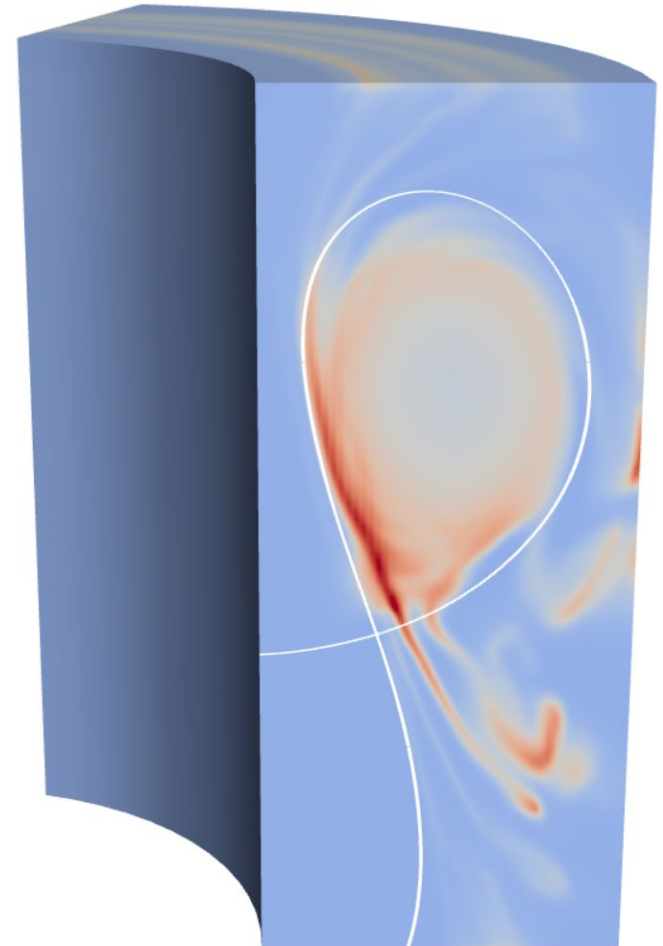


KINetic Deterministic NEutral Solver (KINDNES

-

A kinetic neutrals solver that avoids Monte Carlo noise for turbulent simulations in magnetic confinement devices

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



Plasma simulations need a self-consistent fast neutral model

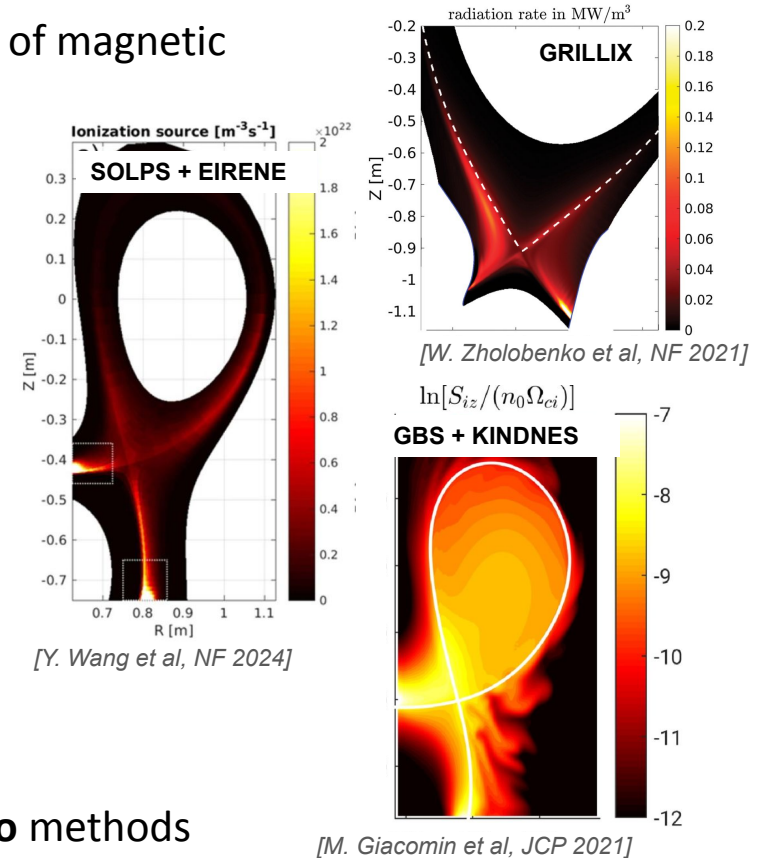
Accurate description of neutral dynamics at the boundary of magnetic confinement devices is fundamental to understand:

- 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, SolEdge, Grillix)
- Kinetic Monte Carlo models (Eirene, Degas2)

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

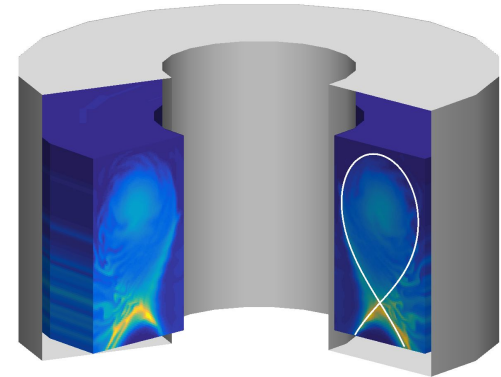
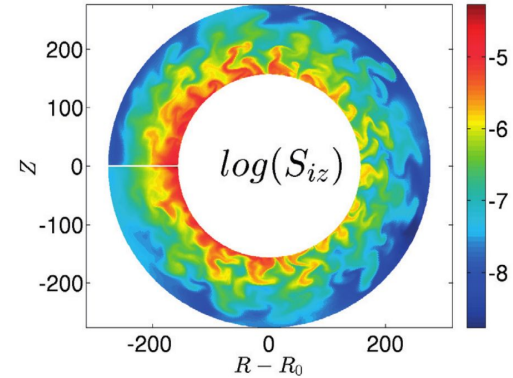


KINDNES born inside GBS, now a standalone library

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



Index

- **The basic elements of the model:**
 - Method of characteristics for kinetic neutrals
 - Implementation on a discrete grid
- The benchmark against EIRENE
- Ongoing developments

Boltzmann equation for neutral particles (one species)

Boltzmann equation for atomic Deuterium:

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

- Different reactions leads to creation/removal of neutrals
- PDE with:
 - decay rates proportional to f_D
 - a source term independent of f_D

Boltzmann equation for neutral particles (one species)

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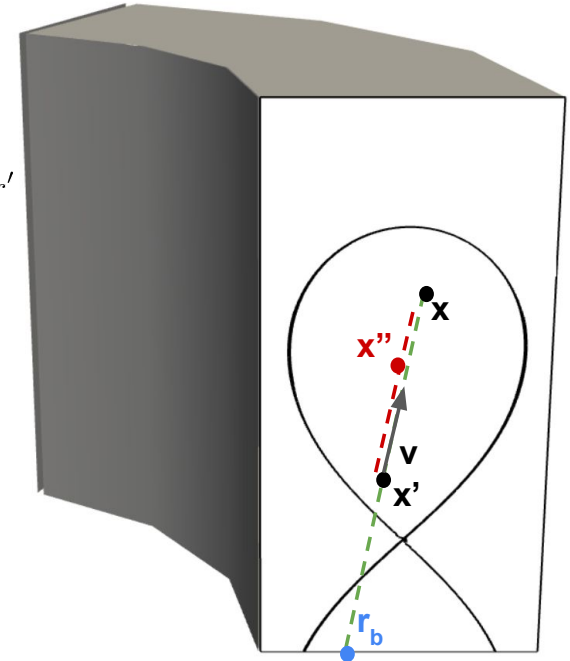
- Different reactions leads to creation/removal of neutrals
- PDE with:
 - decay rates proportional to f_D
 - a source term independent of f_D (but dependent on n_D)

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):

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



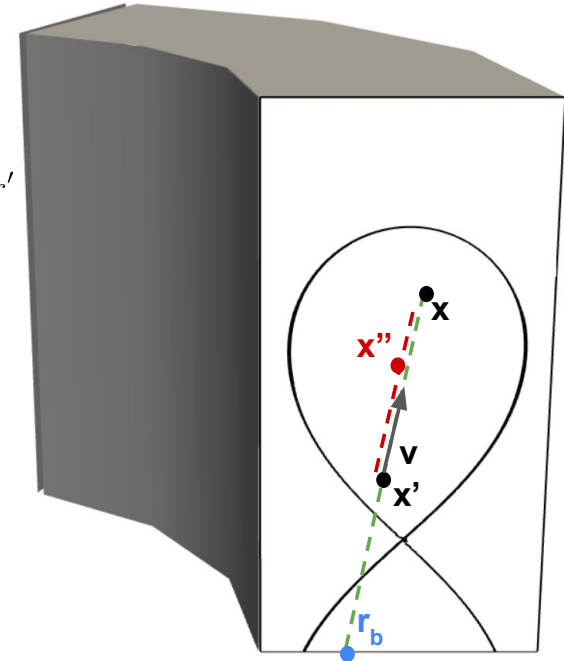
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$$\frac{\partial f_D}{\partial t} + \mathbf{v} \cdot \frac{\partial f_D}{\partial \mathbf{x}} = -\nu_{iz} f_D - \nu_{cx} \left(f_D - \frac{n_D}{n_{D^+}} f_{D^+} \right) + \nu_{rec} f_{D^+}$$

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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 $\nu_{\text{eff},D} = \nu_{iz} + \nu_{cx}$



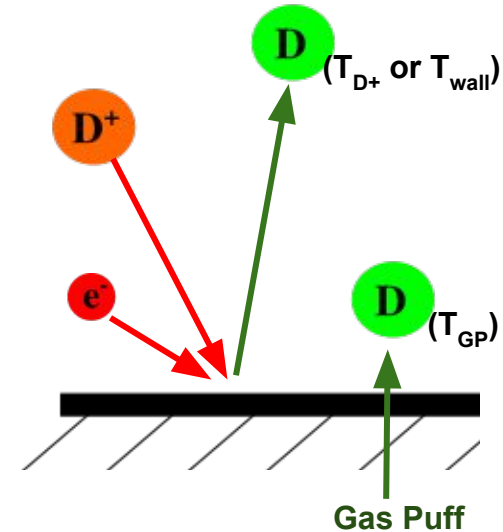
Boundary conditions describe emission, reflection and puffing

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})



Two approximations to simplify the solution

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

- Neutral adiabatic regime $1/\nu_{\text{eff}} < \tau_{\text{turb}} \longrightarrow \partial_t f_D = 0$ [Dropped in G. Drago master thesis, 2025]
- Turbulence anisotropy $\lambda_{\text{mfp}, D} \ll 1/k_{\parallel} \longrightarrow$ Single plane solution
[Dropped in M. Szonyi master thesis, 2026]

Solution algorithm for neutral density

Integrating in velocity space for the first moment of the distribution:

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

Using the explicit boundary condition:

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

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

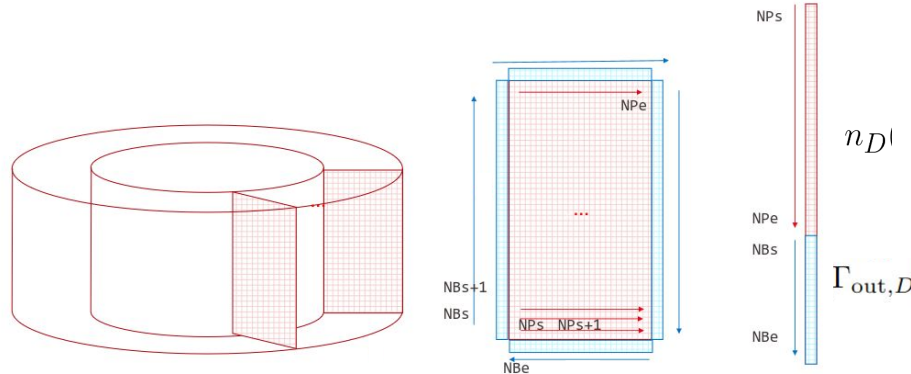
Model solved plane by plane on discrete grid

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

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

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:

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

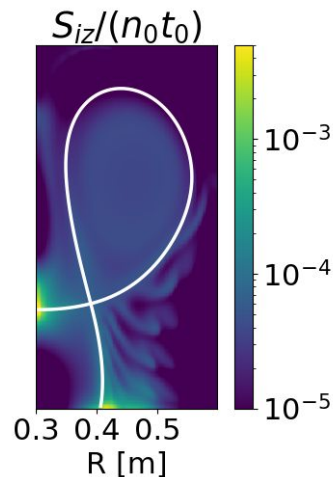
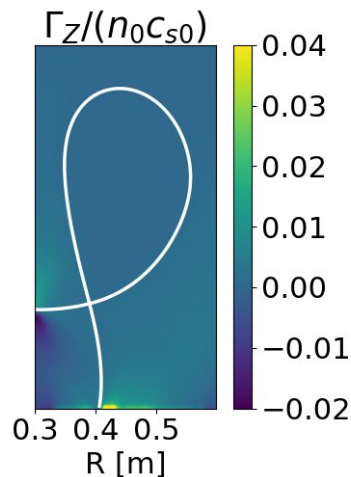
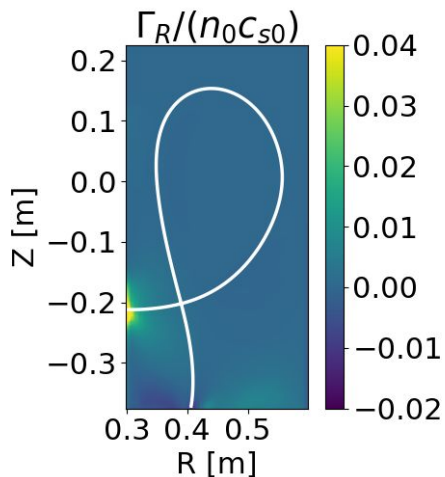
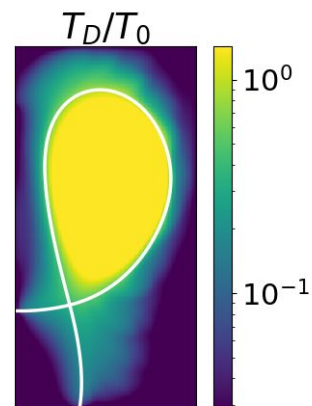
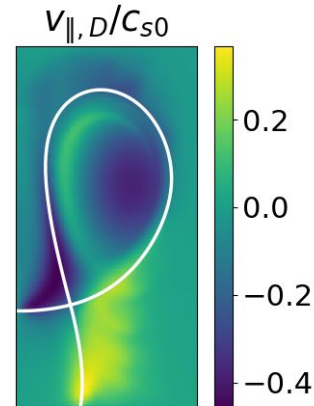
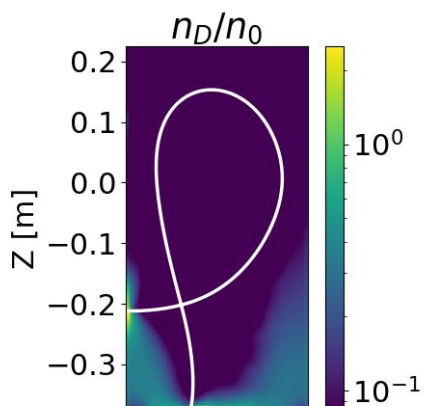
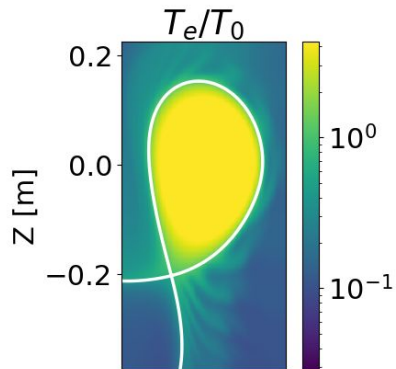
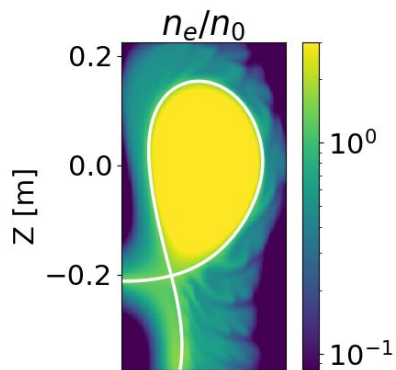
- Neutral density from linear system inversion for each plane: $(\mathbb{1} - K) \mathbf{x} = \mathbf{b}$
- Integrating the previous equation for other moments yields $\mathbf{I}_{D,\perp}, \mathbf{I}_{D,\parallel}, T_D$

Implementation:

- Easy iterative solver with Petsc libraries
- Highly parallelizable $\rightarrow$ plane by plane + each plane parallelized by Petsc

Neutral density solution reflects plasma fluctuations

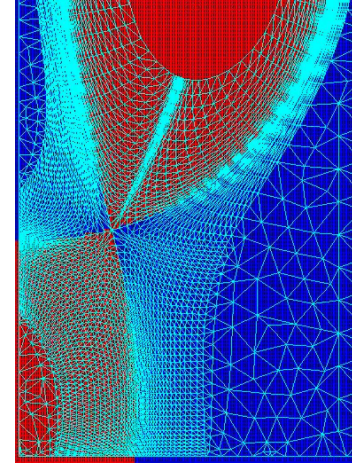
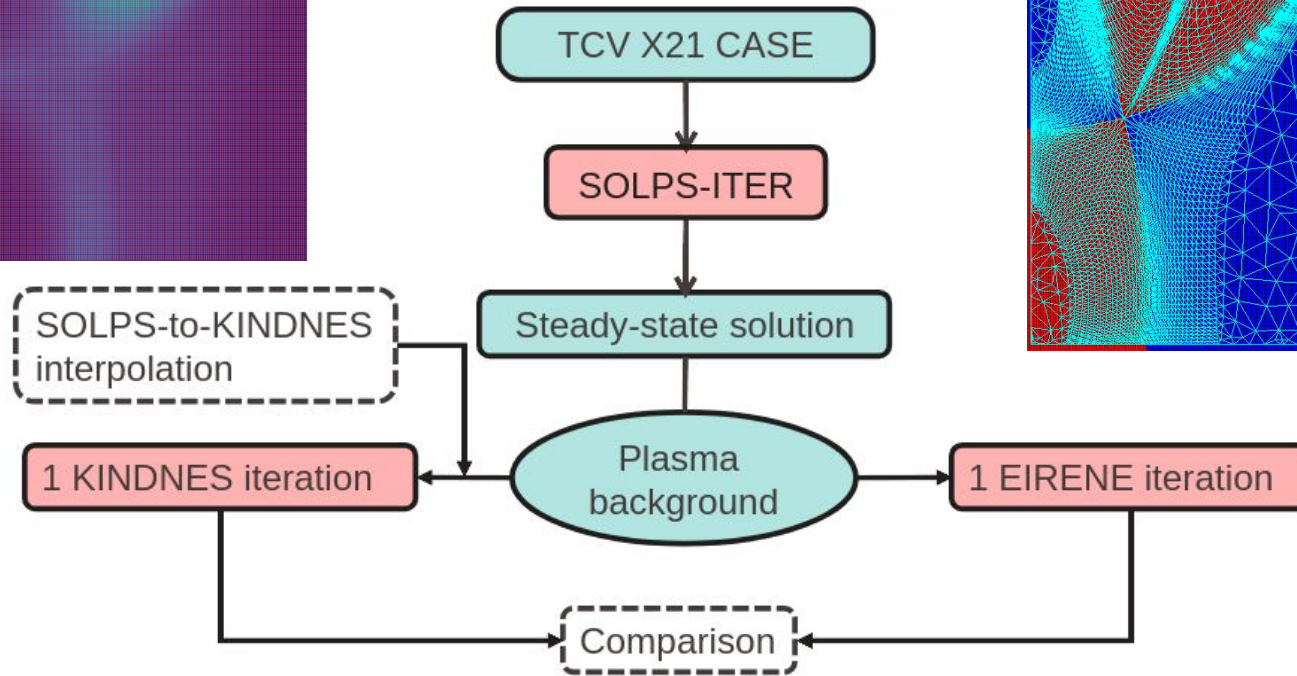
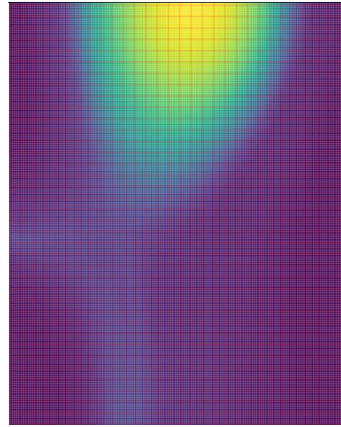
Background plasma:



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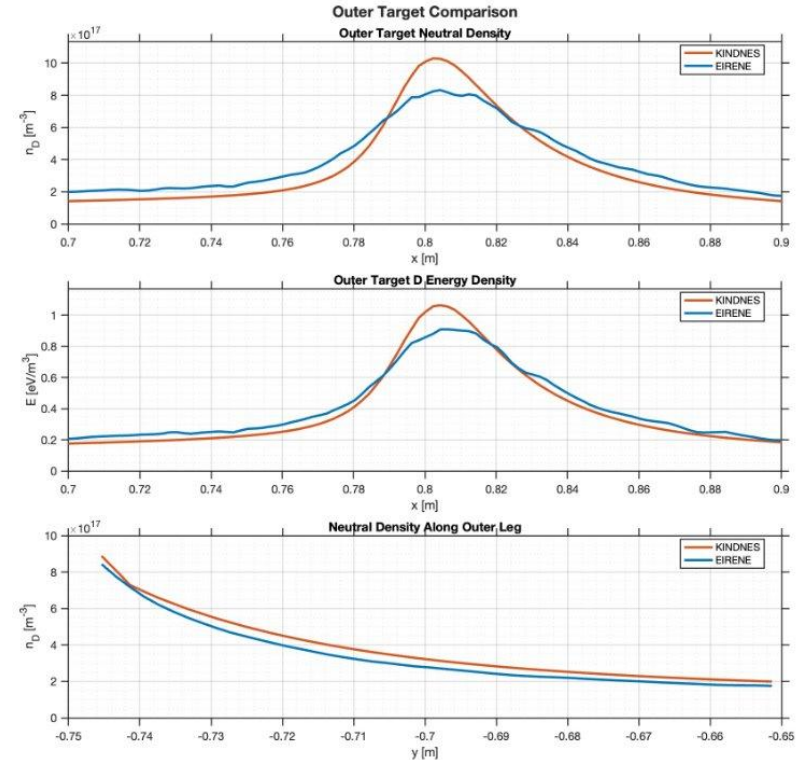
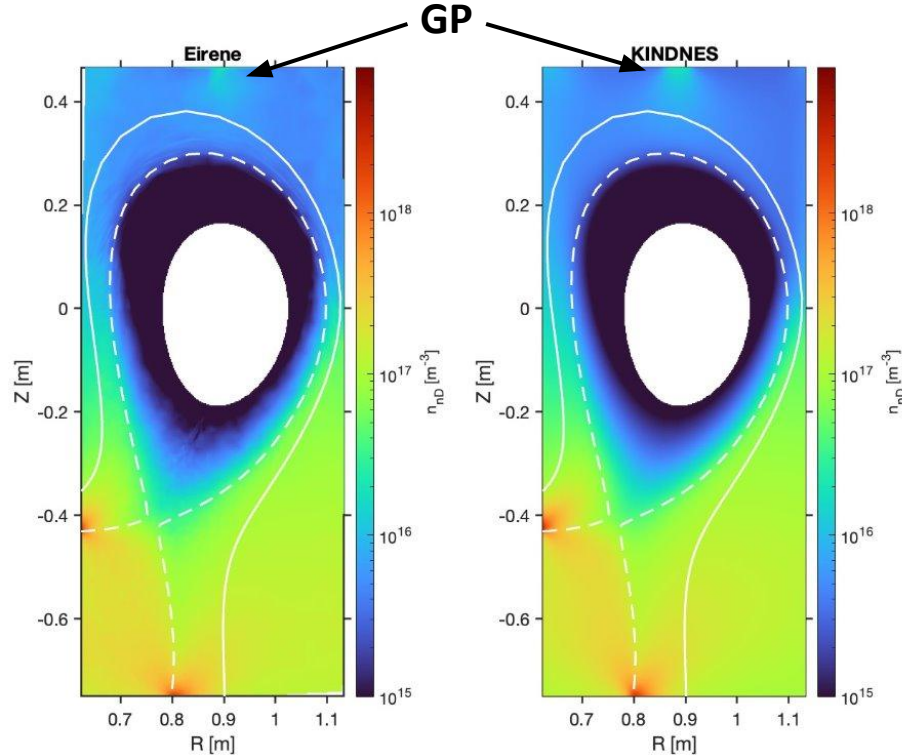
- The basic elements of the model:
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Benchmark based on SOLPS solution for TCV-X21 scenario

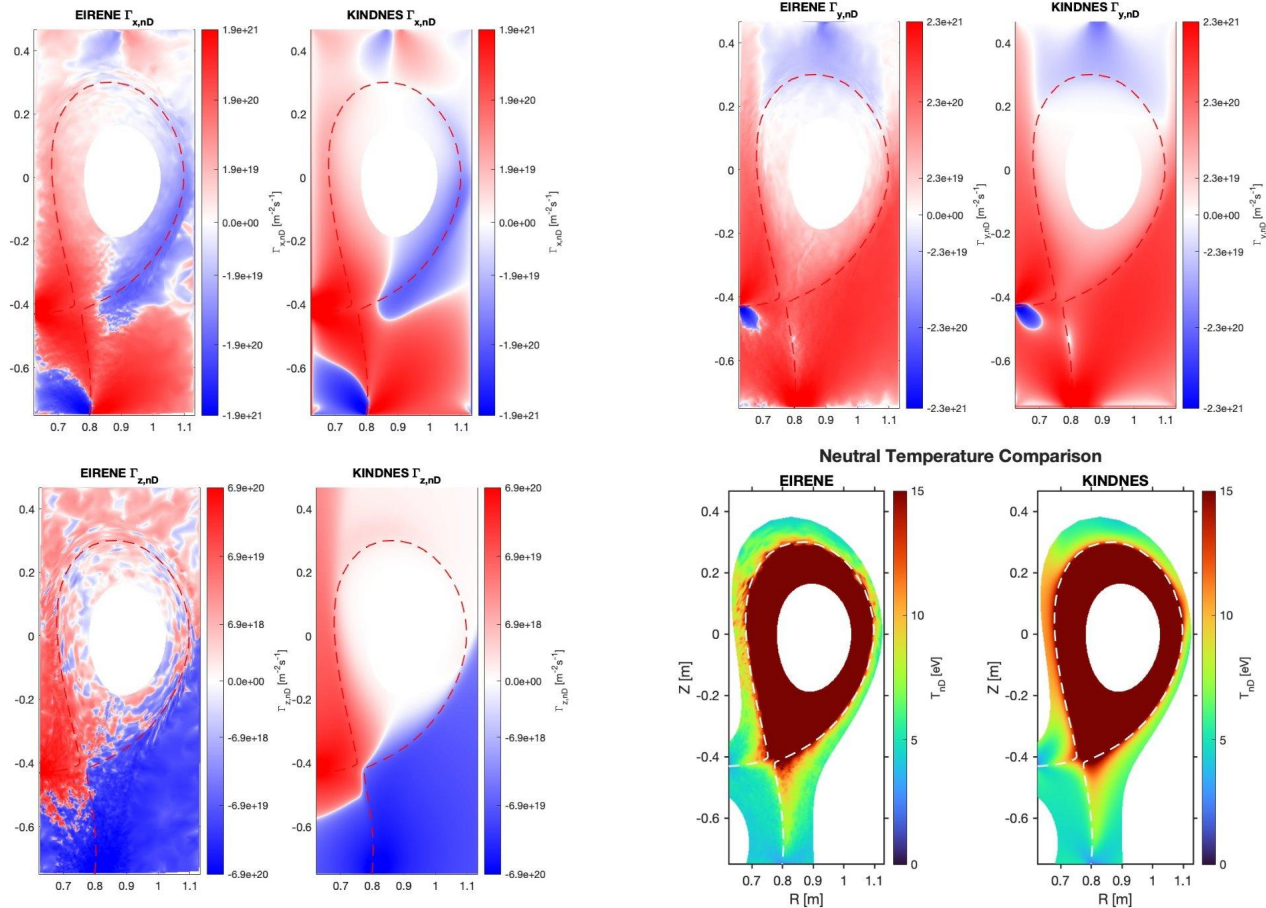


Good agreement between KINDENS and EIRENE

Limiting EIRENE to single ion on a rectangular grid:



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

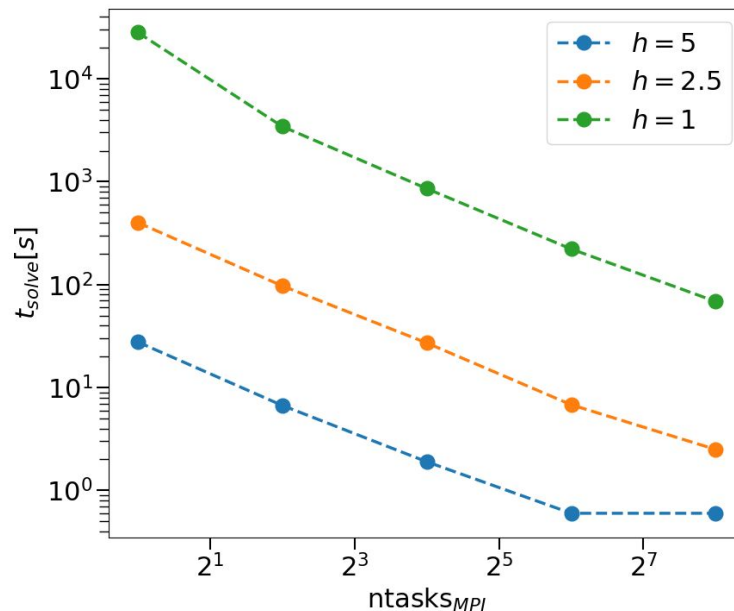
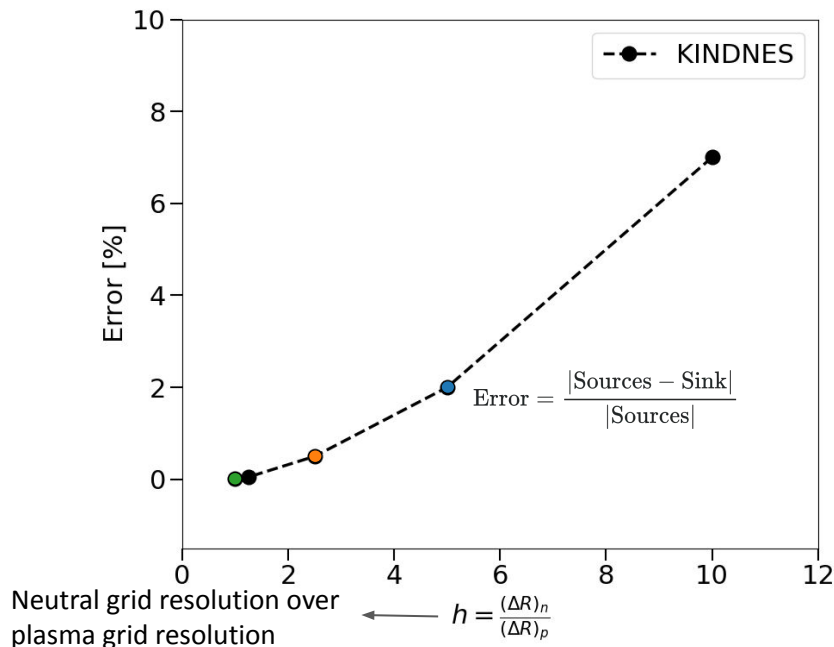


Different way to treat
cx introduces some
differences



KINDNES timings scale well with increasing number of MPI tasks

Tests performed with benchmark case, on 1 Pitagora node

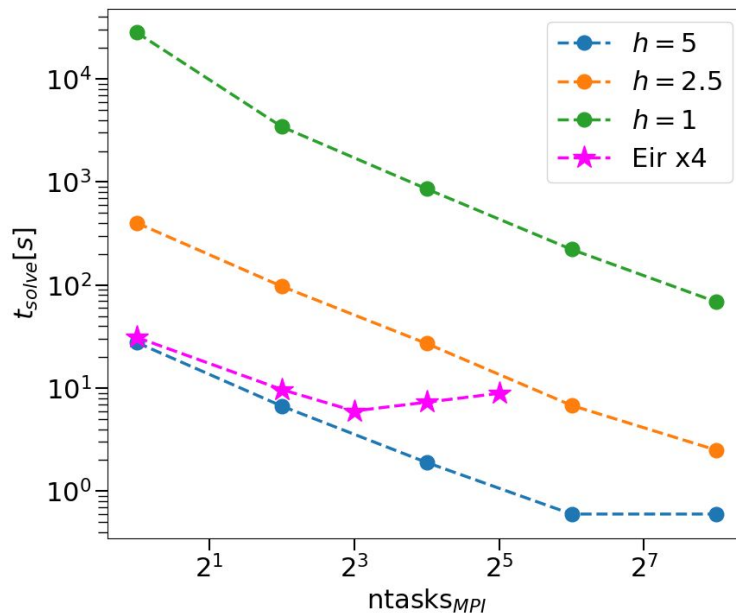
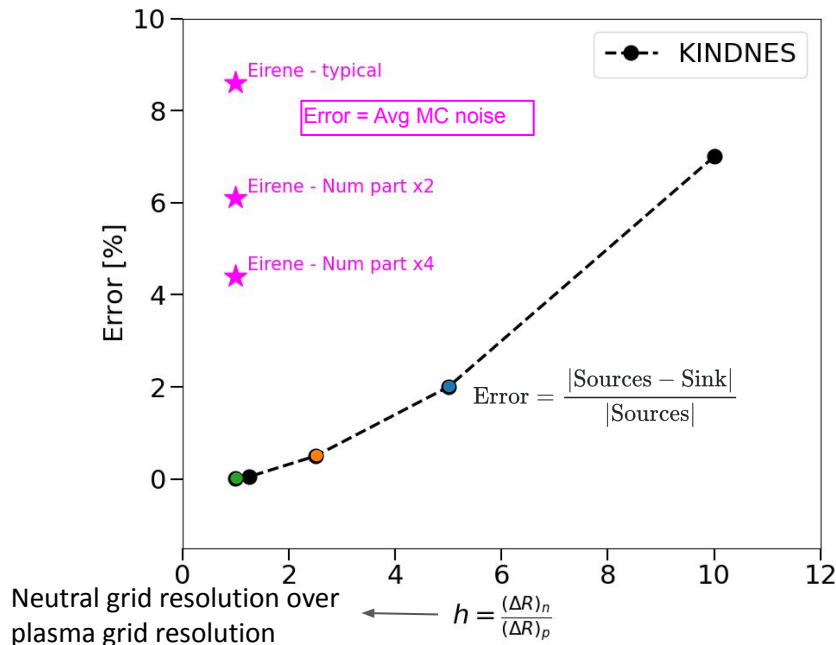


- The error decreases with mesh refinement, while solving time increases
- KINDNES is not limited in the parallelization → New HM solver in development

[M. Guido et al, JCP 2026]

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Extension to multiple species: adding molecular Deuterium D_2

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

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

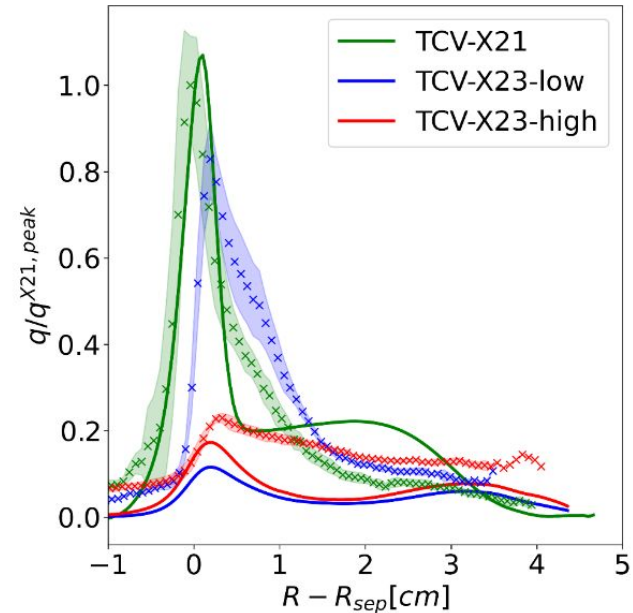
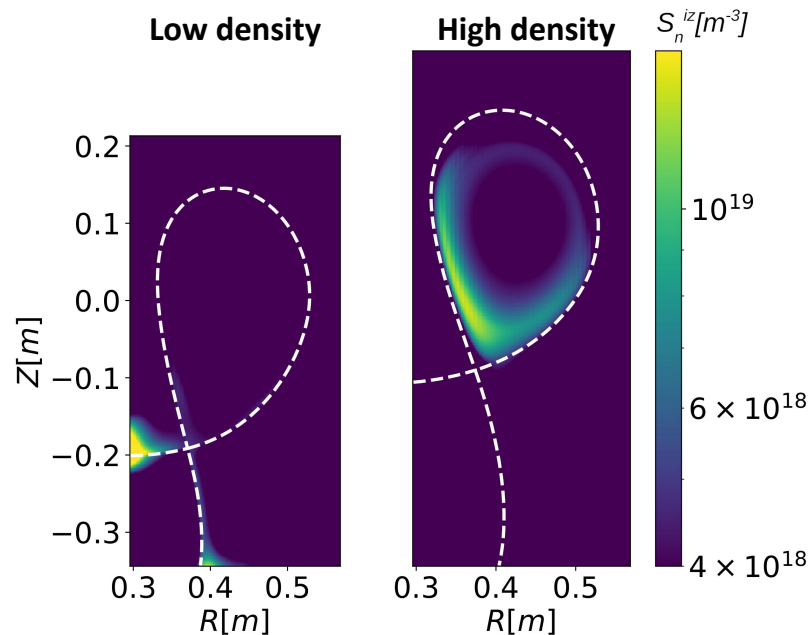
The neutral densities can be obtained by inverting a large linear system:

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

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 strike points $\rightarrow$ detachment

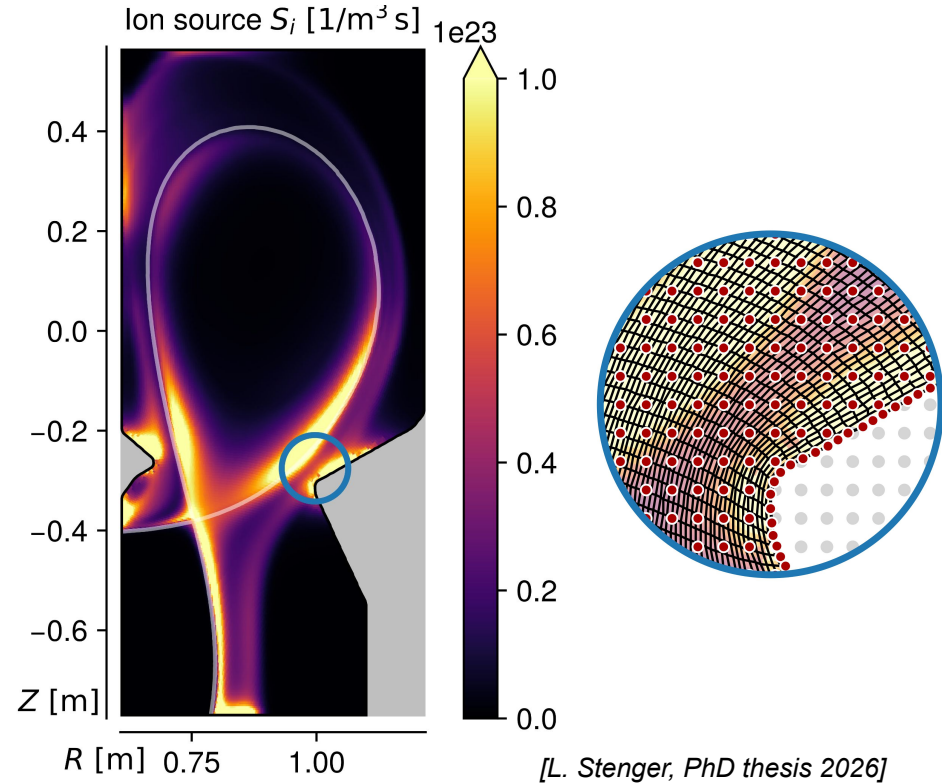
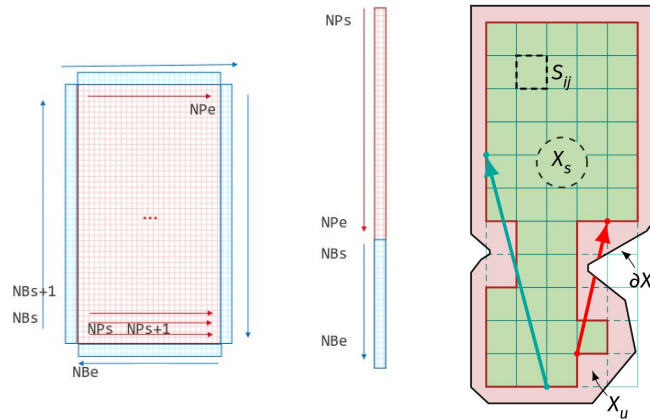


[D. Mancini et al, PPCF 2026]

KINDNES can be solved on arbitrary geometry

Different wall geometry changes only the matrix building :

- Allowed and not allowed paths
- Interpolant between grids
- Solver doesn't need geometry informations



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, dissociation)
- The close agreement of **KINDNES** and **EIRENE** with two independent methods provides strong **cross-verification** of their numerical solutions
- The **direct resolution** of neutrals dynamics guarantees the **absence of numerical noise** introduced by statistical methods
- The features available in GBS are currently under testing and implementation in the **KINDNES** library:
 - New HM solver (90% time reduction on single task)
 - Addition of any neutral species
 - Flexible wall geometry

BACKUP SLIDES

Kernel functions

$$K_{p \rightarrow p}^{D,D^+}(\mathbf{x}_\perp, \mathbf{x}'_\perp) = K_{p \rightarrow p, \text{dir}}^{D,D^+}(\mathbf{x}_\perp, \mathbf{x}'_\perp) + \alpha_{\text{refl}} K_{p \rightarrow p, \text{refl}}^{D,D^+}(\mathbf{x}_\perp, \mathbf{x}'_\perp)$$

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

$$K_{p \rightarrow b, \text{path}}^{D,D^+}(\mathbf{x}_{\perp b}, \mathbf{x}'_\perp) = \int_0^\infty \frac{v_\perp}{r'_\perp} \cos\theta \Phi_\perp[\mathbf{v}_\perp, T_{D^+}](\mathbf{x}'_\perp, \mathbf{v}_\perp) \exp \left[-\frac{1}{v_\perp} \int_0^{r'_\perp} v_{\text{eff},D}(\mathbf{x}''_\perp) dr''_\perp \right] dv_\perp$$

$$K_{b \rightarrow p, \text{path}}^{D, \text{reem}}(\mathbf{x}_\perp, \mathbf{x}'_{\perp b}) = \int_0^\infty \frac{v_\perp}{r'_\perp} \cos\theta' \chi_{\perp, \text{in}, D}(\mathbf{x}'_{\perp b}, \mathbf{v}_\perp) \exp \left[-\frac{1}{v_\perp} \int_0^{r'_\perp} v_{\text{eff},D}(\mathbf{x}''_\perp) dr''_\perp \right] dv_\perp$$

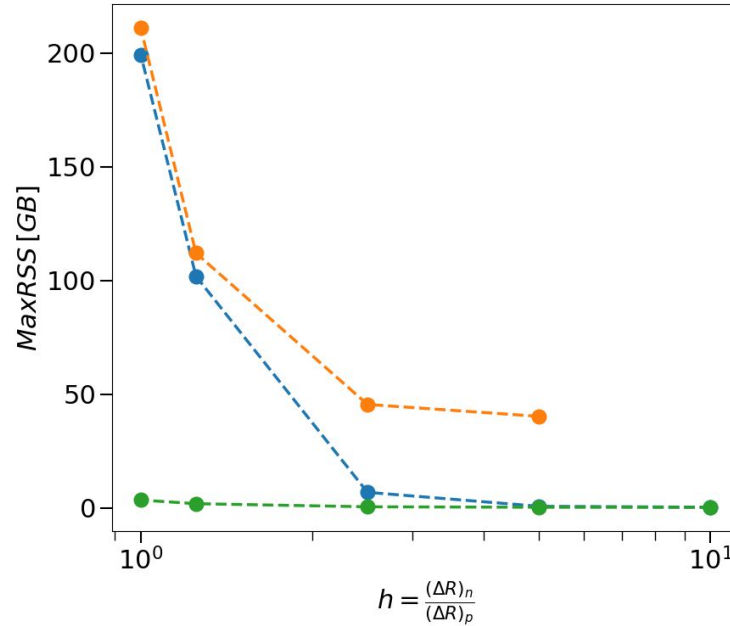
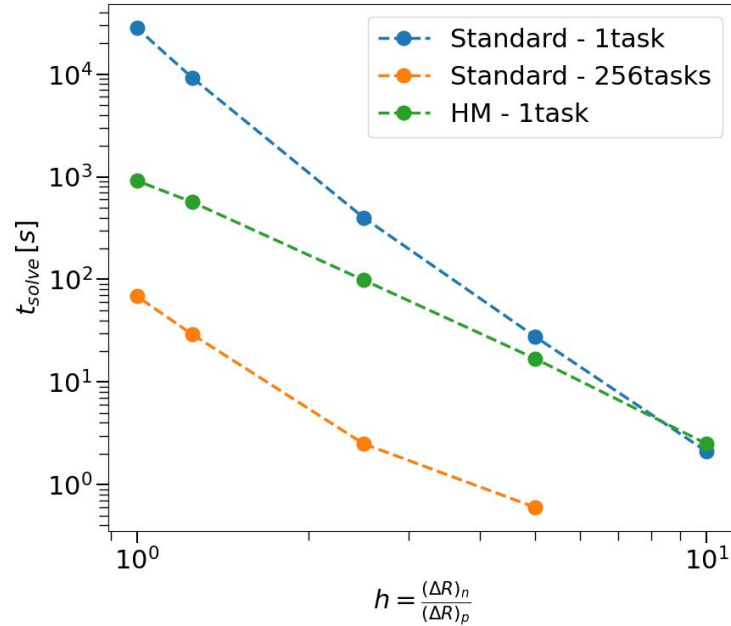
$$K_{b \rightarrow b, \text{path}}^{D, \text{reem}}(\mathbf{x}_{\perp b}, \mathbf{x}'_{\perp b}) = \int_0^\infty \frac{v_\perp^2}{r'_\perp} \cos\theta \cos\theta' \chi_{\perp, \text{in}, D}(\mathbf{x}'_{\perp b}, \mathbf{v}_\perp) \exp \left[-\frac{1}{v_\perp} \int_0^{r'_\perp} v_{\text{eff},D}(\mathbf{x}''_\perp) dr''_\perp \right] dv_\perp$$

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)

New HM solver strongly reduces memory usage and timing

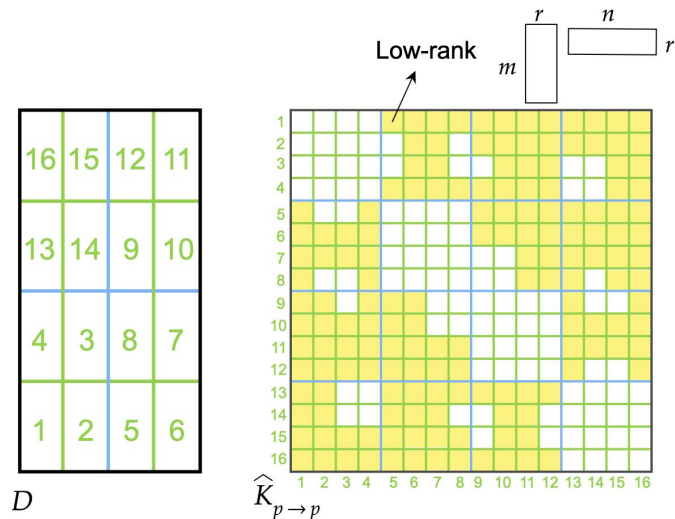


Approximation of most of the matrix elements leads to reduced solver time and memory usage $\longrightarrow$ Parallelization of the method still on-going

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)

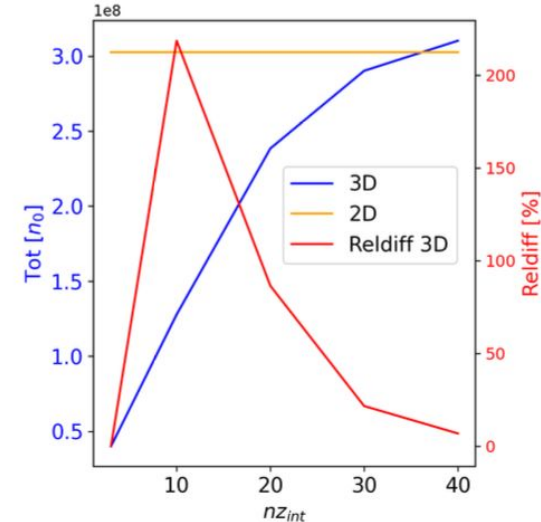
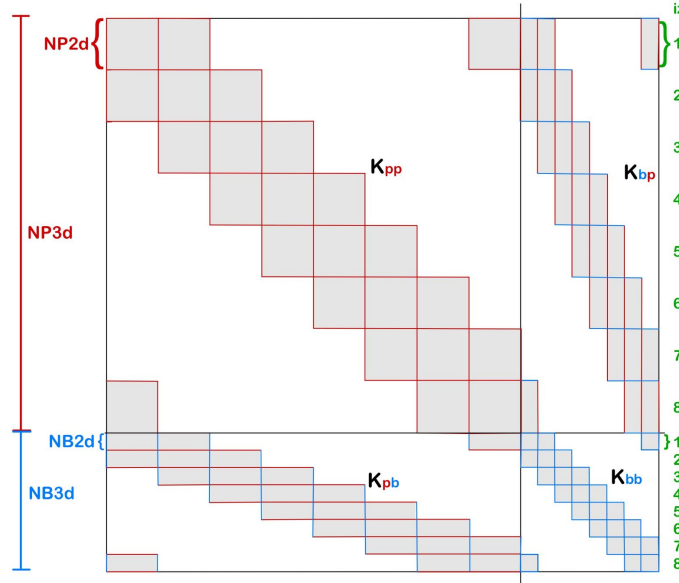
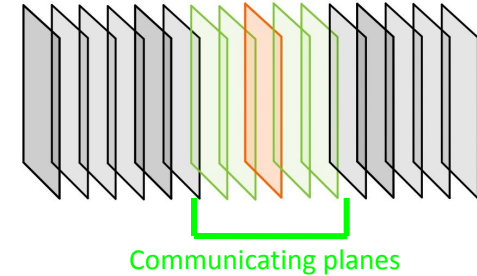


		Time for $\hat{K}_{p \rightarrow p}$ [s]		GMRES time [s]		Memory load
$N_x \times N_y$	N_P	Dense	HM	Dense	HM	
50×100	5000	24.2	6.8	0.5	0.2	27.2 %
80×160	12800	158.5	20.5	8.2	1.3	12.4 %
100×200	20000	396	33.8	12.1	2	8.4 %
150×300	45000	/	92	/	4.3	4.2 %

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



EIRENE MC fluctuations

