For the 4th Technical Meeting on Divertor Concepts 7-10 Nov 2022

EUROfusion

EIRENE modelling with improved CRMs for spectroscopic RT detachment control in EU-DEMO

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JÜLICH Forschungszentrum

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

Outline

1) Collisional-radiative model (CRM) and real time control (RTC) of detachment

2) EIRENE code: CRMs and fluid-kinetic hybridisation (FKH)

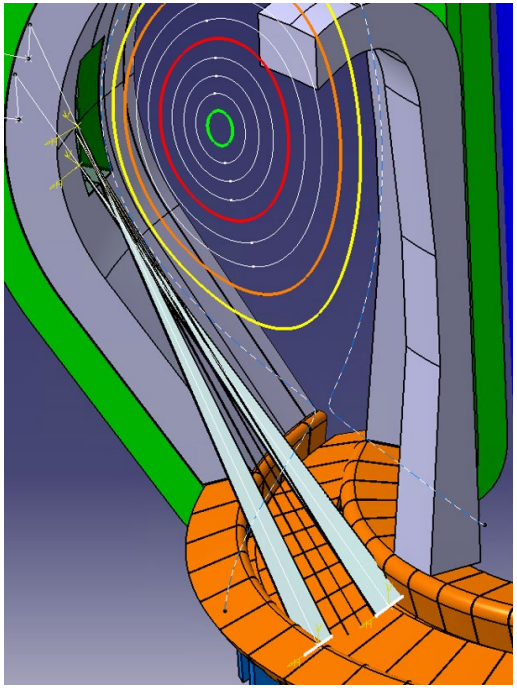
3) EIRENE general development and restructuring: new CRM requirements

4) Standalone CRM for EU-DEMO: branching ratios, vibrostates effect,

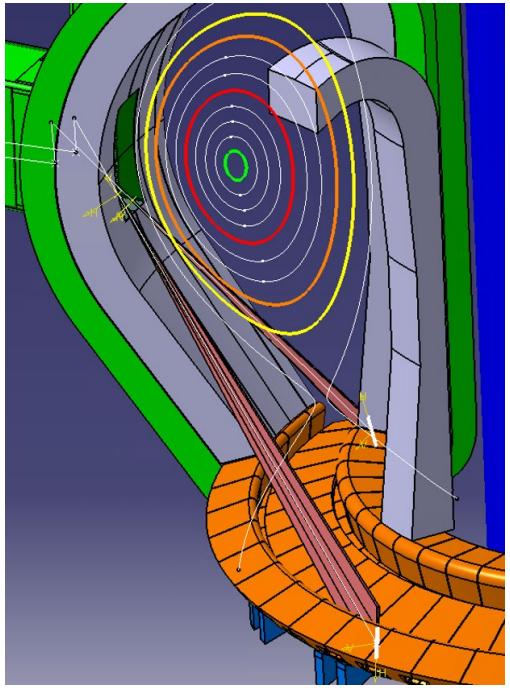
5) HydKin development – A&M data pre-processing

LOS under consideration for EU-DEMO

Inner and outer VT Plasma



Inner and outer VT surface



Courtesy of D.Dunai, I.Katona, EUROfusion WP DC

Modelling for Real-time control (RTC) of detachment:

1) **What spatial resolution and sensitivity is needed?**

2) **Is the current line-of-sight (LOS) choice optimal in general?**

3) **What spectral range and resolution do we need?**

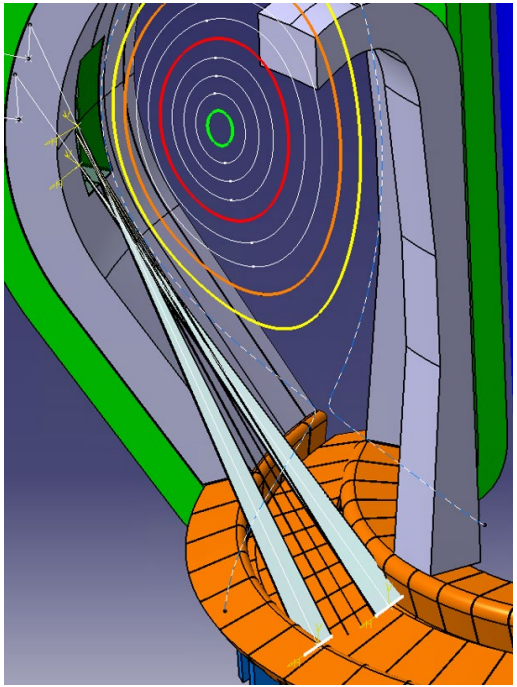
CRM

4) **Which line(s) or line ratios do we choose to characterize the degree of detachment?**
   ➔ Lyman + Balmer lines (H)? Fulcher band (H_2)? Impurity lines?..

1) **What will be effect of opacity (incl. reflection), line blending, etc?**

LOS under consideration for EU-DEMO

Inner and outer VT Plasma



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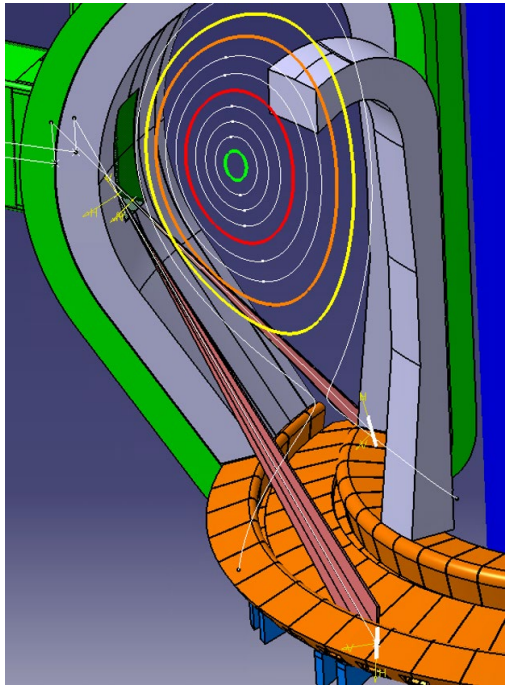

Courtesy of D.Dunai, I.Katona, EUROfusion WP DC

Modelling for Real-time control (RTC) of detachment:

What are the main show-stoppers from the EIRENE (SOLPS-ITER) modelling side?

1) **Sufficient code performance on the DEMO scale**
2) **Including of sufficient physics**
3) **Data consistency and reliability**

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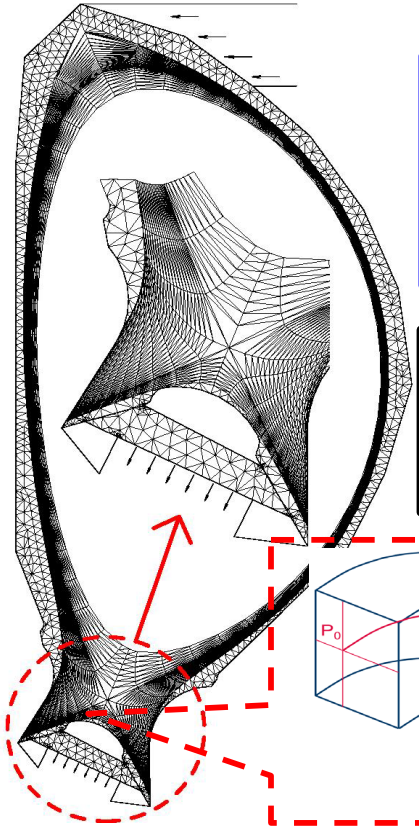
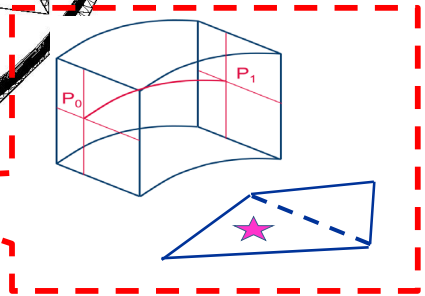
What is EIRENE in a nutshell (e.g. in SOLPS)?..





Macroscopic:

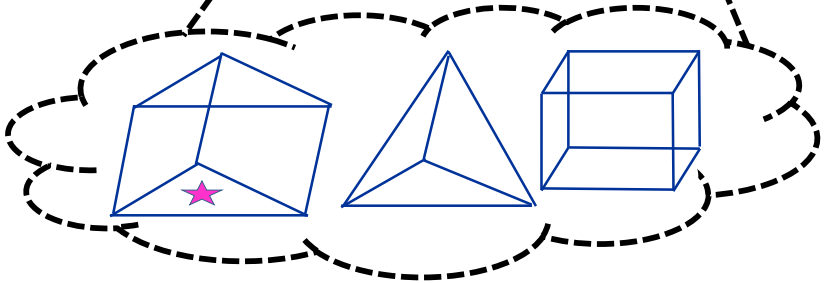
CFD codes (computational **fluid** dynamic): B2, Edge2D, EMC3, SOLEdge3X, etc…

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:

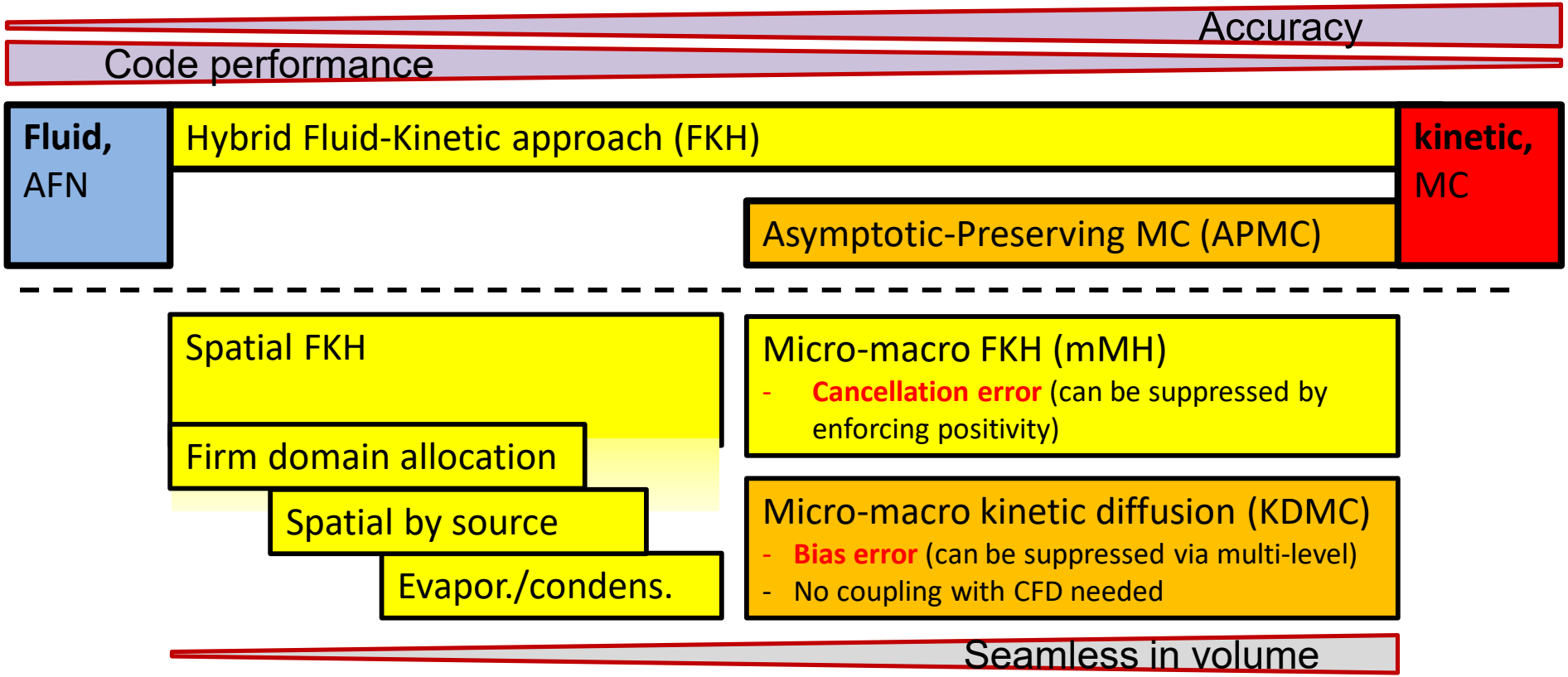
EIRENE-NGM: a 3D3v MC multi-species transport code incl. radiation transfer, **kinetic** or **F-K** hybrid.

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.

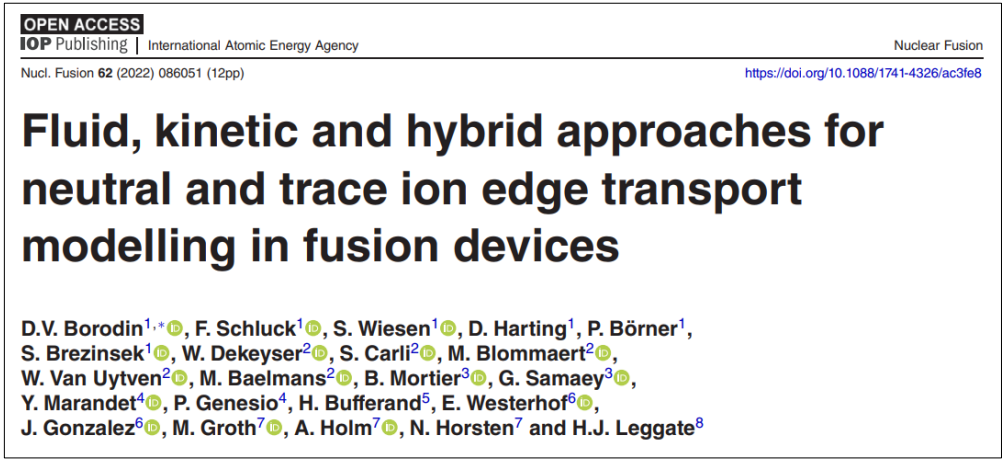
Fluid-kinetic hybridization (FKH)

A hierarchy of neutral models:

D.V. Borodin et al., FEC-2020, NF (2021)



Fluid-Kinetic Hybridisation inside EUROfusion TSVV-5



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IOP Publishing | International Atomic Energy Agency
Nuclear Fusion
Nucl. Fusion 62 (2022) 086051 (12pp)
https://doi.org/10.1088/1741-4326/ac3fe8

Fluid, kinetic and hybrid approaches for neutral and trace ion edge transport modelling in fusion devices

D.V. Borodin[1,*], F. Schluck[1], S. Wiesen[1], D. Harting[1], P. Börner[1], S. Brezinsek[1], W. Dekeyser[2], S. Carli[2], M. Blommaert[2], W. Van Uytven[2], M. Baelmans[2], B. Mortier[3], G. Samaey[3], Y. Marandet[4], P. Genesio[4], H. Bufferand[5], E. Westerhof[6], J. Gonzalez[6], M. Groth[7], A. Holm[7], N. Horsten[7] and H.J. Leggate[8]

The development continues according to the statement in the joint paper

➔ *Combining **mMH/SpH/AFN**, introducing "evaporation/condensation" (fluid ←→ kinetic consideration)*

➔ *Developing **ML-KDMC** (a sort of "asymptotic preserving" MC) as useful alternative*

- **Continuing "brute force approach" for the OpenMP/MPI parallelisation as well as more profound parallelisation based on the "toy" model (EIRON).**
- **General restructuring of the code which includes generalisation of the CRMs**

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General code development of EIRENE

- **Main goals and decisions:**
  - Segregating EIRENE into "starter" and a compact, free of most branching "numeric core"
    - ➔ *Optimisation for HPC, transparency and ease of use.*
  - Unloading the main loop from branching agreed
    - ➔ *Abstractisation of the cell type (removing "geometry" branching)*
    - ➔ *Abstractisation of A&M reactions + tracking of internal states*
  - Version merging scope agreed including synchronisation with SOLPS-ITER
  - Uniform coding style (e.g. variable name conventions, use of OOP, etc.)

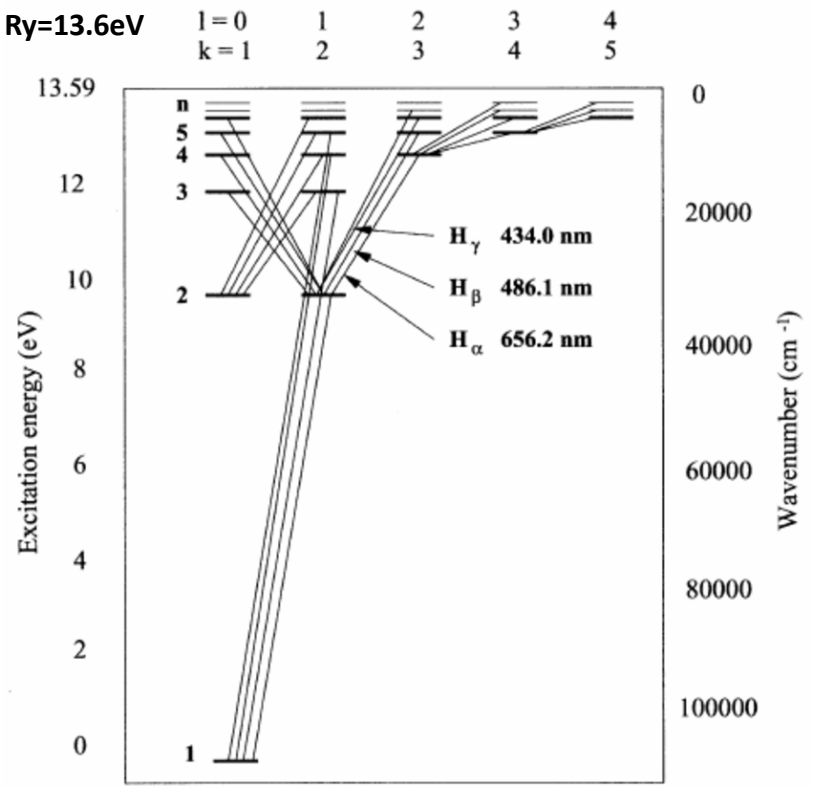
- **With support from the ACHs (Advanced Computing Hubs)**
  - EIRENE "toy model" – EIRON and profiling of EIRENE
    - ➔ *Test of parallelisation schemes incl. domain decomposition options*
    - ➔ *Can be used for other purposes e.g. optimisation of ML-KDMC*
  - EUDAT-based simulation catalogue
    - ➔ *Portfolio of simulation cases*
  - IMASification of the simulation grid (GGD objects) in close contact with ITER (X.Bonnin) and utilizing the positive SOLPS-ITER experience

Eiron

Eirene

Collisional-Radiative Models (CRM)

Grotrian diagram for atomic H (D, T)



Balance equations:

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

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

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

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

$\dots$

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

CRM solvers available

CRM (technically) = reaction data + SOLVER

- Most solvers solve algebraic **stationary** system of equations $\frac{dN_i}{dt} = 0$

➔ in such cases the solver is much less valuable as the A&M data collection

➔ this statement is underlined even by the developers of the very well established and mostly up-to-date YACORA model

D.Wünderlich and U.Fantz, *Atoms* ***2016****, 4(4), 26*

- CRM containing molecular species is even more complex, e.g. one needs to track more processes and more states (vibrational, rotational).

➔ Tracking all the states as separate species demands enormous CPU and memory resources.

- EIRENE pre-calculates rates for each volume cell. It also allows to pre-calculate values for various T_i/T_e ratios.

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

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

- 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).

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

- 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 other 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 AMD Unit: GNAMPP

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

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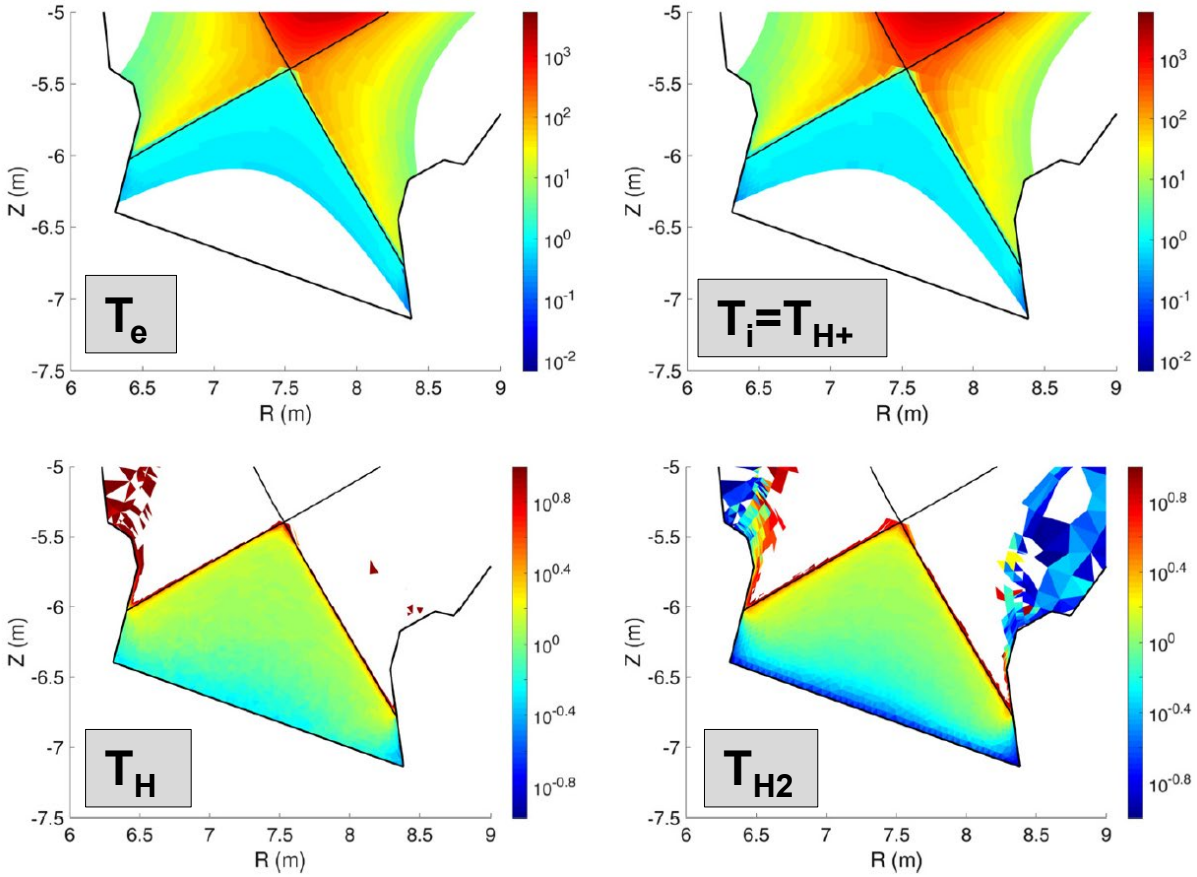
SOLPS-ITER basic simulation case for EU-DEMO

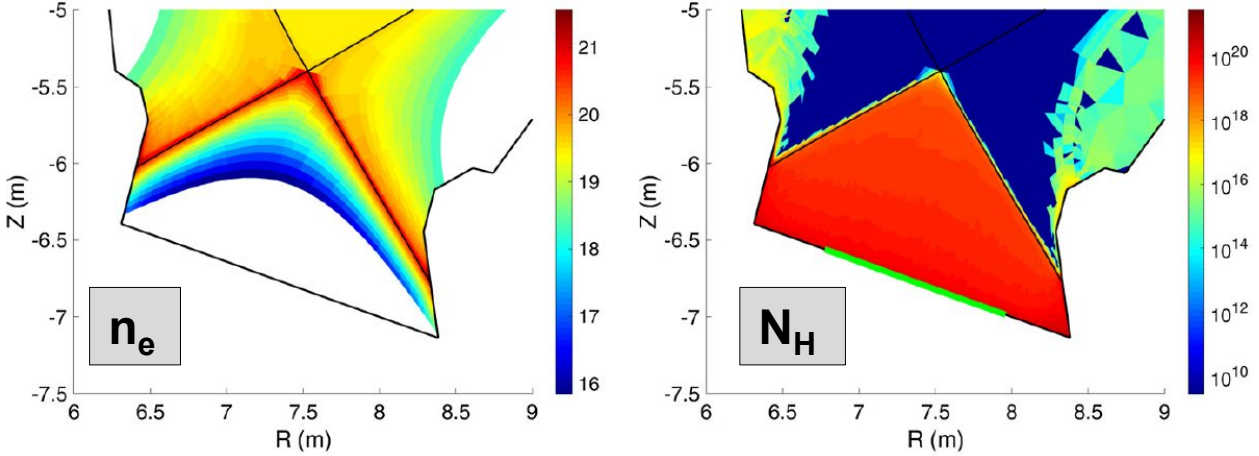


F.Subba et al.,
NF 61 (2021) 106013

Below X-point:

1) $T_e=T_i=10eV$
2) $T(H)=T(H_2)=10eV$
3) $N_e \sim 10e18\ m^{-3}$
4) $N(H)=10e20\ m^{-3}$

SOLPS-ITER basic simulation case for EU-DEMO



F.Subba et al.,
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- **These are semi-detached conditions (1 point)**
  - ➔ Attached vs. detached + 2-3 semidetached cases would be wishful to have!
  - ➔ **We use EIRENE or standalone CRM to identify spectral features useful for the degree of detachment control for this plasma conditions**
- **We can run (and mean to in future!) full EIRENE: SOLPS with a "frozen" fluid side (B2.5)**
  - ➔ This option is not mature enough for meaningful physics results
  - ➔ **We use standalone CRM and vary consrtant plsma conditions around**

YACORA: inclusion molecular source term

- **Stationary run vibrationally resolved:**

YACORA + **Source term adjustable** to the Edge2D-EIRENE

F.Cianfrani, EPS-2022

Particle species

$$p, H_2^+, Z$$
$$H_2(v=0), \ldots, H_2(v=14)$$

Reactions

electron impact

$$H_2 + e \rightarrow H_2(b_{\text{triplet}}) \rightarrow H^+ + H^+ + e + e$$

proton impact

$$H_2 + e \rightarrow H_2^+ + e + e$$

electron impact

$$H_2 + p \rightarrow H_2^+ + p + e$$

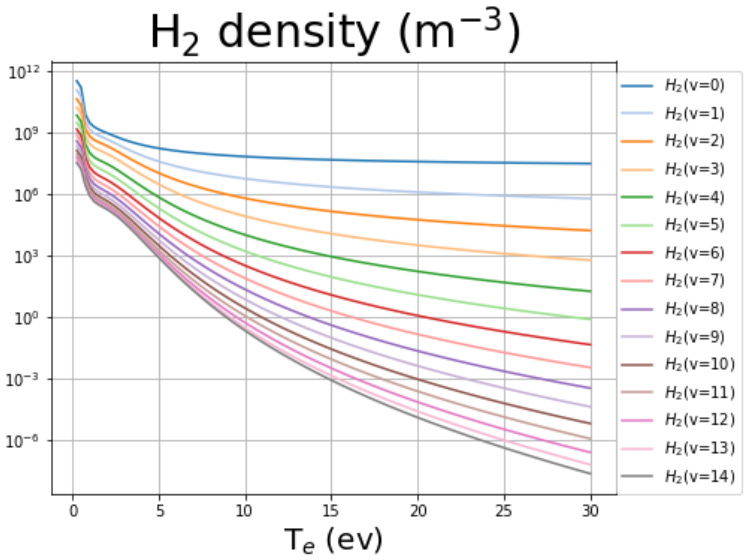
$$H_2 + e \rightarrow H^+ + H^+ + e + e$$

vibrational transitions

$$H_2(v=0) \rightleftharpoons H_2(v=1)$$
$$H_2(v=1) \rightleftharpoons H_2(v=2)$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$
$$H_2(v=13) \rightleftharpoons H_2(v=14)$$

H_2 source term

$$Z \rightarrow H_2(v=0)$$

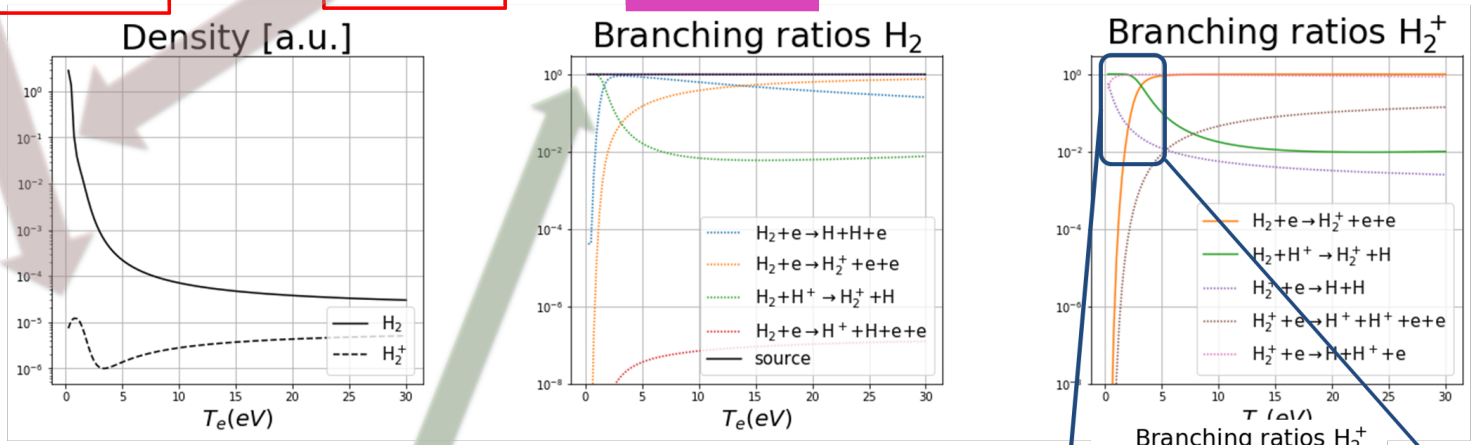


DEMO-relevant conditions – branching ratios

H_2^+ density peak

large H_2 density

EU-DEMO



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

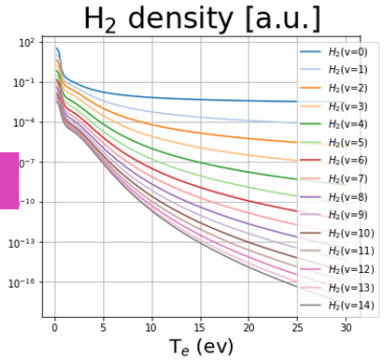
$H_2+H^+ \rightarrow H_2^+ +H$ **MAR** $H_2^+ +e \rightarrow H+H$

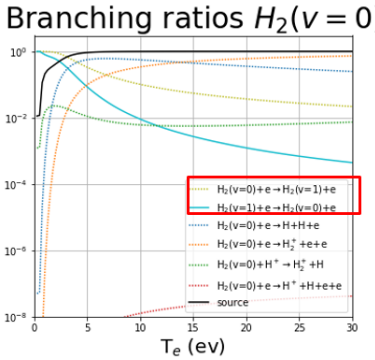
MAR/MAD competition at very low temperature

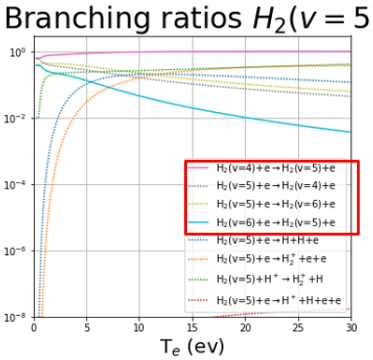
EU-DEMO– effect of resolution by vibrostates

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

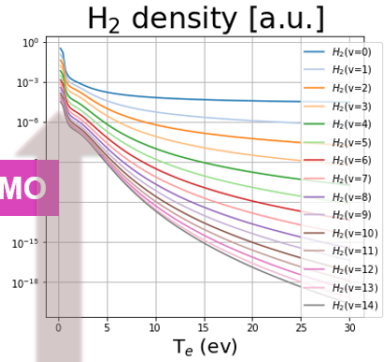
JET

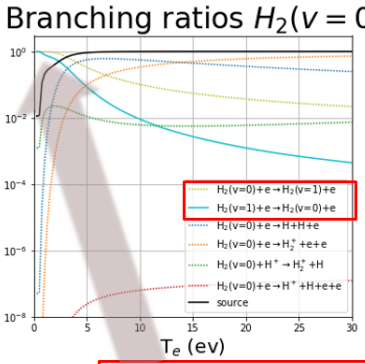


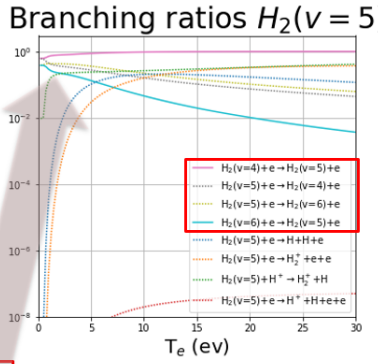




EU-DEMO







- **density:** large at low temperature

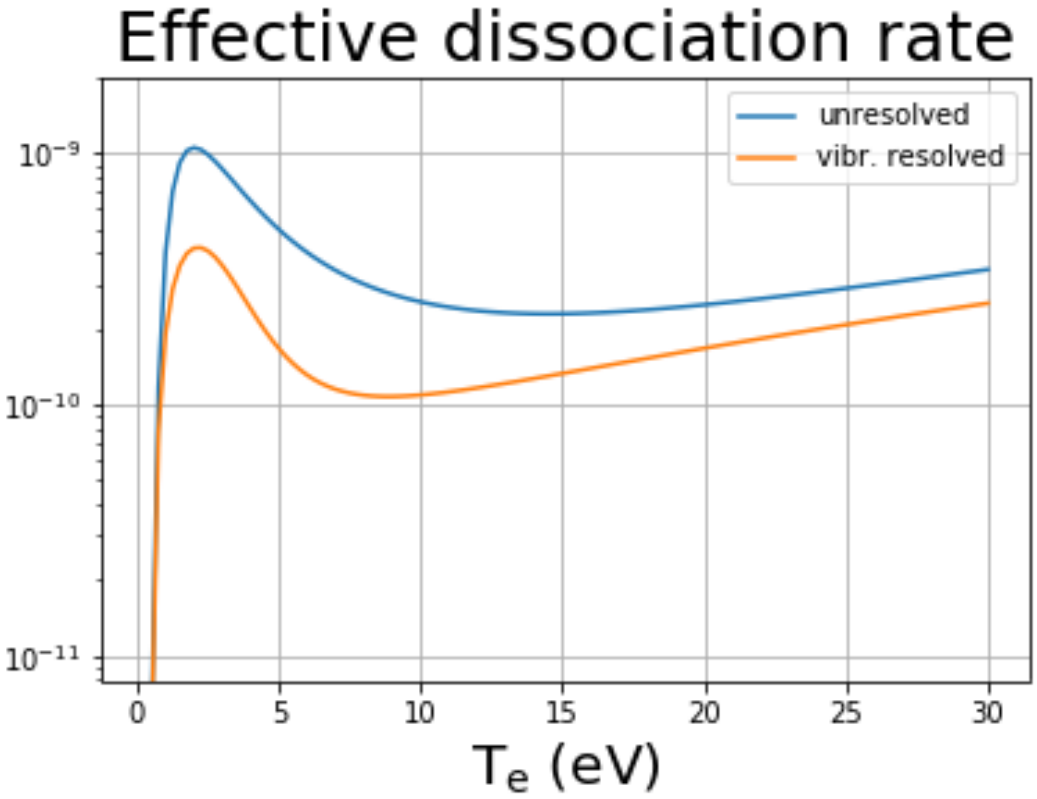
vibrational transitions are the main reaction channels at low temperatures

F.Cianfrani et al., EPS-2022

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

EU-DEMO – effect of resolution by vibrostates



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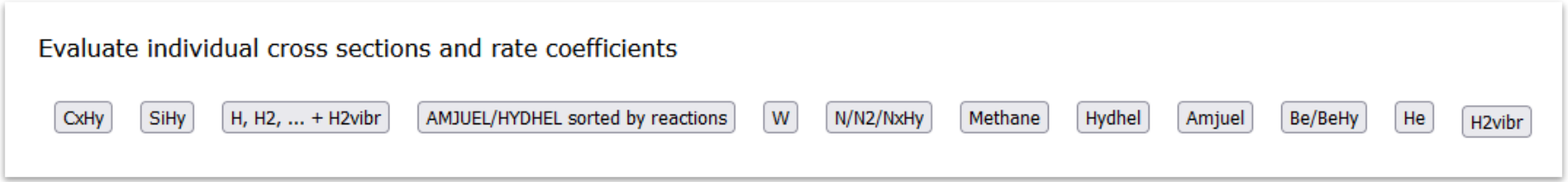
HYDKIN (web-based A&M data tool):

- toolbox for plotting and manipulation of A&M data with a user-friendly graphical interface.

D.Reiter et al., Phys. Scr. 2009

- includes EIRENE databases: AMJUEL, HYDHEL, H2VIBR, METHANE, .. .

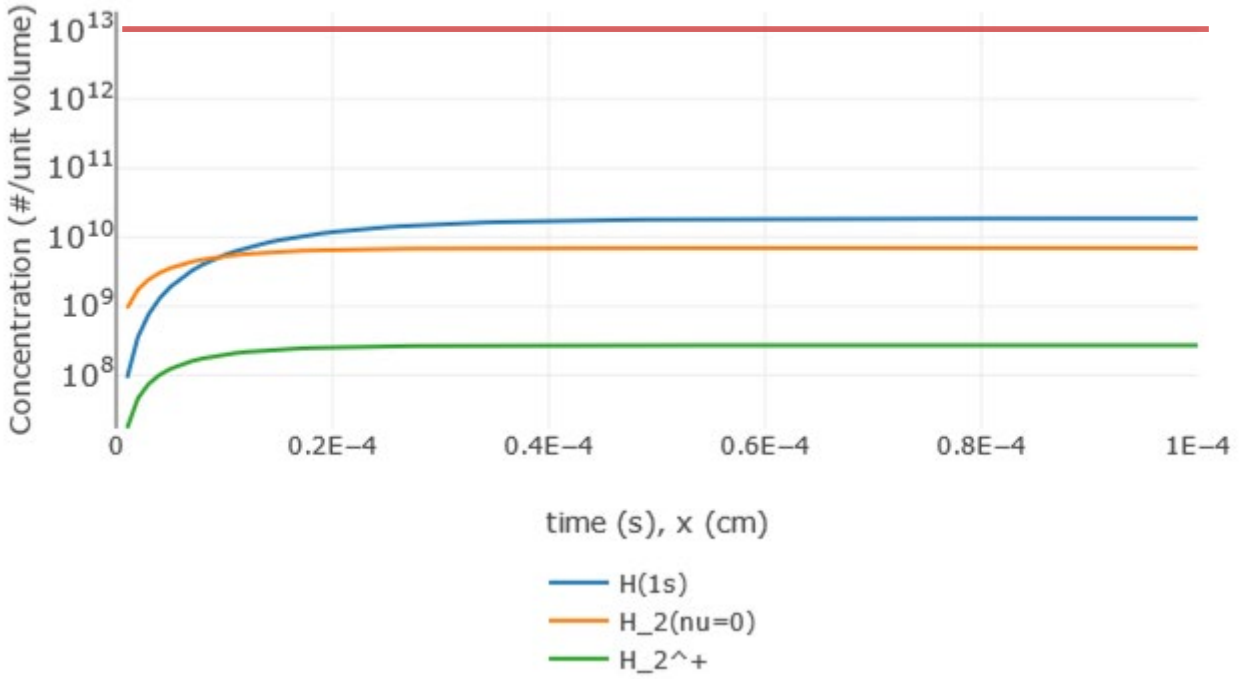


- available at http://www.eirene.de/hydkin/
  Password-protected (for access contact the authors).

F.Cianfrani et al., ICAMDATA-2022

HYDKIN: particle solver (non-stationary)

Default case (see next slides)



reservoir

"infinite reserve" of particles at fixed temperature and density

Development of stationary equilibrium

HYDKIN: what is inside?..

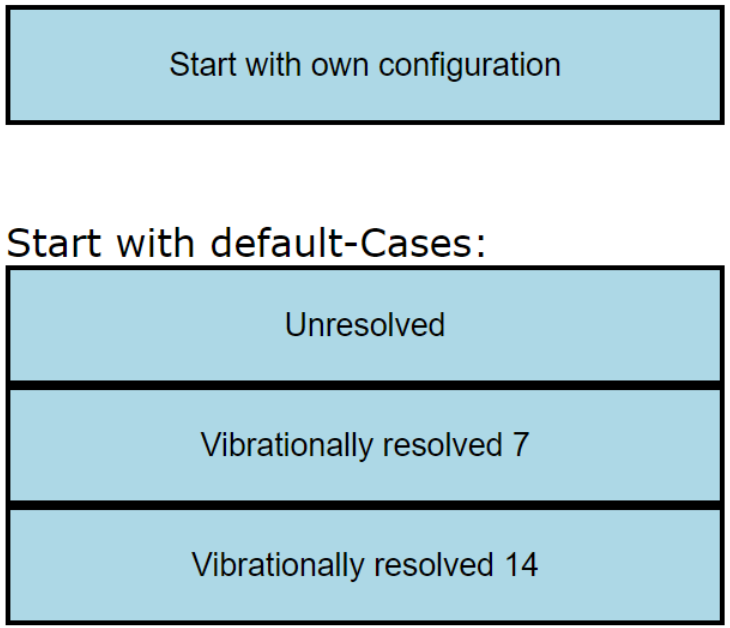
1) **CRM solver (transport excluded, pure A&M side of the problem) with extensive features**
   - ➔ Stationary and **non-stationary** solution (assuming velocity and plasma pars)
   - ➔ Any specie can be treated as "**Reservoir**"
   - ➔ **"Spectral analysis"** based on eigenvalue approach (which reactions are most important?)
   - ➔ **Sensitivity analysis** – vary the plasma parameters, solver settings, reactions, etc.

2) **Plotting, solver results visualisation**
   - ➔ Useful for fast **consistency checks** and trivial analysis while constructing the CRMs
   - ➔ Good for physics analysis in case one follows **established routines**

3) **Flexible reaction tables interconnected with the solver and plotting**
   - ➔ Useful for fast **consistency checks** and trivial analysis while constructing the CRMs
   - ➔ Good for physics analysis in case one follows **established routines**
   - ➔ **Input/output** in various formats (new: JSON) including directly for EIRENE

HYDKIN: using the power of the web-interface

For H_2 case (example):



- **The basis table is highly customisable:**
  1) Deselected reaction can be excluded from the view
  2) User easily selects the level of info for each reaction to be shown
  3) Basic, solver, plotting etc. tables are interlinked

- **All is optimised for checking high amounts of similar data**
  1) Critical things are highlighted
  2) Data is grouped by the reactions (even if comes from various sources)
  3) One can start with initial configuration (standard or custom) and do only essential (e.g. from physics) changes

HYDKIN – new mode (H_2 case)

Version 2022:

AMJUEL/HYDHEL sorted by reactions

Collision with e

not included in solver	selected data unselect all	plot unselect all	Number	reaction	range	reference
◉	○	☑	2.1.1	e + H(1s) → H(2p) + e	E_min: 1.08e+01 - E_max: 2.00e+04	JanevEtAl(1987)
	○	☑		e + H(1s) → H(2p) + e	T_min: 1.26e+00 - T_max: 2.00e+04	JanevEtAl(1987)
○	◉	☑	2.1.2	e + H(1s) → H(2s)+ e	E_min: 1.08e+01 - E_max: 2.00e+04	JanevEtAl(1987)
	○	☑		e + H(1s) → H(2s)+ e	T_min: 1.26e+00 - T_max: 2.00e+04	JanevEtAl(1987)
	○	☐ n=1 -> n'=2 ☐ n=2 -> n'=1		e + H(n) → H(n') + e	T_min: 1.00e-01 - T_max: 1.00e+03 n_min: 1.00e+08 - n_max: 1.00e+16	SawadaFujimoto(199

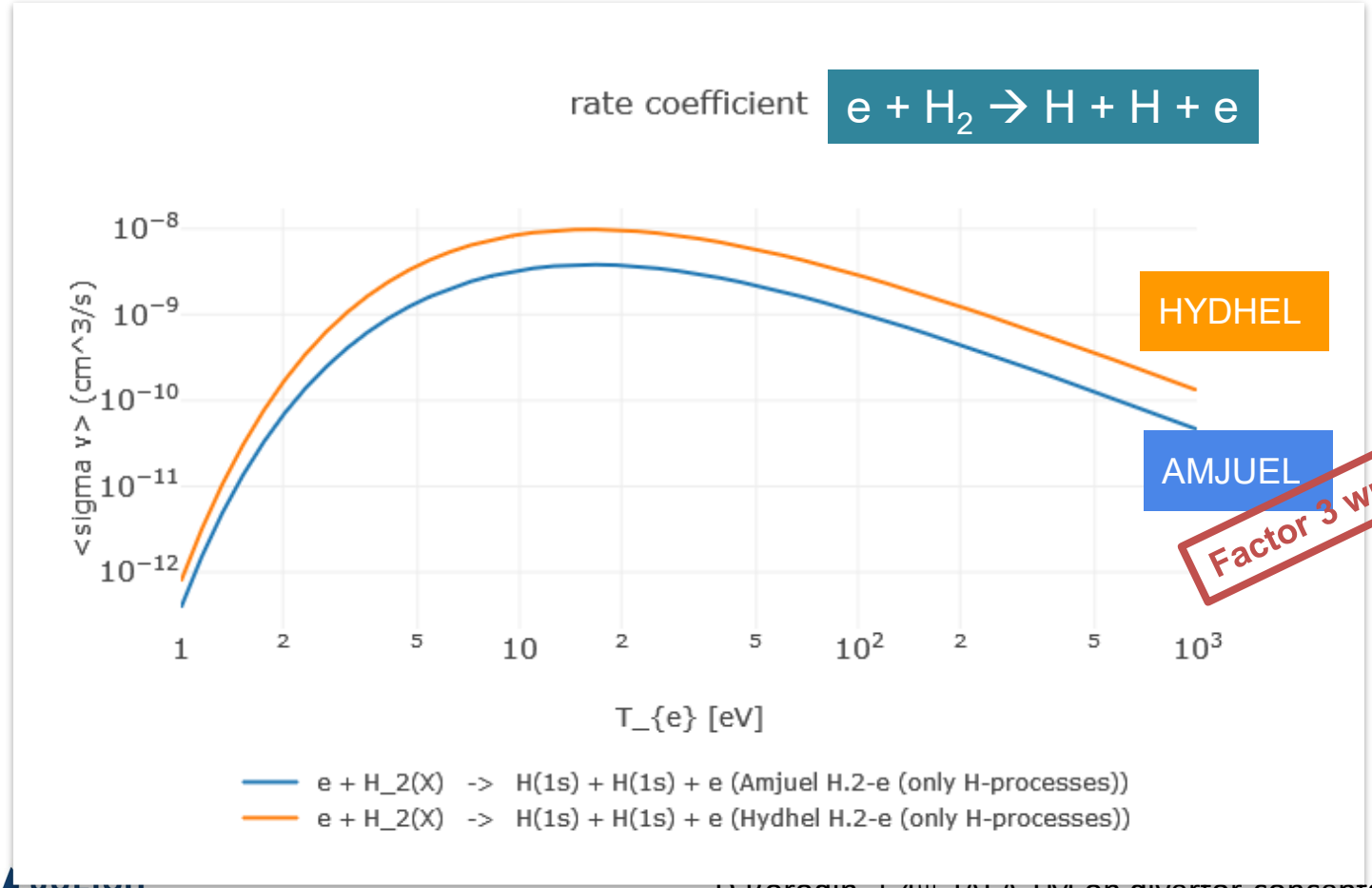
Visibility columns:
reaction: switch to off
range: switch to off
reference: switch to off
data type: switch to off
Peculiar properties: switch to on
generation: switch to on
data origin: switch to on
File/chapter: switch to off

Buttons to adjust table content

show only selected reactions (Groups)

show only selected reactions (rows)

HYDKIN: comparison dissociation rates



HYDKIN can be used to

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

Summary and outlook

1) **The development of EIRENE as "neutral gas module" for the integrated HPC-oriented simulations is ongoing**
   - ➔ 2 lines of **Fluid-Kinetic hybridisation** are exploited
   - ➔ **Parallelisation** is ongoing including testing the parallelisation and domain decomposition schemes with the EIRON "toy"-model and support from the "advanced computing hub".
   - ➔ **Code restructuring** is aimed to remove branching and segregate compact core
   - ➔ **CRM improvement** is very significant part of the improvement

2) **New CRM is concepted and under development**
   - ➔ It should be used both **in EIRENE and standalone**
   - ➔ We use **YACORA** (with additional source introduced) to gain useful experience

3) **HydKin is largely updated and foreseen to be the main A&M pre-processing tool**
   - ➔ All the development is ongoing in a view of **future massive data** extension
   - ➔ It is meant to provide flexible adjustment of CRMs and auto generation of EIRENE input

4) **Application to the EU-DEMO case (P.Subba) shows that**
   - ➔ Even **standalone model is useful** to understand the critical branching ratios
   - ➔ Tracking of **vibrational states** is essential
   - ➔ Full scale SOLPS-ITER runs, thus further development, is needed for tasks like RTC in DEMO

Thanks for the attention!