Atomic Processes in Plasmas,
IAEA, 15-19 May 2023

EUROfusion

Tracking of internal states in collisional-radiative models employed in the transport codes

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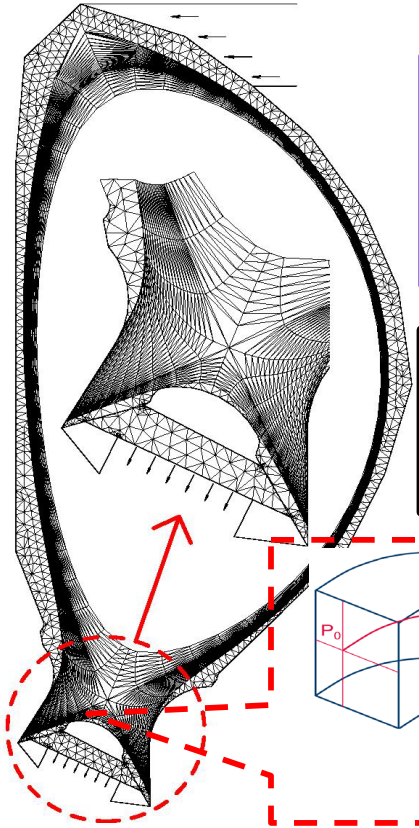
This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect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

Monte-Carlo edge plasma transport codes: EIRENE and ERO

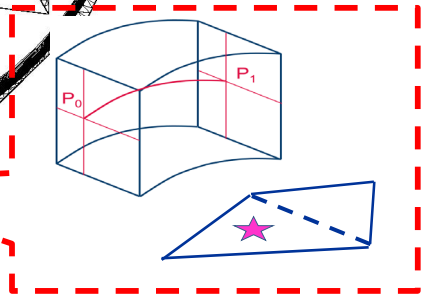
What is EIRENE in a nutshell (e.g. in SOLPS)?..



Macroscopic:

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

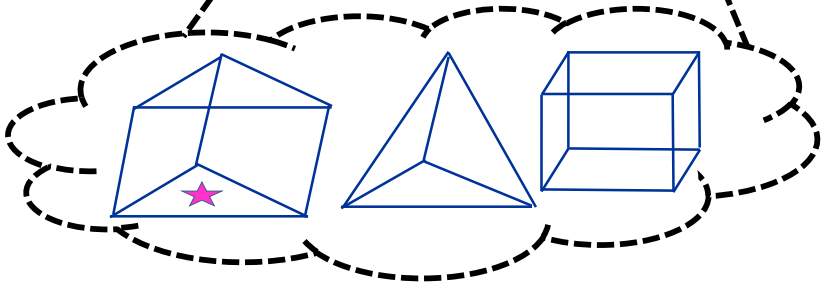
2D or 3D Volume grid (e.g. tetraeder) adopted for current magnetic configuration



Plasma flow parameters

3D EIRENE volume cell

Source terms (Particle, Momentum, Energy)

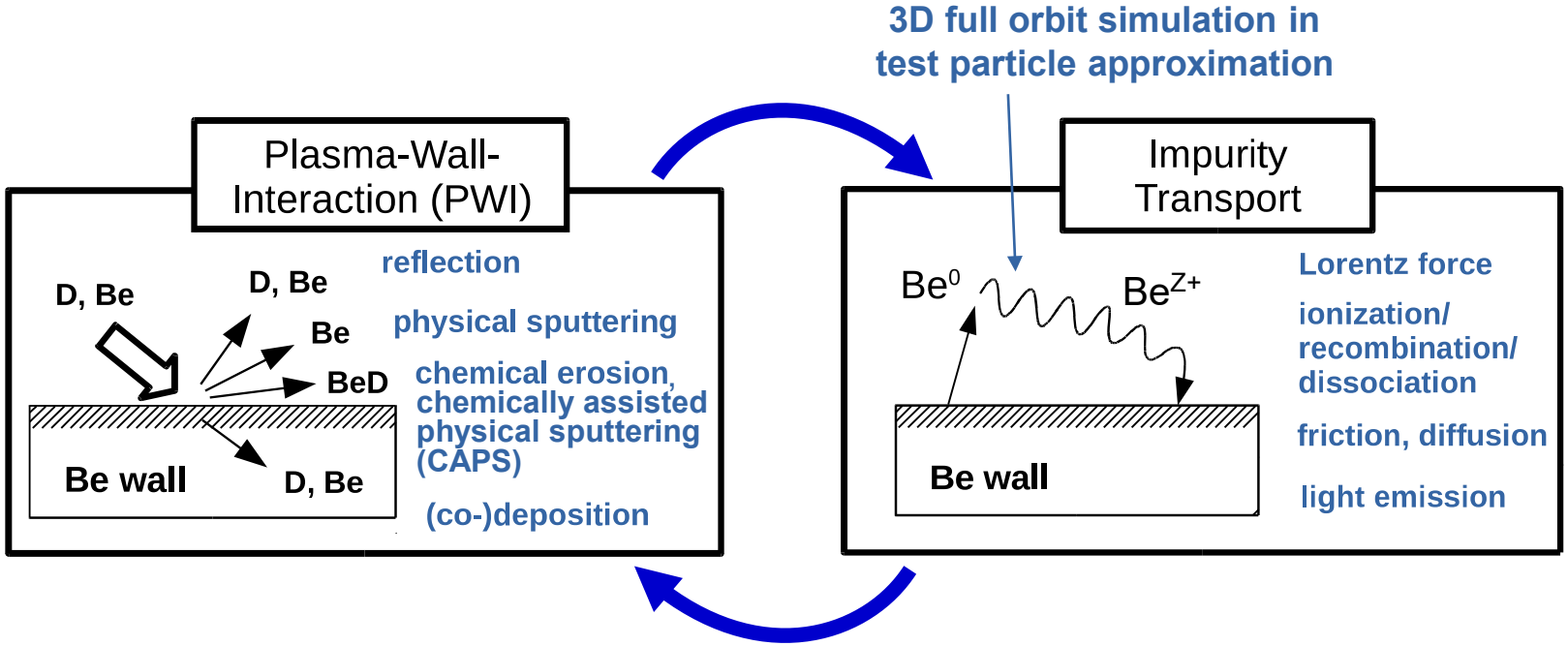


Microscopic:

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.

ERO code: concept and design



Significant code upgrade ERO2.0:

Based on same principles, but allows extending the simulation volume significantly (using HPC)

Transport code variations and commons: CRMs

Property	EIRENE	ERO, ERO2.0
Ab initio	Yes (iterations with fluid code, e.g. with B2.5 → "SOLPS-ITER")	No, test-particle approximation on a given plasma BG (e.g. from SOLPS)
Gyro-motion	Guiding centre approximation	Full-resolved, detailed 3D wall elements, surface sheath
Plasma-wall interaction	Less detailed locally, often no 3D	More detailed: 3D, sheath, etc.
PWI impact on plasma	Yes, also "advanced fluid neutrals", "wall reservoirs" etc.	In general NO (certain effects were introduced…)

Both approaches have clear advantages and range of appropriate tasks, both packages are highly demanded by ITER, EU-DEMO and other fusion-relevant devices!

➔ *Moreover, they often support each other (plasma BGs from various CFD-EIRENE **used and tested** in ERO)*

However, the subtasks for treatment of atomic and molecular processes in plasma are very similar!

- Break-up of the molecular species in plasma
- Ionisation and other processes affecting charge and energy, thus transport
- Synthetic spectroscopy for comparison with diagnostics

Similar A&M process treatment challenges!

Collisional-radiative models (CRMs):

→ **treating none-stationary**

→ **metastables (MS) in atoms**

→ **vibrational states in molecules**

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 than 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.

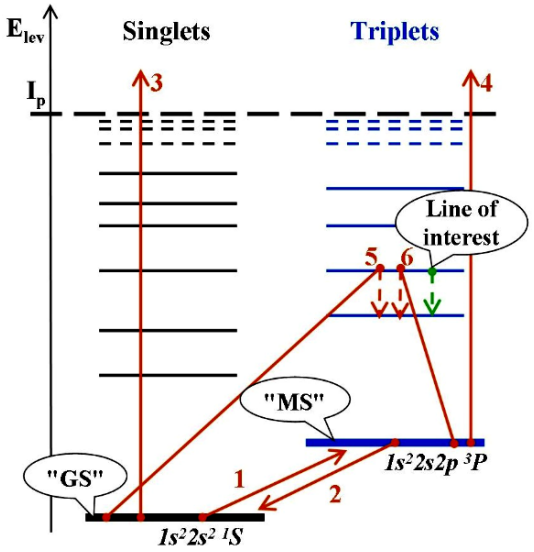
MS-effect for BeI ("generalised" MS 10^{-4}s)

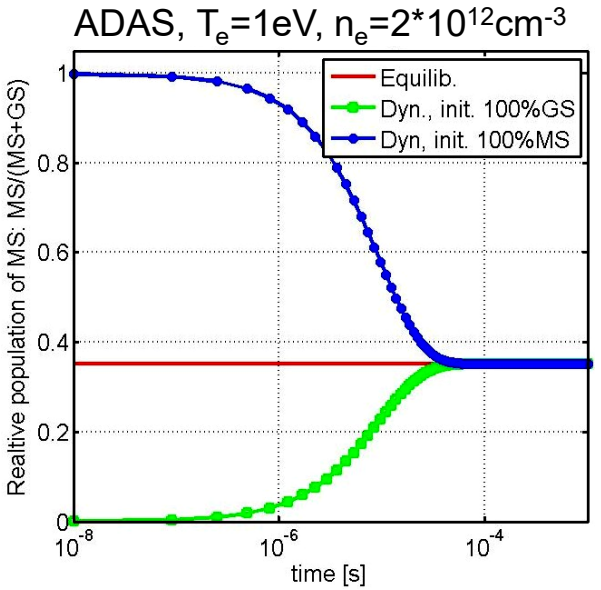
The system of 2 balance equations can be solved analytically . . .

$$\begin{cases} \frac{dN_{GS}}{dt} = -\langle ExGM \rangle N_{GS} - \langle IzG \rangle N_{GS} + \langle ExMG \rangle N_{MS} \\ \frac{dN_{MS}}{dt} = -\langle ExMG \rangle N_{MS} - \langle IzM \rangle N_{MS} + \langle ExGM \rangle N_{GS} \end{cases}$$

$$(C_{1i}, C_{2i}, \lambda_p, \lambda_m \text{ determined by rates}):$$

$$dN_i(t) = C_{1i} \exp(-\lambda_p t) + C_{2i} \exp(-\lambda_m t)$$





Effective rates:

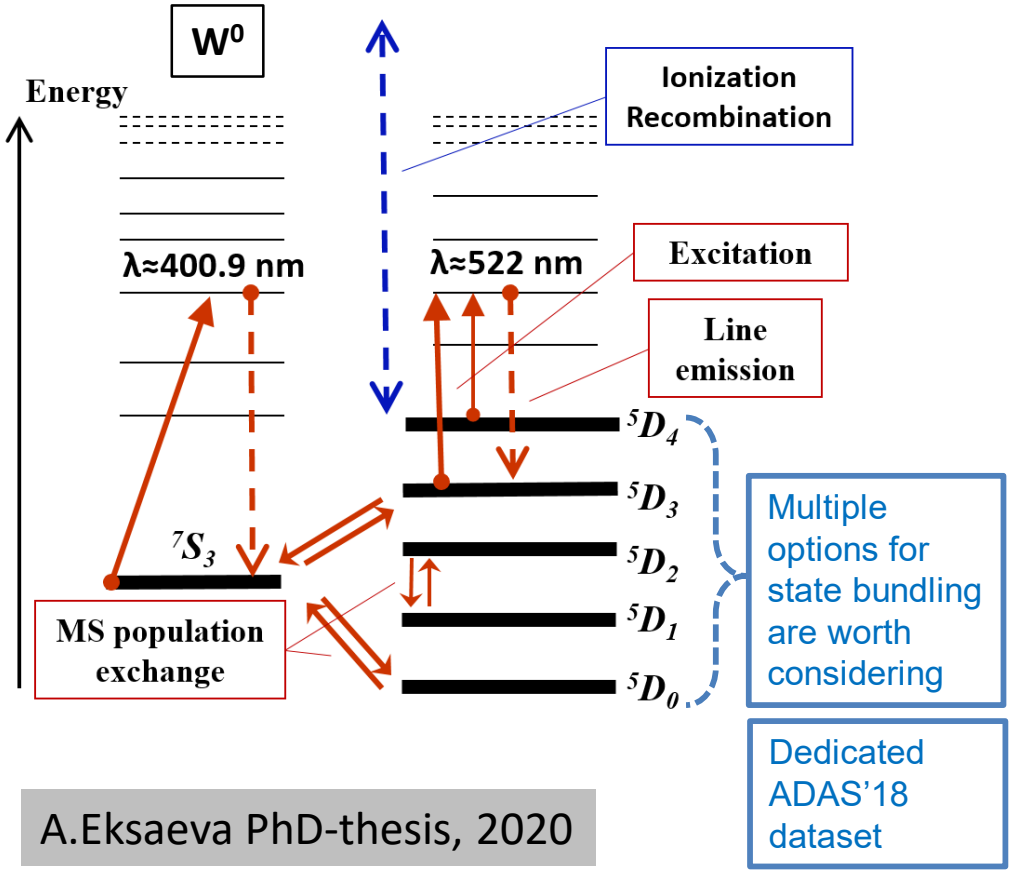
1,2) transitions <Ex..> between "GS" and "MS"

3,4) ionizations <Iz..> from "GS" and "MS"

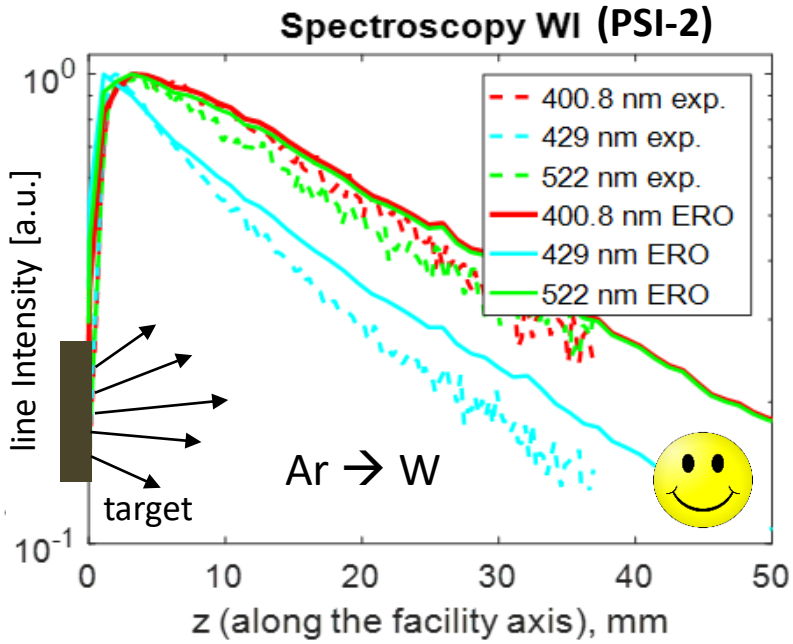
5,6) line intensity (PEC – photon emission coefficient), contributions from "GS" and "MS"

- MS-population tracking was introduced into ERO and demonstrated to be of significance by applications to PISCES-B, PSI-2 and JET-ILW **(neutral Be, He, W)**
- For WI dedicated ADAS dataset was developed; various lower states bundling options (~10) tested etc.

MS-effect for WI (PSI-2 linear plasma device, JET)

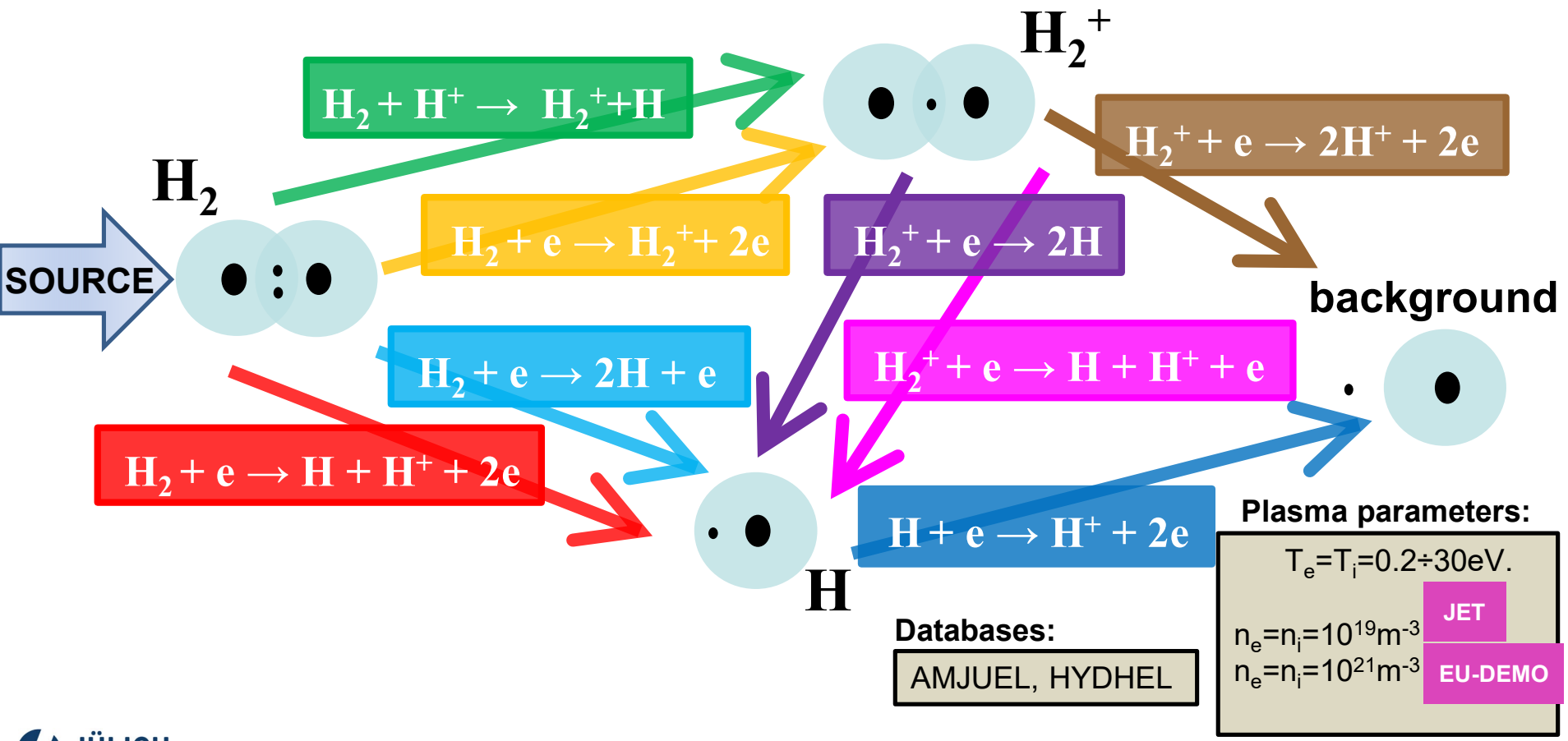


A.Eksaeva PhD-thesis, 2020

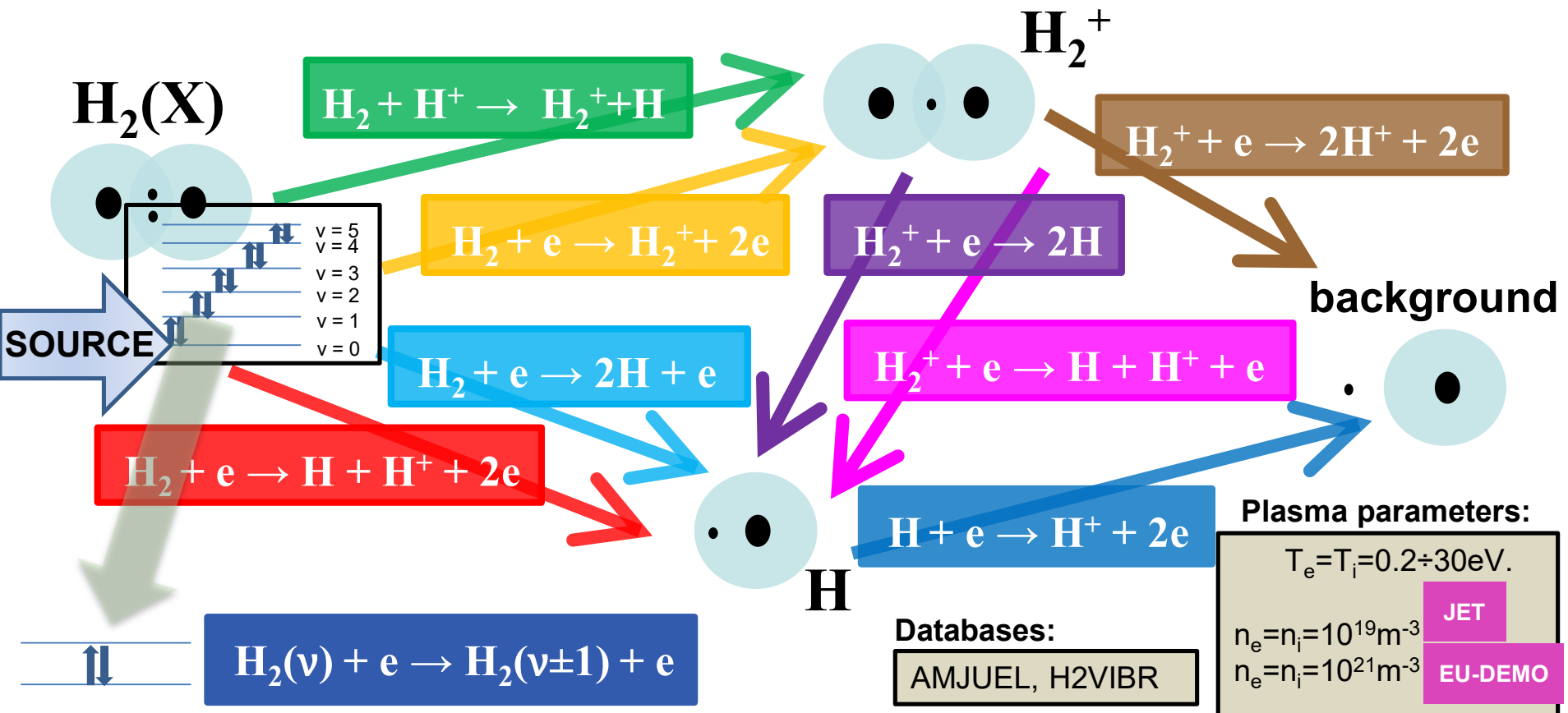


✓ **Test in tokamak (JET ITER-like Wall):** MS tracking reduces simulated line intensity by x1.7!

CRM FOR MOLECULES



CRM FOR MOLECULES : vibral resolution

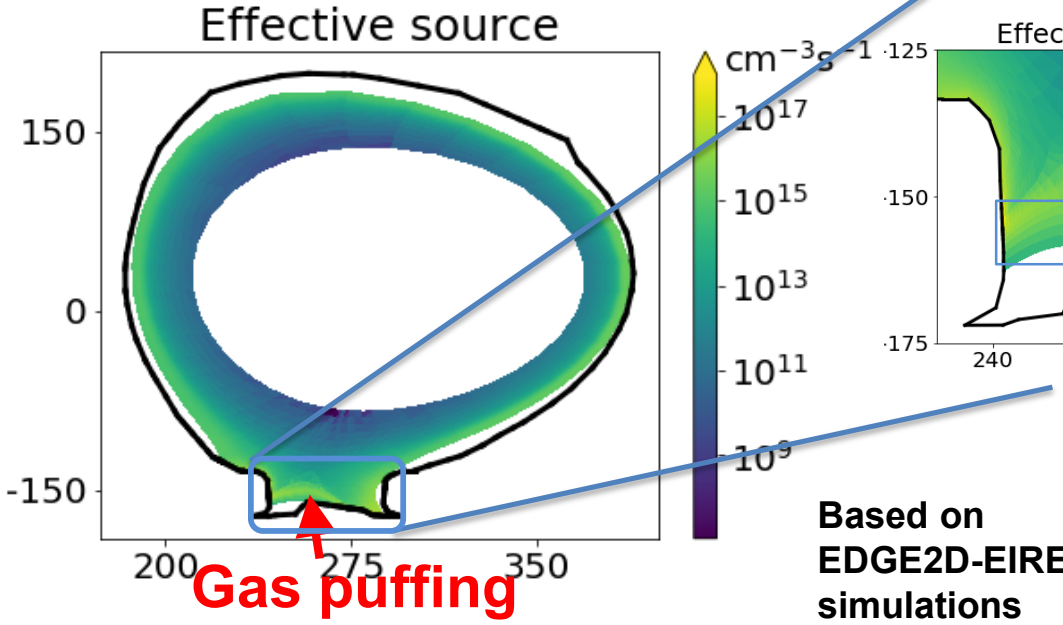


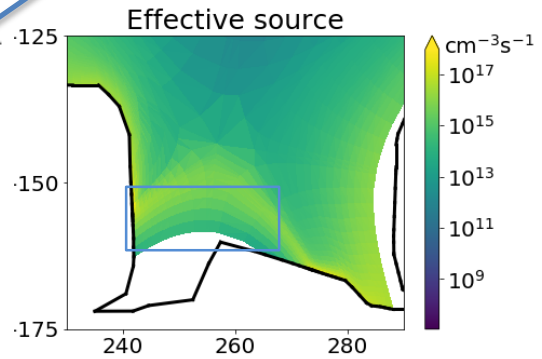
Standalone CRM vs EIRENE: Effective source (JET)

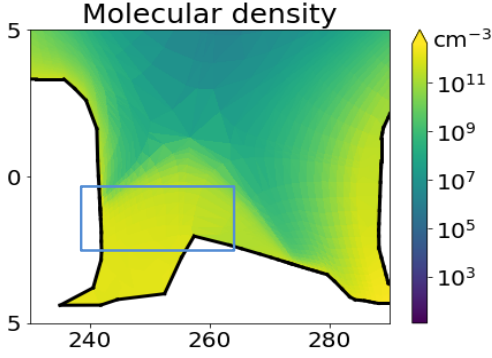
- CRM in each simulation cell: molecule density scales linearly with the source →

with isotope rescaling

$$\frac{density(edge2D)}{density(CRM)} = \frac{\boldsymbol{effective\ source(edge2D)}}{reference\ source(CRM)}$$





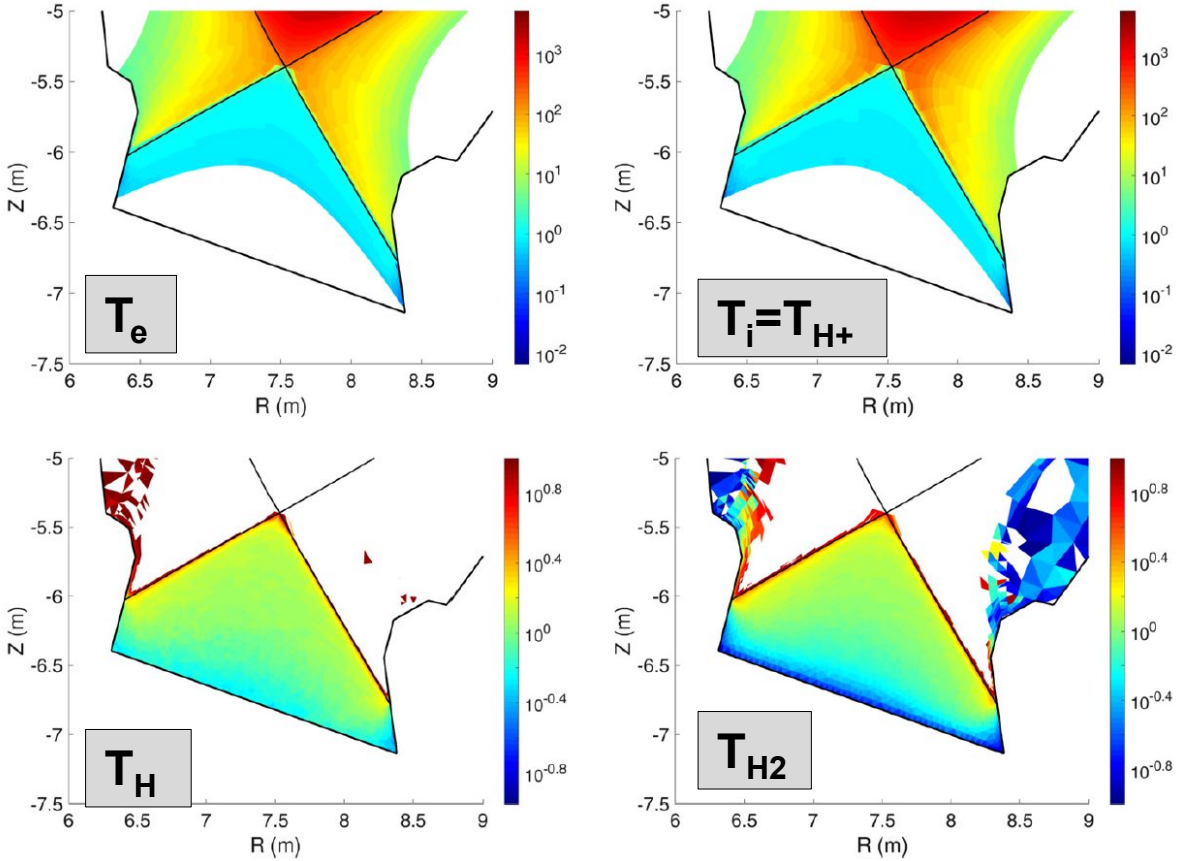


Based on EDGE2D-EIRENE simulations
JET shot 81472

M Groth et al. NF 2013

- **divertor region**: iny → novel physical conditions (dominance of CX reactions at low temperature)`

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) $N(H)=10e20\ m^{-3}$
5) . . .

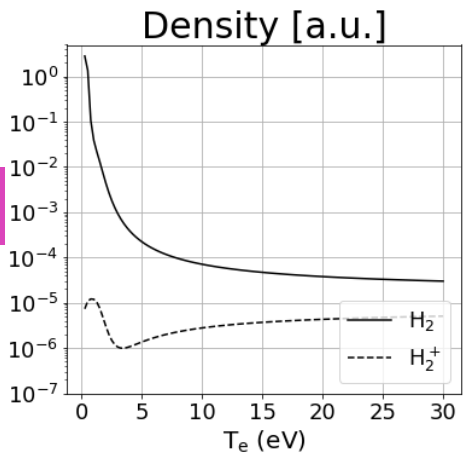
We can do the following:

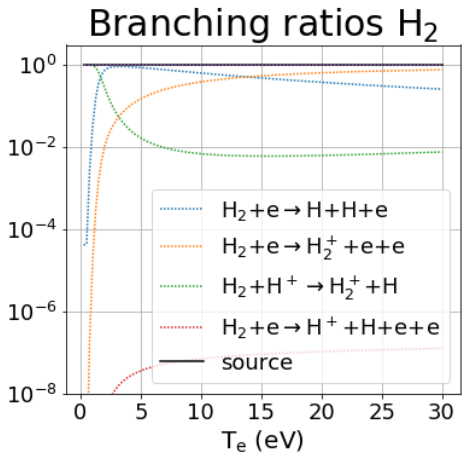
a) run full EIRENE: SOLPS with a "frozen" fluid side (B2.5)

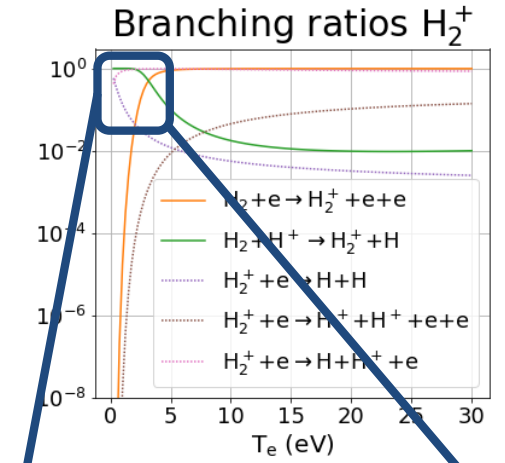
b) try to get some results from the standalone approach (mostly neglecting transport)

CRM FOR MOLECULES: leading reactions

EU-DEMO

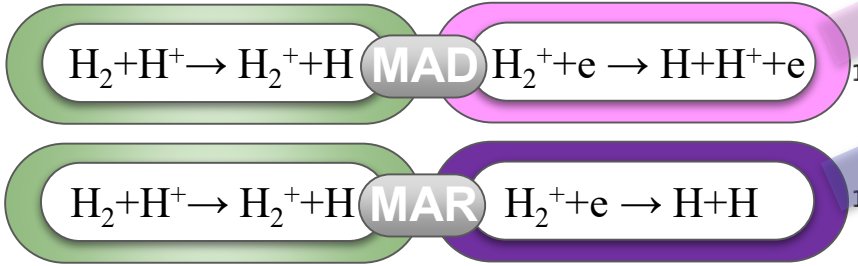


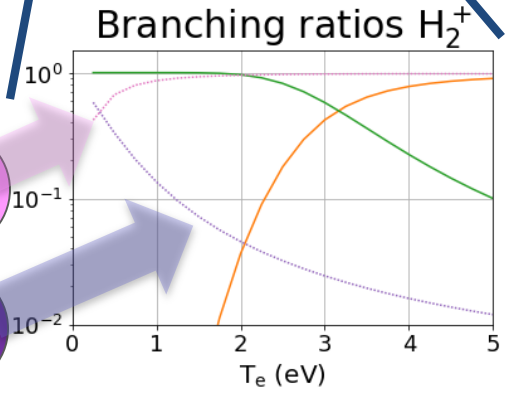




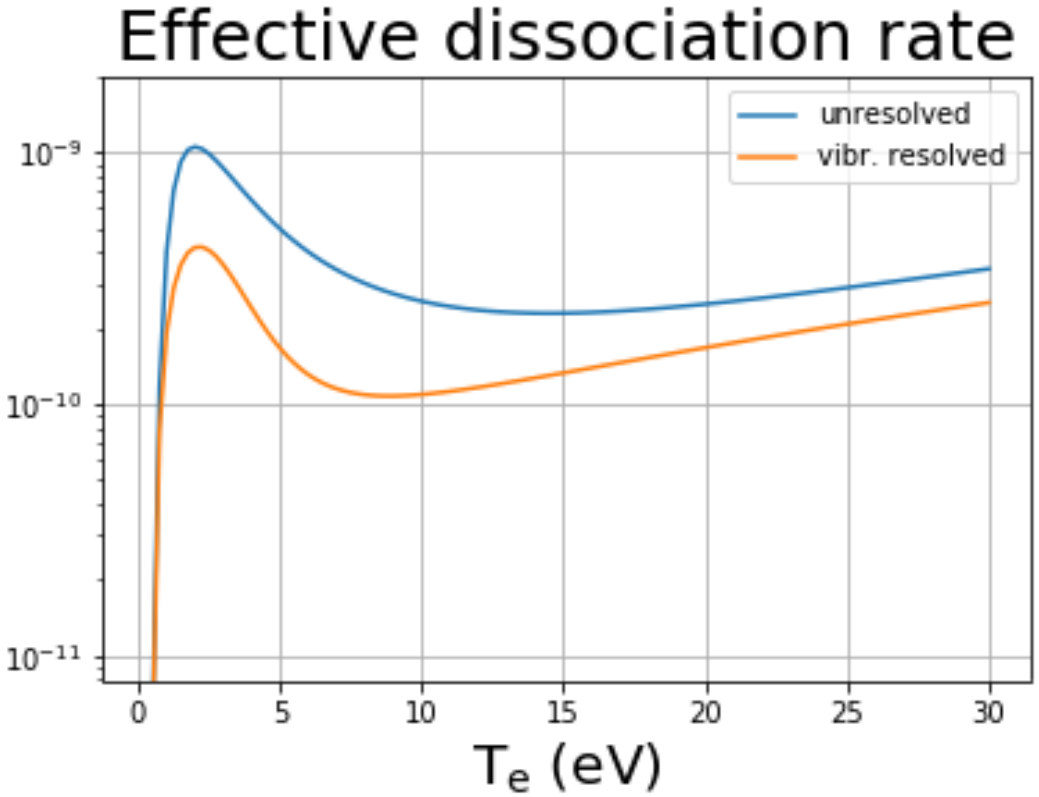
low temperature (T < 2eV) leading reaction chains:

MAR/MAD competition at very low temperature





EU-DEMO – effect of resolution by vibrostates



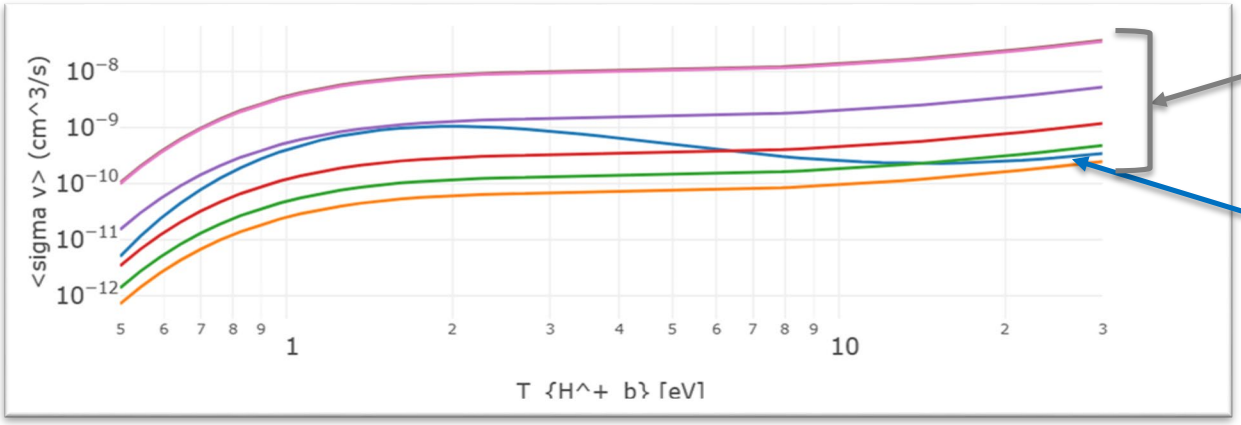
F.Cianfrani et al.,
EPS-2022

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"

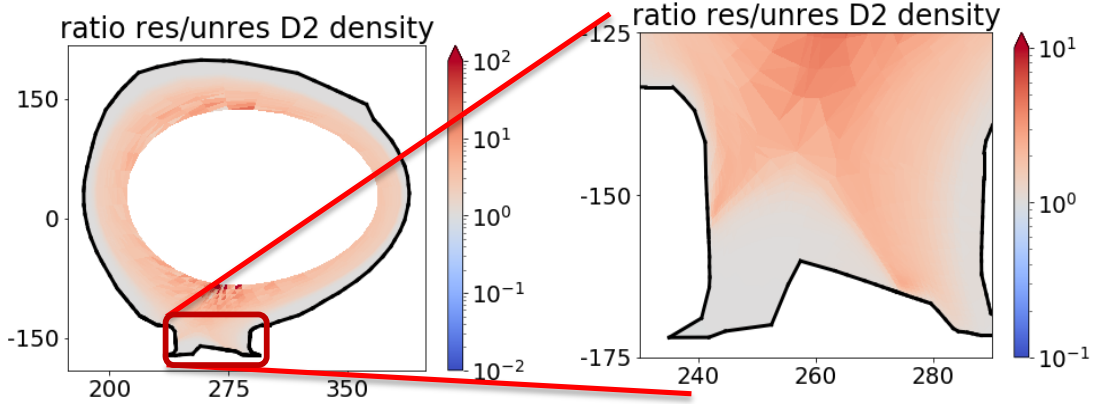
A.Holm, M.Groth, et al.,
PET, CPP 2021

Resolved vs. unresolved on vibrostates CRM in EIRENE



H2VIBR: resolved

AMJUEL: unresolved

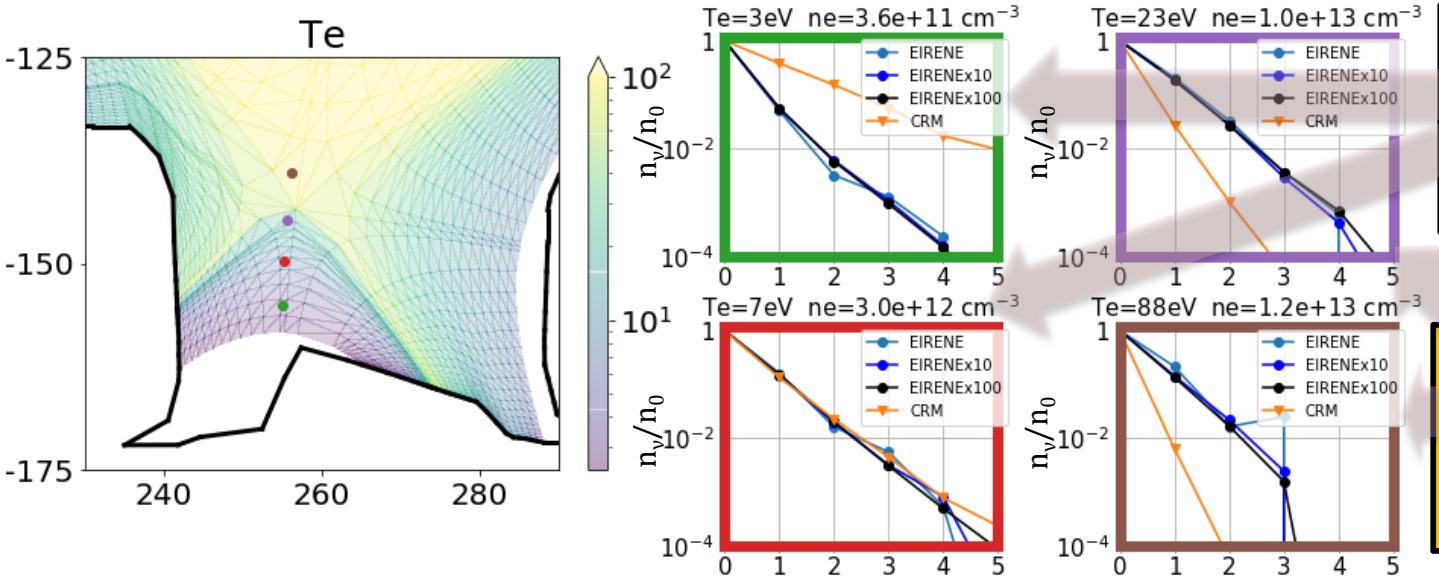


Larger molecular density (factor≃2÷3) along the separatrix with vibr. resolution.

Standalone CRM vs EIRENE - 1

Simulations: **SOURCE v=0**

EIRENE: 793'300 histories
EIRENEx10: 7'933'000 histories
EIRENEx100: 79'330'000 histories



CRM overestimates excited state population at low temperature

CRM underestimates excited state population at large temperature

Standalone CRM vs EIRENE - 2

The deviations from CRM are determined by **molecular sources**:

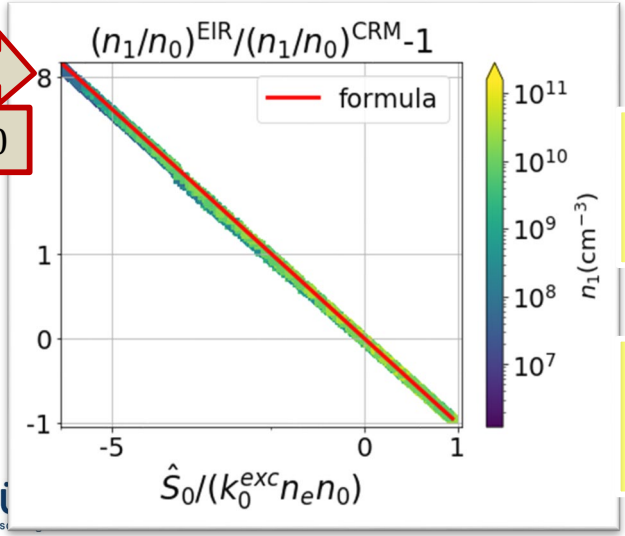
$k_\nu^{exc/dex}$: excitation/de-excitation rate

$$\left(\frac{n_{\nu+1}}{n_\nu}\right)^{EIR} = \left(\frac{n_{\nu+1}}{n_\nu}\right)^{CRM}\left(1 - \frac{\hat{S}_\nu}{k_\nu^{exc}\, n_e\, n_\nu}\right)$$

$$\hat{S}_\nu = \sum_{\bar{\nu}=\nu+1}^{N} S_{\bar{\nu}}^{EIR}\left(\frac{n_{\bar{\nu}}}{n_{\nu+1}}\right)^{CRM} \frac{k_{\bar{\nu}}^{dex}\cdot\ldots\cdot k_{\nu+2}^{dex}}{k_{\nu+1}^{exc}\cdot\ldots\cdot k_{\bar{\nu}-1}^{exc}}$$

$\bar{\nu} - \nu - 1$

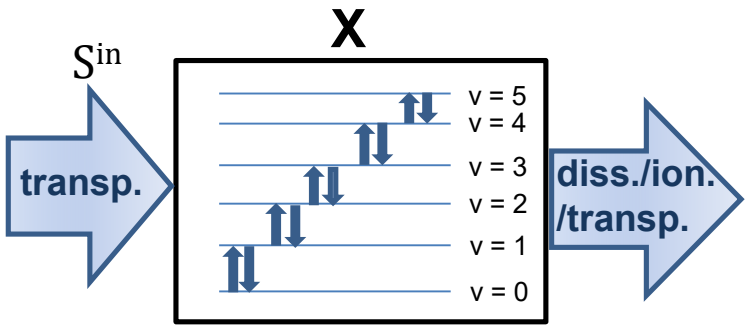
$\nu = 0$



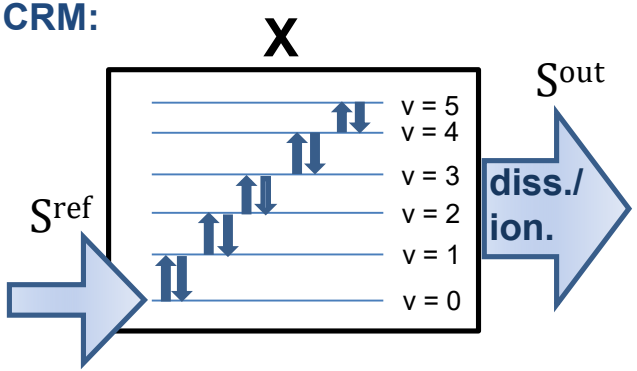
positive deviations at **sinks**

negative deviations at **sources**

EIRENE:



CRM:



Standalone CRM vs EIRENE - 3

The deviations from CRM are determined by **molecular sources**:

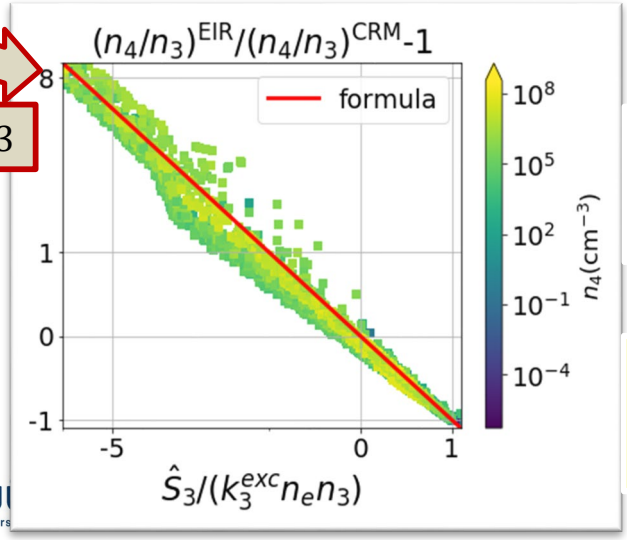
$k_\nu^{exc/dex}$ ⇅ : excitation/de-excitation rate

$$\left(\frac{n_{\nu+1}}{n_\nu}\right)^{EIR} = \left(\frac{n_{\nu+1}}{n_\nu}\right)^{CRM}\left(1 - \frac{\hat{S}_\nu}{k_\nu^{exc}\, n_e\, n_\nu}\right)$$

$$\hat{S}_\nu = \sum_{\bar{\nu}=\nu+1}^{N} S_{\bar{\nu}}^{EIR}\left(\frac{n_{\bar{\nu}}}{n_{\nu+1}}\right)^{CRM} \frac{k_{\bar{\nu}}^{dex}\cdot\ldots\cdot k_{\nu+2}^{dex}}{k_{\nu+1}^{exc}\cdot\ldots\cdot k_{\bar{\nu}-1}^{exc}}$$

$\bar{\nu} - \nu - 1$

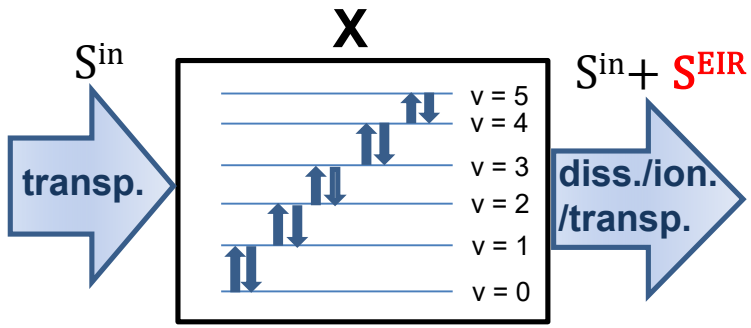
$\nu = 3$



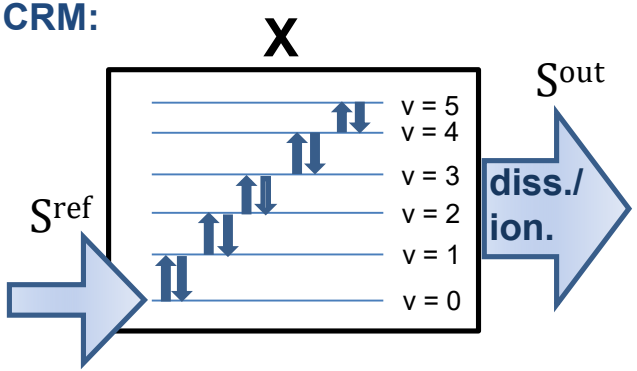
positive deviations at **sinks**

negative deviations at **sources**

EIRENE:



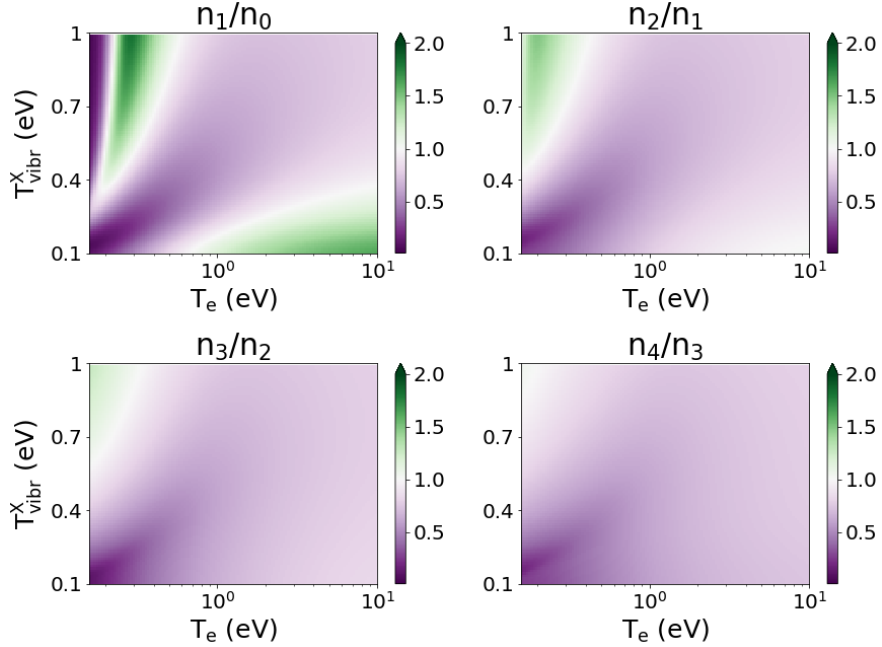
CRM:

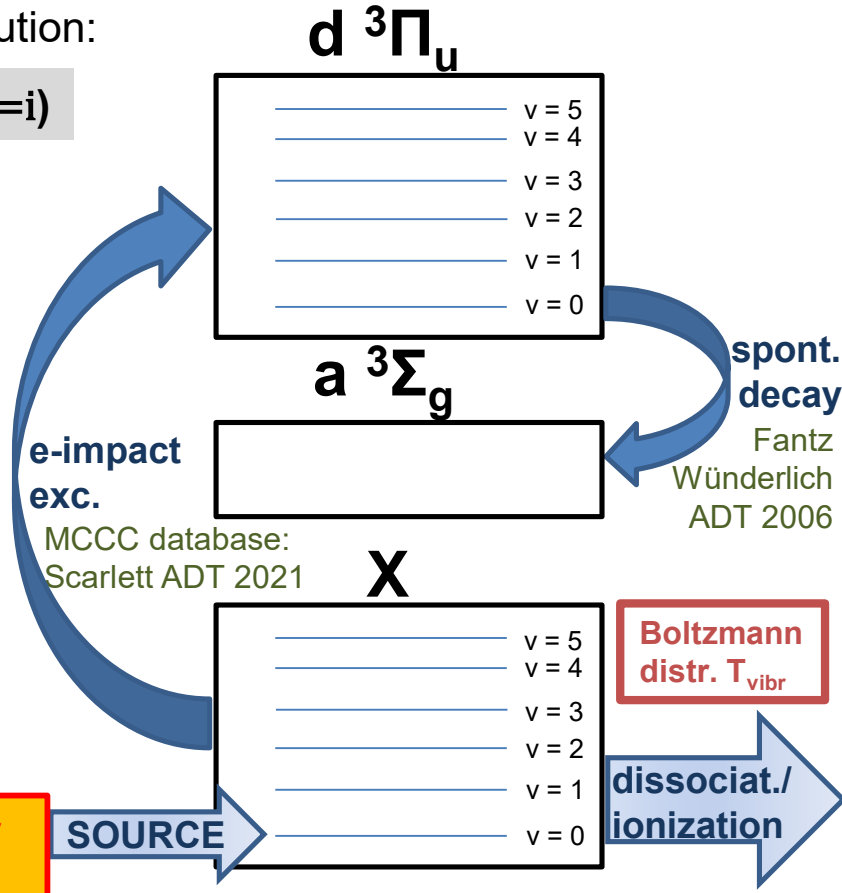


EXCITED MOLECULAR STATES

Model for excited states on top of ground state distribution:

- population coeff. excited state **d $^3\Pi_u$:** $n_i = n(d,v=i)$



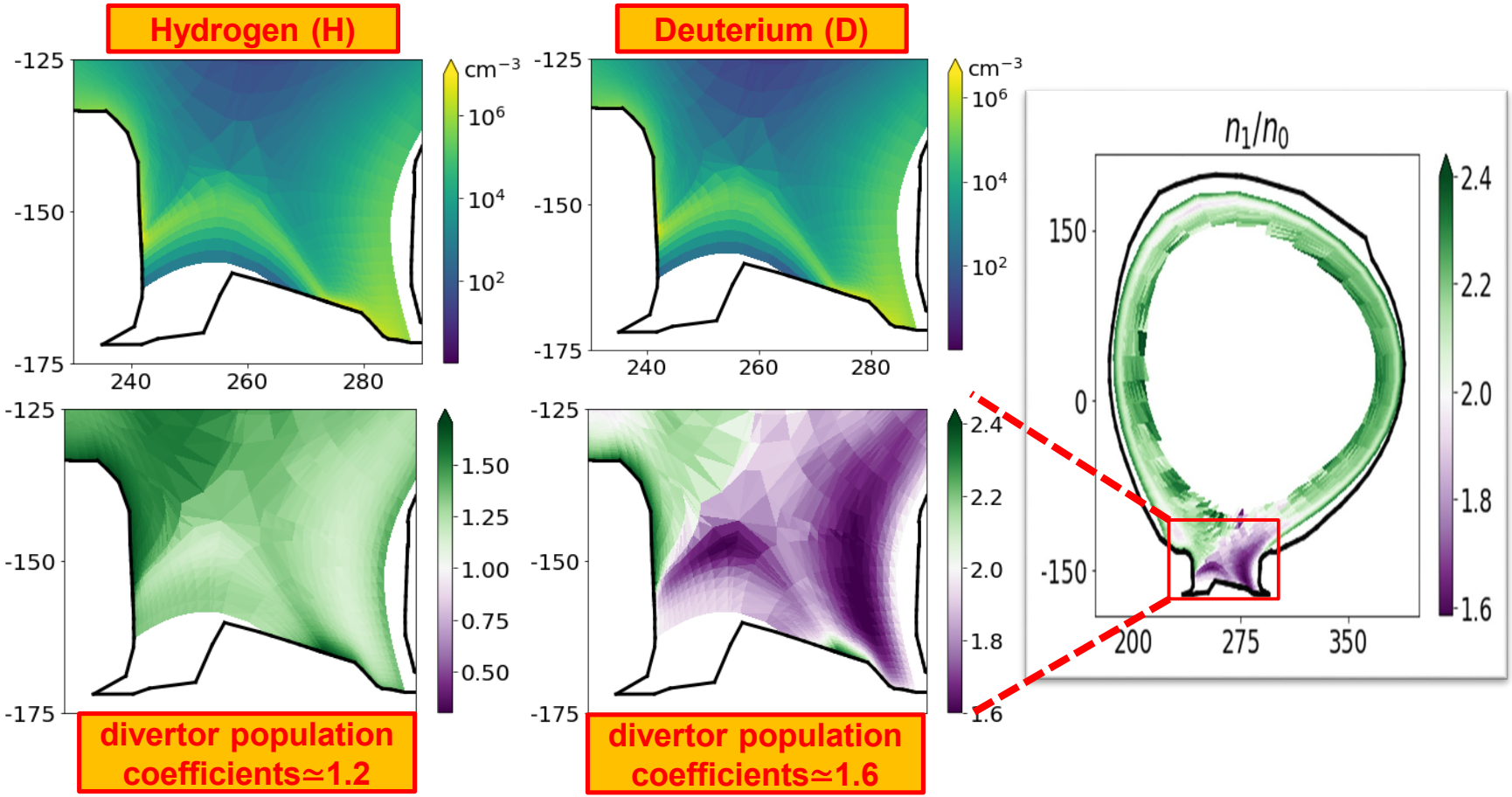


ratio of Fulcher band intensities as a proxy for ground state vibr. distribution

EIRENE: exited molecular states in divertor

excited state **d $^3\Pi_u$**:

Vibro-state popu-lation ratio **n_1/n_0**:



New (or updated) modelling tools:

→ **Ploutos**

→ **ModCR**

Standalone CRM - Ploutos: what is inside?..

Earlier known as “HydKin”

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**
   - ➔ Optimised for **consistency checks** and trivial analysis while constructing the CRMs
   - ➔ **Input/output** in various formats (new: **JSON**) including directly for EIRENE
   - ➔ Critical things are highlighted, **level of information** detail **controlled** by the user.
   - ➔ Data is **grouped by the reactions** (even if from various sources).
   - ➔ Standard or custom **initial configurations**

Power of web-based Interface!

PLOUTOS can be used to

www.eirene.de

Both statues are at Glyptothek, Munich.

EIRENE

- **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)*

PLOUTOS – (H_2 2022/23 case)

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)

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!

New code (also library for EIRENE): “ModCR”

- **Should provide BOTH standalone and build-in CRM for EIRENE**
  - Therefore written in modern Fortran
  - Linked with Ploutos (uses the same JSON files for I/O)

    (AMJuel, HydHel, H2Vibr, etc are already inside, moreover under flexible web-powered control)
  - Non-stationary approach utilising up-to-date Sundails solver (CVODE) for stiff ODE systems

    (algebraic stationary option also available for control)

- **The whole specie-state and reaction basis is inside, however the code should form the list of “active states”**
  - Determined by user in JSON parameter file (for a few simulations)
  - Provide different resolution on states being tracked
  - Provide flexible border for tracking of MC species and internal state populations as variables

This is unique and justifies creation of the new code

ODE Solver for ModCR

- **SUNDIALS:** SUite of Nonlinear and DIfferential/ALgebraic Equation Solvers

Developed at LLNL - awarded the 2023 SIAM/ACM Prize in Computational Science and Engineering

git repository: https://github.com/LLNL/sundials

Package	Purpose
CVODE	solves initial value problems for ordinary differential equation (ODE) systems.
CVODES	solves ODE systems and includes sensitivity analysis capabilities (forward and adjoint).
ARKODE	solves initial value ODE problems with additive Runge-Kutta methods, including support for IMEX methods.
IDA	solves initial value problems for differential-algebraic equation (DAE) systems.
IDAS	solves DAE systems and includes sensitivity analysis capabilities (forward and adjoint).
KINSOL	solves nonlinear algebraic systems.

Modern, powerful and flexible – still it is available in FORTRAN (so suits to EIRENE)

Summary and outlook

1) **CRMs are essential and potentially common part of the plasma MC transport codes**

2) **Transport and A&M sides of MC transport codes are NOT separable, however using the standalone approach is often extremely useful**
   - ➔ Gives insight into the A&M physics
   - ➔ Allows more control, looking into details and straightforward answers
   - ➔ Particular valuable if standalone and external CRM would be just the same
   - ➔ Isotope (D vs. H) effect demonstrates the significance of vibro-resolved MCCC data

3) **New CRM (ModCR) is concepted and under development**
   - ➔ PLOUTOS will keep and even strengthen its role as data pre-processor
   - ➔ It is aimed to provide flexible “border” between particles treated as MC species or variables characterising the internal state

4) **Opacity and other effects should be available in ModCR, but it is too early to talk about that at the current stage.**

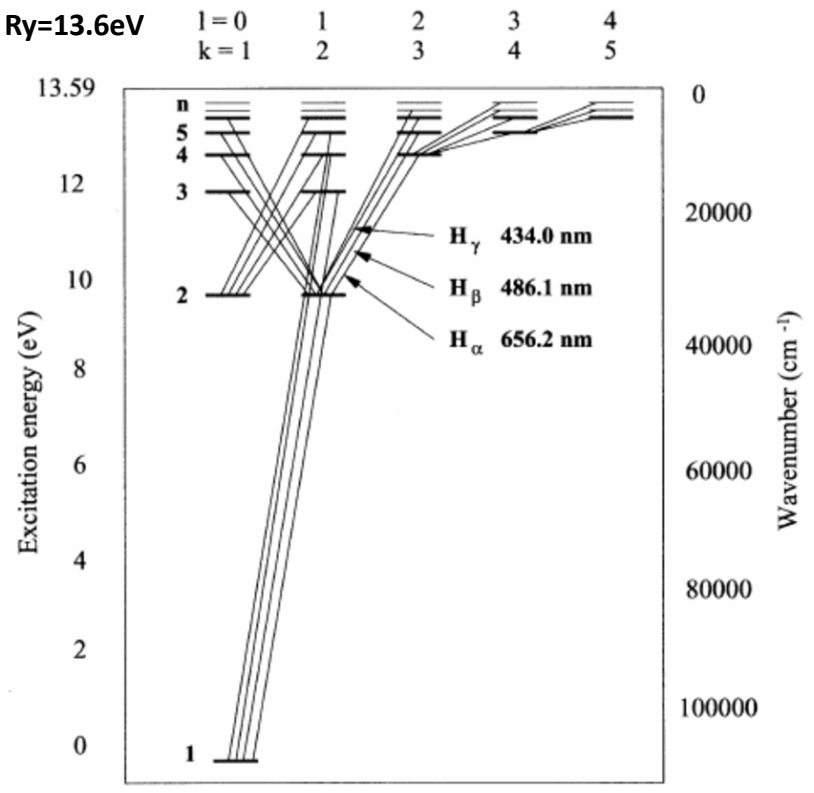
Further details at www.eirene.de

Thanks for the attention!

Special thanks to
1) ADAS (M.O'Mullane et al.) for constant support
2) YACORA developers (U.Fanz, D.Wunderlich, et al.) for consultations
3) MCCC developers (D.V.Fursa et al.) for providing the database

Collisional-Radiative Models (CRM)

Grotrian diagram for atomic H (D, T)



Balance equations:

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

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

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

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

$\ldots$

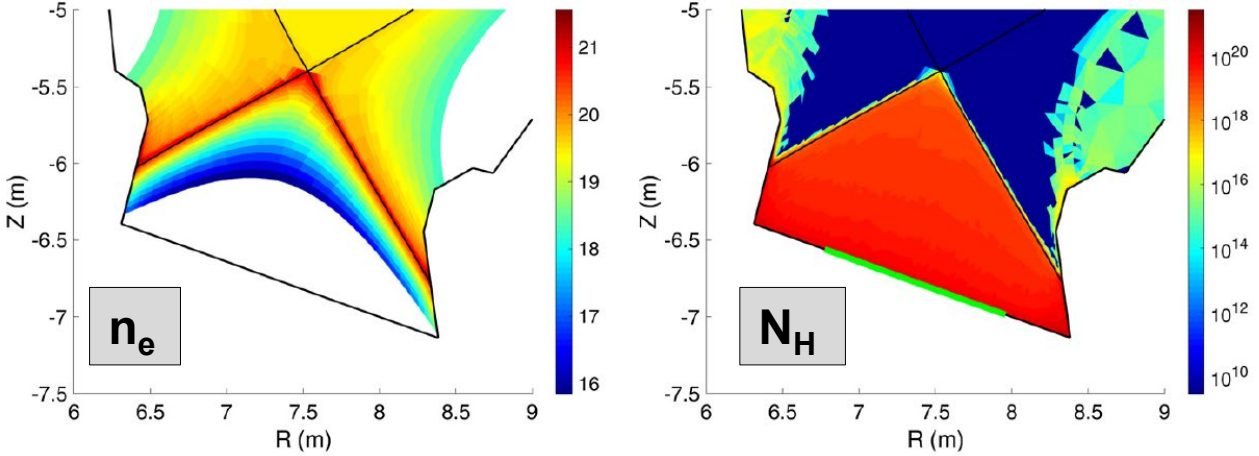
j, k, l, m, z, … states can be fine-superfine ***resolved*** *or, opposite, bundled into few quasi-* ***metastables*** *(MS)*

CRM = list of states + transition data

Often used:

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

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) $N(H)=10e20\ m^{-3}$

- **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 constant plasma conditions around**

SOLVER

- **SUNDIALS:** SUite of Nonlinear and DIfferential/ALgebraic Equation Solvers

written in C++: **Modern Fortran interface** (modules)

$$\dot{y} = f(t, y)\,, \quad y(t_0) = y_0$$

- **CVODE:** solution of IVP variable-step multistep methods:

$$\sum_{i=0}^{K_1} \alpha_{n,i} y^{n-i} + h_n \sum_{i=0}^{K_2} \beta_{n,i} \dot{y}^{n-i} = 0$$

  - ADAMS-MOULTON FORMULAS
  - BACKWARDS DIFFERENTIATION FORMULAS → stiff problems

Nonlinear solve:

- default: Newton iteration based on linear solver
- user-defined

Linear solver families:

- *direct* for dense, banded, or sparse matrices
- *spils:* scaled preconditioned iterative (Krylov) linear solvers.

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

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