

KINetic Deterministic NEutral Solver (KINDNES) - A kinetic neutrals solver that avoids Monte Carlo noise for turbulent simulations in magnetic confinement devices

D. Mancini and P. Ricci



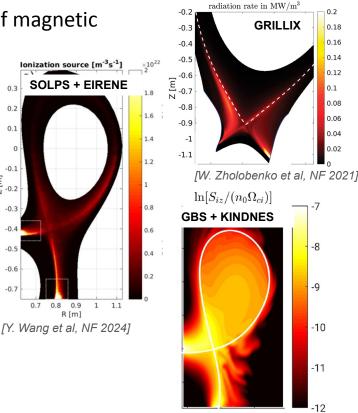
### D. Mancini | TSVV-K | 22-8-2025

### Plasma simulations need a self-consistent fast neutral model

**EPFL** 

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]



[M. Giacomin et al, JCP 2021]

Page 2

### Plasma simulations need a self-consistent fast neutral model

**EPFL** 

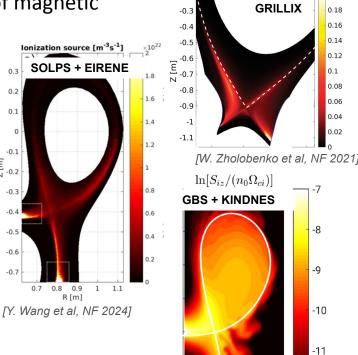
Accurate description of neutral dynamics at the boundary of magnetic

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

[M. Giacomin et al, JCP 2021]

radiation rate in MW/m<sup>3</sup>

Page 3

### Index



- The basic elements of the model:
  - Method of characteristics for kinetic neutrals
  - Extension to multiple species
- On-going developments:
  - Flexible wall geometry
  - Memory reduction with hierarchical matrices
  - Full 3D reconstruction
  - Decoupling KINDNES from GBS

### . Mancini I TSVV-K I 22-8-2025

### Boltzmann equation for neutral particles (one species)



Boltzmann equation for atomic Deuterium:

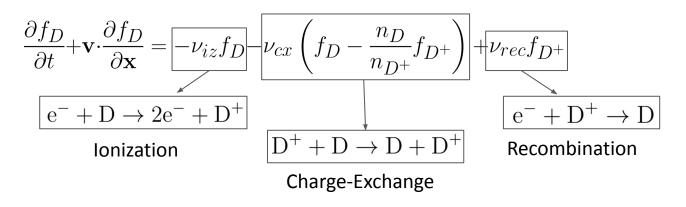
$$\frac{\partial f_D}{\partial t} + \mathbf{v} \cdot \frac{\partial f_D}{\partial \mathbf{x}} = -\nu_{iz} f_D - \nu_{cx} \left( f_D - \frac{n_D}{n_{D^+}} f_{D^+} \right) + \nu_{rec} f_{D^+}$$

- Different reactions leads to creation/removal of neutrals
- PDE with:
  - $\circ$  decay rates proportional to  $f_{\scriptscriptstyle D}$
  - $\circ$  a source term independent of  $f_D$

### **Boltzmann equation for neutral particles (one species)**



Boltzmann equation for atomic Deuterium:



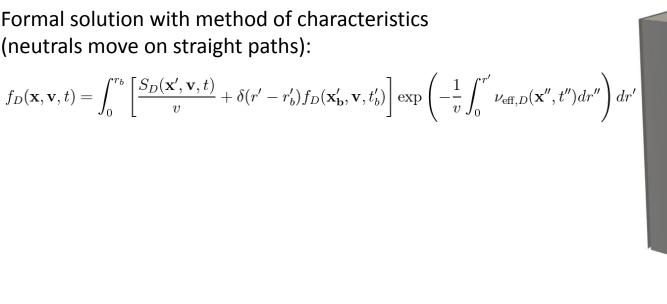
- Different reactions leads to creation/removal of neutrals
- PDE with:
  - decay rates proportional to  $f_D$
  - a source term independent of  $f_D$  (but dependent on  $n_D$ )

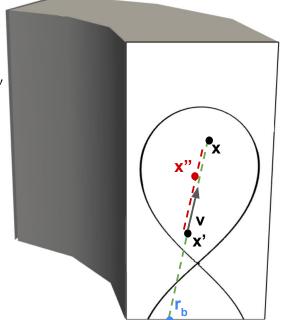
### Solution based on deterministic algorithm avoiding statistical noise of Monte Carlo methods



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

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





# C707-0-77 | V-0.40

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

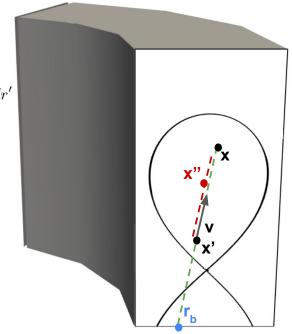


$$\frac{\partial f_D}{\partial t} + \mathbf{v} \cdot \frac{\partial f_D}{\partial \mathbf{x}} = -\nu_{iz} f_D - \nu_{cx} \left( f_D - \frac{n_D}{n_{D^+}} f_{D^+} \right) + \nu_{rec} f_{D^+}$$

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

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

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



## D. Mancini | TSVV-K | 22-8-2025

### Boundary conditions describe emission, reflection and puffing

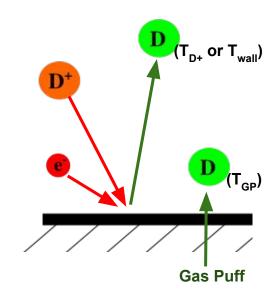


### For the points on the boundary $\mathbf{x}_{b}$ :

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

### 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 ( $\chi_{in}$ )
- Additional sources like gas puff  $(\chi_{GP})$



### 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  $1/
  u_{
  m eff} < au_{
  m turb} \longrightarrow \partial_t f_D = 0$
- Turbulence anisotropy  $\,\lambda_{{
  m mfp},D}\ll 1/k_{\parallel}\,\,$  Single plane solution

### Solution algorithm for neutral density



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

$$n_{\mathrm{D}} = \int d\mathbf{v} \ f_D(\mathbf{x}, \mathbf{v}, t) = \iint_0^{r_b} \left[ \frac{S_D(\mathbf{x}', \mathbf{v}, t)}{v} + \delta(r' - r_b') f_D(\mathbf{x}_b', \mathbf{v}, t_b') \right] \exp\left(-\frac{1}{v} \int_0^{r'} \nu_{\mathrm{eff}, D}(\mathbf{x}'', t'') dr''\right) dr' \ d\mathbf{v}$$

Using the explicit boundary condition:

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

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

### Solution algorithm for neutral density



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

$$n_{\mathrm{D}} = \int d\mathbf{v} \ f_D(\mathbf{x}, \mathbf{v}, t) = \iint_0^{r_b} \left[ \frac{S_D(\mathbf{x}', \mathbf{v}, t)}{v} + \delta(r' - r_b') f_D(\mathbf{x}_b', \mathbf{v}, t_b') \right] \exp\left(-\frac{1}{v} \int_0^{r'} \nu_{\mathrm{eff}, D}(\mathbf{x}'', t'') dr''\right) dr' \ d\mathbf{v}$$

Using the explicit boundary condition:

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

$$\Gamma_{\mathrm{out}, D}(\mathbf{x}_b) = \int_{\Sigma} \widehat{n_{D}(\mathbf{x}')} \nu_{\mathrm{cx}}(\mathbf{x}') \underbrace{K_{p \to b}(\mathbf{x}_b, \mathbf{x}')} d\Sigma + \int_{\partial \Sigma} \Gamma_{\mathrm{out}, D}(\mathbf{x}'_b) \underbrace{K_{b \to b}(\mathbf{x}_b, \mathbf{x}'_b)} d\sigma_b + \Gamma_{\mathrm{out}, \mathrm{rec}}(\mathbf{x}_b) + \Gamma_{\mathrm{out}, \mathrm{D}^+}(\mathbf{x}_b) + \Gamma_{\mathrm{out}, \mathrm{GP}}(\mathbf{x}_b)$$

- System of two integral equations to evaluate  $n_{p}$
- Velocity integrals hidden in the 4 kernel functions  $K_{pp}$ ,  $K_{pb}$ ,  $K_{bp}$ ,  $K_{bb}$

### Model solved plane by plane on discrete grid

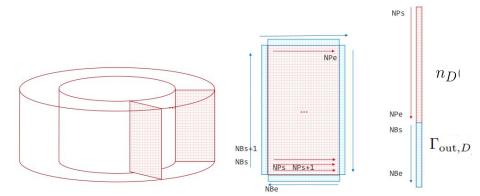


$$n_{D}(\mathbf{x}) = \int_{\Sigma} n_{D}(\mathbf{x}') \nu_{\text{cx}}(\mathbf{x}') K_{p \to p}(\mathbf{x}, \mathbf{x}') d\Sigma + \int_{\partial \Sigma} \Gamma_{\text{out}, D}(\mathbf{x}'_b) K_{b \to p}(\mathbf{x}, \mathbf{x}'_b) d\sigma_b + n_{D, \text{rec}}(\mathbf{x}) + n_{D, \text{GP}}(\mathbf{x})$$

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

Discretized as a system on a linearized grid:

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



### Model solved plane by plane on discrete grid



Discretized as a system on a linearized grid:

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

- Neutral density from linear system inversion for each plane: (1 K)x = b
- Integrating the previous equation for other moments yields  $m{\Gamma}_{D..L'}m{\Gamma}_{D..L'}$ ,  $m{T}_{D..L'}$

### Implementation:

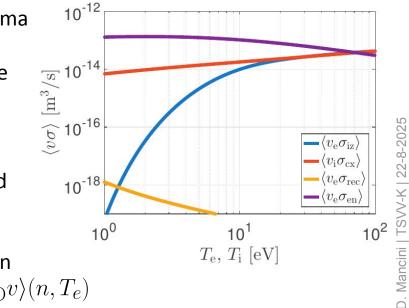
- Easy iterative solver with Petsc libraries
- Highly parallelizable  $\rightarrow$  plane by plane + each plane parallelized by Petsc

### KINDNES was born coupled with GBS



### The current GBS code structure is:

- Short cycling scheme: neutrals solved every N plasma steps (typically 100 < N < 5000)</li>
  - Plasma density, temperature and fluxes to the wall interpolated on a cartesian neutral grid
  - System solved on the neutral grid
  - Neutral moments interpolated on plasma grid



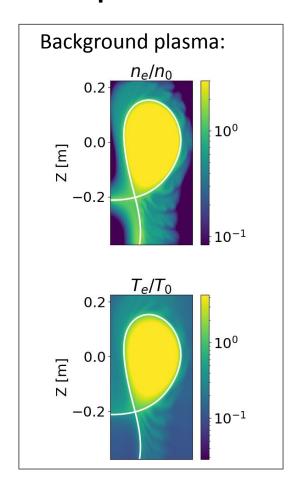
• Plasma sources updated at every step with reaction rates evaluated as Krook operators  $\,
u_{\rm iz,D}=n\langle\sigma_{\rm iz,D}v\rangle(n,T_e)\,$ 

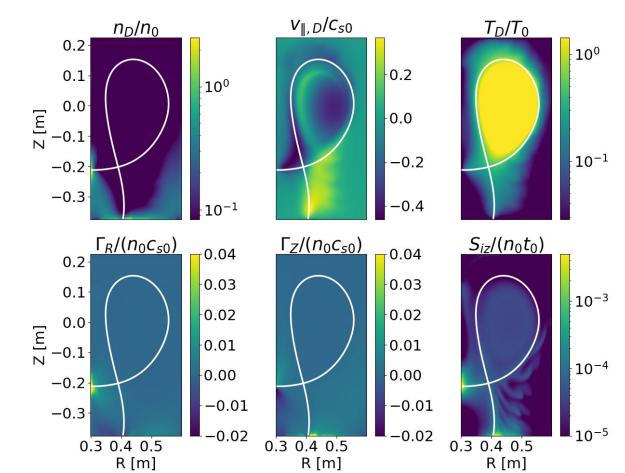
[C. Wersal and P. Ricci 2015 NF, OpenAdas data http://open.adas.ac.uk]

### **EPFL**

D. Mancini | TSVV-K | 22-8-2025

### Example of the solution in a standard TCV-X21 attached L-mode case





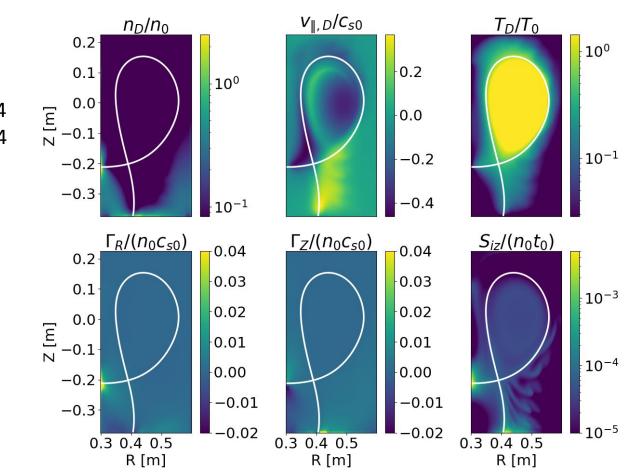
### Example of the solution in a standard TCV-X21 attached L-mode case

### **EPFL**

### Some numbers:

- Plasma grid 150 x 300 x 64
- Neutrals grid 50 x 100 x 64
- Time to solution on 5 x 4 x 64 cpu (Pitagora)
  - = 16s (one neutral update every 1000 plasma step)

Grid resolution scalings and unit testing of the code described in [M. Giacomin et al., JCP, 2022]



### . Mancini | TSVV-K | 22-8-2025

### Extension to multiple species: adding molecular Deuterium D<sub>2</sub>

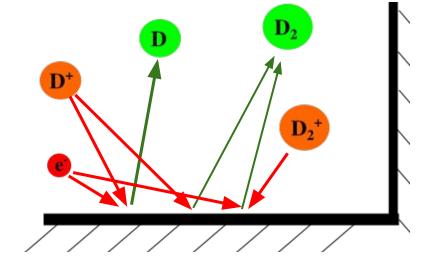


### Two coupled PDEs:

$$\frac{\partial f_{D^{+}}}{\partial t} + \mathbf{v} \cdot \frac{\partial f_{D^{+}}}{\partial \mathbf{x}} = v_{\mathrm{iz,D}} f_{\mathrm{D}} - v_{\mathrm{rec,D^{+}}} f_{D^{+}} - v_{\mathrm{cx,D}} \left( \frac{n_{\mathrm{D}}}{n_{\mathrm{D^{+}}}} f_{D^{+}} - f_{\mathrm{D}} \right) + v_{\mathrm{cx,D-D_{2}^{+}}} f_{\mathrm{D}} - v_{\mathrm{cx,D_{2}-D^{+}}} \frac{n_{\mathrm{D_{2}}}}{n_{\mathrm{D^{+}}}} f_{D^{+}} + \dots 
\frac{\partial f_{\mathrm{D_{2}^{+}}}}{\partial t} + \mathbf{v} \cdot \frac{\partial f_{\mathrm{D_{2}^{+}}}}{\partial \mathbf{x}} = v_{\mathrm{iz,D_{2}}} f_{\mathrm{D_{2}}} - v_{\mathrm{rec,D_{2}^{+}}} f_{\mathrm{D_{2}^{+}}} - v_{\mathrm{cx,D_{2}}} \left( \frac{n_{\mathrm{D_{2}}}}{n_{\mathrm{D_{2}^{+}}}} f_{\mathrm{D_{2}^{+}}} - f_{\mathrm{D_{2}}} \right) - v_{\mathrm{cx,D_{2}-D^{+}}} f_{\mathrm{D_{2}}} - v_{\mathrm{cx,D-D_{2}^{+}}} \frac{n_{\mathrm{D}}}{n_{\mathrm{D_{2}^{+}}}} f_{\mathrm{D_{2}^{+}}} + \dots$$

### 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<sub>2</sub>



$$\frac{\partial f_{D^{+}}}{\partial t} + \mathbf{v} \cdot \frac{\partial f_{D^{+}}}{\partial \mathbf{x}} = v_{\text{iz,D}} f_{D} - v_{\text{rec,D^{+}}} f_{D^{+}} - v_{\text{cx,D}} \left( \frac{n_{D}}{n_{D^{+}}} f_{D^{+}} - f_{D} \right) + v_{\text{cx,D-D}_{2}^{+}} f_{D} - v_{\text{cx,D}_{2}-D^{+}} \frac{n_{D_{2}}}{n_{D^{+}}} f_{D^{+}} + \dots 
\frac{\partial f_{D_{2}^{+}}}{\partial t} + \mathbf{v} \cdot \frac{\partial f_{D_{2}^{+}}}{\partial \mathbf{x}} = v_{\text{iz,D}_{2}} f_{D_{2}} - v_{\text{rec,D_{2}^{+}}} f_{D_{2}^{+}} - v_{\text{cx,D_{2}}} \left( \frac{n_{D_{2}}}{n_{D_{2}^{+}}} f_{D_{2}^{+}} - f_{D_{2}} \right) - v_{\text{cx,D_{2}-D^{+}}} f_{D_{2}} - v_{\text{cx,D-D}_{2}^{+}} \frac{n_{D}}{n_{D_{2}^{+}}} f_{D_{2}^{+}} + \dots$$

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

(cx, iz, diss)

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

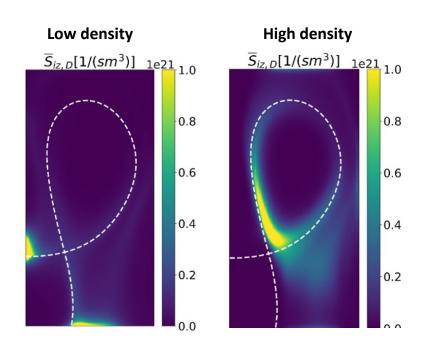
[A. Coroado and P. Ricci 2022 NF]

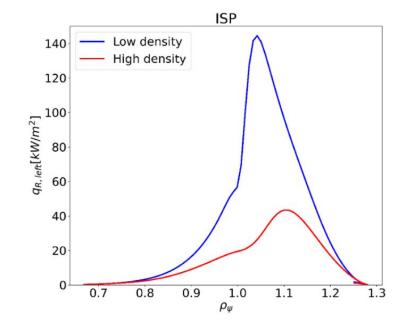
### GBS simulations of detached plasma with molecules



### 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





### Index



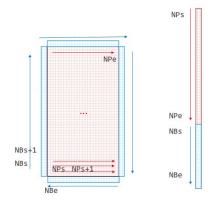
- The basic elements of the model:
  - Method of characteristics for kinetic neutrals
  - Extension to multiple species
- On-going developments:
  - Flexible wall geometry
  - Memory reduction with hierarchical matrices
  - Full 3D reconstruction
  - Decoupling KINDNES from GBS

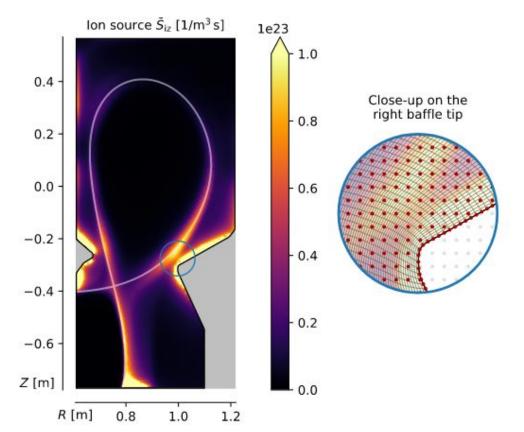
### On-going: flexible wall geometry

**EPFL** 

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)





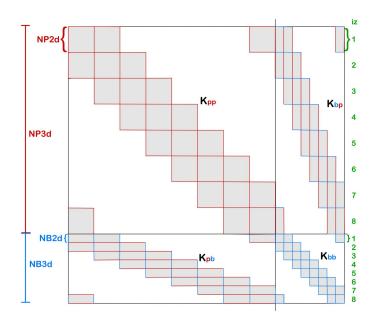
[L. Stenger et al, in preparation]

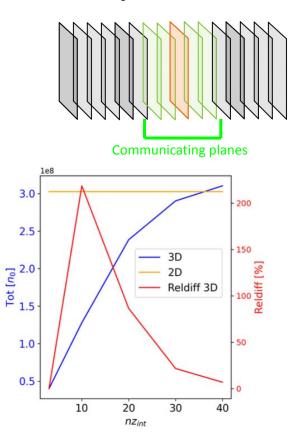


### On-going: coupling between planes for non-uniform phenomena

Single solution for the whole tokamak:

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



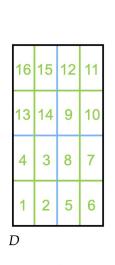


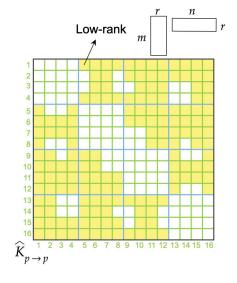
### On-going: efficiency increased using hierarchical matrices (HM)



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



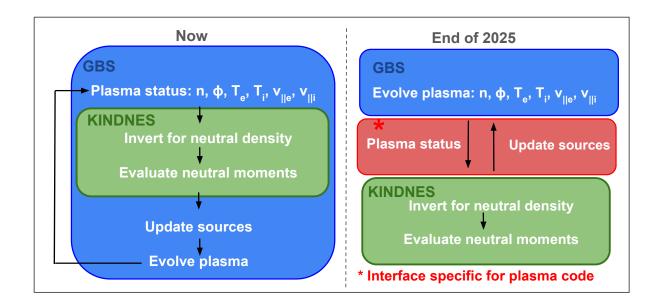


		Time to	or $K_{p  o p}$ [s]	GMRES	time [s]	
$N_x \times N_y$	$N_P$	Dense	НМ	Dense	НМ	Memory load
50 × 100	5000	24.2	6.8	0.5	0.2	27.2 %
80 × 160	12800	158.5	20.5	8.2	1.3	12.4 %
100 × 200	20000	396	33.8	12.1	2	8.4 %
150 × 300	45000	/	92	/	4.3	4.2 %



### On-going: decoupling KINDNES from GBS and GPU implementation

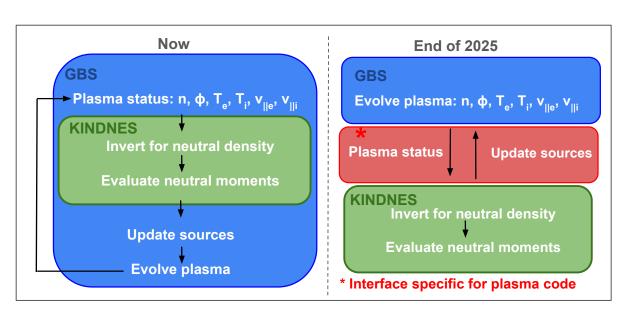
- KINDNES supported by EPFL Advance Computing Hub and applied math groups
- The code runs on all EUROfusion GPU HPC and beyond
- GBS ported on GPU, currently:
  - Plasma evolution on GPU
  - KINDNES on CPU





### On-going: decoupling KINDNES from GBS and GPU implementation

- KINDNES supported by EPFL Advance Computing Hub and applied math groups
- The code runs on all EUROfusion GPU HPC and beyond
- GBS ported on GPU, currently:
  - Plasma evolution on GPU
  - $\circ$  KINDNES on CPU  $\rightarrow$  matrix inversion can be implemented on GPU, interesting with HM



	Time fo	or $\hat{K}_{p ightarrow p}$ [s]
$N_P$	Dense	НМ
5000	24.2	6.8
12800	158.5	20.5
20000	396	33.8
45000	/	92

### **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)
- It is possible to extend it with any neutral species, selecting the relevant reactions (increase of memory usage)
- Implementation highly parallelizable on CPU and portable to GPU
- Code implementation verified and tested
- Decoupling from GBS ongoing (end of 2025)

### **Proposed projects for TSVV-K:**

- Verify on a test case against Advanced Fluid Neutrals and Kinetic Monte Carlo (put in the context of other methods and codes, see D.V. Borodin et al 2022)
- Validation against experimental results
- Further future: extension to additional species

### **Kernel functions**



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

$$\begin{split} K_{p\rightarrow p,\mathrm{path}}^{\mathrm{D,D^{+}}}(\mathbf{x}_{\perp},\mathbf{x}_{\perp}') &= \int_{0}^{\infty} \frac{1}{r_{\perp}'} \Phi_{\perp}[\mathbf{v}_{\perp,\mathrm{D^{+}}},T_{\mathrm{D^{+}}}]}(\mathbf{x}_{\perp}',\mathbf{v}_{\perp}) \exp\left[-\frac{1}{\nu_{\perp}} \int_{0}^{r_{\perp}'} v_{\mathrm{eff,D}}(\mathbf{x}_{\perp}'') dr_{\perp}''\right] dv_{\perp} \\ K_{p\rightarrow b,\mathrm{path}}^{\mathrm{D,D^{+}}}(\mathbf{x}_{\perp \mathrm{b}},\mathbf{x}_{\perp}') &= \int_{0}^{\infty} \frac{v_{\perp}}{r_{\perp}'} \cos\theta \Phi_{\perp}[\mathbf{v}_{\perp,\mathrm{D^{+}}},T_{\mathrm{D^{+}}}]}(\mathbf{x}_{\perp}',\mathbf{v}_{\perp}) \exp\left[-\frac{1}{\nu_{\perp}} \int_{0}^{r_{\perp}'} v_{\mathrm{eff,D}}(\mathbf{x}_{\perp}'') dr_{\perp}''\right] dv_{\perp} \\ K_{b\rightarrow p,\mathrm{path}}^{\mathrm{D,reem}}(\mathbf{x}_{\perp},\mathbf{x}_{\perp \mathrm{b}}') &= \int_{0}^{\infty} \frac{v_{\perp}}{r_{\perp}'} \cos\theta' \chi_{\perp,\mathrm{in,D}}(\mathbf{x}_{\perp \mathrm{b}}',\mathbf{v}_{\perp}) \exp\left[-\frac{1}{\nu_{\perp}} \int_{0}^{r_{\perp}'} v_{\mathrm{eff,D}}(\mathbf{x}_{\perp}'') dr_{\perp}''\right] dv_{\perp} \\ K_{b\rightarrow b,\mathrm{path}}^{\mathrm{D,reem}}(\mathbf{x}_{\perp \mathrm{b}},\mathbf{x}_{\perp \mathrm{b}}') &= \int_{0}^{\infty} \frac{v_{\perp}^{2}}{r_{\perp}'} \cos\theta \cos\theta' \chi_{\perp,\mathrm{in,D}}(\mathbf{x}_{\perp \mathrm{b}}',\mathbf{v}_{\perp}) \exp\left[-\frac{1}{\nu_{\perp}} \int_{0}^{r_{\perp}'} v_{\mathrm{eff,D}}(\mathbf{x}_{\perp}'') dr_{\perp}''\right] dv_{\perp} \end{split}$$

### **List of Deuterium reactions**



Collisional process	Equation	Reaction Frequency
Ionization of D	$e^{-} + D \rightarrow 2e^{-} + D^{+}$	$v_{\rm iz,D} = n_{\rm e} \langle v_{\rm e} \sigma_{\rm iz,D}(v_{\rm e}) \rangle$
Recombination of D <sup>+</sup> and e <sup>-</sup>	$e^- + D^+ \rightarrow D$	$v_{\rm rec,D^+} = n_{\rm e} \langle v_{\rm e} \sigma_{\rm rec,D^+}(v_{\rm e}) \rangle$
e <sup>-</sup> – D elastic collisions	$e^- + D \rightarrow e^- + D$	$v_{\text{e-D}} = n_{\text{e}} \langle v_{\text{e}} \sigma_{\text{e-D}}(v_{\text{e}}) \rangle$
Ionization of $D_2$	$e^- + D_2 \rightarrow 2e^- + D_2^+$	$v_{\rm iz,D_2} = n_{\rm e} \left\langle v_{\rm e} \sigma_{\rm iz,D_2}(v_{\rm e}) \right\rangle$
Recombination of $D_2^+$ and $e^-$	$e^- + D_2^+ \rightarrow D_2$	$v_{\text{rec},D_2^+} = n_e \left\langle v_e \sigma_{\text{rec},D_2^+}(v_e) \right\rangle$
e <sup>-</sup> – D <sub>2</sub> elastic collisions	$e^- + D_2 \rightarrow e^- + D_2$	$v_{\text{e-D}_2} = n_{\text{e}} \langle v_{\text{e}} \sigma_{\text{e-D}_2}(v_{\text{e}}) \rangle$
Dissociation of D <sub>2</sub>	$e^- + D_2 \rightarrow e^- + D + D$	$v_{\rm diss,D_2} = n_{\rm e} \langle v_{\rm e} \sigma_{\rm diss,D_2}(v_{\rm e}) \rangle$
Dissociative ionization of $D_2$	$e^- + D_2 \rightarrow 2e^- + D + D^+$	$v_{\text{diss-iz,D}_2} = n_e \langle v_e \sigma_{\text{diss-iz,D}_2}(v_e) \rangle$
Dissociation of $D_2^+$	$e^- + D_2^+ \rightarrow e^- + D + D^+$	$v_{\mathrm{diss},\mathrm{D}_2^+} = n_\mathrm{e} \left\langle v_\mathrm{e} \sigma_{\mathrm{diss},\mathrm{D}_2^+}(v_\mathrm{e}) \right\rangle$
Dissociative ionization of $D_2^+$	$e^- + \mathrm{D}_2^+ \rightarrow 2e^- + 2\mathrm{D}^+$	$v_{\text{diss-iz},D_2^+} = n_e \left\langle v_e \sigma_{\text{diss-iz},D_2^+}(v_e) \right\rangle$
Dissociative recombination of $D_2^+$	$e^- + D_2^+ \rightarrow 2D$	$v_{\text{diss-rec},D_2^+} = n_e \left\langle v_e \sigma_{\text{diss-rec},D_2^+}(v_e) \right\rangle$
Charge-exchange of D <sup>+</sup> , D	$D^+ + D \rightarrow D + D^+$	$v_{\rm cx,D} = n_{\rm D^+} \left\langle v_{\rm D^+} \sigma_{\rm cx,D^+} (v_{\rm D^+}) \right\rangle$
Charge-exchange of $\mathrm{D}_2^+, \mathrm{D}_2$	$D_2^+ + D_2 \rightarrow D_2 + D_2^+$	$v_{\text{cx,D}_2} = n_{\text{D}_2^+} \left\langle v_{\text{D}_2^+} \sigma_{\text{cx,D}_2^+} (v_{\text{D}_2^+}) \right\rangle$
Charge-exchange of D <sub>2</sub> +, D	$D_2^+ + D \rightarrow D_2 + D^+$	$v_{\text{cx,D-D}_2^+} = n_{\text{D}_2^+} \left\langle v_{\text{D}_2^+} \sigma_{\text{cx,D-D}_2^+} (v_{\text{D}_2^+}) \right\rangle$
Charge-exchange of D <sub>2</sub> , D <sup>+</sup>	$D_2 + D^+ \rightarrow D_2^+ + D$	$v_{\rm cx,D_2-D^+} = n_{\rm D^+} \langle v_{\rm D^+} \sigma_{\rm cx,D_2-D^+} (v_{\rm D^+}) \rangle$

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