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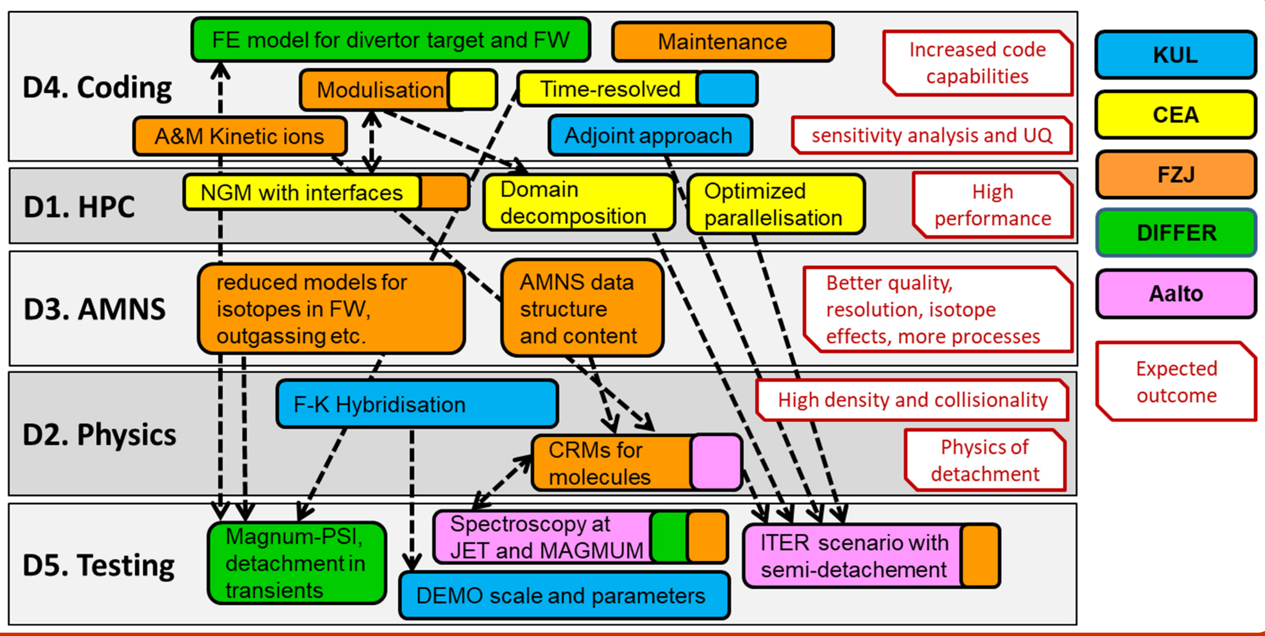
TSVV-5: Neutral gas dynamics in the edge

General task deliverables

- **D1**. Neutral gas code that allows for an efficient use of HPC resources (towards exoscale systems and/or HPC booster techniques) through suitable parallelization methods.
- **D2**. Revised and extended physics basis for the neutral gas model. Further development of the radiative-collision model towards the full vibrational resolution for all hydrogen isotopes and specific impurities for seeding.
- **D3**. Improved (in contents and structure) Atomic and Molecular database for volumetric and surface processes. Database access through generalized interfaces to, e.g., atomic, molecular, nuclear and surface (AMNS) physics data.
- **D4**. Interfaces and boundary conditions necessary for future applications; modularization of the neutral gas code to facilitate coupling to computation fluid dynamics (CFD) codes (2D or 3D codes, turbulence codes, time-dependent) and possibly also to gyro-kinetic/gyrofluid plasma codes.
- **D5**. Strategy towards a validated predictive capability for integrated fusion reactor modelling for (semi-)detached divertor plasmas. Liaison with TSVV Tasks 3 and 4.

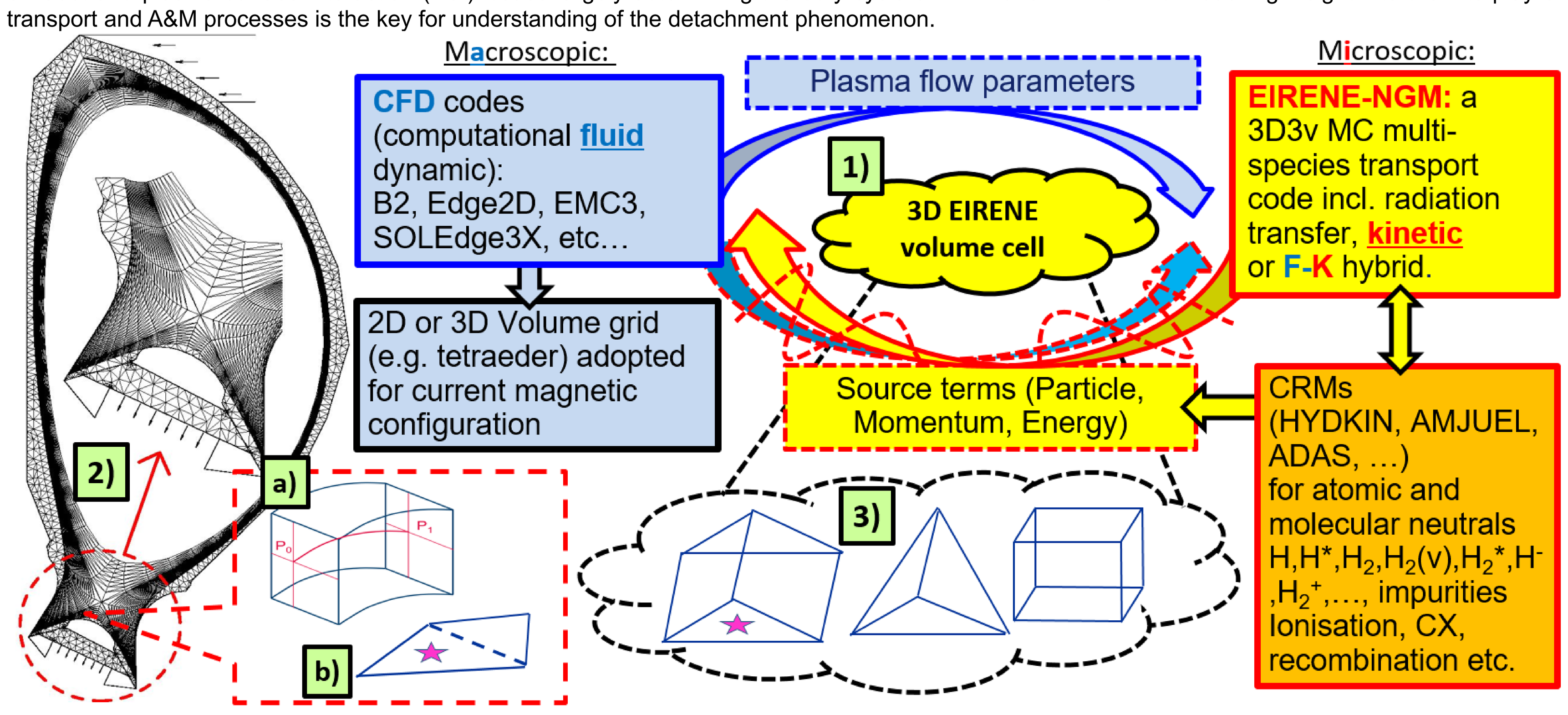


ACH support and other external cooperation

- **ACH-MPG.** Profiling and **parallelisation** (hybrid MPI/OpenMP) of EIRENE, code refactoring and streamlining, code repository: **CI and versioning** (e.g. EPL, manual, coding guidelines and changelog versions are synchronised via git hooks), support in **ModCR development**.
- **ACH-VTT. EIRON** "toy-model" – skeleton of EIRENE code in 2D slab geometry especially developed for testing of various **parallelization and domain decomposition** schemes.
- **ACH-IPPLM. IMASification of EIRENE.** EIRENE treats multiple grid types - we go from GGD objects defined for SOLPS-related "triangles" to more generalized ones aimed to cover all of EIRENE cell types.
- **Links with other TSVVs (in particular TSVV-3 and TSVV-7)** are under joint discussion, we do presentations at joint meetings incl. the code camps. The focuses are the **interfaces** between the codes as well as jointly defined **reference simulation cases**.
- Due to **SOLPS-ITER package** we maintain strong direct contact with **ITER**. The EIRENE repositories at FZJ and ITER are mirrored, but the code **forking** was significant – now **reduced** to minimum (it was a pre-condition for the recent "milestone version" **(MsV) release**).

EIRENE-NGM package

The **EIRENE** code [1][2] also known as Neutral Gas Module (NGM) is a **multi-purpose Boltzmann-equation Monte-Carlo (MC) solver** typically employed in an iterative scheme with a Computational Fluid Dynamics code (CFD). It can track atomic and molecular (A&M) neutrals and ions kinetically, however ions are mostly handled on the CFD (EDGE2D, EMC3, SOLEDG3X, etc.) side. EIRENE provides in return the momentum, energy and particle sources. A number of such CFD-EIRENE code packages e.g. SOLPS-ITER [4] (B2.5-EIRENE) are employed by the fusion community. An essential part of the NGM are the collisional-radiative models (CRMs) for A&M processes involving main-plasma species and impurities. This includes ionization-dissociation-recombination and elastic processes. Numerical simulations with EIRENE-NGM are indispensable for both understanding and predicting the fuel and impurity transport in the edge and divertor areas of fusion devices. The transport determines impurity penetration towards the core, plasma exhaust and plasma-surface interaction (PSI) issues largely determining the duty cycle of ITER and DEMO. The modelling insight into the interplay of transport and A&M processes is the key for understanding of the detachment phenomenon.



EIRENE-NGM iterative scheme with the CFD codes [2]. *1) The NGM runs simulations for a number of volume cells; 2) The CFD side determines magnetic configuration and runs itself on a grid optimized for it - the cell shape typically mimics the magnetic field line geometry; this grid may be 3D like in EMC3 a) or 2D, for instance quadrangular plasma cells b) split into triangles in SOLPS-ITER; 3) The EIRENE cells, always 3D, correspond to (or approximate) the CFD cells; for 2D CFD cells an extra dimension is provided (magenta stars mark corresponding triangles in 2D SOLPS and 3D EIRENE cells). EIRENE can run fully kinetic or, alternatively, a fraction of neutrals can be treated as fluid providing higher simulation performance; the corresponding fluid calculations are typically provided by the CFD side. In case of APMC hybridisation no direct coupling with CFD is necessary.*

Collisional-radiative models (inside EIRENE and support tools)

Balance equations:

$$\frac{dN_i}{dt} = \sum_{j\neq i} A_{ji}N_j + n_e \cdot (EXCIT + IZ + CX + REC)$$

$$EXCIT = \sum_{j\neq i}\langle v\sigma_{ji}\rangle N_j$$

$$IZ = \sum_m \langle v\sigma_{mi}\rangle N_m^- + \sum_z \langle v\sigma_{zi}\rangle N_z^{2-} + \ldots$$

$$REC = \sum_k \langle v\sigma_{ki}\rangle N_k^+ + \sum_l \langle v\sigma_{li}\rangle N_l^{2+} + \ldots$$

$\ldots$

*j, k, l, m, z, … states can be fine-superfine **resolved** or, opposite, bundled into few quasi-**metastables** (MS)*

CRM = list of states + transition data

Often used:
$\langle v\sigma_{ji}\rangle(T_e, n_e)$- effective Maxwellian averaged rates

EIRENE: collisional-radiative model (CRM) challenges:

- **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)** $\boxed{\frac{dN_i}{dt} \neq 0}$

?

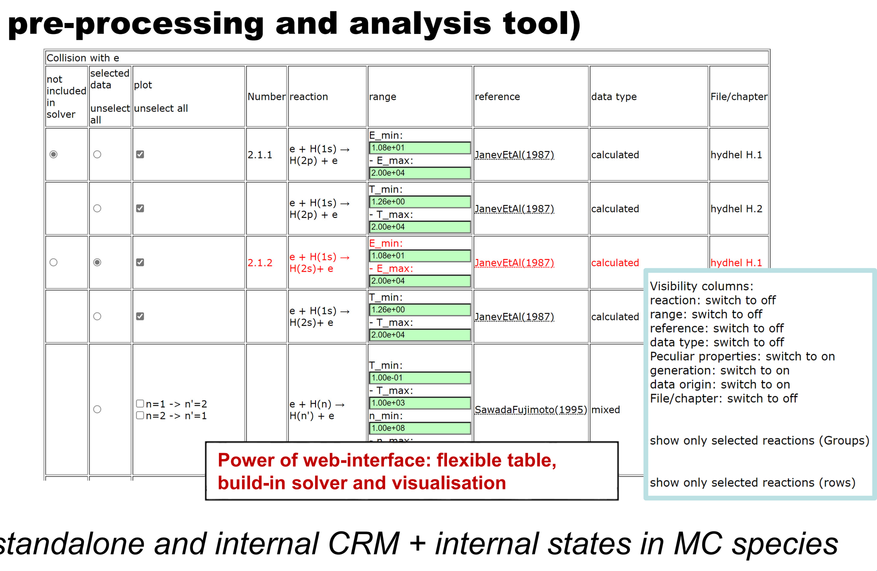
- **improving performance for simulations on ITER/DEMO scales**
- **facilitate UQ and design with EIRENE**
- **control the exploding amounts of data**

EIRENE often uses effective ("condensed") rates tabulated from a CRM. It can be also done internally ("ColRad" routine) and include photon trancing (opacity) [7].

PLOUTOS (web-based A&M data pre-processing and analysis tool)

*EIRENE with **PLOUTOS** 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**
- **to perform sensitivity studies:**
  - *understand A&M side of the problem and identify the most significant processes (among the selected ones)*

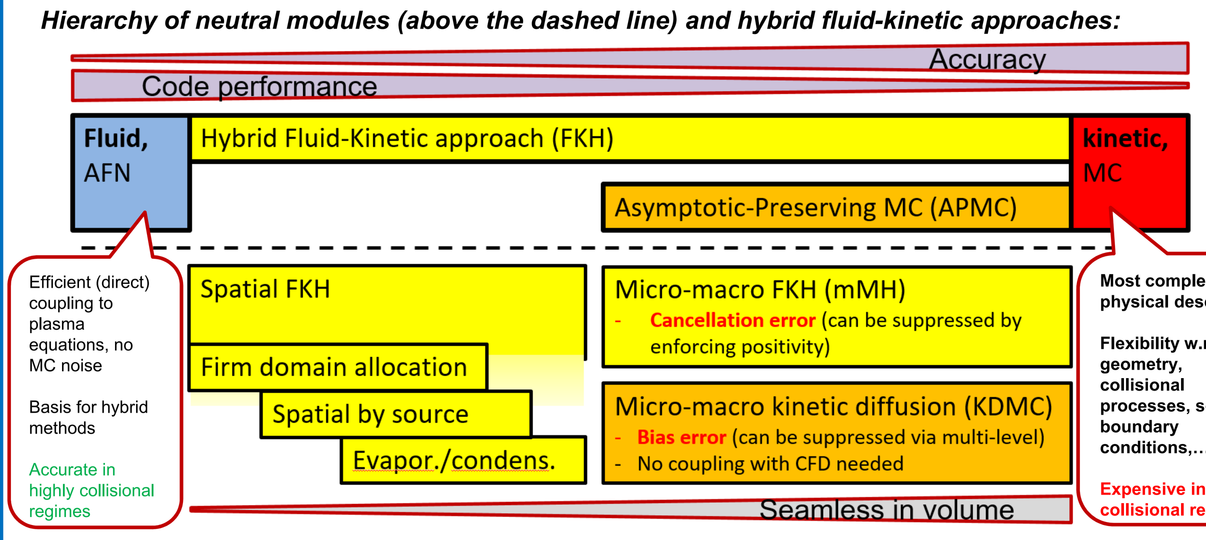


Power of web-interface: flexible table, build-in solver and visualisation

New: ModCR (CRM module as library with API) – *both standalone and internal CRM + internal states in MC species*

Fluid-kinetic hybridisation (FKH) approaches relation and basic theory [2]

Hierarchy of neutral modules (above the dashed line) and hybrid fluid-kinetic approaches:



*Most developed and tested **AFN/SpH/mMH branch**:*

mMH assumption:

$$f = \sum_i f_i = \sum_i f_i^k + f^f + f^\delta$$

f^f - equivalent to AFN, f_i^k- kinetic terms calculated kinetically by MC approach, f^δ - "kinetic correction", seamless in the entire simulation volume.

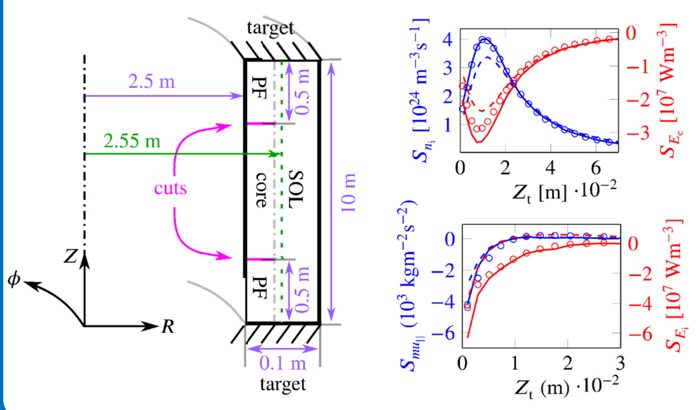
SpH assumption:

$$\sum_i f_i \approx \sum_i f_i^k + f^f$$

f_i^k assumed negligible in all simulation domains where Knudsen number K_n is sufficiently small, thus AFN is valid (firm allocation) or, alternatively, more flexible approach [21] with evaporation/condensation terms $S_{f\to k}$ and $S_{k\to f}$ is used:

$$\frac{\partial f^k}{\partial t} + v \cdot \nabla f^k = S_c + S_v(f^k) + S_{f\to k} - S_{k\to f}$$

$$\frac{\partial f^f}{\partial t} + v \cdot \nabla f^f = S_v(f^f) - S_{f\to k} + S_{k\to f}$$



An example of FKH simulation (JET-relevant slab, mMH):

- *hybrid solution approaches the full kinetic one by the accuracy.*
- *Spead-up factor 5-10 demonstrated*
- *Similar tests (accuracy and performance) were performed also for other FKH approaches*

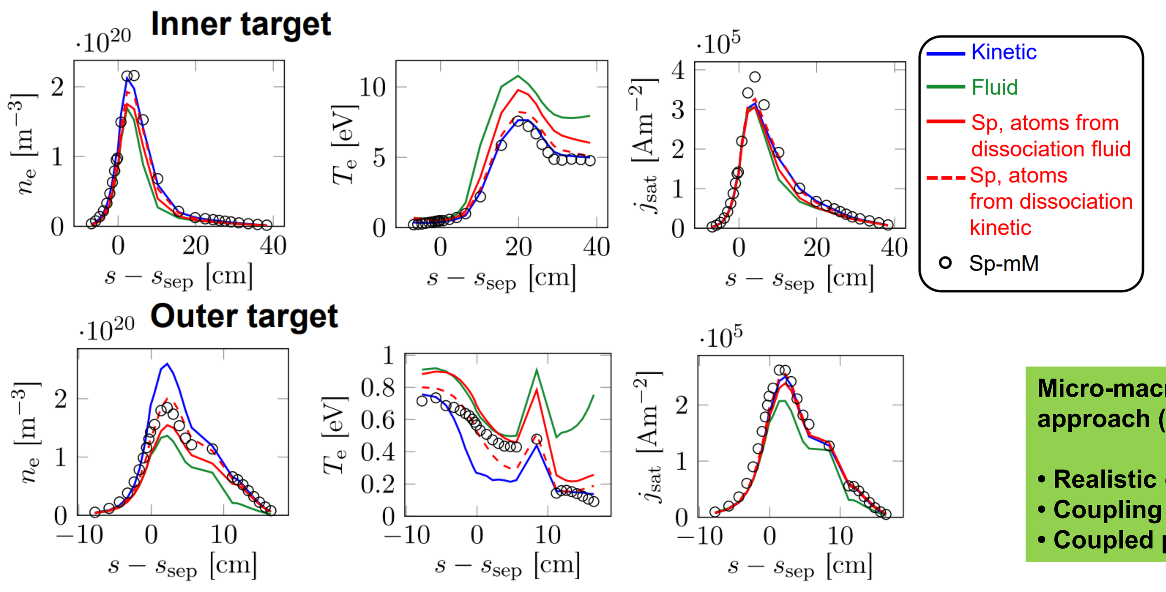
N.Horsten et al., "A hybrid fluid-kinetic neutral model …", **CPP, vol. 60, no. 5-6, p. e201900132, 2020**

Hybrid SpH and mMH methods are subject to ongoing research.

Examples of obtained results

Progress with FKH - JET L-mode case:

N.Horsten et al., *"Application of spatially hybrid fluid–kinetic neutral model on JET L-mode plasmas",* **NME 27 (2021) 100969 and PET-2021 oral**



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

2021

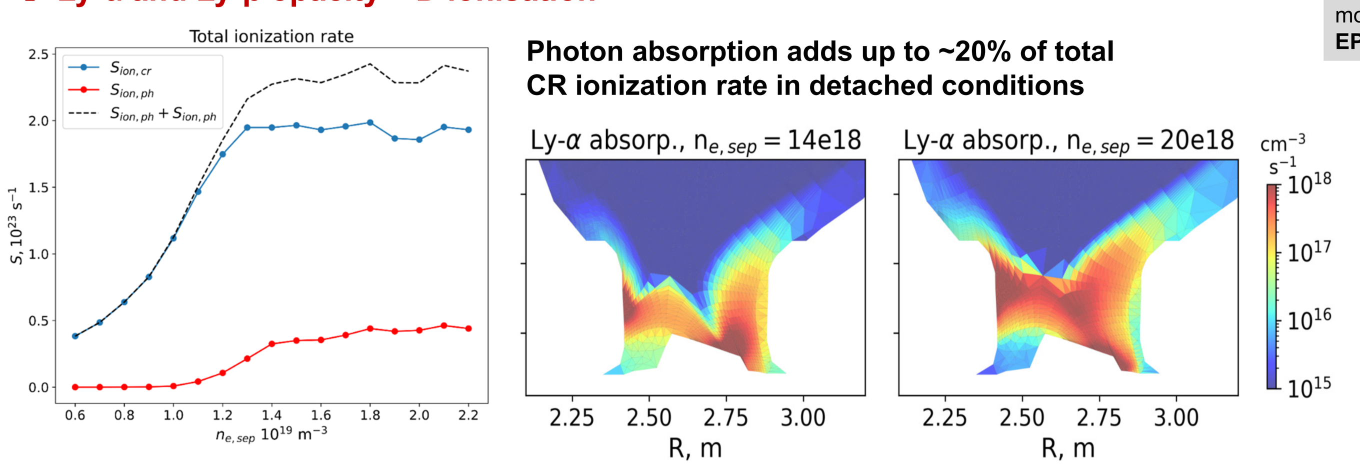
Micro-macro approach combined with spatially hybrid approach (Sp-mM)

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

Ly-α and Ly-β opacity – D ionisation

R. Chandra et al. "Radiation transport modelling in EIRENE revisited **EPS 2023 P1-001**

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



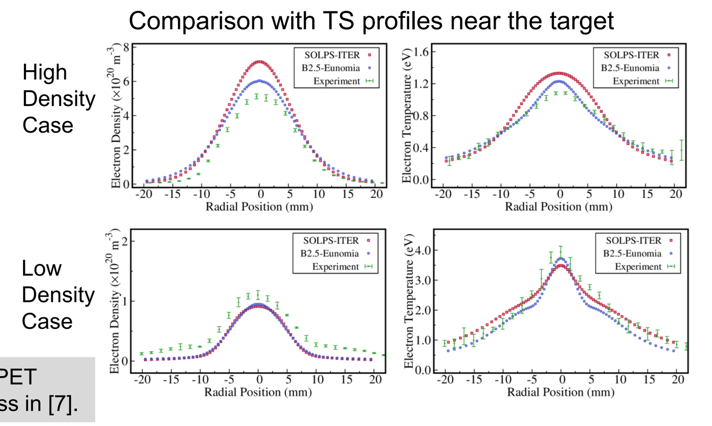
'Extra' ionization contribution from Ly-α and Ly- β photon absorption:
- increases population of excited D neutrals
- extra ionisation

Further development and full theory published in 2024 [6].

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.*

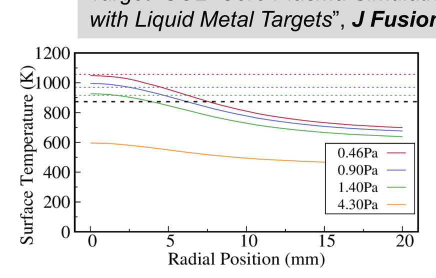
Comparison with TS profiles near the target



J.Gonzalez, E.Westerhof, et al., PET 2021, CPP (2022) Further progress in [7].

- **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)*

Nallo, G.F., Gonzalez, J., *et al. "Towards Integrated Target–SOL–Core Plasma Simulations for Fusion Devices with Liquid Metal Targets"*, ***J Fusion Energ* 42, 41 (2023).**

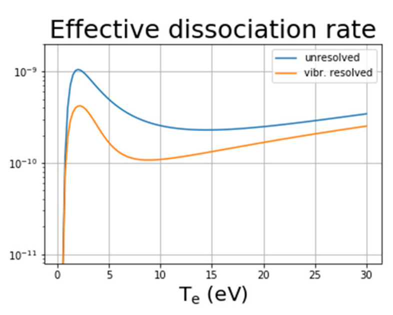


Surface temperature from SOLPS-FEM (solid line) and pyrometer measurements at the target centre (dashed line) for different neutral pressures in the target chamber.

Impact of resolution by vibrational states in H_2

- **Edge2D-EIRENE modelling for JET:** "Up to **40% reduction in effective dissociation rate** due to transport of vibrational states".

A.Holm, M.Groth, et al., *"Impact of vibrationally resolved H2 on particle balance in Eirene simulations",* **CPP (2022), https://doi.org/10.1002/ctpp.202100189**



F.Cianfrani, et al., *"Collisional-radiative model for transport simulations of neutrals in detached conditions"* **EPS-2022, P2a.105**

The study was continued in **[5].**

- The same is captured by the standalone CRM.
- The turnover T_e for **MAD or MAR branching ratios** domination at JET and EU-DEMO relevant conditions in detached divertor depends on number of vibrational states (0, 7 or 14) included.

Current status and plans for 2025

Significant progress is reached along main lines of the project – physics (FKH and CRMs) as well as code refactoring and infrastructure improvement (the license "EPL", IMASification, webpages, CI and version merging, documentation etc.). **1st MsV** ("Milestone Version") is **released** in Oct-2024 (following a beta-version in 2023). Some unplanned additional developments ("EIRON" toy-model for testing of parallelization and domain composition concepts, new universal CRM module "ModCR" etc.) were started.

The main focuses for 2025 are:

1. **Final merge and polishing** of the existing code branches, finalize the list of **reference** simulation (ITER SimDB) and CI **cases**, **validation** (where experiment data is available) or verification of those cases, final profiling and optimization of the EIRENE-NGM code for performance, universal framework and particular **interfaces** to other codes in related TSVVs.
2. Perform predictive runs for ITER and DEMO (utilizing the improved CRMs and A&M data basis as well as the FKH) **demonstrating new capabilities.** Demonstrate a meaningful simulation case with ~1 billion volume cells. ACH HPC support is expected.
3. Writing **joint overview papers** (or reports/preprints) regarding the a) HPC ready modular EIRENE-NGM with interfaces for the IM and its performance optimization from by parallelization as well as algorithmic improvement; b) improved AMNS and CRMs; c) EIRENE-NGM validation, UQ and predictive power.

More detailed working plans will be elaborated at Code Camp in Nov-2024 with participation from ITER and related TSVVs (3 and 7).

Possible directions for development in 2026-2027

1. Further **code refactoring and modulisation** e.g. segregation of the plasma-wall interaction into as dedicated module containing also a coupled FEM (fuel retention and outgassing, impact on erosion etc.) already demonstrated to bring added value to EIRENE.
2. Continuation with the **refinement of CRMs** (internal routines like ColRad, external tools Ploutos and new ModCR module):
   a. Adding new datasets recently available from data producers (more species, better accuracy and resolution incl. **vibrational and rotational states** in molecules, bundling and quasi-metastable schemes in atoms; test also **non-stationary approach** in CRMs.
   b. Improving the models e.g. providing the **reflections** in photon tracing, or further investigation of **CXN** parameter distributions.
   c. Prepare **validated datasets** for particular fusion-relevant tasks e.g. characterisation of detachment degree by spectroscopy.
3. Further improvement of EIRENE-NGM **performance** (at ITER and DEMO scales)
   a. Improving **parallelisation and domain decomposition schemes** utilizing **EIRON** (toy-model) tests and new modular structure.
   b. Consideration of further **FKH schemes** (algorithm development) with related result quantification (incl. use of EIRON).
4. Systematic treatment of **D, H, T, He and mixed plasmas :** providing validated isotope-resolved data, demonstrating sufficient performance at ITER and DEMO scales as well as capturing of main physical effects including time-dependent runs.
5. Providing **code interfaces** with the codes from other TSVVs (e.g. improving treatment of turbulence and PSI effects). Continuation with the deeper IMASification of EIRENE. Establishing of further reference simulation cases utilizing the SimDB-based data server.

References

[1] D. Reiter, M. Baelmans and P. Börner, "The EIRENE and B2-EIRENE Codes", Fusion Science and Technology, no. 47:2, pp. 172-186, 2005.
[2] D.V.Borodin et al., *"Fluid, kinetic and hybrid approaches for neutral and trace ion edge transport modelling in fusion devices",* 2022 Nucl. Fusion 62 086051
[3] D. Reiter et al., *"EIRENE-related data: AMJUEL, HYDKIN, HYDHEL, H2VIBR",* http://www.eirene.de
[4] Wiesen, S. at al., *"The new SOLPS-ITER code package",* J. Nucl. Mat. 463, pp 480-484 (2015)
[5] F.Cianfrani, D.V. Borodin & B.Küppers, *"Data processing and visualization tool for atomic and molecular data for collisional radiative models",* Eur. Phys. J. D 77, 139 (2023).
[6] R.Chandra et al., *"Lyman line opacities in tokamak divertor plasmas under high-recycling and detached conditions",* NME (2024), doi: https://doi.org/10.1016/j.nme.2024.101794
[7] J Gonzalez et al., "Coupled simulations with SOLPS-ITER and B2.5-Eunomia for detachment experiments in Magnum-PSI", 2023 Plasma Phys. Control. Fusion 65 045009

Acknowledgement

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