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Aalto University School of Science

DIFFER Dutch Institute for Fundamental Energy Research

EUROfusion

WP PWIE meeting 2025

# TSVV Task 5: *"Neutral Gas Dynamics in the Edge"*

***27.03.2025***

**D. Borodin et al.**

JÜLICH Forschungszentrum

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.

# The EIRENE MC code: related packages and tools

***EIRENE code (PLOUTOS and other tools)***
http://www.eirene.de/

FZJ is EIRENE origin, however fluid side of EIRENE-CFD packages often are developed elsewhere, e.g.:
- 2D **SOLPS-ITER** (B2.5-***EIRENE***)
- 3D **EMC3-*EIRENE***
- **SOLEdge3X-*EIRENE*** (with turbulence)
- *many others …*

***The atomic/molecular data*** *accumulations were for decades supported by IAEA*
***Hydhel, H2Vibr, AMJuel, Hydkin - PLOUTOS*** *(new)*
***ADAS (external)***

**Eirene** with the infant Ploutos

*Statue by Cephisodotus the Elder*

*Glyptothek, Munich.*

# TSVV-5: Neutral Gas Dynamics in the Edge

***Main simulation tool:***
***EIRENE code (and EIRENE-CFD packages)***
http://www.eirene.de/

**We aim to transform it to IM- and HPC-ready neutral gas module (*EIRENE-NGM*) suitable for simulations on ITER and DEMO scale with large focus on (semi)detached divertor plasmas**

***FP-9 deliverables:***

1. Ne… …vards exa… …rallelization me…
2. Revised and extended physics basis f… …towards the full dev… vibrational resolution for all hydrogen isotopes and spe… …for seeding.
3. Imp… …ole… vol… …through gen…ed interfaces to, …molecular, nuclear and surface (AMNS) physics data.
4. Interfaces and ha… mo… …fluid dyn… …turbulence codes, time-dependent) and possibly also to gyro-kinetic/gyrofluid plasma…
5. Str… …ed fusion reactor mo… …detached divertor plasmas. Liaison with TSVV Tasks 3 and 4.

**Code performance, parallelization, refactoring, domain decomposition, I/O for HPC, …**

**Fluid-kinetic hybridisation (FKH) and improved CRMs**

**Improved AMNS data, both in structure/physics and content**

**physics**

**EIRENE as NGM – restructuring, interfaces to other codes, time-dependent runs, kinetic ions**

**Validation with experiments and test of predictive capabilities for ITER and DEMO**

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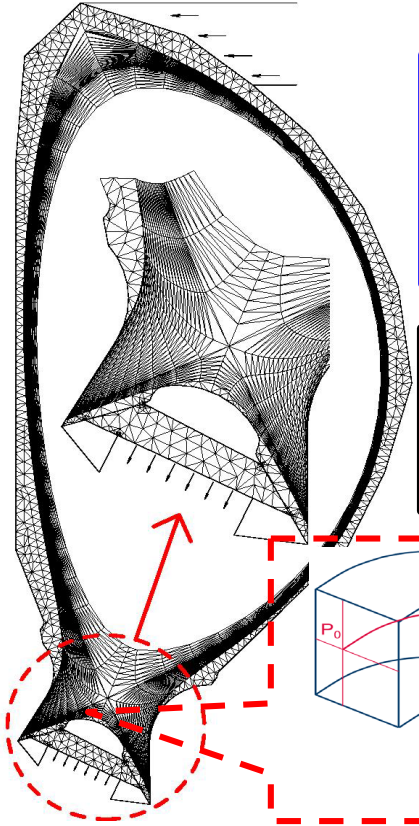
# What is EIRENE in a nutshell (e.g. in SOLPS)?..



Macroscopic:

**CFD** codes (computational **fluid** dynamic): B2, Edge2D, EMC3, SOLEdge3X, etc…

2D or 3D Volume grid (e.g. tetraeder) adopted for current magnetic configuration

Plasma flow parameters

3D EIRENE volume cell

Source terms (Particle, Momentum, Energy)

Microscopic:

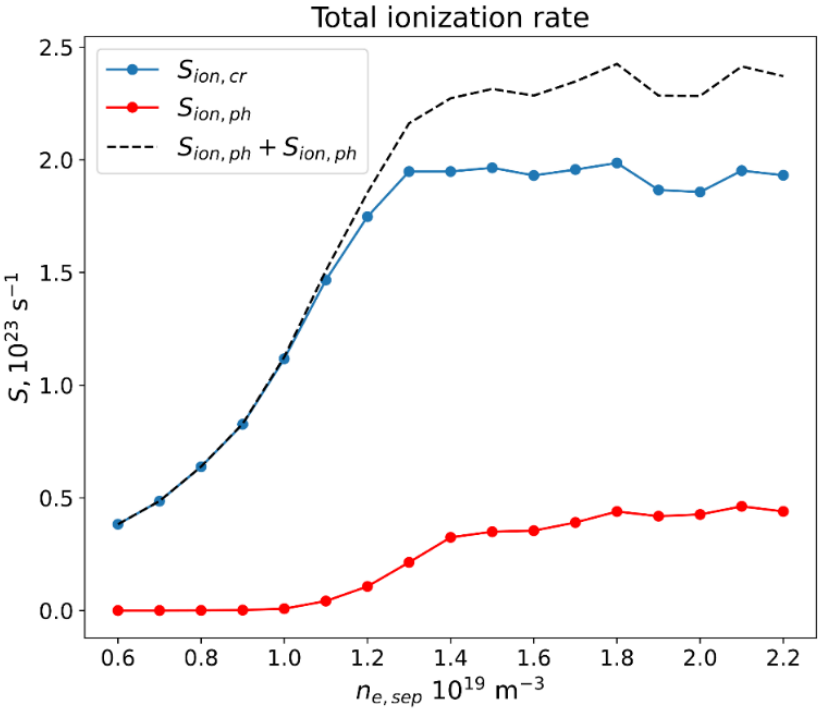
**EIRENE-NGM:** a 3D3v MC multi-species transport code incl. radiation transfer, **kinetic** or **F-K** hybrid.

**CRMs** (HYDKIN, AMJUEL, ADAS, …) for atomic and molecular neutrals $H, H^*, H_2, H_2(v), H_2^*, H^-, H_2^+$,…, impurities Ionisation, CX, recombination etc.

**Photon tracing** opacity, extra ionisation, ….

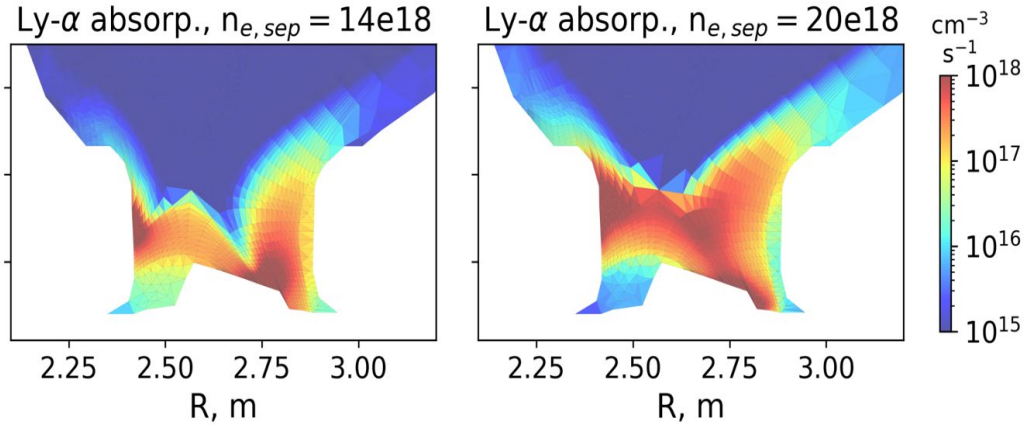
R.Chandra et al., EPS-2023

# Photon tracing: Ly-α and Ly-β opacity → D ionisation




***R. Chandra et al. EPS 2023 P1-001***

**Photon absorption adds up to ~20% of total CR ionization rate in detached conditions**



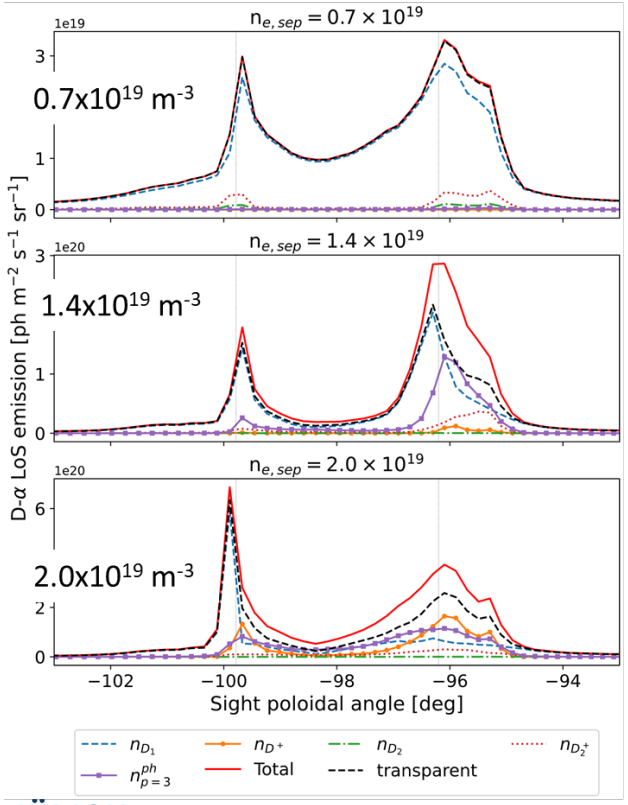

**'Extra' ionization** contribution from Ly-**α** and Ly- **β** photon absorption:

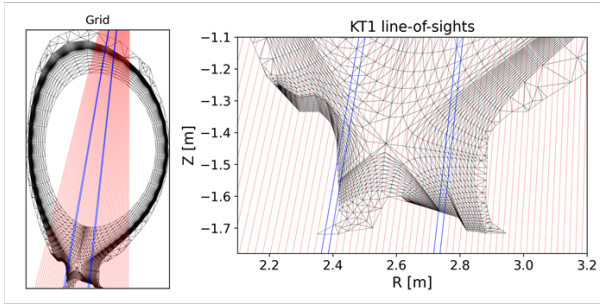
➔ increases population of excited D neutrals

➔ extra ionisation

# Photon tracing: Ly-lines opacity → Balmer emission

## Ly-β opacity enhances $D_\alpha$ emission by 50%-100% in the LFS strike point of JET-ILW L-mode plasmas in high-recycling and detached conditions




Sight lines of the vertically viewing scanning mirror VUV-vis imaging spectroscopy system (KT1) in JET-ILW superimposed on the SOLPS-ITER grid. Blue lines are strike point locations.

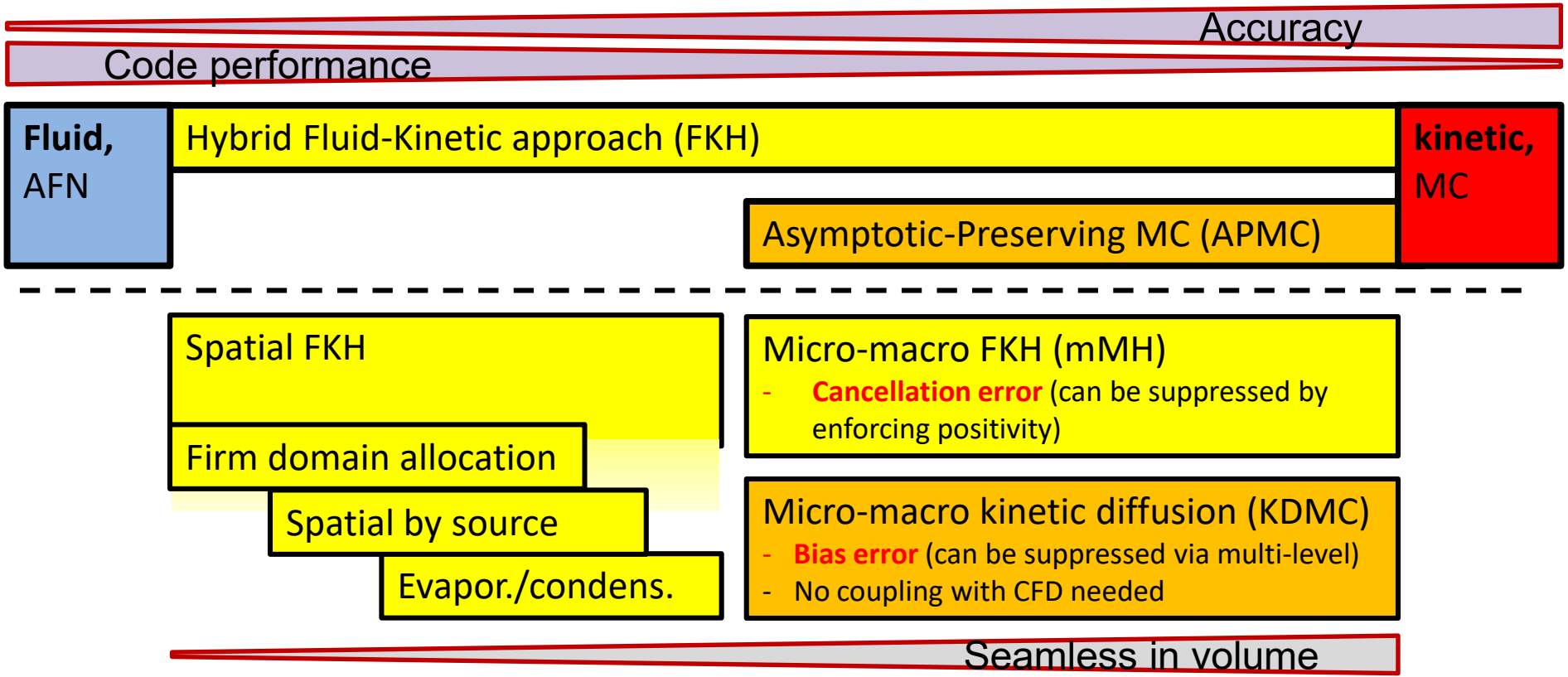
- EIRENE Ly-$\alpha$ and Ly-$\beta$ photons tracing module applied to JET-ILW SOLPS-ITER L-mode plasma stationary solutions with increasing $n_{e,sep}$ densities
- Line-integrated D-$\alpha$ emission using KT1 sightlines, separated by contributions from external densities and by Ly-$\beta$ absorption ($n_{ph,p=3}$), negligible effects on the inner strike point

R. Chandra et al., PSI 2024

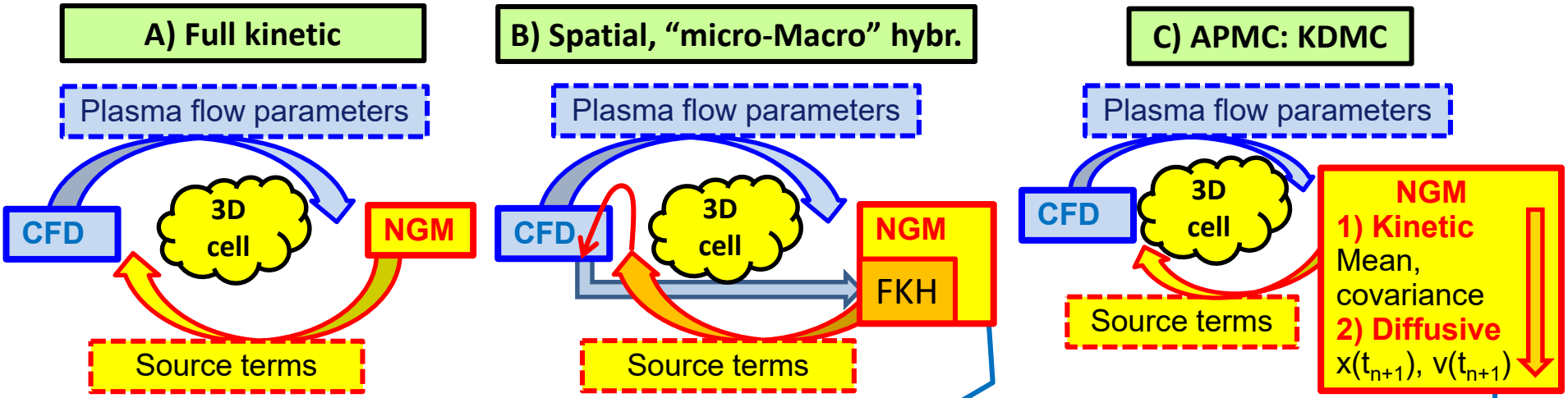
# Fluid-kinetic hybridization (FKH)

**A hierarchy of neutral models:**

D.V. Borodin et al., FEC-2020, NF (2022)



# F-K Hybridisation approaches utilized in EIRENE-NGM



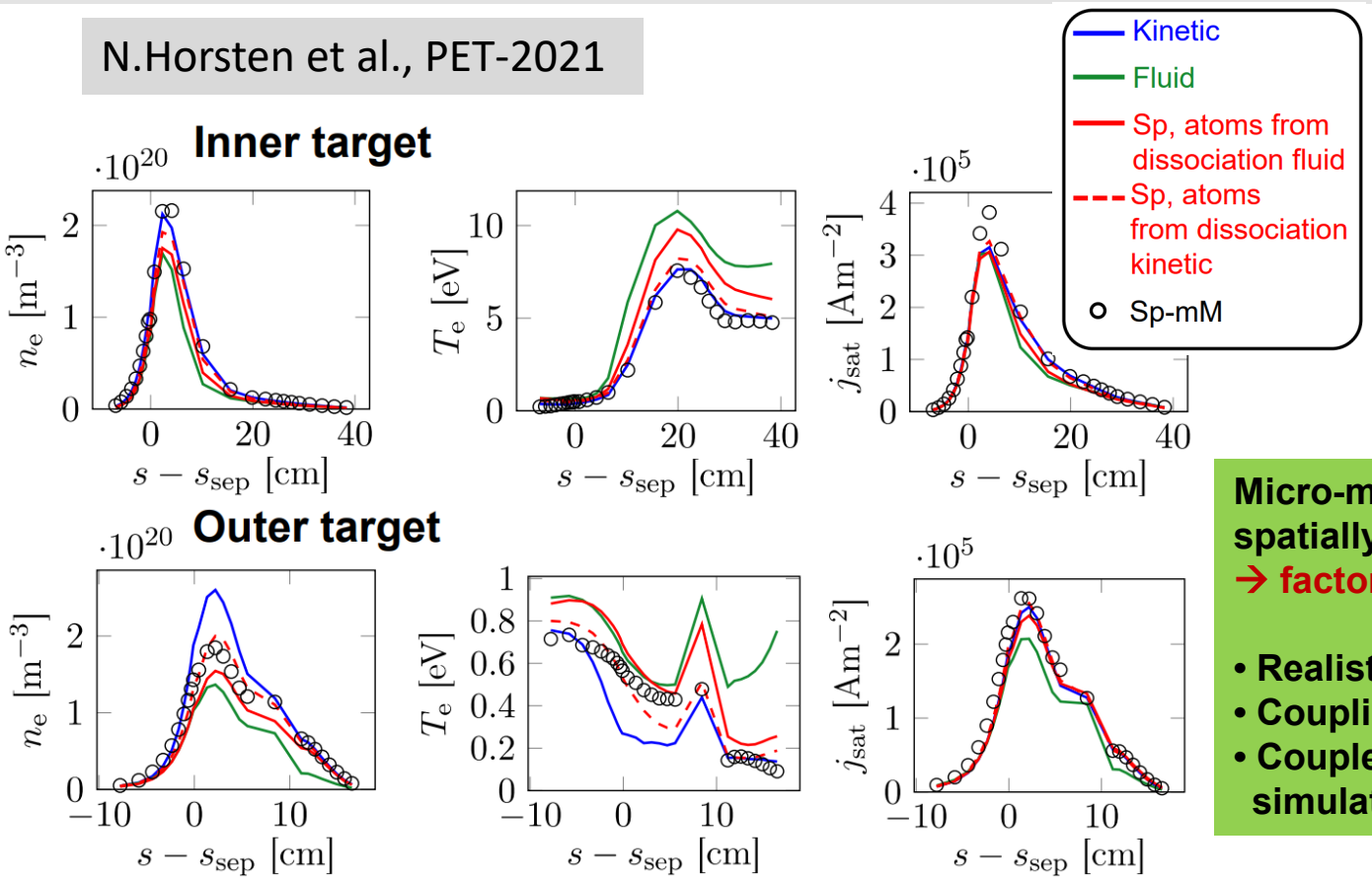

f= $f_F$ + $f_K$, optionally with evaporation/condensation:

$$\frac{\partial f_{K,F}}{\partial t} + \vec{v} \cdot \overrightarrow{\nabla f}_{K,F} = S_{iz}^{K,F} + S_{rc}^{K,F} + S_{cx}^{K,F} + S_{mol}^{K,F} \pm S_{F\to K} \pm S_{K\to F}$$

**Kinetic step** with constant velocity followed by **random walk** with appropriate parameters

# Recent progress with micro-Macro (JET L-mode case)

N.Horsten et al., PET-2021



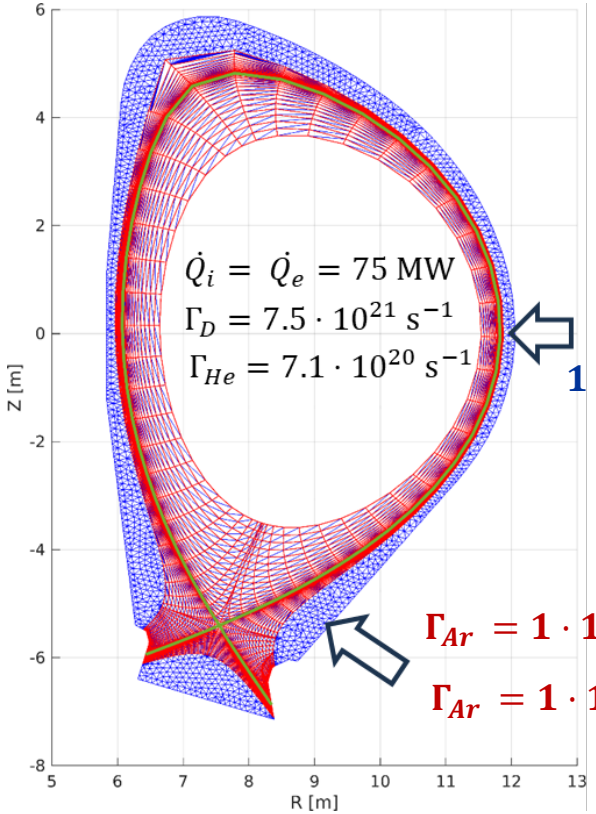

**Purely micro-macro (mM) approach for rectangular slab geometry with fixed background plasma**

2021

**Micro-macro combined with spatially hybrid approach (Sp-mM)**
**→ factor 5-10 faster than full kinetic!**

- **Realistic geometry, void regions**
- **Coupling to kinetic molecules**
- **Coupled plasma-neutral simulations**

# Actual DEMO simulations (with NCC) [KU Leven]




$$\epsilon_{num} = \epsilon_d + \epsilon_c + \epsilon_b + \epsilon_s$$

[K. Ghoos analysis scheme]

**statistical error**
*(direct result of noisy MC sources)*

**finite sampling bias error**
*(deterministic error due to noise + non-linearity)*

**convergence error**
*(non-zero residuals)*

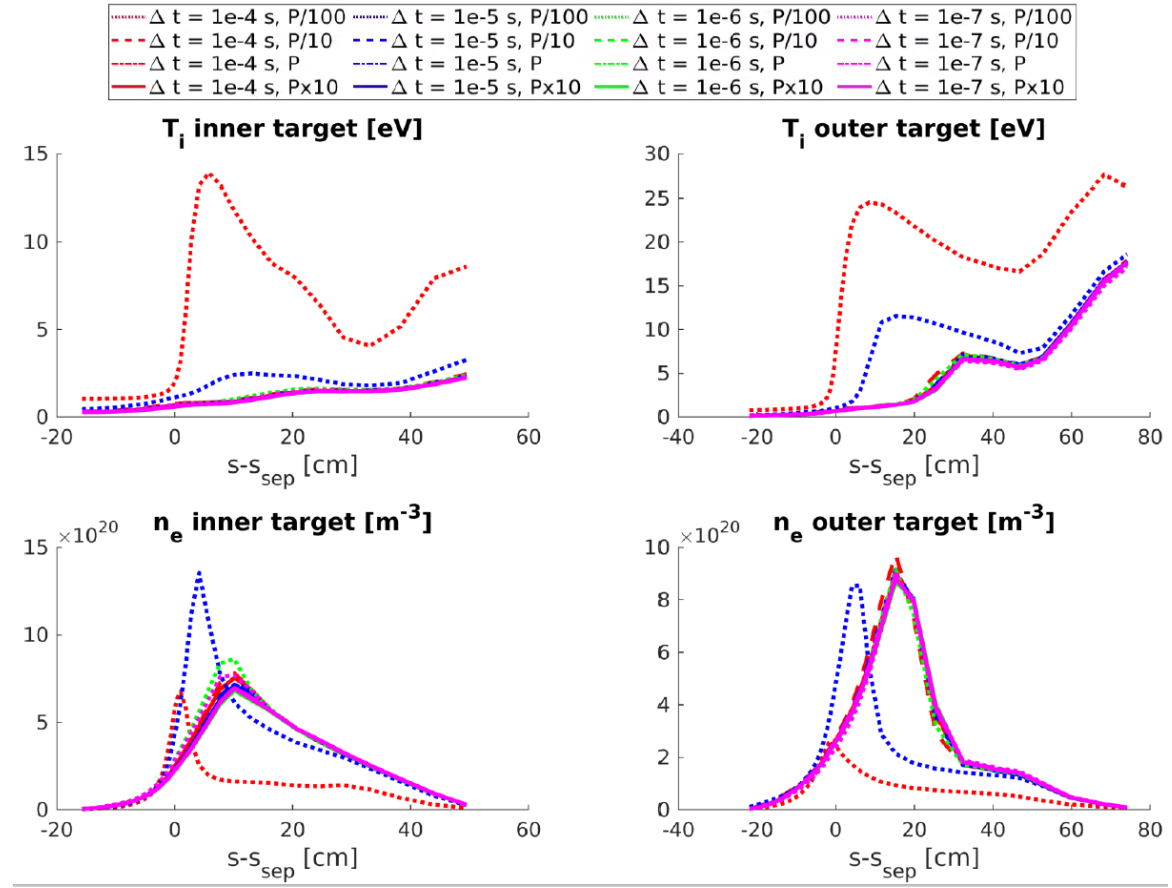
**discretisation error**
*(finite grid resolution)*

**Goal:**

**acceptable numerical errors for DEMO SOLPS cases (e.g. < 10%) as cheaply as possible**

W.Dekeyser, W Van Uytven
N.Horsten, et al.

# DEMO simulations – actual results [KU Leven]



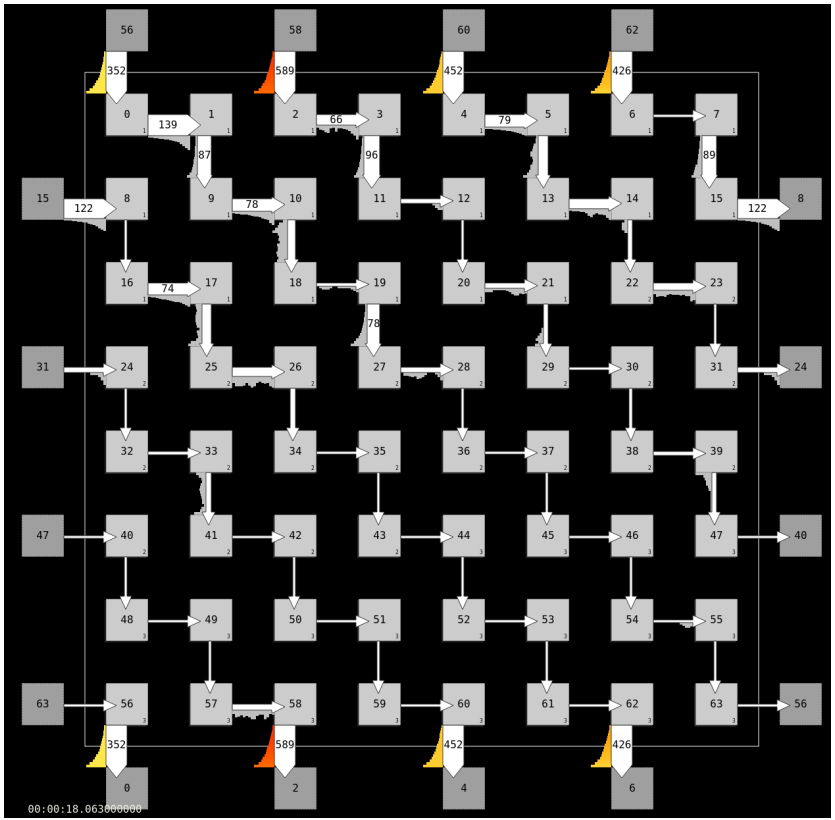

**“D-only” case:**

- ➔ only time steps $1^e$-4s and $1^e$-5s for P/100 lead to a qualitatively wrong solution
- ➔ no noticeable effect of n-n collisions on convergence behaviour
- ➔ bias decreases monotinically with $\Delta t$

**Preliminary:** Multi-species cases appear to have much larger bias than D-only case. Improved source averaging and time stepping schemes under investigation

# General code development of EIRENE – EIRON (ACH-VTT)

## On the right: the data flow between subdomains



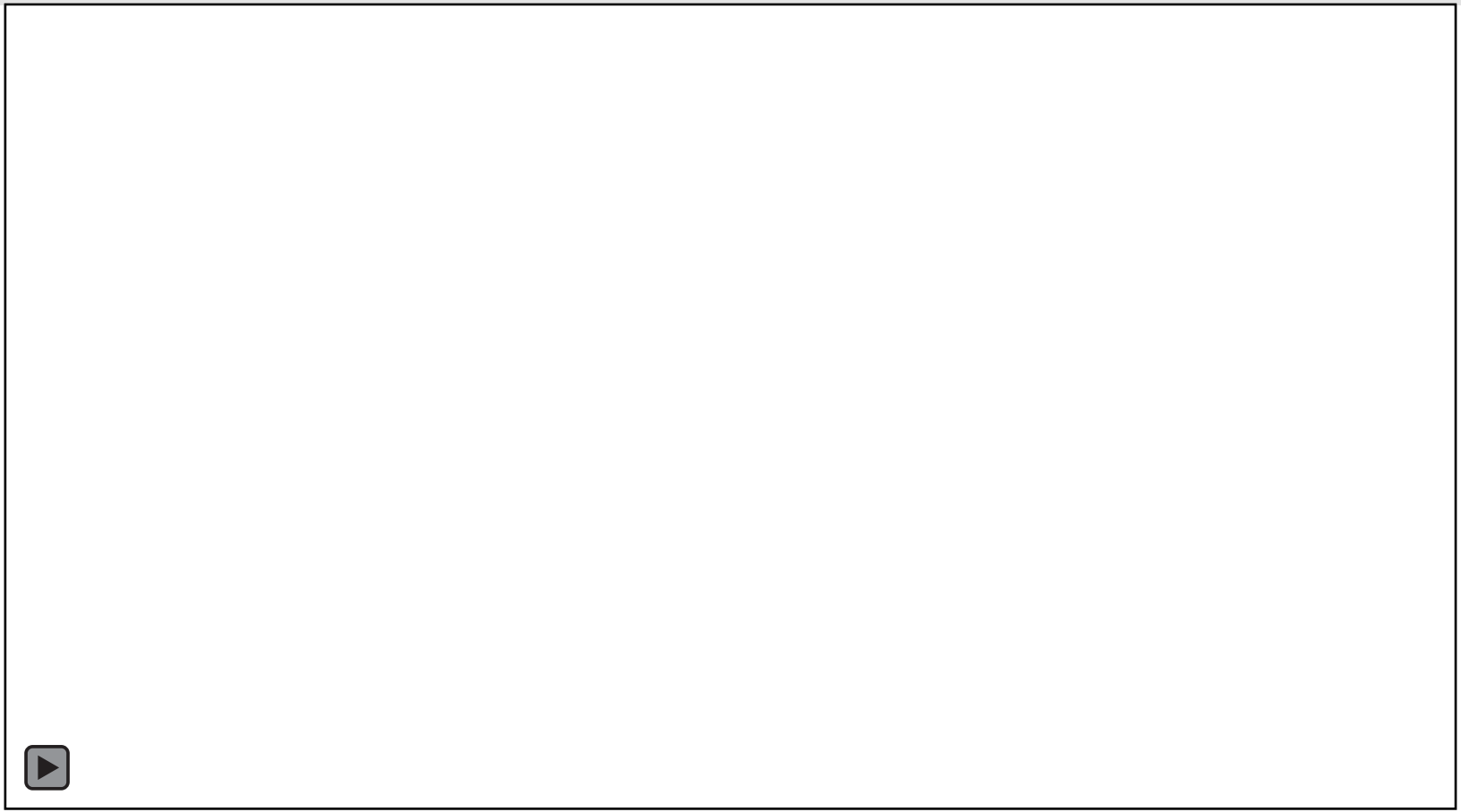

If a histogram is yellow or red, it indicates a bottleneck.

- **EIRENE "toy model" – EIRON and profiling of EIRENE**
- ➔ *Test of parallelisation and domain decomposition schemes*
- ➔ *Can be used for other purposes e.g. optimisation of ML-KDMC*

Eiron

Eirene

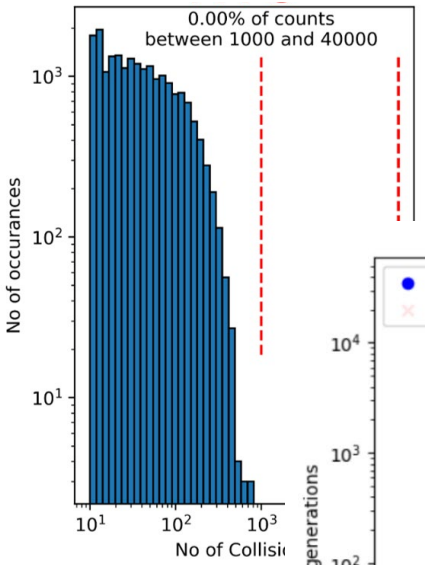
# EIRON (ACH-VTT, O.Lappi) – bottleneck analysis



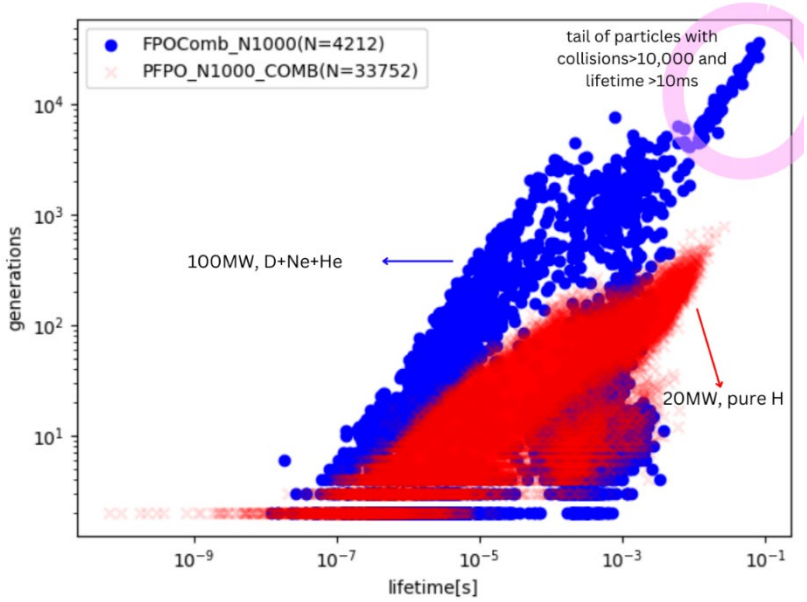
# First runs on ITER scale – performance challenges [AMU/CEA]

- Lifetime vs No of generations for each Eirene particle in log log scale
- FPO (blue dots) vs PFPO (red crosses)
- Very few particles have a linear relationship between generations and lifetimes
- Impact of this linear section on the plasma solution?

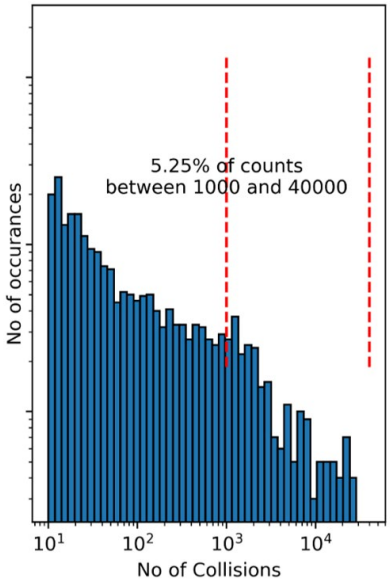
**20MW, pure H (PFPO)**




***SOLEDGE3X-EIRENE, TSVV-3 ⇔ TSVV-5***



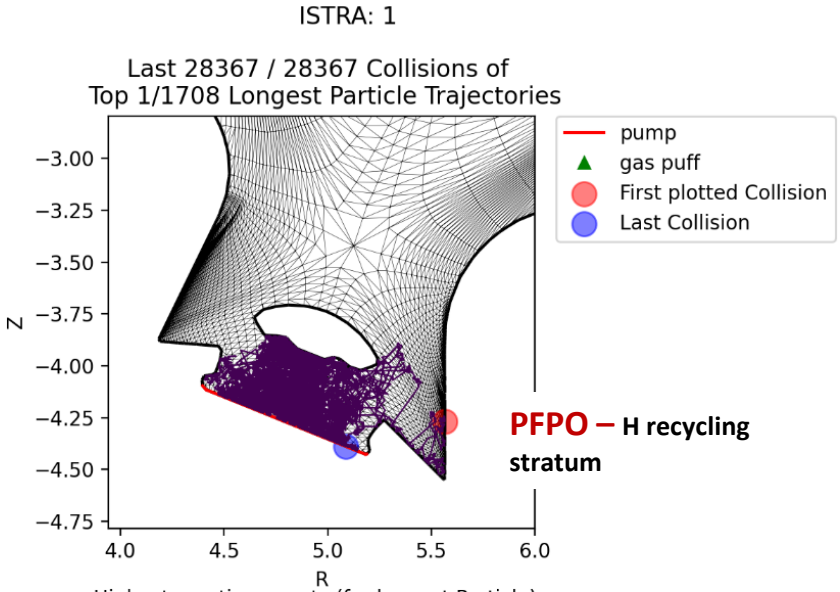

**100MW, Burning plasma (FPO)**

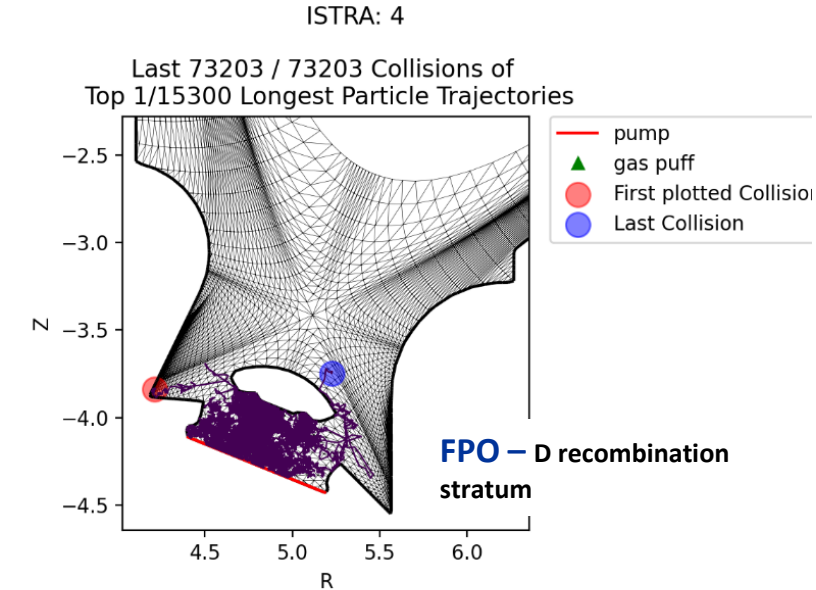



*Courtesy*
Y.Marandet,
S.Kumar

# ITER FPO performance challenges – analysis [S.Kumar, CEA]

***Longest trajectories simillar and dominated by elastic neutral-neutral collisions***




- Longest trajetories are for recombination and recycling strata for particles trapped under the dome.
- Elastic collisions dominate the collision count for the longest trajectories.
- Trajectories much shorter when turning off neutral-neutral collisions.

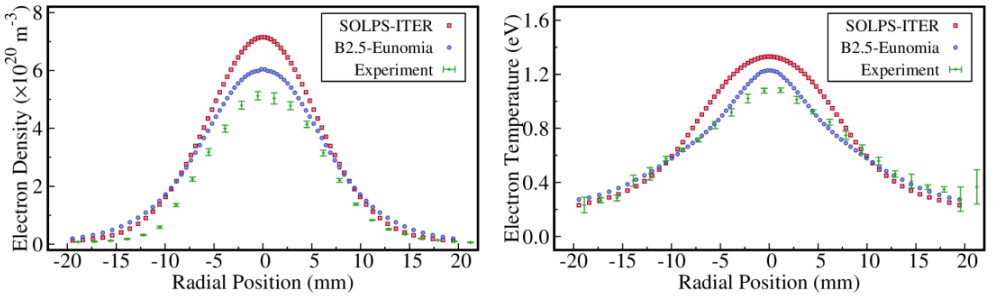
# EIRENE application to Magnum-PSI

- **Comparison of SOLPS-ITER (B2.5-EIRENE) with**
- **B2.5-ENOMIA**
  - ***Aim:*** *transfer all the useful development into EIRENE*
  - *Main differences are identified to be in* ***CRMs (MAR, EI, EC)*** *– direct comparison is often not possible.*

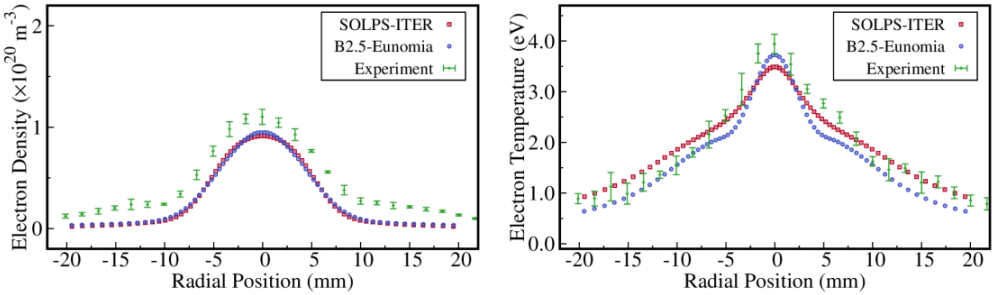
- **New FEM model for PWI in EIRENE** *(based on FreeFem++)*
  - ***Aim:*** *treat self-consistently temperature and sputtering, absorption and outgassing, recycling, transients (time-dependent simulations)*

Comparison with TS profiles near the target

High Density Case




Low Density Case




J. Gonzalez, E. Westerhof, et al., PET 2021, CPP (2022)

# EIRENE: collisional-radiative model (CRM) challenges

***EIRENE often uses effective ("condensed") rates tabulated from a CRM.***

→ **isotopes: $D_2$, $T_2$, $H_2$, DT, HD, …, Be-H/D/T, N-xxx, …**

→ **vibrational (and rotational) states in molecules**

→ **treating non-stationary effects e.g. metastables (MS) in atoms (e.g. He)**

→ **improving performance for simulations on ITER/DEMO scales**

→ **facilitate UQ and design with EIRENE**

→ **control the exploding amounts of data**

# PLOUTOS web-based tool for A&M data processing (FZJ)

www.eirene.de

EIRENE

*Both statues are at Glyptothek, Munich.*

- **to import/export data (JSON, tabular, etc.)**
- **to produce input data for EIRENE and for other codes with CRMs**
  ➔ *load/improve/save the developed configuration (selected reactions and parameters) including starting from the standard pre-sets*
- **to check data for consistency and abnormal features**
- **do sensitivity studies:**
  ➔ *understand A&M side of the problem and identify the most significant processes (among the selected ones)*

**The table contains data sources and type(s), "generation", other info …**
➔ *we plan adding simulation case references.*

# PLOUTOS interface – ($H_2$ 2022/23 case)

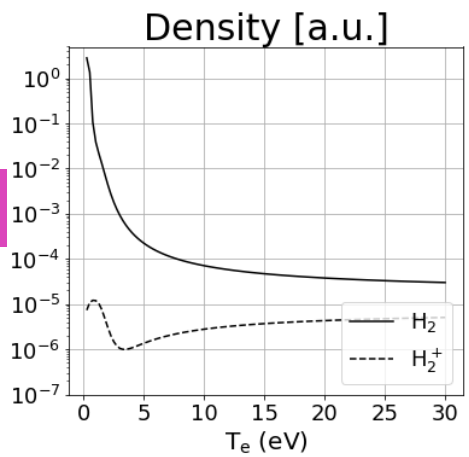
Collision with e

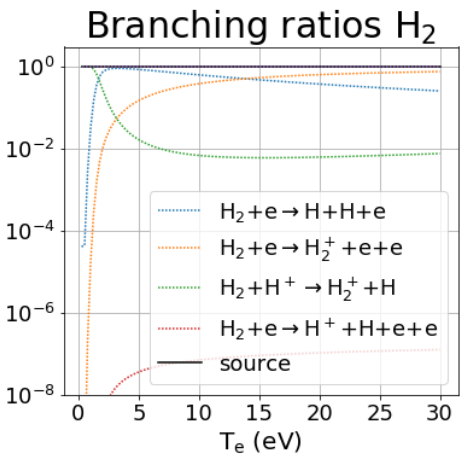
| not included in solver | selected data<br>unselect all | plot<br>unselect all | Number | reaction | range | reference | data type | File/chapter |
|---|---|---|---|---|---|---|---|---|
| ◉ | ○ | ☑ | 2.1.1 | e + H(1s) → H(2p) + e | E_min: 1.08e+01<br>- E_max: 2.00e+04 | JanevEtAl(1987) | calculated | hydhel H.1 |
| | ○ | ☑ | | e + H(1s) → H(2p) + e | T_min: 1.26e+00<br>- T_max: 2.00e+04 | JanevEtAl(1987) | calculated | hydhel H.2 |
| ○ | ◉ | ☑ | 2.1.2 | e + H(1s) → H(2s)+ e | E_min: 1.08e+01<br>- E_max: 2.00e+04 | JanevEtAl(1987) | calculated | hydhel H.1 |
| | ○ | ☑ | | e + H(1s) → H(2s)+ e | T_min: 1.26e+00<br>- T_max: 2.00e+04 | JanevEtAl(1987) | calculated | hydhel H.2 |
| | ○ | ☐ n=1 -> n'=2<br>☐ n=2 -> n'=1 | | e + H(n) → H(n') + e | T_min: 1.00e-01<br>- T_max: 1.00e+03<br>n_min: 1.00e+08<br>- n_max: 1.00e+16 | SawadaFujimoto(1995) | mixed | h2vibr H.4<br>2.1.5[cd] |

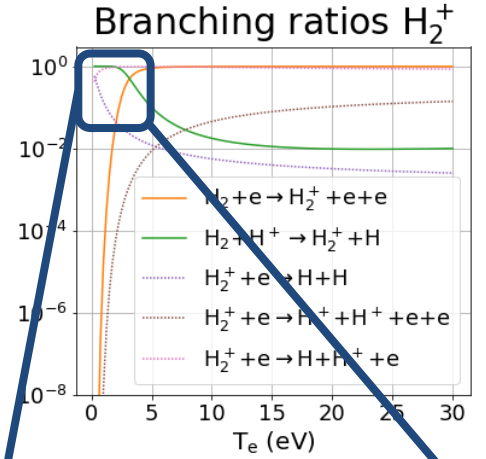
- **All columns can be turned on/off**
- **Reactions grouped by types**
- **Rows: one can turn on/off only selected for the CRM**

# CRM FOR MOLECULES: leading reactions

EU-DEMO

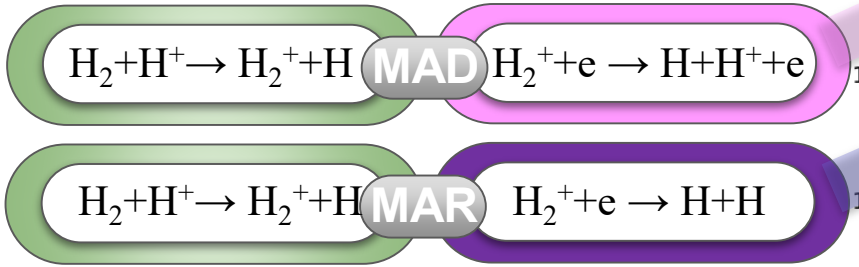


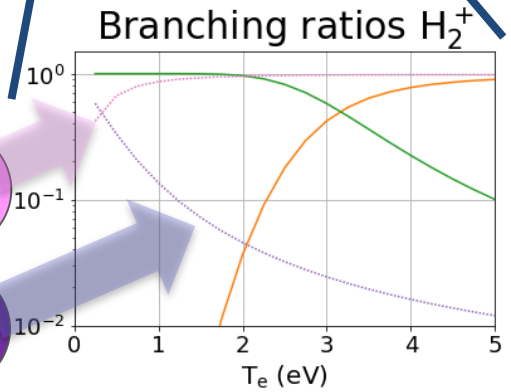




**low temperature** (T < 2eV) leading reaction chains:

**MAR/MAD competition at very low temperature**

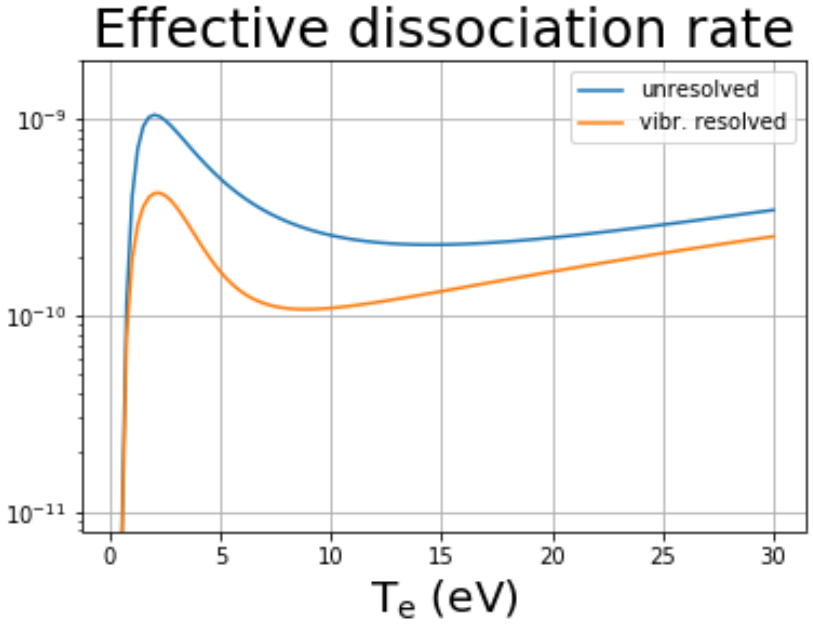


# EU-DEMO and JET – effect of resolution by vibrostates

➔ MAR/MAD branching ration modelling results significantly depend on resolution by vibrational states in $H_2$

➔ So as other parameters such as total ionisation rate in the volume




F.Cianfrani et al.,
EPS-2022

**Fully in line with the EIRENE and other CRMs:**

**JET modelling:**
"Up to **40% reduction in effective dissociation rate** due to transport of vibrational states"

A.Holm, M.Groth, et al.,
PET, CPP 2021

# New CRM Solver for EIRENE – "ModCR"

- This CRM is aimed to precompute rate coefficients accounting for **all parametric dependences** ($n_e$, $T_e$, but also $T_i$, …) in contrast with currently used polynomial fits (AMJUEL, …) + add a number of levels/processes not accounted for at this time
- The **internal states** (e.g. rovibrational states in molecular species) are to be tracked with a flexible a flexible control over this resolution (as separate specie or variable).
- The **nonstationary solution** for balance equations should be the default one (with the stationary only as a useful option).
- The solver should be **modular**, thus **usable standalone** or even in **various codes**.
- The **improved A&M data input** (encapsulated data - JSON, potentially also HDF5). We need **tools for visualisation and testing**.
  - ***Meet the exploding amounts of data for molecules (with resolution by rovibrational states)***

$$T_i \neq T_e, \; etc.$$

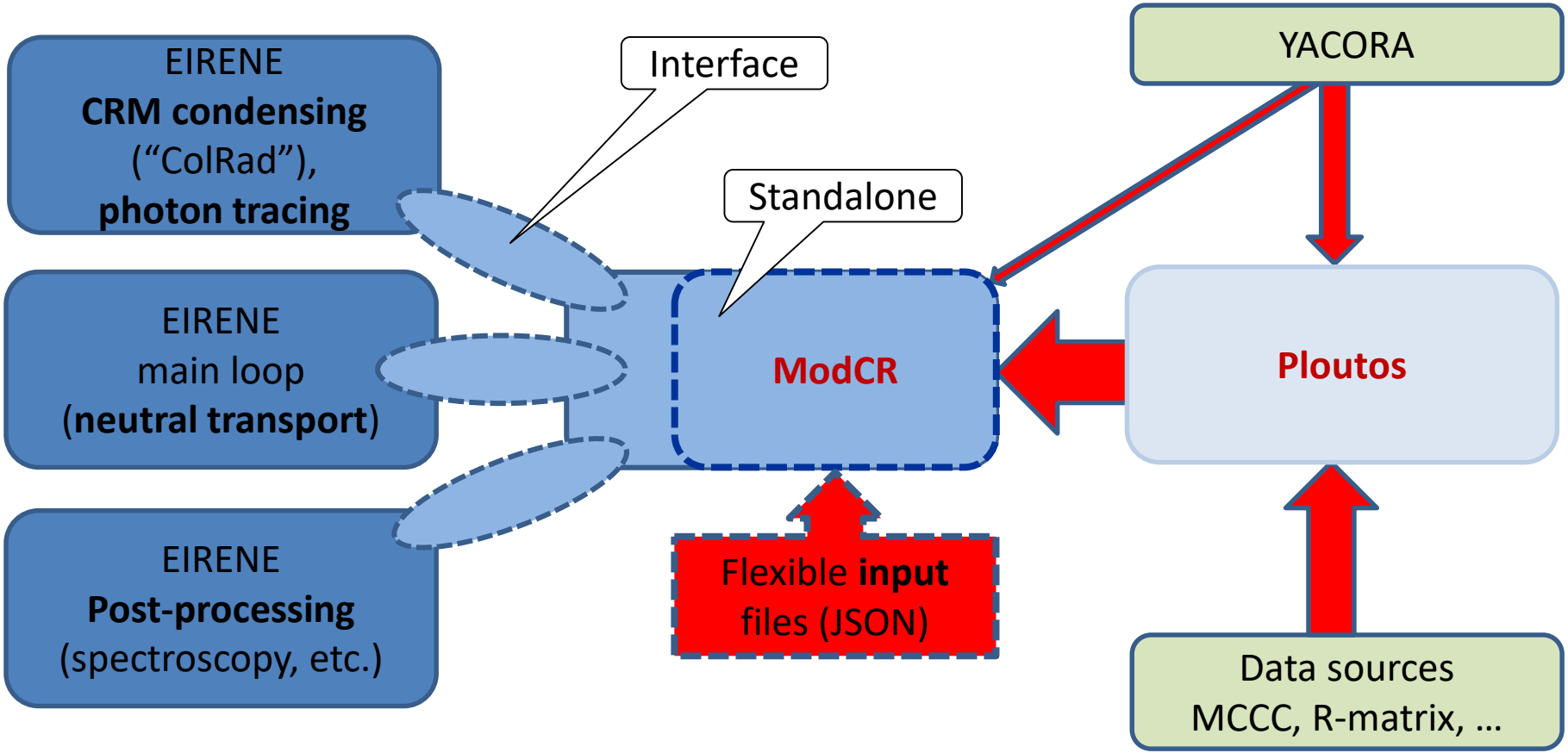
$$\frac{dN_i}{dt} \neq 0$$

***Why not also ERO?..***


**Not only performance and reliability, but additional physics can be provided!**

➔ *For instance, what if detachment is caused by non-stationary effects?!..*

# ModCR interaction with EIRENE and other tools



# Summary: TSVV-5 progress and plans

## ❑ Physics

- ***F**luid-**k**inetic **h**ybridisation **(FKH)** development successfully continues – incl. new branches (KDMC)*
- ***A&M CRM** extension and refinement (Ploutos + ModCR, photon tracing - opacity)*
- *Establishing **simulation cases** (validation at JET, Magnum-PSI, verification **at ITER and EU-DEMO scales** with realistic geometry) – in progress incl. with new features - FKH etc.*

Time-dep. runs
see M.Groth talk

## ❑ Code development

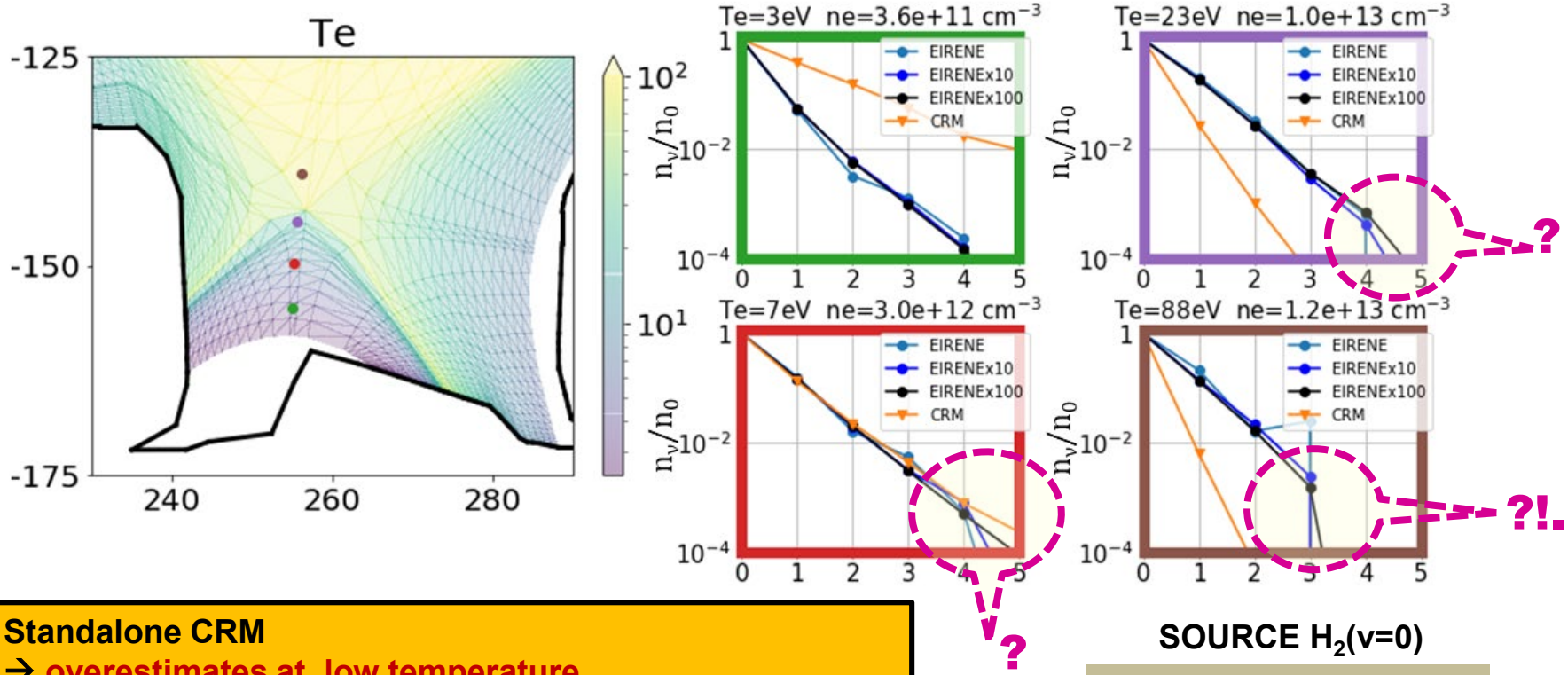
- ***Parallelisation:** OpenMP-MPI hybrid (related code refactoring done; **EIRON** "toy"-model (ACH-VTT) allows testing CPU loading and domain decomposition approaches so as new FKH options)*
- ***Code streamlining** (Segregation of the numeric core, etc.) – good progress, new big changes (e.g. ModCR substituting CRM part in the inner loop) – concepted and progressing.*
- *Merging all existing versions into first milestone one (**MsV**) – released in Nov 2024*
- *Improved I/O (JSON/HDF5), visualisation, **IMAS**ification, etc. – done or in good progress (with ACH)*

## ❑ Organisational and techical items

- ***New EIRENE license**, "infectious open source", **Coding guidelines**, ChangeLog, **JSON schema** (←STYX), **improved CI** - available at [www.Eirene.de](http://www.Eirene.de) and as part of EIRENE Git repo, good progress*
- ***Regular VCs and annual Code Camps, also strong and regular communication with ITER, IAEA and neighbour TSVVs** (mostly 3 and 7, but also others).*

# Thanks for the attention!

# Standalone CRM vs EIRENE (statistic issues)




**Standalone CRM**
→ **overestimates at low temperature**
→ **underestimates at large temperature**
**the excited state population**

**SOURCE $H_2$(v=0)**

| | |
|---|---|
| **EIRENE:** | 793'300 histories |
| **EIRENEx10:** | 7'933'000 histories |
| **EIRENEx100:** | 79'330'000 hist. |