KU LEUVEN

Aix*Marseille université Initiative d'excellence

cea

Aalto University School of Science

DIFFER Dutch Institute for Fundamental Energy Research

EUROfusion

Final review for E-TASC SB

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

28.01.2026

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.

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

KU LEUVEN
Aalto University School of Science
Aix*Marseille université
cea
DIFFER Dutch Institute for Fundamental Energy Research
JÜLICH Forschungszentrum

FP-9 deliverables:

1. Ne… wards … exa… rallelization … me…

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

2. Revised and extended physics basis f… dev… model towards the full vibrational resolution for all hydrogen isotopes and specific impurities for seeding.

Fluid-kinetic hybridisation (FKH) and improved CRMs

physics

3. Im… olec… vol… through generalized interfaces to, … molecular, nuclear and surface (AMNS) physics data.

Improved AMNS data, both in structure/physics and content

4. Interfaces and … mo… fluid dy… turbulence codes, time-dependent) and possibly also to gyro-kinetic/gyrofluid plasma cod…

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

5. Str… ed fusion reactor mo… (semi)detached divertor plasmas. Liaison with TSVV Tasks 3 and 4.

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

EIRENE-NGM DEVELOPERS (TSVV-5)

D.V. BORODIN, F. CIANFRANI, D. HARTING, P.BÖRNER, B.KÜPPERS, M.GORDON
Forschungszentrum Jülich, Institut für Energie- und Klimaforschung – Plasmaphysik, Germany

W. DEKEYSER, S. CARLI, M. BLOMMAERT, N. HORSTEN, W. VAN UYTVEN, M. BAELMANS
KU Leuven, Department of Mechanical Engineering, Belgium

B. MORTIER, G. SAMAEY, E. LOEVBACK, TH.STEEL, V.MAES
KU Leuven, Department of Computer Science, Belgium

Y. MARANDET, P. GENESIO, J.DENIS, N.RIVALS
Aix-Marseille Univ., France

H. BUFFERAND
CEA, IRFM, France

E. WESTERHOF, J.G. MUNOZ, P.W. GROEN
DIFFER - Dutch Institute for Fundamental Energy Research, Eindhoven, the Netherlands

M. GROTH, A. HOLM , R.CHANDRA
Department of Applied Physics, Aalto University, Espoo, Finland

\+ ACH-VTT: **O.LAPPI**

\+ ACH-MPG: **H.J.LEGGATE**

\+ ACH-IPPLM: **D.YADYKIN**, **YU.YAKOVENKO**, **P.CHMIELEWSKI**, **M.OWSIAK**, **B.POGODZIŃSKI**

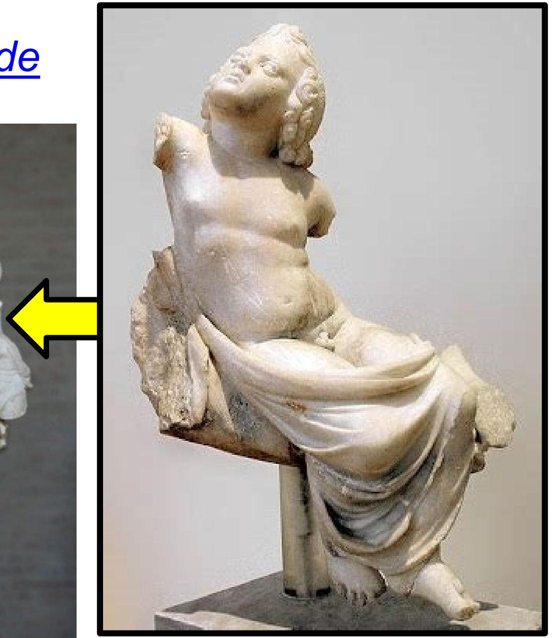
\+ ITER Organisation: **X.BONNIN**

Eirene with the infant Ploutos

PLOUTOS (web-based tool) can be used to

www.eirene.de

EIRENE

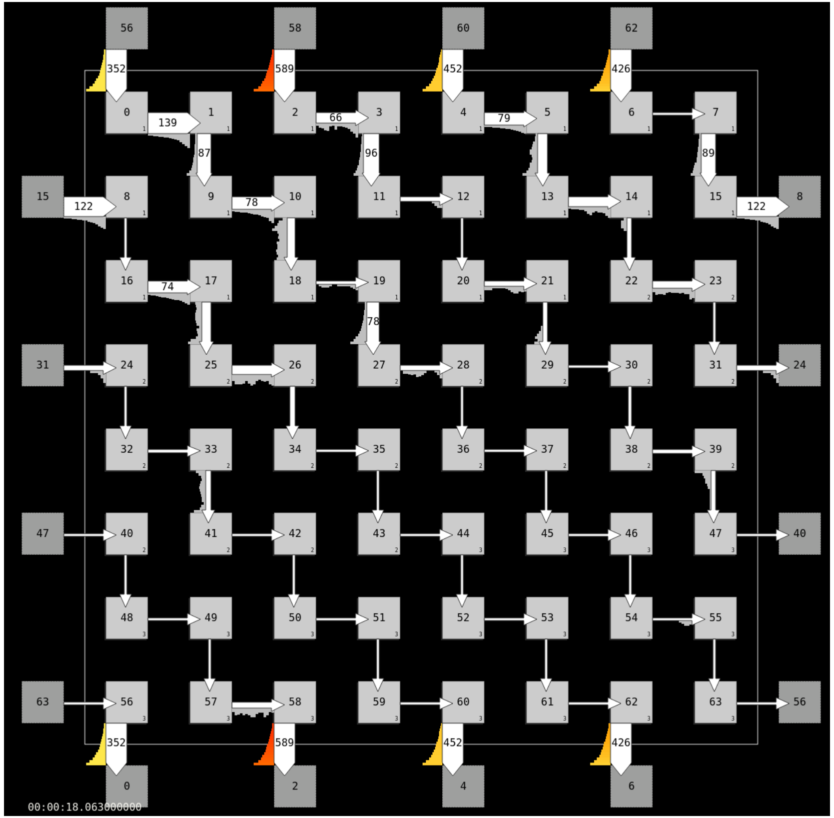


Both statues are at Glyptothek, Munich.

- **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)*

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

On the right: the data flow between subdomains



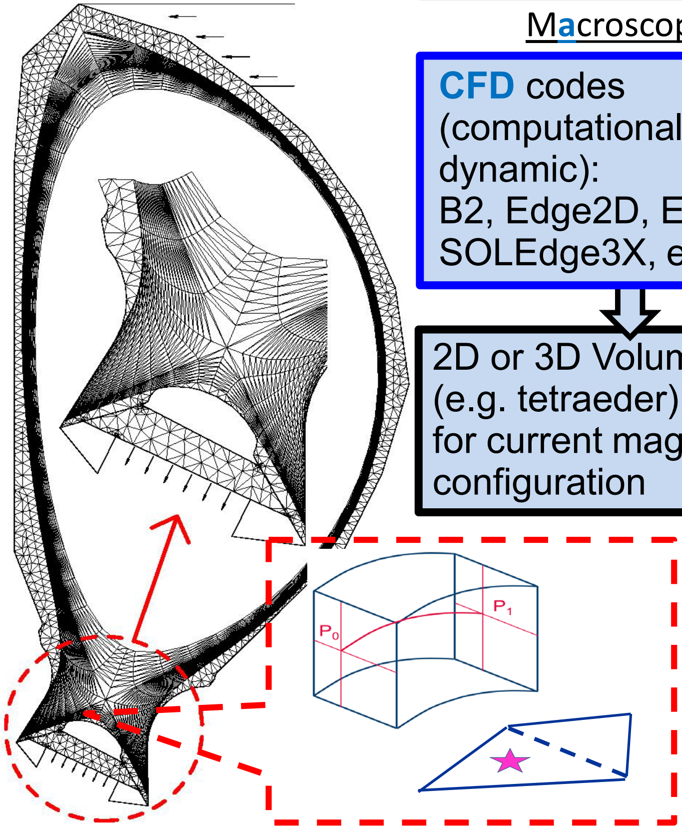
If a histogram is yellow or red, it indicates a bottleneck.

- **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

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

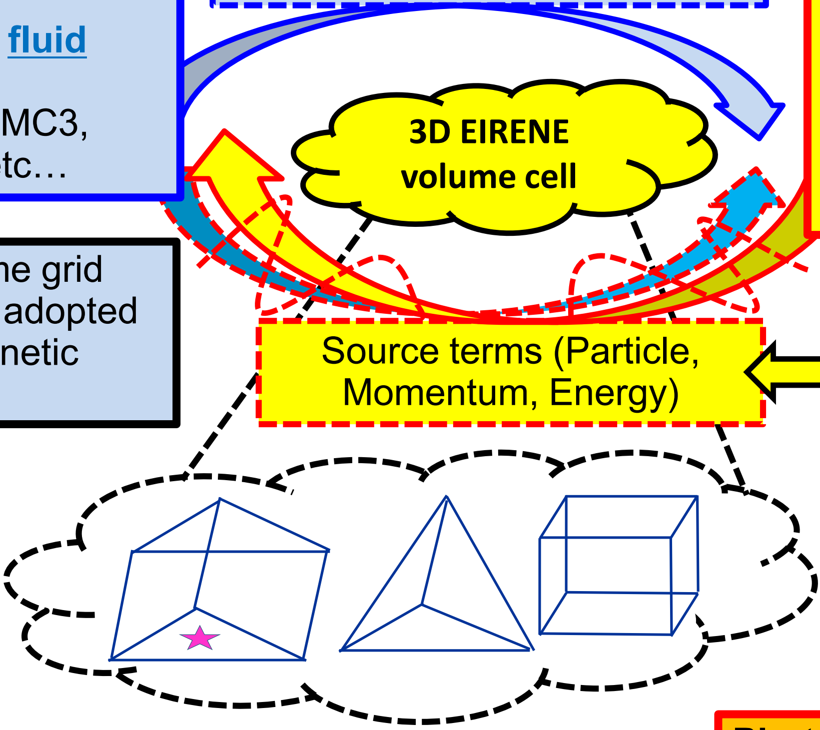


Macroscopic:

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



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

A&M data and CRMs in EIRENE

- *Photon trapping (opacity)*
- *ModCR module*

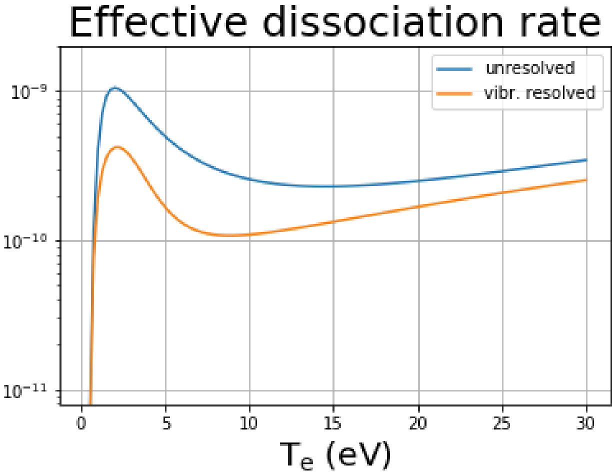
Total volume effects from CRM *(local effects much stronger!)*

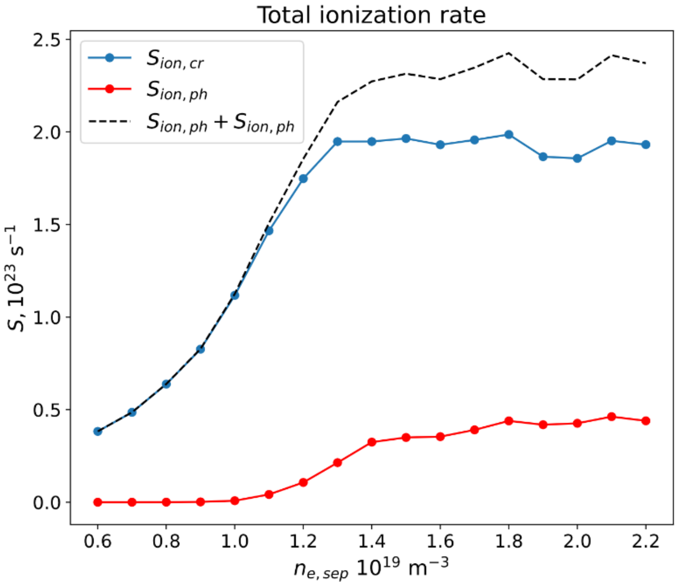
1) **Photon tracing – opacity effects**

2) **Resolution by vibrational states in H_2 *(D_2, DT, …)***

- **Photon absorption adds up to ~20% of total CR ionization rate in detached conditions**
- **Ly-β opacity enhances D-α emission at LFS SP by 50-100% (JET-ILW detached L-mode)**

- **Up to 40% reduction in effective dissociation rate due to transport of vibrational states (for JET)**





Cianfrani, F., Borodin, D.V. & Küppers, B. Eur. Phys. J. D 2023. https://doi.org/10.1140/epjd/s10053-023-00722-5

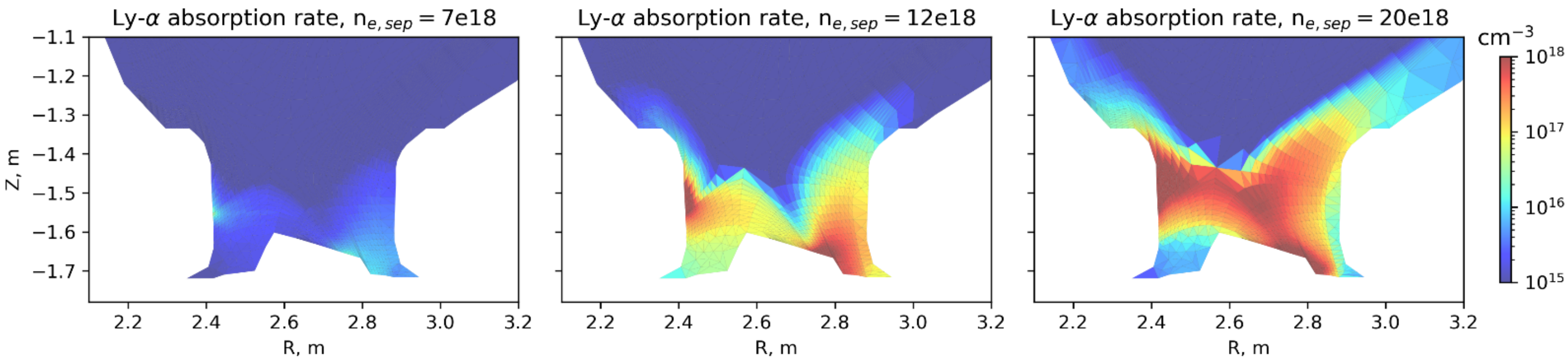
R. Chandra, M.Groth et al. NME 2024 https://doi.org/10.1016/j.nme.2024.101794

Ly-α absorption is poloidally non-uniform and cannot be captured with a single population escape factor requiring photon tracing and opacity

(R.Chandra, M.Groth - Aalto)

JET81472 (D plasma), SOLPS-ITER

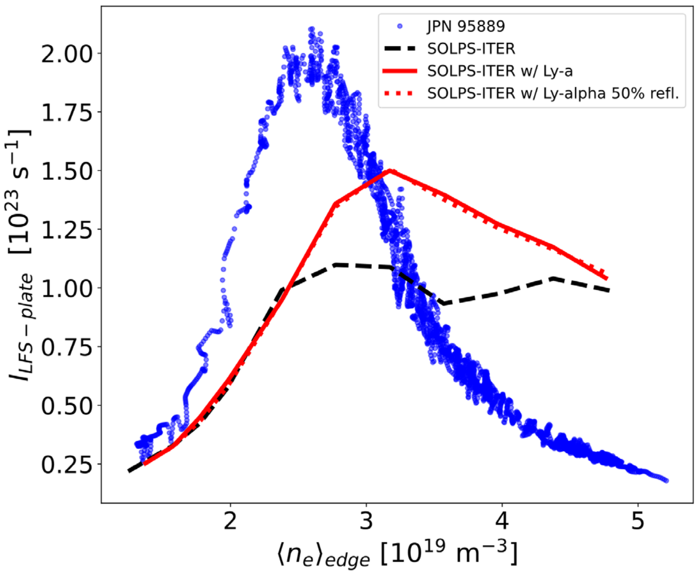
low-recycling | high-recycling | detached

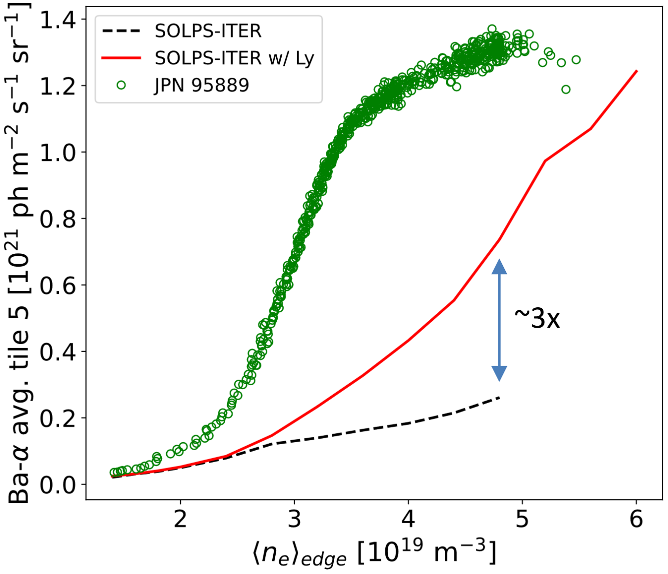


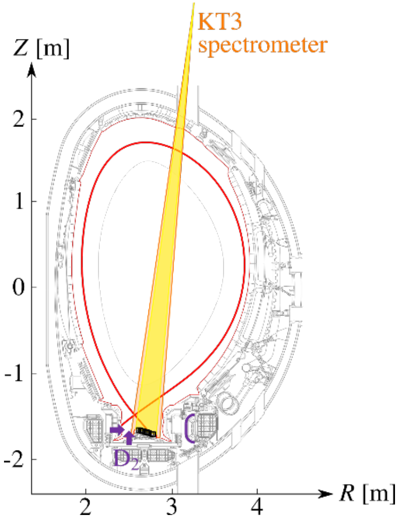
Lyman absorption ➔ increases population of excited D atoms ➔ increased Da emission ➔ more consistent with JET-ILW measurements

Fully coupled plasma-gas-photon: prediction of LFS-plate peak values improved by ~30% and increased Ba-α emission by 3x with Lyman trapping

JET81472 D SOLPS-ITER







Lyman absorption ➔ increases population of excited D atoms ➔ increased Da emission ➔ more consistent with JET-ILW measurements

R. Chandra, et al. PET-20, 2025

EIRENE: collisional-radiative model (CRM) challenges

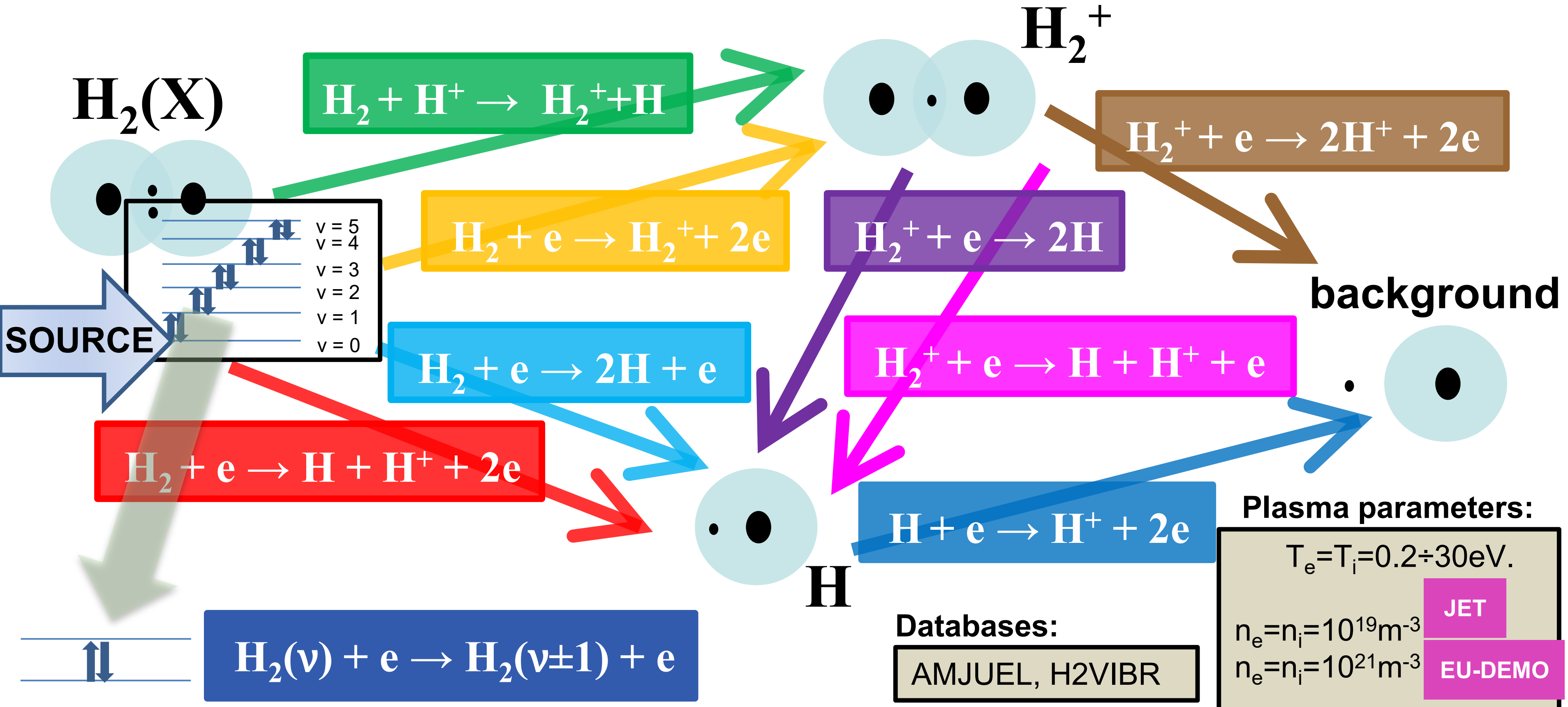
EIRENE often uses effective ("condensed") rates tabulated from a CRM.

- → 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), so as photon trapping (opacity)

?

- → improving performance for simulations on ITER/DEMO scales
- → facilitate UQ and design with EIRENE
- → control the exploding amounts and quality of data

CRM FOR MOLECULES : vibral resolution



Databases:

AMJUEL, H2VIBR

Plasma parameters:

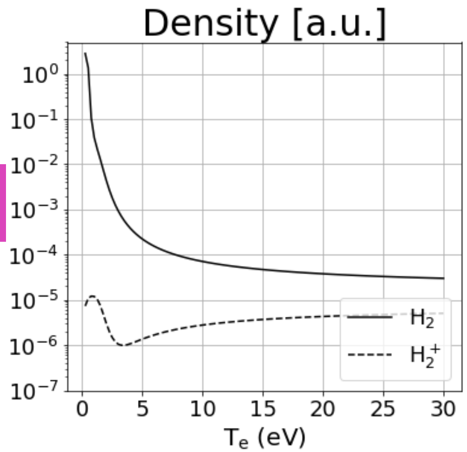
$T_e=T_i=0.2\div30$eV.

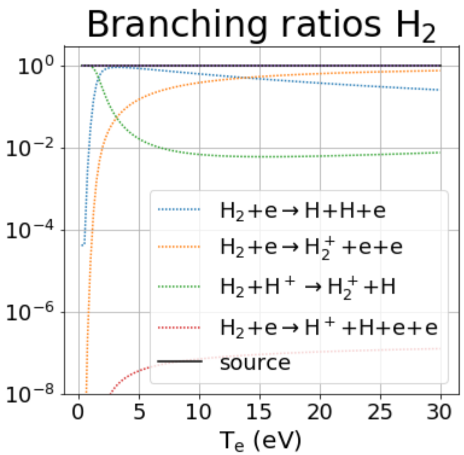
$n_e=n_i=10^{19}m^{-3}$ JET

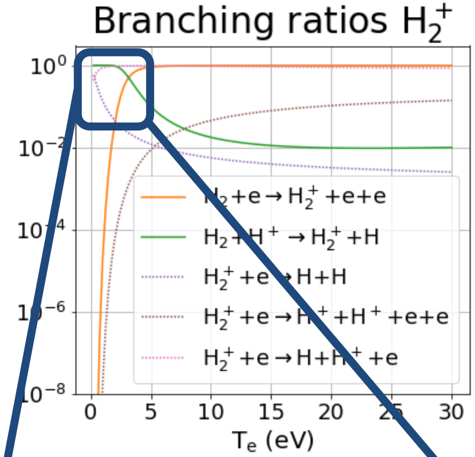
$n_e=n_i=10^{21}m^{-3}$ EU-DEMO

CRM FOR MOLECULES: leading reactions

EU-DEMO





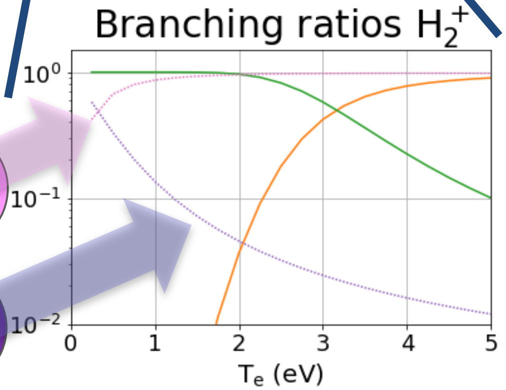


low temperature (T < 2eV) leading reaction chains:

MAR/MAD competition at very low temperature

$H_2+H^+ \rightarrow H_2^+ +H$ **MAD** $H_2^+ +e \rightarrow H+H^+ +e$

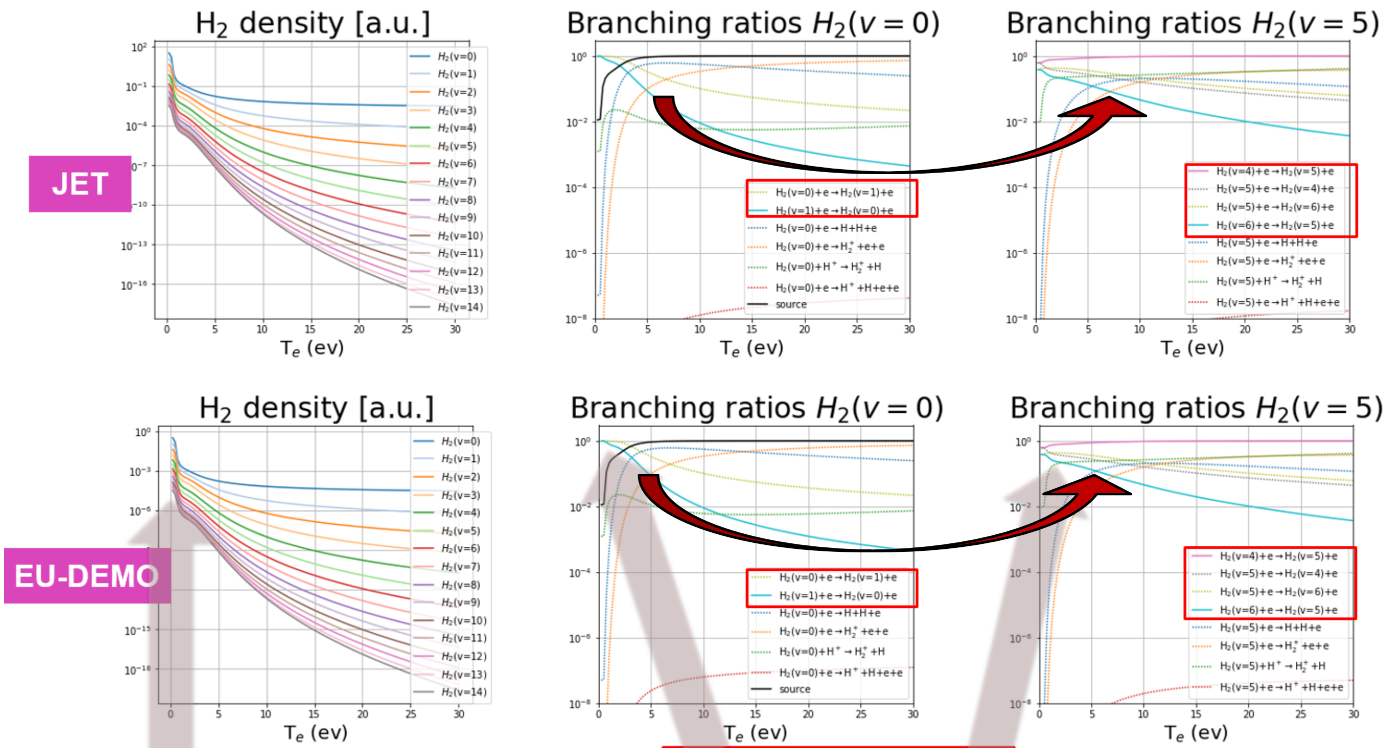
$H_2+H^+ \rightarrow H_2^+ +H$ **MAR** $H_2^+ +e \rightarrow H+H$



Effect of resolution by vibrostates

$$H_2(v) + e \rightarrow H_2(v\pm1) + e$$ rates H2vibr[5]

F.Cianfrani et al., EPS-2022



- **density:** **large at low temperature**

vibrational transitions are the main reaction channels at low temperatures

Fully in line with the EIRENE and other CRMs:
"Up to **40% reduction in effective dissociation rate** due to transport of vibrational states"

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

‘StoichioMatr’ approach for balance equations

N_s = Number of Species, N_r = Number of Reactions, k_r = Rate coefficient for Reaction r

Reactions

$$\sum_{s=1}^{N_s} \nu'_{s,r} X_s \xrightarrow{k_r} \sum_{s=1}^{N_s} \nu''_{s,r} X_s$$

Rate Laws

$$\frac{\partial [X_s]}{\partial t} = \sum_{r=1}^{N_r} \nu_{s,r} k_r \prod_{p=1}^{N_s} [X_p]^{\nu'_{p,s}}$$

Stoichiometric Matrix

$$\nu_{s,r} = \nu''_{s,r} - \nu'_{s,r}$$

<u>Reiser, D.,</u> von Keudell, A. & Urbanietz, T.
Determining Chemical Reaction Systems in Plasma-Assisted Conversion of Methane Using Genetic Algorithms.
Plasma Chem Plasma Process ***41****, 793–813 (2021).*

➔ *Very good fits with the Ploutous-like CRM files*

➔ *General and **<u>abstract</u>** (no problem to treat e, p, e-e etc. driven transitions inside single matrix – “reservoirs”)*

- ❖ Abstractisation of reactions in the main loop of EIRENE is one of the ModCR goals. **Aim: <u>minimise branching</u>** by reaction type

➔ *Extra step with “StoichioMatr’” will allow keeping the basic database on particular solver run (can be several even by single ModCR start)*

➔ *No linearity is implied*

New CRM Solver for EIRENE concepted

- 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** should be readable and structured (for starters JSON, potentially also HDF5). It should be pre-processed mostly automatic and easily exchanged with other codes and tools. We need **tools for visualisation and testing**.
  - The only way to meet the exploding amounts of data from RMPS and CCC for molecules (with resolution by rovibrational states)
  - IAEA GNAMPP assists, but also reveals the challenges

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

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

Why not also ERO?..

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

Policy proposal on management of AMNS data

Policy proposal formulated as it spined off from the decennial IAEA meeting on Atomic, Molecular and surface data in 2024.

+3 additional events at FZJ and IAEA
Including 28th Meeting of the Atomic and Molecular Data Centres Network (DCN28) (1-3 October 2025): Timetable ·

(F.A.I.R data and metadata)

- GitHub: https://github.com/D-V-Borodin/AMDPolicyDoc (public for the time being. We count on change requests to be submitted as "pull requests")
  git clone https://github.com/D-V-Borodin/AMDPolicyDoc.git
  or git clone git@github.com:D-V-Borodin/AMDPolicyDoc.git

AFN, FKH, KDMC

Hierarchy of (partially reduced) models…

Fluid-kinetic hybridization (FKH)

A hierarchy of neutral models:

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

Accuracy

Code performance

Fluid, AFN

Hybrid Fluid-Kinetic approach (FKH)

Asymptotic-Preserving MC (APMC)

kinetic, MC

Not fully rigorous, speedup >100

Spatial FKH

Firm domain allocation

Spatial by source

Evapor./condens.

Flexible domain border - tested

Micro-macro FKH (mMH)

- **Cancellation error** (can be suppressed by enforcing positivity)

Typical speedup ~10 (or less)

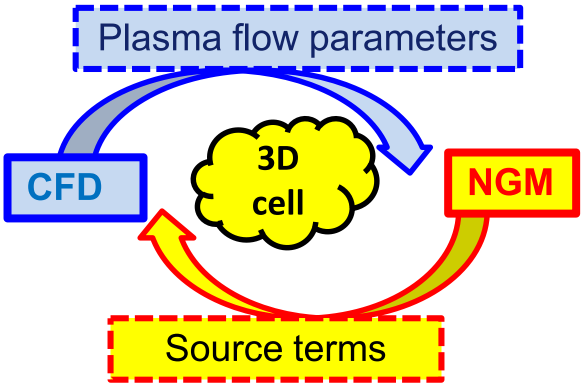
Micro-macro kinetic diffusion (KDMC)

- **Bias error** (can be suppressed via multi-level)
- No coupling with CFD needed

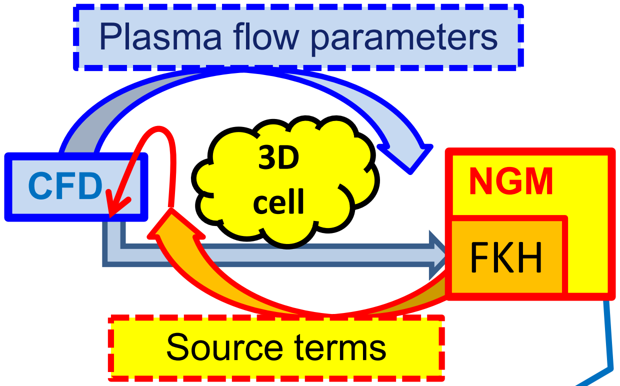
Seamless in volume

F-K Hybridisation approaches utilized in EIRENE-NGM

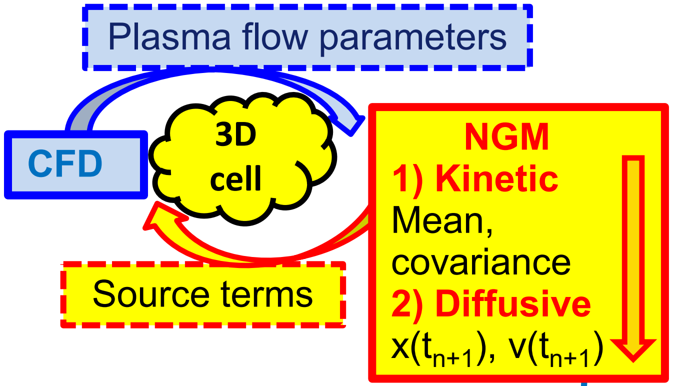
A) Full kinetic



B) Spatial, "micro-Macro" hybr.



C) APMC: KDMC



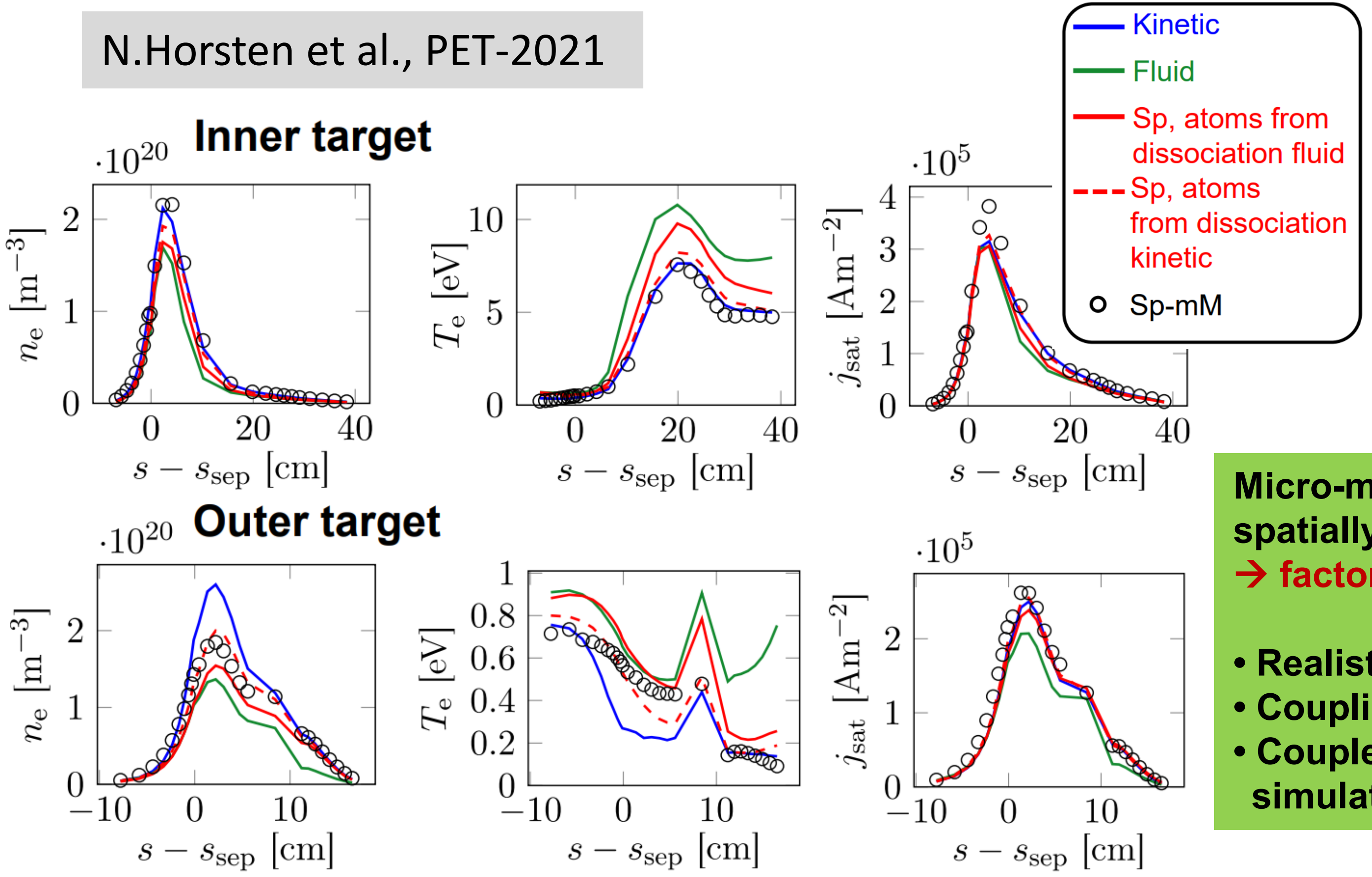
$f = f_F + f_K$, optionally with evaporation/condensation:

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

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!

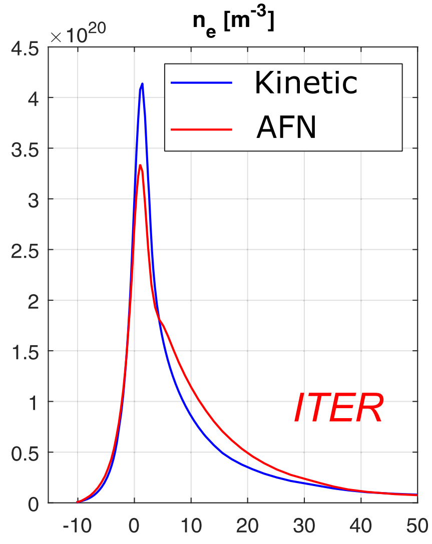
- **Realistic geometry, void regions**
- **Coupling to kinetic molecules**
- **Coupled plasma-neutral simulations**

AFN: mature, accurate fluid model for H/D/T atoms

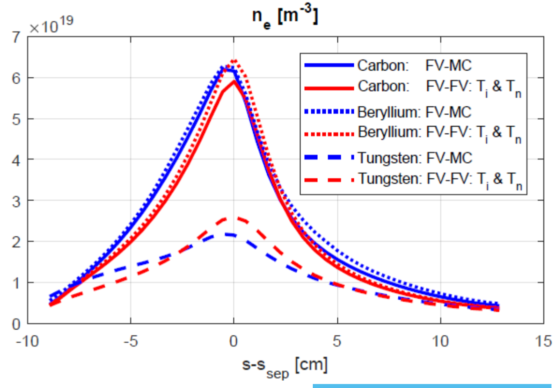
[N. Horsten et al, NF 2017; W. Van Uytven et al., NME 2022;…]

- **Consistency with fully kinetic simulation without tuning parameters**
  - Transport coefficients and BCs based on AMJUEL/HYDHEL/TRIM
  - Including effects of drifts, n-n collisions, …
  - Rigorous comparison with fully kinetic simulations (EIRENE) on various devices/geometries
- **Integration in various codes**
  - Default model in SOLPS-ITER extended grids version. Relevant input files automatically generated.
  - Basic AFN models (***but not yet BCs (!)***) implemented in various European turbulence codes (link TSVV3/B), incl. SOLEDGE3X, GRILLIX, and also gyrokinetic code GENE-X (link TSVV4/C)
- **Applied to simulate multiple machines**, incl. TCV, AUG, JET, ITER, DEMO (link WP TE, WP DES)
- **Next step**
  - Fluid model for molecules: first AFN-like model based on ion-molecule collisions gives promising results

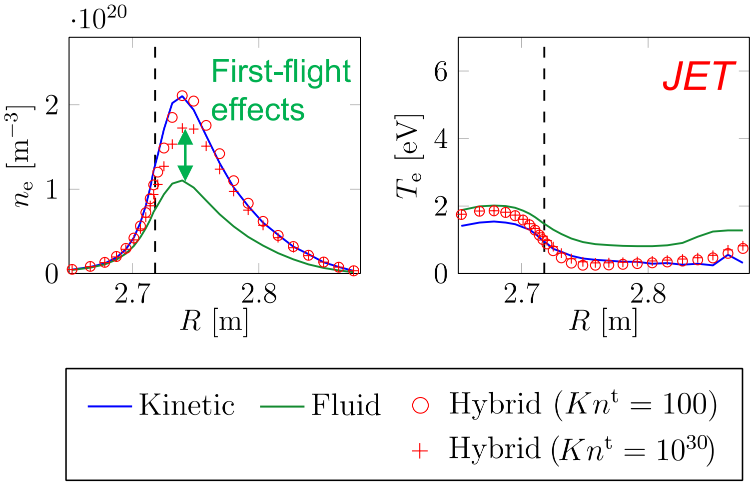
➔ **AFN matured in its use and linked to other TSVVs**



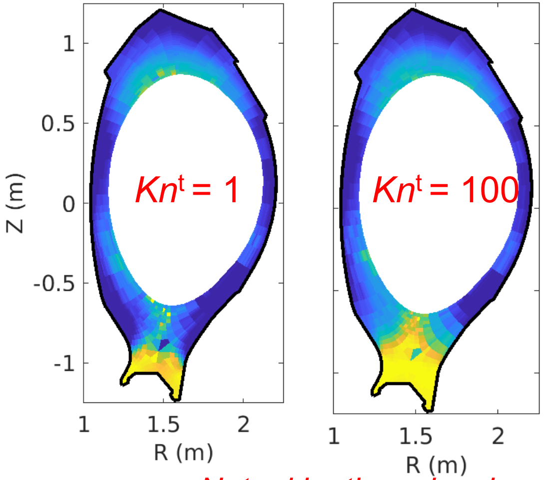
[W. Van Uytven et al., NF 62 (2022).]

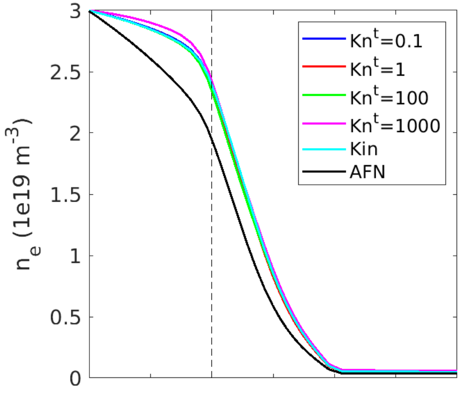


Spatially hybrid modeling (SpH) to balance accuracy and computational cost



[N. Horsten et al., NME 33 (2022).]





[W. Dekeyser et al., PET 2025.]

Note: kinetic molecules present in hybrid simulations; molecules become computational bottleneck

- Kinetic effects corrected by SpH
  - Coupling to void regions beyond plasma grid
  - Coupling to molecules and impurity neutrals
  - Kinetic effects in low-collisional regions
- ***Trade-off accuracy vs. speed: up to factor 10 faster than fully kinetic simulations***

- Method:
  - Launch all neutrals kinetically (first flight effects!)
  - Transfer atoms to fluid (AFN) population when

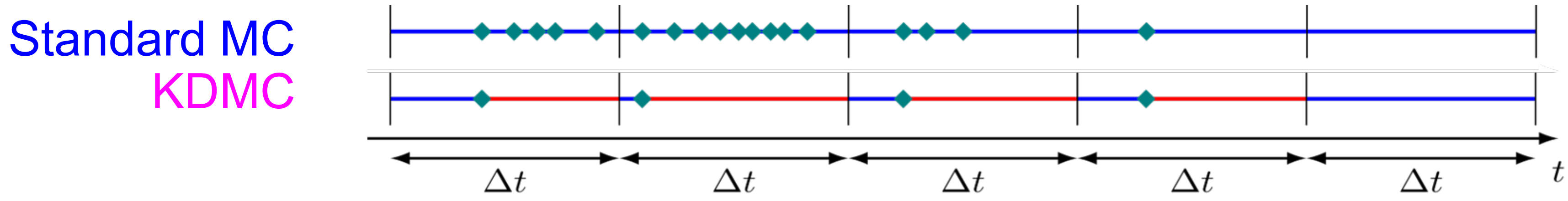
Particle Knudsen number

$$Kn^p < Kn^t$$

User imposed transition criterion

KU LEUVEN

KDMC – Kinetic Diffusion Monte Carlo: An asymptotic-preserving particle method



- The method:
  - Alternative, fully particle-based, hybrid method
  - Alternate between normal kinetic steps and diffusive (fluid) steps
  - Couple with AFN model for QOI estimation (plasma sources)
  - Optionally, MLMC for increased speedup
- Optimized basic implementation (EIRON)
  - **Demonstrated that the claimed speed-ups are also visible in optimized code**
  - Identified practical issues in combining domain decomposition and KDMC to be resolved
- **3D implementation with unstructured mesh (NEPTUNE-MC)**
  - Identified and resolved problems with boundary conditions
  - Steps taken to validate scheme on "real" test cases (WIP)
  - **Outlook, TSVV-K:** Good candidate for coupling to turbulence codes (TSVV-B/C)
- New variant with significantly reduced bias under development

KU LEUVEN

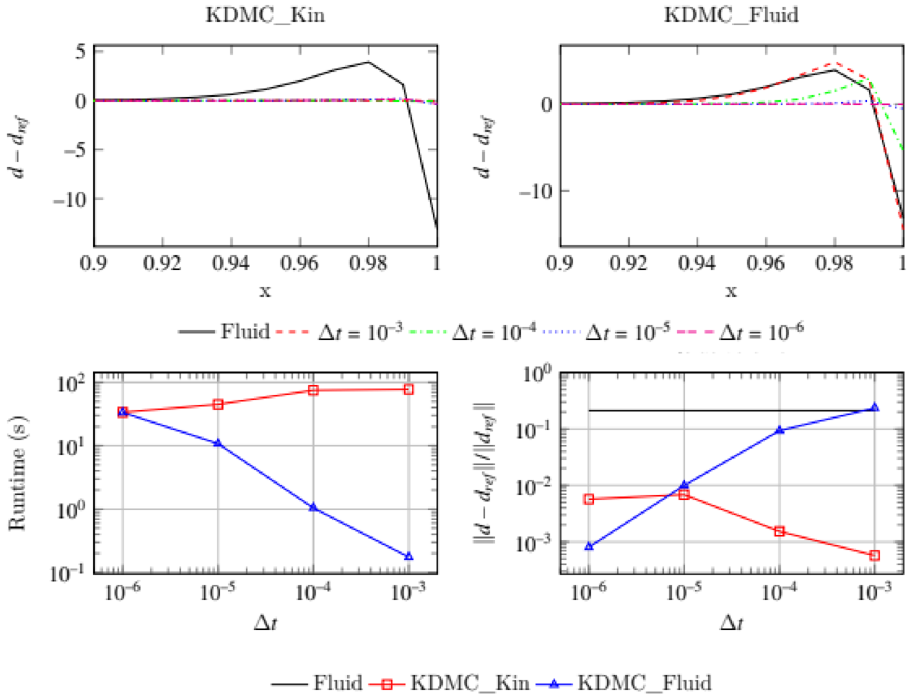
KDMC: boundary conditions

- **Problem: the standard derivation of KDMC only works when not close to the boundary**

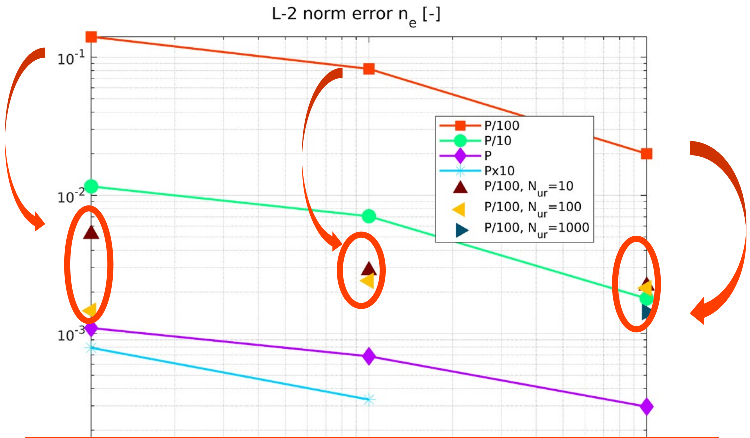
- **Solution 1:**
  - If the new sampled position is outside the domain, throw it away and simulate that timestep kinetically
  - Simple to implement, but expensive and may be inaccurate, especially when there is drift away from the boundary

- **Solution 2 (new):**
  - Analytically calculate the correct distribution that takes the boundary condition into account and sample from it.
  - Cheap to simulate and an accurate approximation of the fluid equations, but more difficult to implement, and occasionally less accurate than the fully kinetic BC of solution 1

➔ **KDMC algorithm is ready for upscaling**

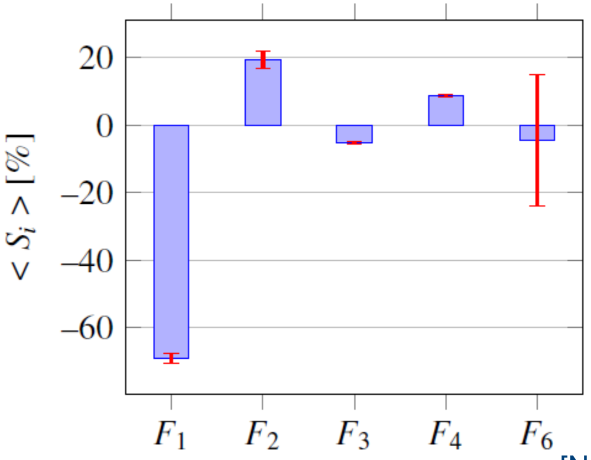


Error analysis, code coupling and sensitivity studies



1-2 order-of-magnitude bias reduction due to underrelaxation

[W. Van Uytven et al., PET 2025]



i	Reaction
1	$D + e \rightarrow D^+ + 2e$
2	$D + D^+ \rightarrow D^+ + D$
3	$D_2 + e \rightarrow D_2^+ + 2e$
4	$D_2 + e \rightarrow 2D + e$
5	$D_2 + e \rightarrow D + D^+ + 2e$

[N. Horsten et al., CPP 2024]

AD sensitivities of neutral density w.r.t. reaction rate coeffs.

- FHK model development supported through theoretical model development and extensive error analysis studies (e.g. [V. Maes et al.])
- Error reduction and code-speed up through improved plasma-neutral coupling strategies (e.g. [W. Van Uytven et al., PET 2025])

- Application of Algorithmic Differentiation to compute sensitivities of EIRENE output quantities w.r.t. code inputs ([N. Horsten et al., CPP 2024])

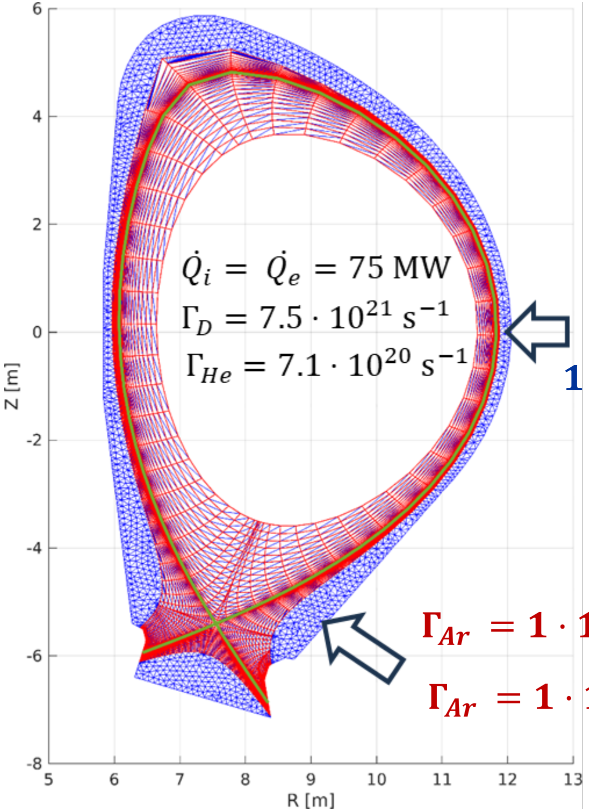
➔ **Accurate and faster models and algorithms are available**

KU LEUVEN

Actual DEMO simulations (with NCC)

KU LEUVEN

D +(He + Ar)



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

[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)*

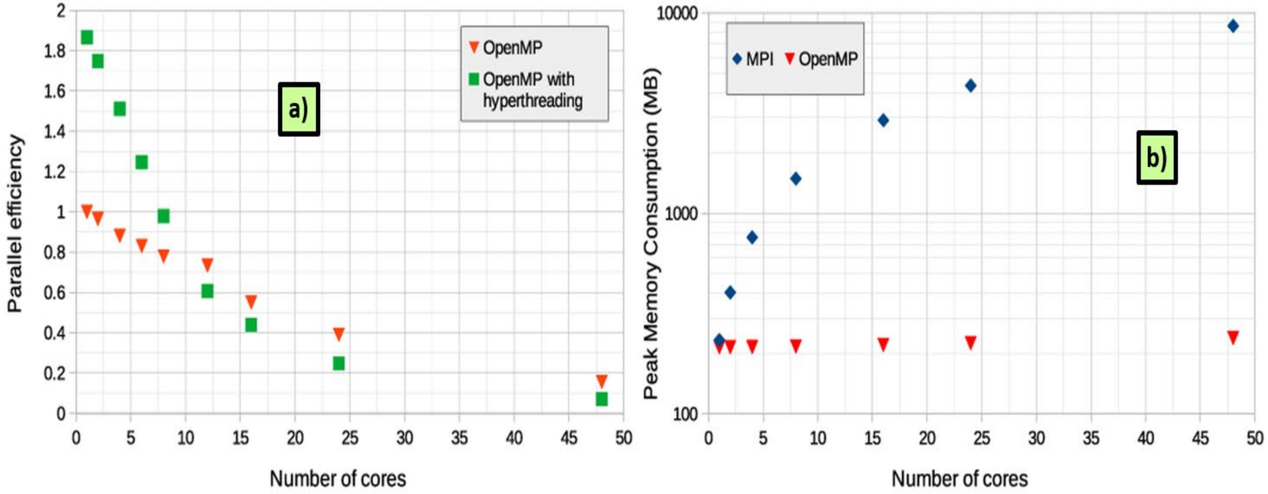
Goal:
acceptable numerical errors for DEMO SOLPS cases (e.g. < 10%) as cheaply as possible

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

EIRENE performance on ITER/DEMO scale

EIRENE parallelization

- OpenMP parallelization layer added (now hybrid MPI/OpenMP) for Monet Carlo particles, using shared memory for tallies
  → reduce memory footprint w.r.t. pure MPI approach



- Works very well memory wise
- Efficiency degrades strongly after 12 cores, investigated with EIRON (memory bottleneck, next slide)

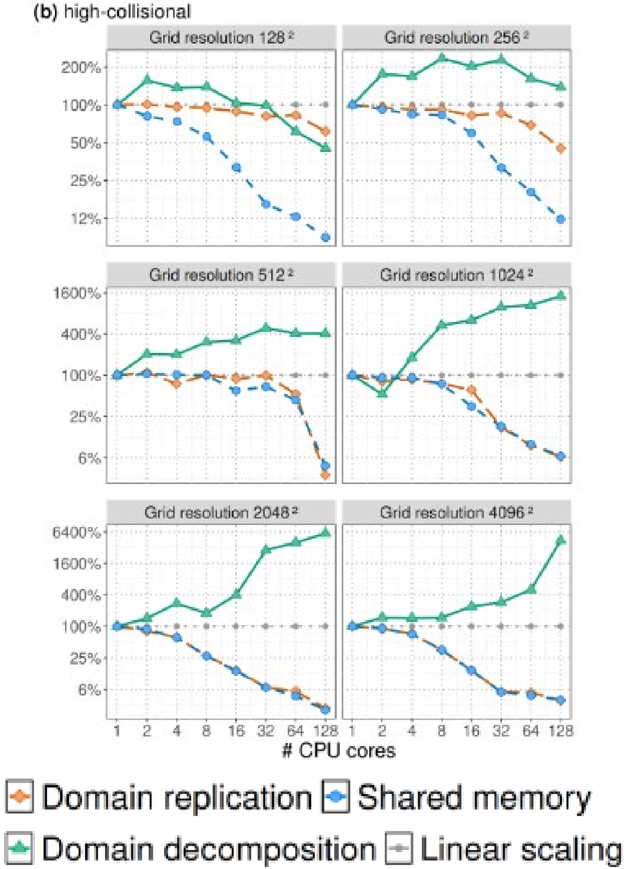
D.V.Borodin et al., NF 2022

Achieves a x10 memory footprint reduction with good efficiency

- MPI parallelization of A&M data rate calculations (in view of CRM usage : 1 solve/grid cell/time step before MC run); computational domain divided in blocks sent to separate CPUs

Domain Decomposition tested in EIRON

- To reduce memory load per node, split the computational grid in subdomains and distribute domains among cores
- These methods have been investigated in other fields, such as neutronics
  - ➔ *origin of OpenMC*
- Different algorithms depending on communciation scheme, termination scheme, …
- Algorithm with original efficient termination scheme (fully asynchronous) implemented and tested in EIRON
- Superlinear behaviour observed (efficiency > 100%) and related to cache behavior (e.g. when subdomains are small enough to fit in cache)
- Provides a blueprint for implementation in EIRENE
- **Next big item** : load balancing, requires calibration runs on coarser grid to allocate domains to processors in an optimal way
- EIRON also reproduces similar to REIRENE the efficiency drop when using
  - → OpenMP shared memory

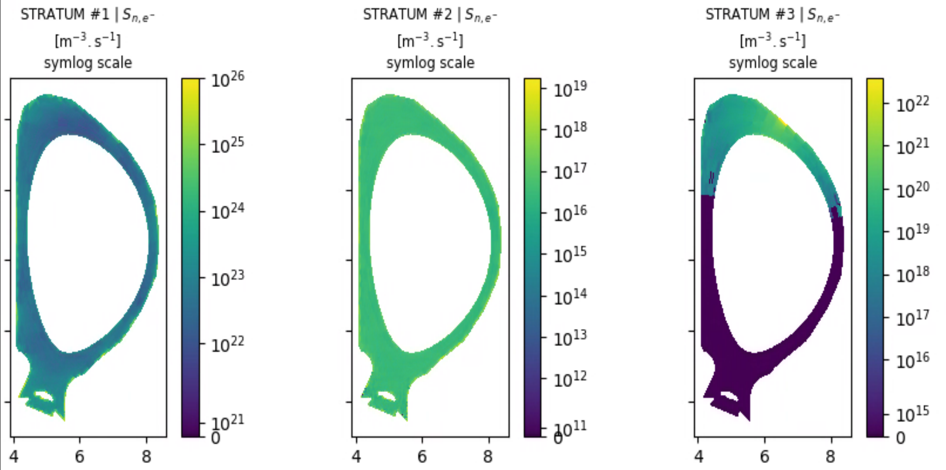


STYX2.0 generic interface to fluid codes

- Joint work with TSVV3, STYX1.0 is the interface used in Soledeg3X-EIRENE since more than 10 years
- STYX2.0 redevelopped from scratch to improve maintanability (separate repos), modularity, fluidity of data exchange, input format (JSON), HDF5 output.
- Basic version in final testing
- Test with other plasma solver foreseen in TSVV-K, making all the TSVV5 models available
- The interpolation routines between the EIRENE grid and the fluid code grids have to be developped on the plasma code side
- TSSV-K : decoupling the plasma code grid and the EIRENE grid (avoid over-resolution and strongly reduce memory footprint)

SOLEDGE3X-STYX2.0 coupled run test run:

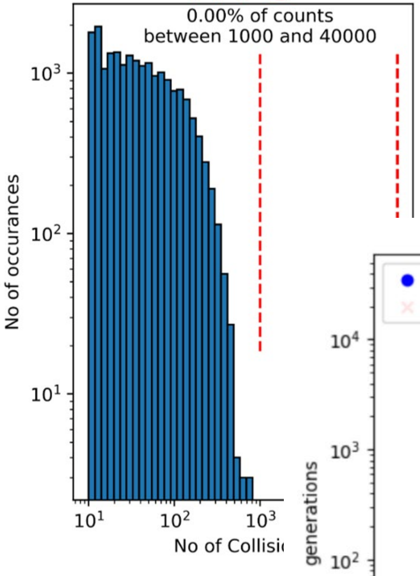
Particle source per stratum



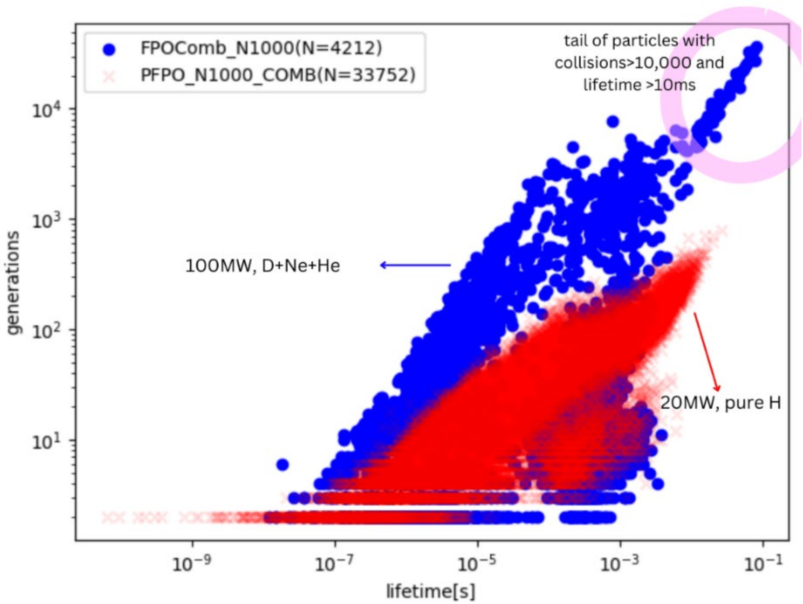
First runs on ITER scale – performance challenges [AMU/CEA]

- 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?

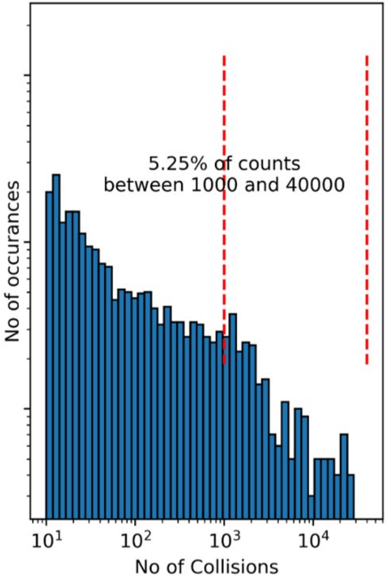
20MW, pure H (PFPO)



SOLEDGE3X-EIRENE, TSVV-3 ⇔ TSVV-5



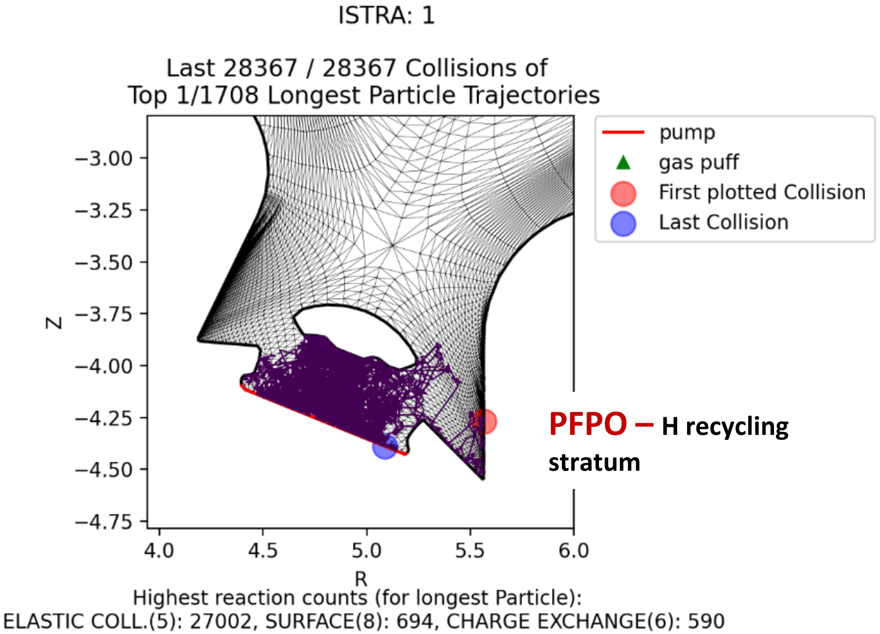
100MW, Burning plasma (FPO)



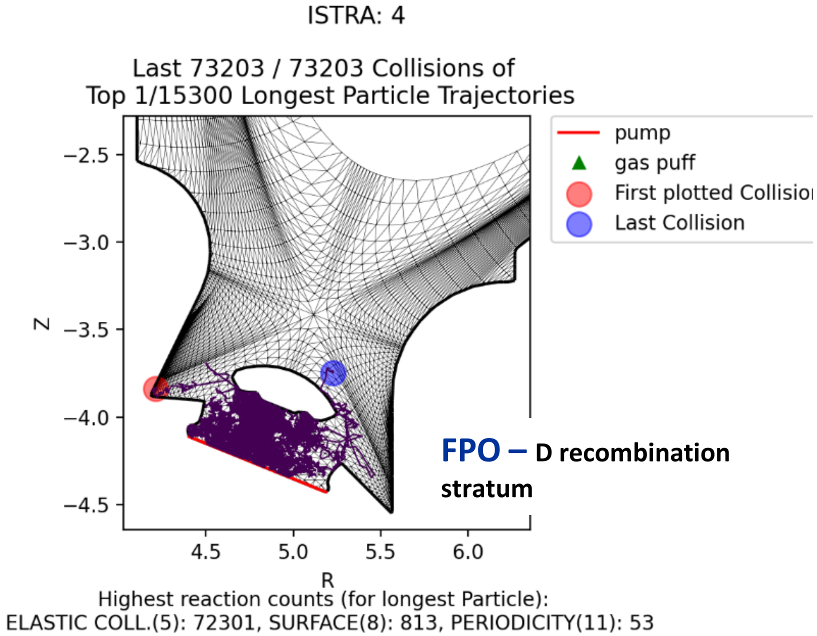
Courtesy S. Sureshkumar, Y. Maranadet

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

Longest trajectories simillar and dominated by elastic neutral-neutral collisions



PFPO – H recycling stratum



FPO – D recombination stratum

- 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 validation

JET-ILW, Magnum-PSI, etc.

Contents lists available at ScienceDirect

Nuclear Materials and Energy

journal homepage: www.elsevier.com/locate/nme

Validation of SOLPS-ITER and EDGE2D-EIRENE simulations for H, D, and T JET ITER-like wall low-confinement mode plasmas

N. Horsten [a],*, M. Groth [b], V.-P. Rikala [b], B. Lomanowski [c], A.G. Meigs [d], S. Aleiferis [d], X. Bonnin [e], G. Corrigan [d], W. Dekeyser [a], R. Futtersack [d], D. Harting [f], D. Reiter [g], V. Solokha [b], B. Thomas [d], S. Van den Kerkhof [a], N. Vervloesem [a], JET Contributors [1]

N.Horsten et al., Nuclear Materials and Energy 42 (2025) 101842

EIRENE application to Magnum-PSI

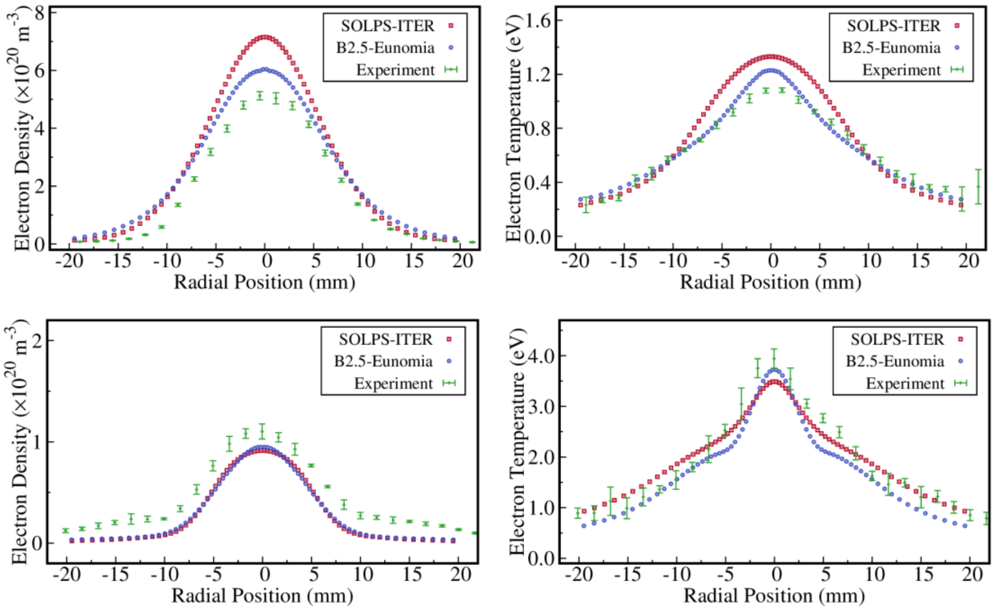
- **Comparison of SOLPS-ITER (B2.5-EIRENE) with**
- **B2.5-ENOMIA**
  - ➢ ***Aim:** transfer all the useful development into EIRENE*
  - ➢ *Main differences are identified to be in **CRMs (MAR, EI, EC)** – direct comparison is often not possible.*

- **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

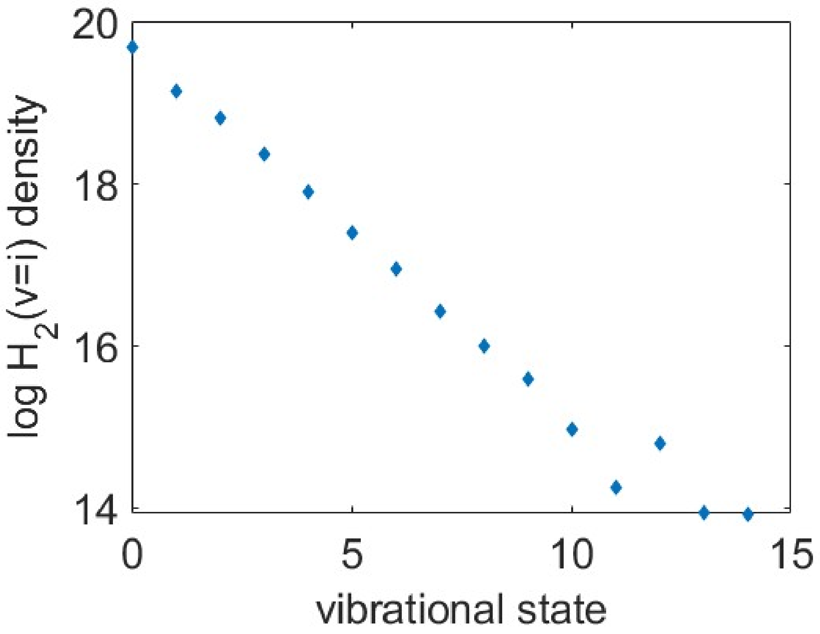


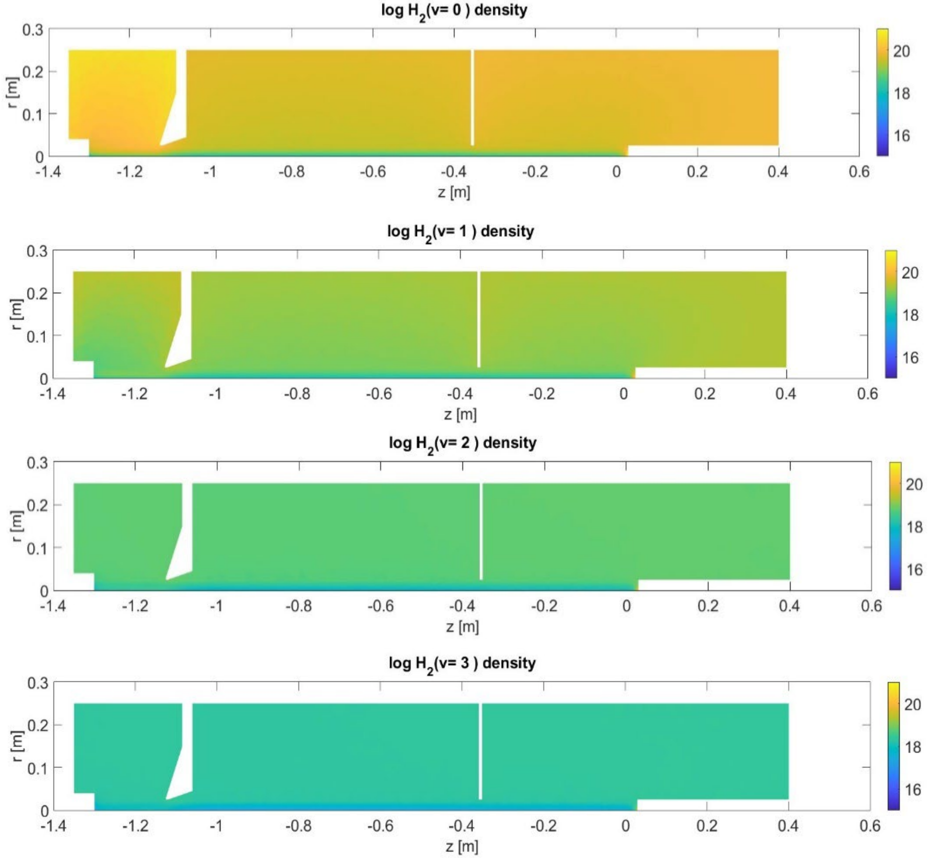
J. Gonzalez, E. Westerhof, et al., PET 2021, CPP (2022)

Magnum-PSI simulations with vibrationally resolved H2

Based on high density (0.47 Pa) case from Chandra and Gonzalez et al.

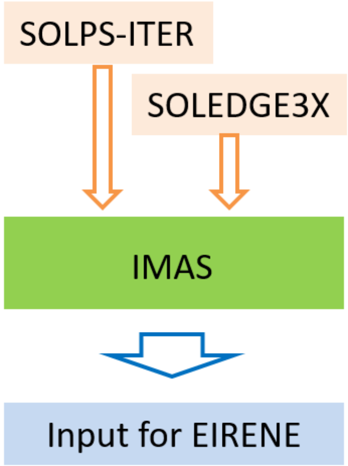
vibrational distribution around plasma beam





General code development and IMASification

IMASification of EIRENE (with ACH-IPPLM)



Codes with interface to EIRENE on 2D poloidal are first priority (like SOLPS), yet 3D packages like EMC3-EIRENE will profit from it as well.

Following steps were selected to be done first place:

- Develop standardized IMAS interfaces for EIRENE input based on output data from SOLEDGE3X and SOLPS-ITER codes.
- Create a universal interface enabling data transfer from IMAS to EIRENE.
- Adapt SOLPS-ITER output data to the corresponding EIRENE IMAS Interface Data Structures (IDSs).
- Adapt SOLEDGE3X output data to the relevant IMAS IDSs.

Outcome:

- EIRENE interfaces developed generating geometry files (grid nodes, triangles, and triangle neighbours) from IMAS IDSs for SOLPS-ITER and SOLEDGE3X; interface module enabling the generation of initial tallies for EIRENE based on data stored in IMAS IDSs developed.
- EIRENE simulations can be launched using input data stored in IMAS IDSs with full compatibility with the EUROfusion Integrated Modelling framework - validation tests on the New Gateway.
- Simplified coupling with other IMAS-ified edge and core plasma codes is now available.
- The concept of IMAS-ified EIRENE output for future implementation as a subroutine executed directly within the EIRENE code is defined.
- Documentation and a demo version of the EIRENE interface provided.

ACH-IPPLM:
P.Chmielewski,
D.Yadykin
M.Owsiak
B.Pogodziński

Code development

- Roughly 20 different code versions (FZJ, ITER, …) have been analysed and merged together. Following features are included.

- The main loop of EIRENE was significantly cleaned up from legacy constructions, useless branching etc. Many variables were grouped into structures mimicking the I/O in main routines.

- 1st **EIRENE MsV released in NOV 2024;** already in use by ITER and other colleagues.

- Most part of the code is now in modern FORTRAN. We actively use ModCR as a testbed for new technologies (e.g. we use now actively UML diagrams and OOP).

- ModCR development started (standalone code), large parts (e.g. LTE approach, data processing) are already available.

We hope to continue that development in TSVV-K…

EIRENE licencing – new User Agreement (UA)

www.eirene.de/EPL

Dual with open source **CC BY-NC-ND 4.0**

New UA "EPL (EIRENE public license)"

- Based on copyleft licence (however GPL3.0 occurs to be not suitable).
- Similar declarative statements as in the old FZJ UA.
- More clear statement about the EIRENE-based publications.
- Developers and users are divided into "basic" (BD) and "associated" ones (AD).
- NEW: commercial use of executable by any AD groups.

→ *ADs get more rights on decision-making, direct access to the repository, etc.*

← *ADs must keep to the "Developer Code of Conduct" of one of self-governed communities.*

Current status: *License is broadly accepted by over 20 parties including ITER ("B2" legal forms provided), 154 "basic developers" registered*

Summary and outlook

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.*

*➔ new: **SimDB** repo in FZJ…*

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.) –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)*
- *Interfaces (IMAS, codes of related TSVVs, STYX2.0)…*

Organisational and technical items

- ***New EIRENE license**, "infectious open source", **Coding guidelines**, ChangeLog, **improved CI** - available at 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!