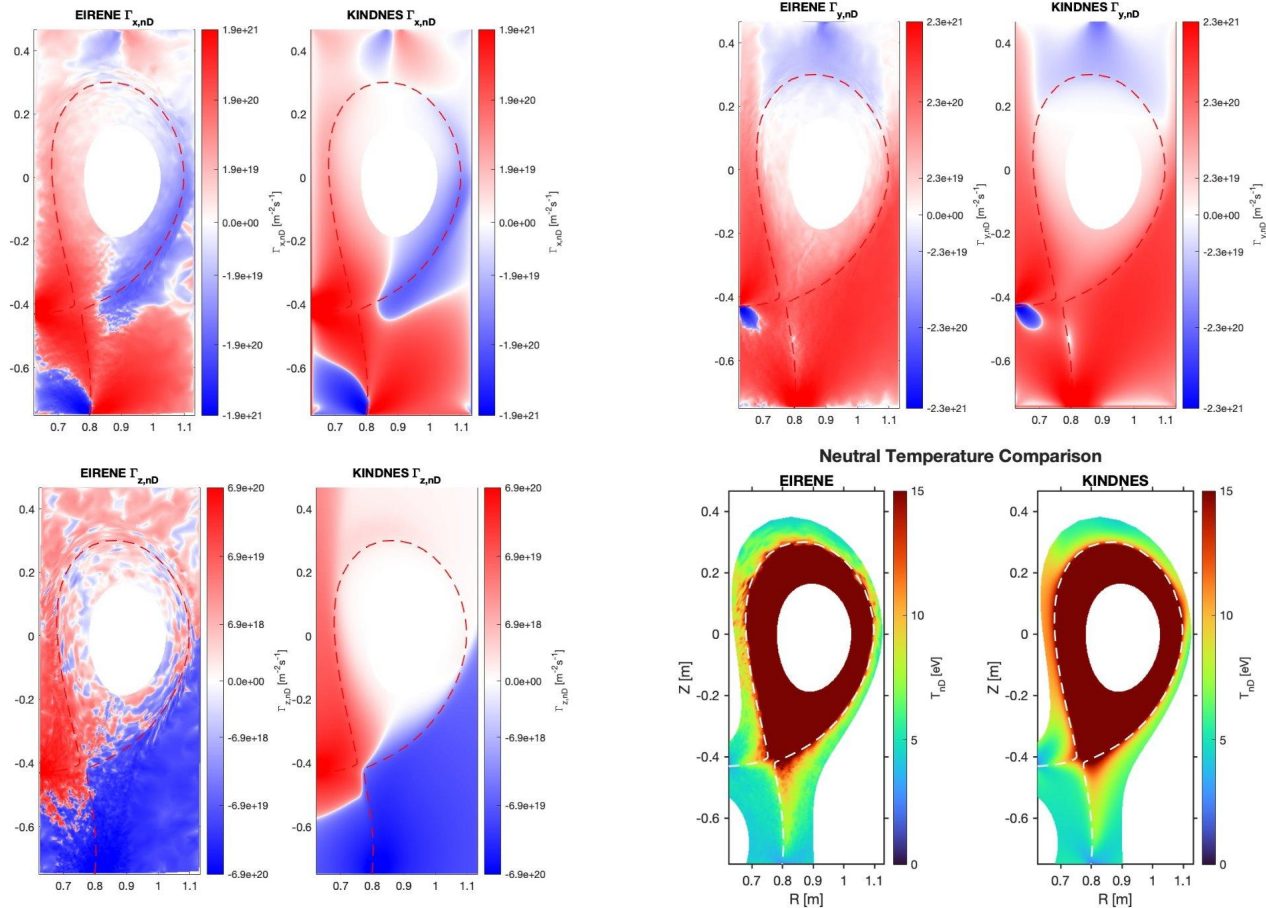
Benchmark based on SOLPS solution for TCV-X21 scenario



Very good agreement for neutral density



Agreement between the two codes up to EIRENE's numerical noise

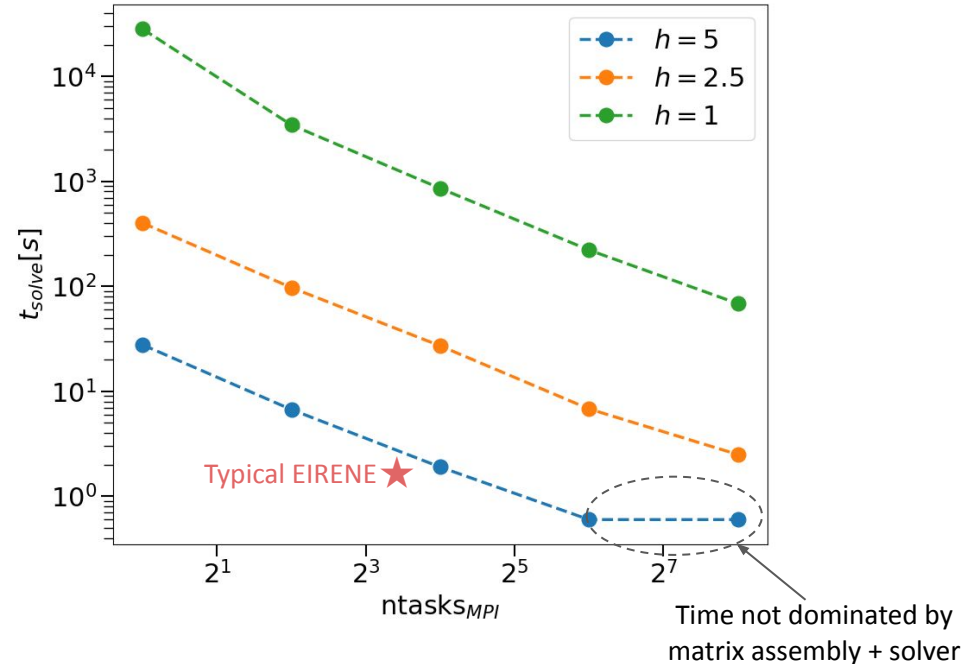
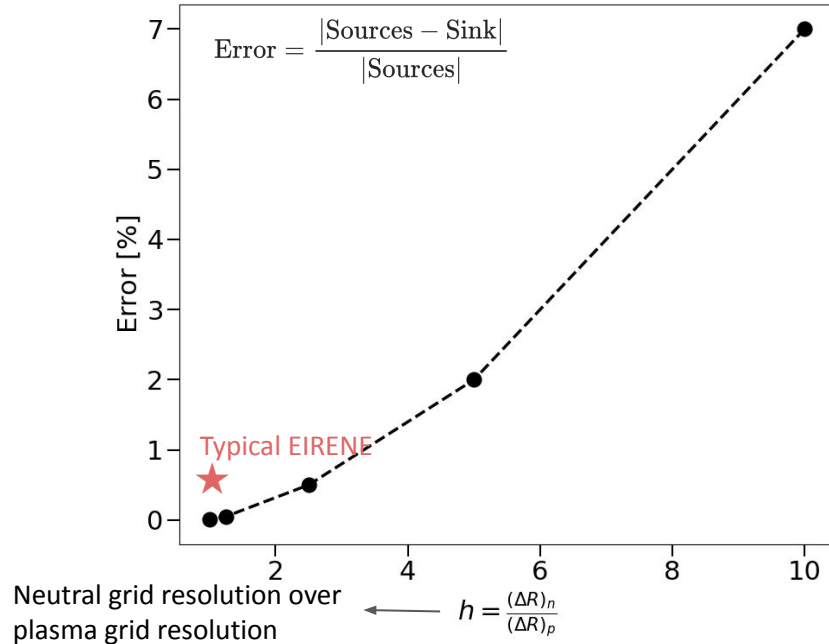


Different way to treat
cx introduces some
differences



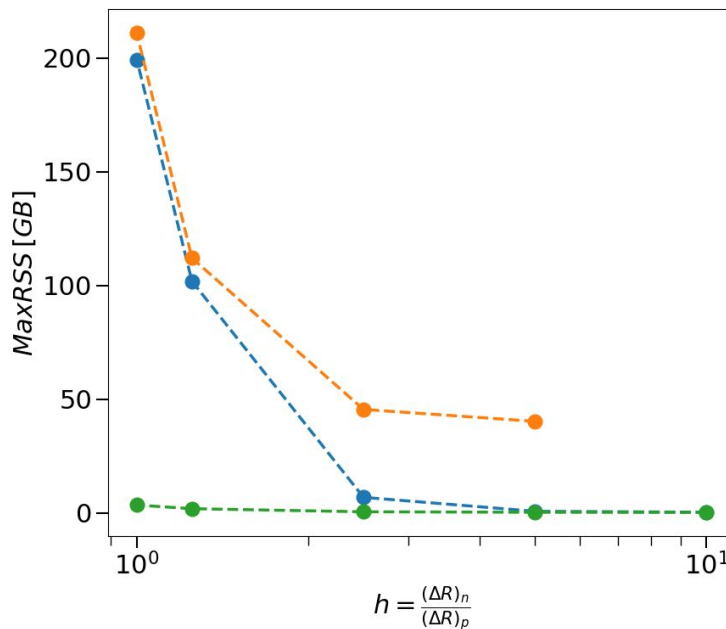
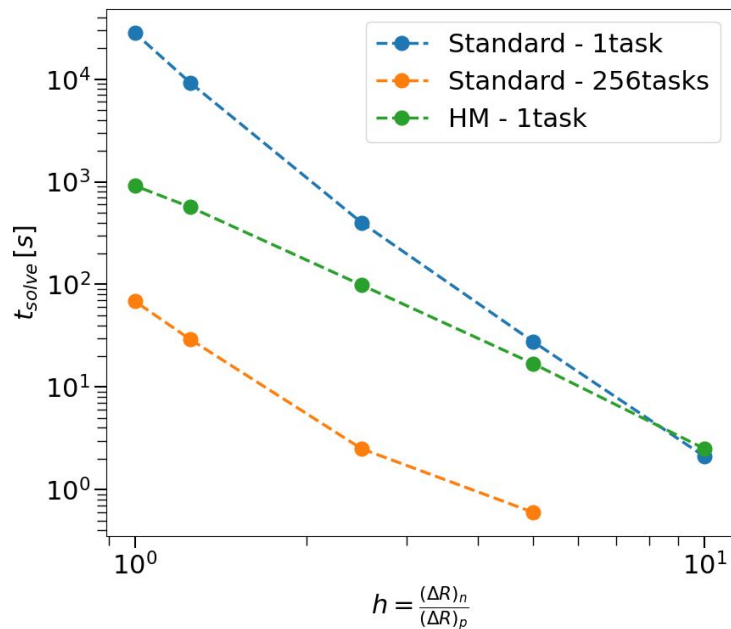
KINDNES timings scale well with increasing number of MPI tasks

Tests performed with benchmark case, on 1 Pitagora node



- The error decreases with mesh refinement, while solving time increases
- KINDNES is not limited in the parallelization (scales well up to $t_{\text{solve}} < 0.6\text{s}$)

New HM solver strongly reduces memory usage and timing



Approximation of most of the matrix elements leads to reduced solver time and memory usage $\longrightarrow$ Parallelization of the method still on-going

Conclusions

KINDNES enables self-consistent **kinetic neutrals** simulations without Monte Carlo noise:

- The model describes **neutral recycling**, reflection and re-emission at the wall, together with all the **most relevant reactions** in the boundary of magnetic fusion devices (ionization, charge-exchange, recombination)
- It is possible to extend it with **any** neutral **species**, selecting the relevant reactions (increase of memory usage)
- Implementation **highly parallelizable** on CPU solver shows good scalability with increasing MPI tasks
- **Standalone library created**, verified and tested
- Testing of the library shows **good agreement with EIRENE** simulation

Ongoing work

- Finish porting all GBS features in the library (flexible grid, additional species)
- Parallelize HM method to decrease solver timing

Extension to multiple species: adding molecular Deuterium D_2

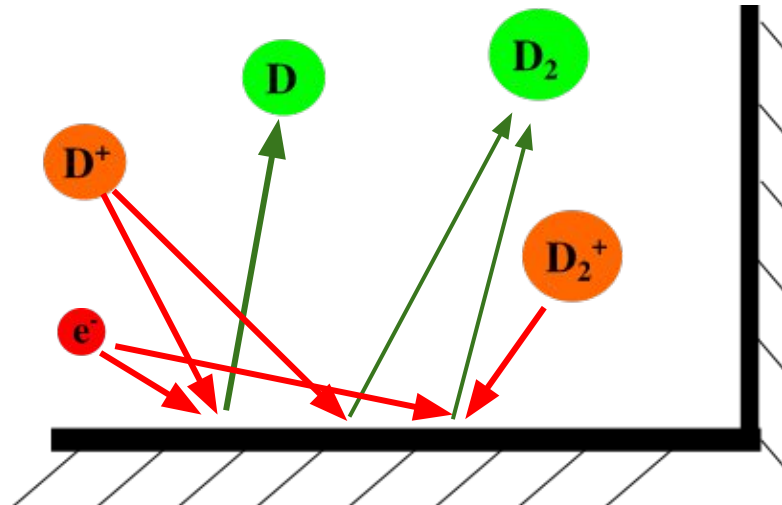
Two coupled PDEs:

$$\frac{\partial f_{D^+}}{\partial t} + \mathbf{v} \cdot \frac{\partial f_{D^+}}{\partial \mathbf{x}} = \nu_{iz,D} f_D - \nu_{rec,D^+} f_{D^+} - \nu_{cx,D} \left(\frac{n_D}{n_{D^+}} f_{D^+} - f_D \right) + \nu_{cx,D-D_2^+} f_D - \nu_{cx,D_2-D^+} \frac{n_{D_2}}{n_{D^+}} f_{D^+} + \dots$$

$$\frac{\partial f_{D_2^+}}{\partial t} + \mathbf{v} \cdot \frac{\partial f_{D_2^+}}{\partial \mathbf{x}} = \nu_{iz,D_2} f_{D_2} - \nu_{rec,D_2^+} f_{D_2^+} - \nu_{cx,D_2} \left(\frac{n_{D_2}}{n_{D_2^+}} f_{D_2^+} - f_{D_2} \right) - \nu_{cx,D_2-D^+} f_{D_2} - \nu_{cx,D-D_2^+} \frac{n_D}{n_{D_2^+}} f_{D_2^+} + \dots$$

Boundary conditions:

- Neutral recycling due to total ion flux to the wall (including **parallel** and **drift velocity**)
- Reflection, re-emission, and association



Extension to multiple species: adding molecular Deuterium D_2

$$\frac{\partial f_{D^+}}{\partial t} + \mathbf{v} \cdot \frac{\partial f_{D^+}}{\partial \mathbf{x}} = \nu_{iz,D} f_D - \nu_{rec,D^+} f_{D^+} - \nu_{cx,D} \left(\frac{n_D}{n_{D^+}} f_{D^+} - f_D \right) + \nu_{cx,D-D_2^+} f_D - \nu_{cx,D_2-D^+} \frac{n_{D_2}}{n_{D^+}} f_{D^+} + \dots$$

$$\frac{\partial f_{D_2^+}}{\partial t} + \mathbf{v} \cdot \frac{\partial f_{D_2^+}}{\partial \mathbf{x}} = \nu_{iz,D_2} f_{D_2} - \nu_{rec,D_2^+} f_{D_2^+} - \nu_{cx,D_2} \left(\frac{n_{D_2}}{n_{D_2^+}} f_{D_2^+} - f_{D_2} \right) - \nu_{cx,D_2-D^+} f_{D_2} - \nu_{cx,D-D_2^+} \frac{n_D}{n_{D_2^+}} f_{D_2^+} + \dots$$

The neutral densities can be obtained by inverting a large linear system:

$$\begin{pmatrix} n_D \\ \Gamma_{out,D} \\ n_{D_2} \\ \Gamma_{out,D_2} \end{pmatrix} = \underbrace{\begin{pmatrix} M_{11} & M_{12} & M_{13} & 0 \\ M_{21} & M_{22} & M_{23} & 0 \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{pmatrix}}_{\text{Interactions with plasma (cx, iz, diss)}} \begin{pmatrix} n_D \\ \Gamma_{out,D} \\ n_{D_2} \\ \Gamma_{out,D} \end{pmatrix} + \underbrace{\begin{pmatrix} n_D^{rec,D^+} + n_D^{diss,D_2^+} \\ \Gamma_D^{rec,D^+} + \Gamma_{out,D}^{D^+} \Gamma_D^{refl,D^+} \\ n_{D_2}^{rec,D^+} \\ \Gamma_{D_2}^{rec,D_2^+} + \Gamma_{D_2}^{refl,D_2^+} \Gamma_{D_2}^{refl,D^+} \end{pmatrix}}_{\text{Neutrals from rec, diss and puffing}}$$

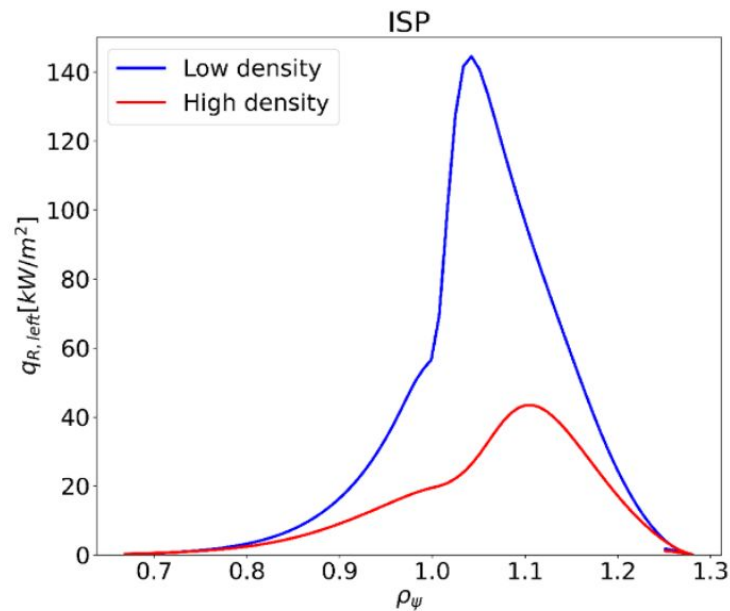
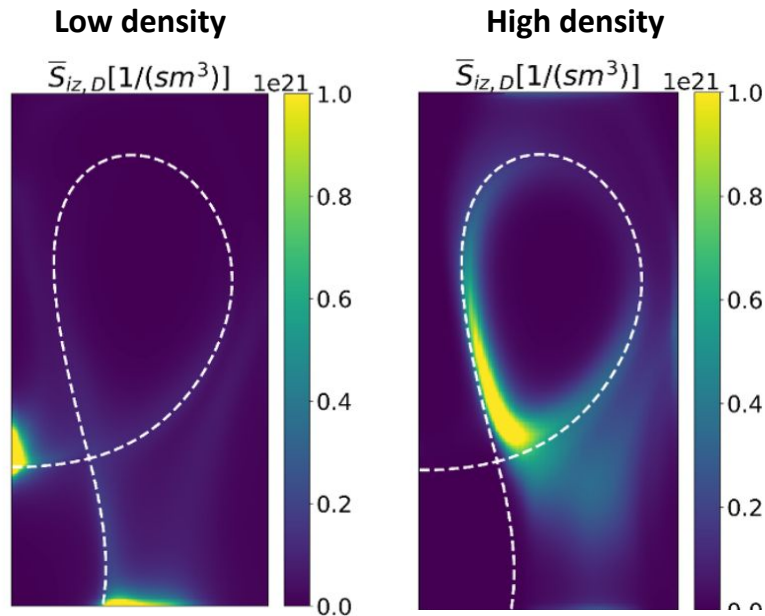
Interactions with plasma
(cx, iz, diss)

Neutrals from rec, diss and puffing

GBS simulations of detached plasma with molecules

Going from low to high density:

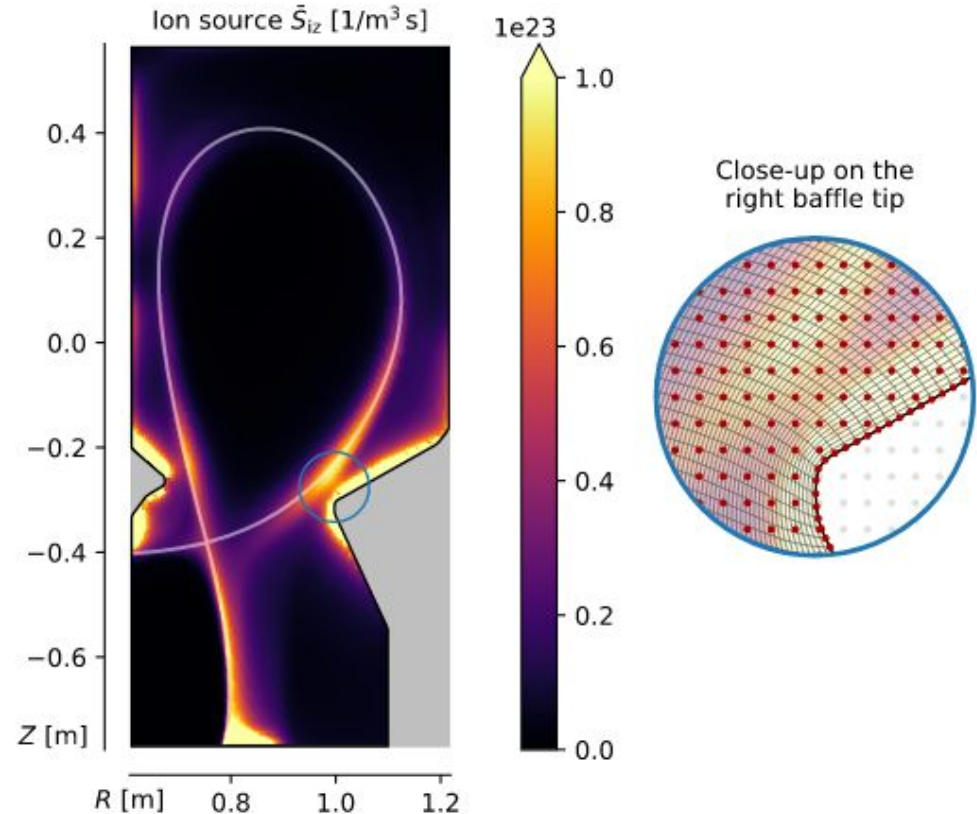
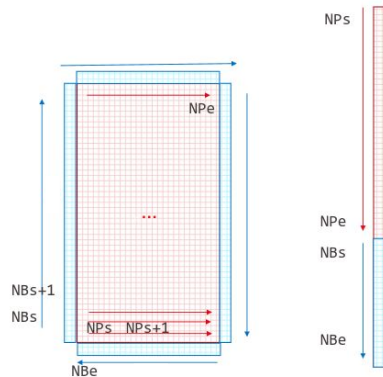
- Ionization front moves in the core
- Strong decrease of heat flux at the inner strike point (ISP) $\rightarrow$ detachment of inner target



Flexible wall geometry

Implementation on arbitrary boundary
+ cartesian grid:

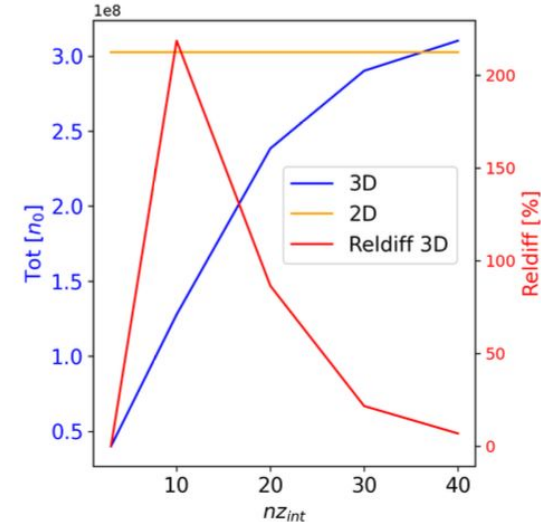
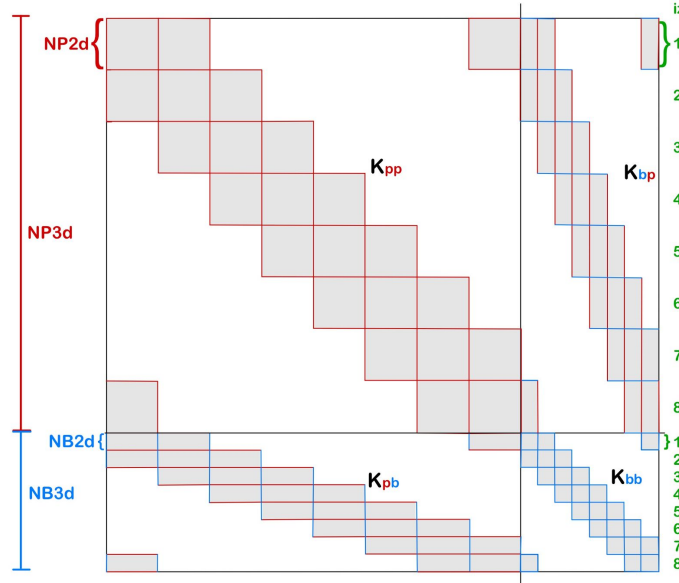
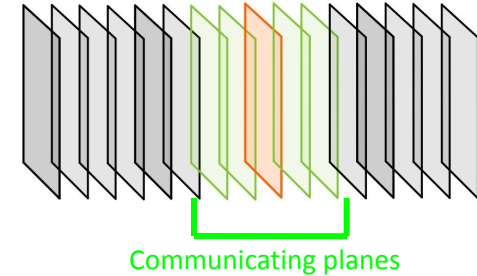
- Decoupling inner and boundary grid, given as inputs
- Higher number of boundary points needed (slightly larger matrix to invert)



On-going: coupling between planes for non-uniform phenomena

Single solution for the whole tokamak:

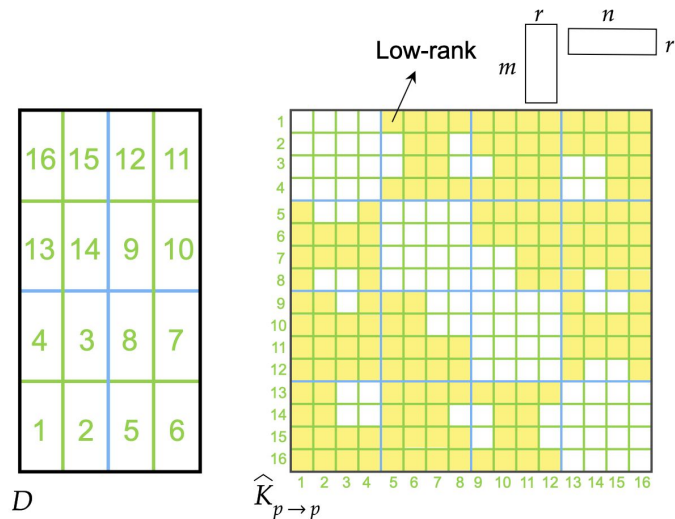
- Drop of approximation $\lambda_{\text{mfp},D} \ll 1/k_{\parallel}$
- Null elements for distant planes $\rightarrow$ sparse matrix
- Large increase of matrix dimension



On-going: efficiency increased using hierarchical matrices (HM)

Approximation of the matrix elements when corresponding points are distant in space:

- Great reduction of number of elements evaluated
→ reduced memory and time
- Allows high neutrals grid resolution
- Not yet parallelized on a single plane
(new phd student A. Laville)



		Time for $\hat{K}_{p \rightarrow p}$ [s]		GMRES time [s]		Memory load
$N_x \times N_y$	N_P	Dense	HM	Dense	HM	
50×100	5000	24.2	6.8	0.5	0.2	27.2 %
80×160	12800	158.5	20.5	8.2	1.3	12.4 %
100×200	20000	396	33.8	12.1	2	8.4 %
150×300	45000	/	92	/	4.3	4.2 %

List of Deuterium reactions

Collisional process	Equation	Reaction Frequency
Ionization of D	$e^- + D \rightarrow 2e^- + D^+$	$\nu_{iz,D} = n_e \langle \nu_e \sigma_{iz,D}(\nu_e) \rangle$
Recombination of D^+ and e^-	$e^- + D^+ \rightarrow D$	$\nu_{rec,D^+} = n_e \langle \nu_e \sigma_{rec,D^+}(\nu_e) \rangle$
$e^- - D$ elastic collisions	$e^- + D \rightarrow e^- + D$	$\nu_{e-D} = n_e \langle \nu_e \sigma_{e-D}(\nu_e) \rangle$
Ionization of D_2	$e^- + D_2 \rightarrow 2e^- + D_2^+$	$\nu_{iz,D_2} = n_e \langle \nu_e \sigma_{iz,D_2}(\nu_e) \rangle$
Recombination of D_2^+ and e^-	$e^- + D_2^+ \rightarrow D_2$	$\nu_{rec,D_2^+} = n_e \langle \nu_e \sigma_{rec,D_2^+}(\nu_e) \rangle$
$e^- - D_2$ elastic collisions	$e^- + D_2 \rightarrow e^- + D_2$	$\nu_{e-D_2} = n_e \langle \nu_e \sigma_{e-D_2}(\nu_e) \rangle$
Dissociation of D_2	$e^- + D_2 \rightarrow e^- + D + D$	$\nu_{diss,D_2} = n_e \langle \nu_e \sigma_{diss,D_2}(\nu_e) \rangle$
Dissociative ionization of D_2	$e^- + D_2 \rightarrow 2e^- + D + D^+$	$\nu_{diss-iz,D_2} = n_e \langle \nu_e \sigma_{diss-iz,D_2}(\nu_e) \rangle$
Dissociation of D_2^+	$e^- + D_2^+ \rightarrow e^- + D + D^+$	$\nu_{diss,D_2^+} = n_e \langle \nu_e \sigma_{diss,D_2^+}(\nu_e) \rangle$
Dissociative ionization of D_2^+	$e^- + D_2^+ \rightarrow 2e^- + 2D^+$	$\nu_{diss-iz,D_2^+} = n_e \langle \nu_e \sigma_{diss-iz,D_2^+}(\nu_e) \rangle$
Dissociative recombination of D_2^+	$e^- + D_2^+ \rightarrow 2D$	$\nu_{diss-rec,D_2^+} = n_e \langle \nu_e \sigma_{diss-rec,D_2^+}(\nu_e) \rangle$
Charge-exchange of D^+, D	$D^+ + D \rightarrow D + D^+$	$\nu_{cx,D} = n_{D^+} \langle \nu_{D^+} \sigma_{cx,D^+}(\nu_{D^+}) \rangle$
Charge-exchange of D_2^+, D_2	$D_2^+ + D_2 \rightarrow D_2 + D_2^+$	$\nu_{cx,D_2} = n_{D_2^+} \langle \nu_{D_2^+} \sigma_{cx,D_2^+}(\nu_{D_2^+}) \rangle$
Charge-exchange of D_2^+, D	$D_2^+ + D \rightarrow D_2 + D^+$	$\nu_{cx,D-D_2^+} = n_{D_2^+} \langle \nu_{D_2^+} \sigma_{cx,D-D_2^+}(\nu_{D_2^+}) \rangle$
Charge-exchange of D_2, D^+	$D_2 + D^+ \rightarrow D_2^+ + D$	$\nu_{cx,D_2-D^+} = n_{D^+} \langle \nu_{D^+} \sigma_{cx,D_2-D^+}(\nu_{D^+}) \rangle$

Average always over the
faste species: electrons or
ions (for cx)