TSVV-K: FZJ contribution

ModCR, Ploutos, A&M, SimDB, ACHs, IMAS, …

D. Borodin et al.

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New CRM Solver for EIRENE – "ModCR"

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

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

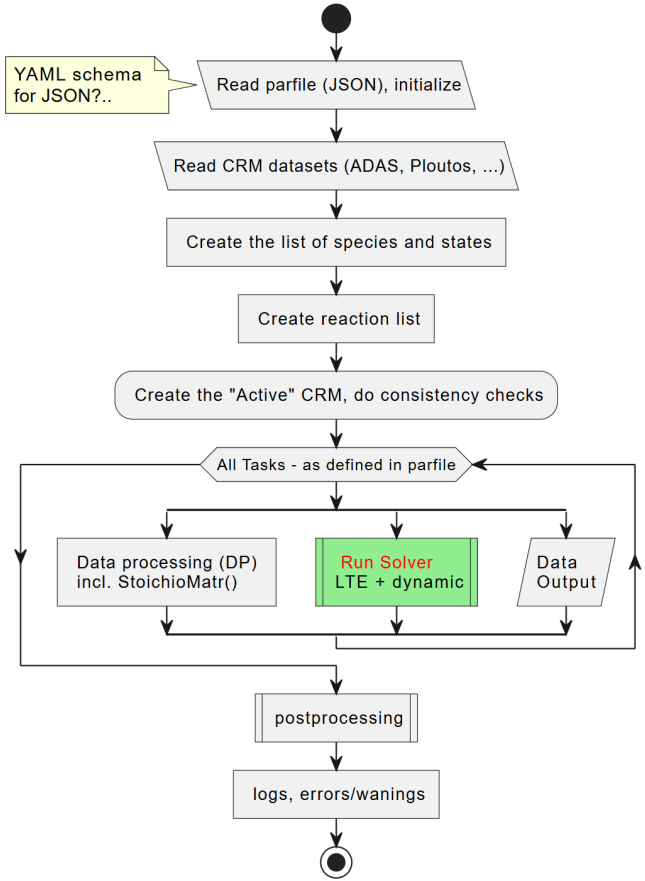
$$\frac{dN_i}{dt} \neq 0$$

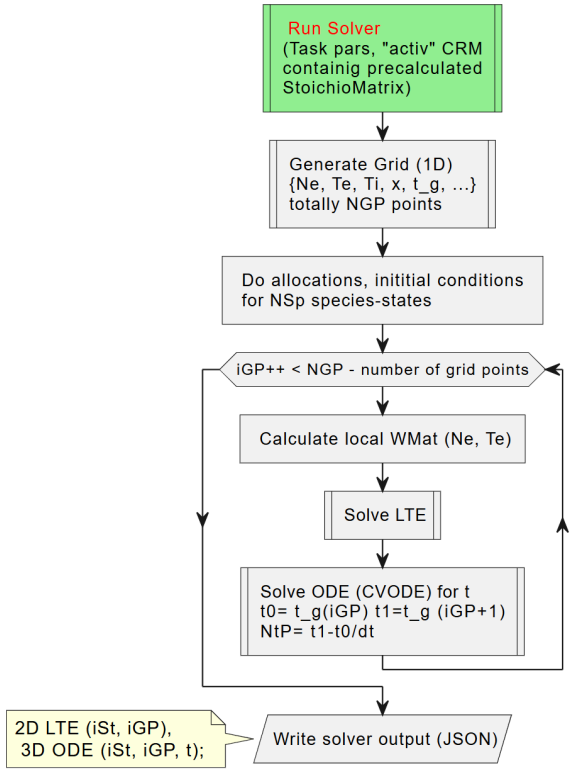
Why not also ERO?..

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

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

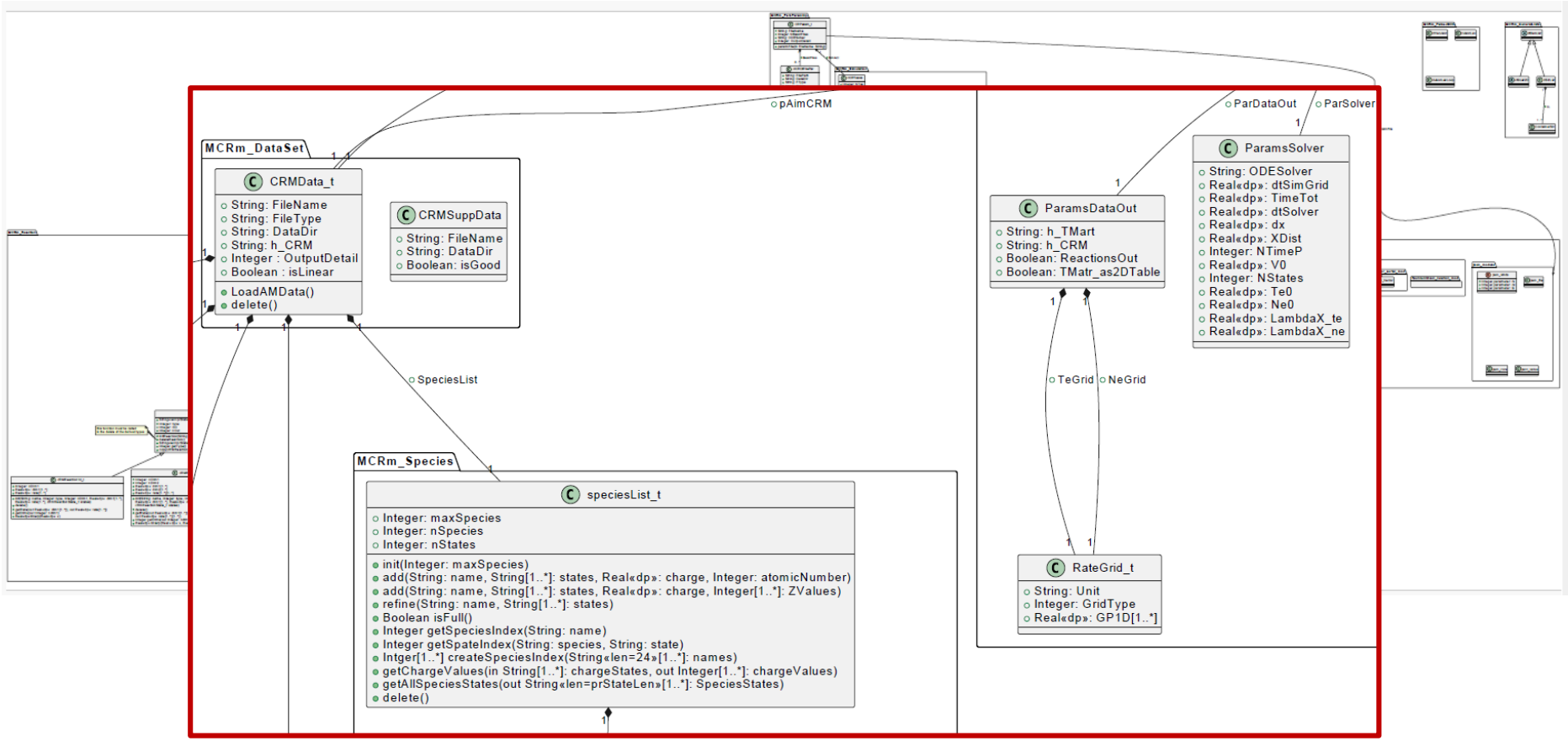
UML for ModCR –crude version of “action diagram”





➔ Other diagrams ***(e.g. “class diagram”)*** allow optimisation of workflow and data structure…

UML Class Diagramm of ModCR



Policy proposal on management of AMNS data

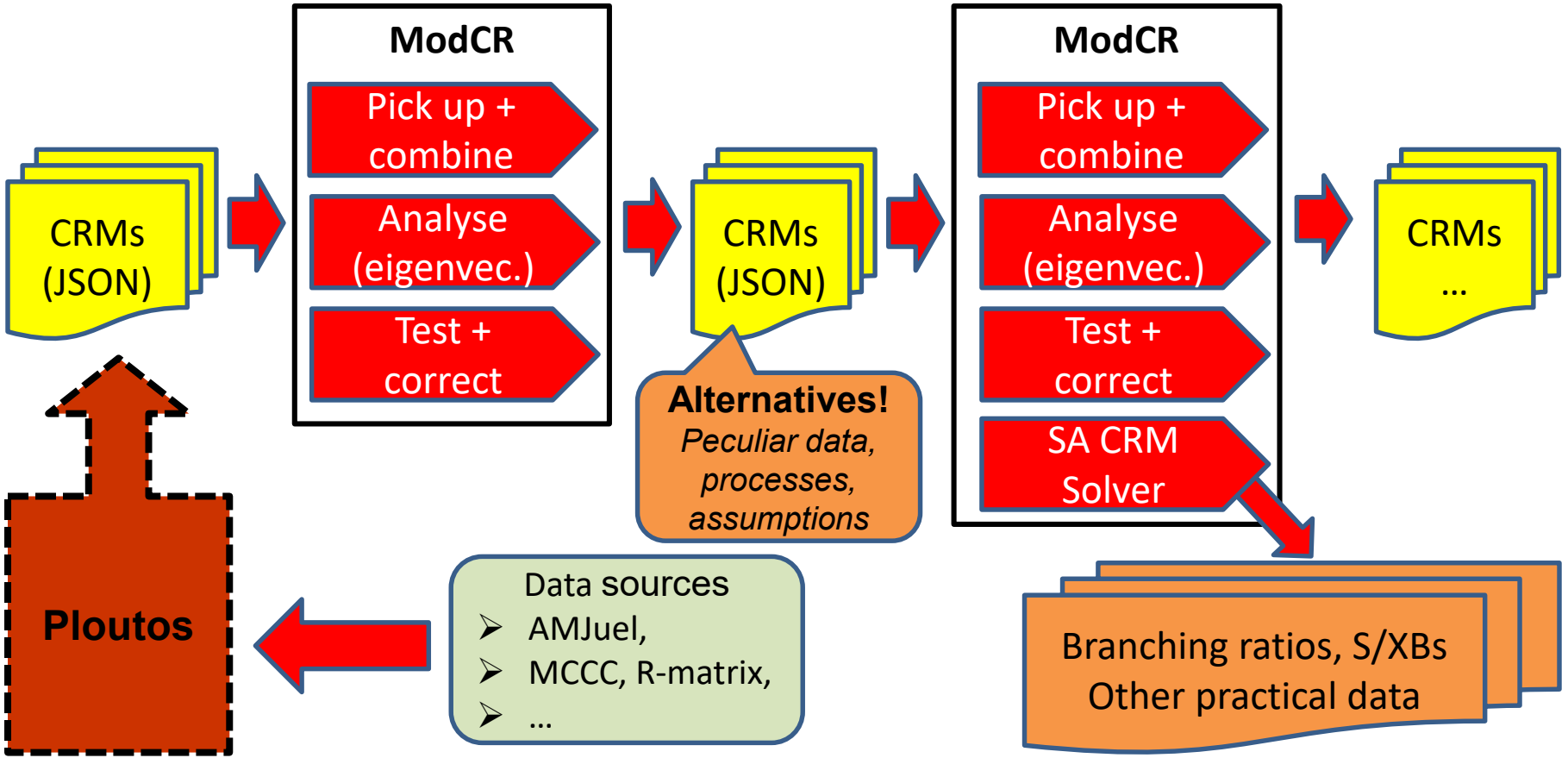
Policy proposal formulated as it spinned off from the decennial IAEA meeting on Atomic, Molecular and surface data in 2024.

+3 additional events at FZJ and IAEA
Inluding 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

Pipelenes of CRMs



MAD/MAD (Kevin Verhaegh)

Resolving errors in predictive simulations

- Power loss
- Momentum loss
- Particle loss

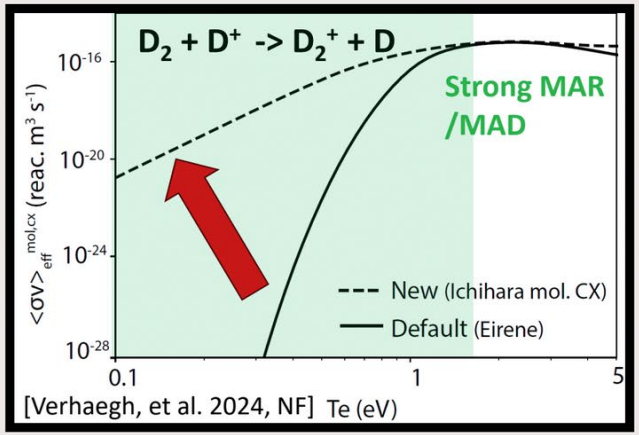
New rate calculation -> orders-of-magnitude higher molecular CX (for deuterium)

MAR: $D_2 + D^+ \rightarrow D_2^+ + D$; $D_2^+ + e^- \rightarrow D + D^*$

MAD: $D_2 + D^+ \rightarrow D_2^+ + D$; $D_2^+ + e^- \rightarrow D^* + D^+ + e^-$

'Tip of the iceberg':
many inaccuracies rates
Improved CRM calculations needed
(using data from Fursa, Laporta, …)

New rates using 'Eirene-like' CRM
Only $< \sigma v >_v^{H_2,CX}$ changed (Ichihara, 2000, J phys B)



D⁻ also missing. Using Laporta, et al. + CRUMPET – further raises MAR +20%

17b/24 Improving predictive simulations

UK Atomic Energy Authority TU/e

Isotope-dependent!

MAR preference v=4 is for D! (v=2 for H, v=10 for T)!

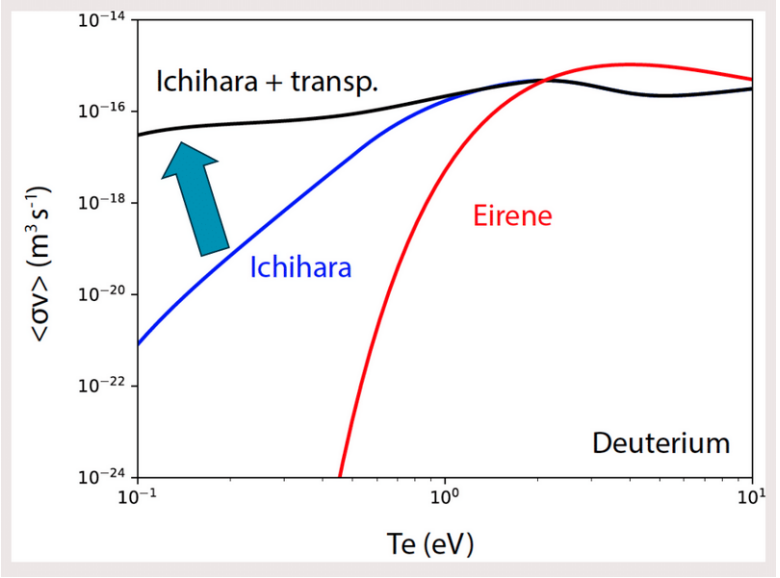
https://amdis.iaea.org/CRP/molecules

New CRMs (ModCR/Ploutos) - data

- **Do studies of CRM for molecules dependent on local wall temperature**
  - ➔ Simulation case still to be defined – with ITER?...
  - ➔ Good existing case for validation? Linear devices?

PET 2025 N. Horsten et al., PSI 2024
Is related?...

- **New D2 (H,T) CRM:**
- Do Ishihara/Kevin rates incorporation
- Include vibrostates (consider what need/can be done)
- MCCC+ Ion Schneider (also collegues)
- Alternative CRM: Vincenzo Laporta (Bari)
- Keep contact with YACORA team

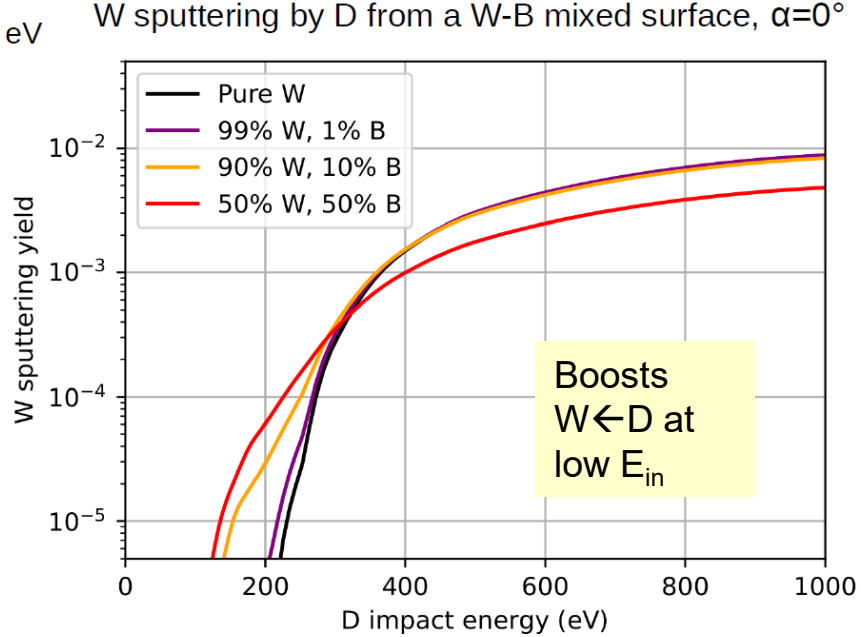


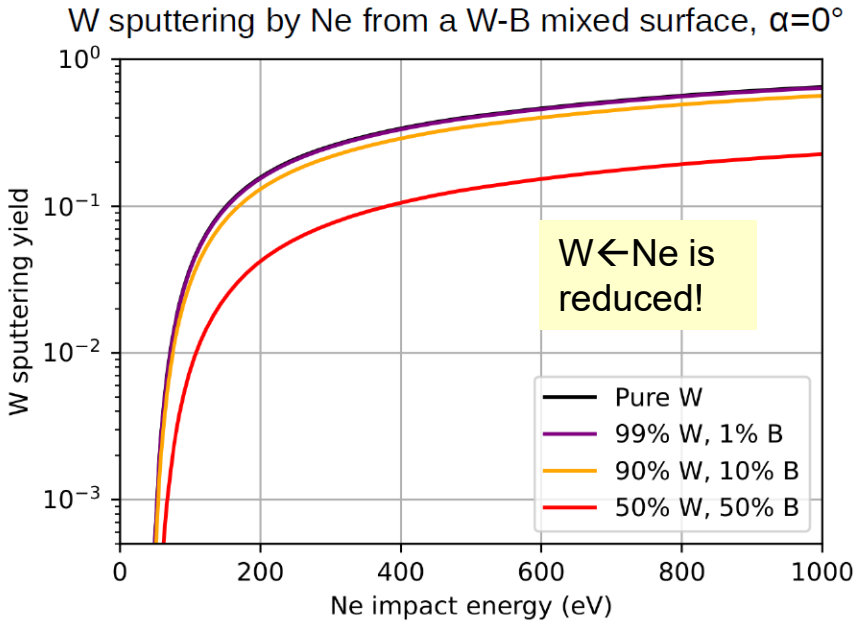
https://conferences.iaea.org/event/442/

Recent updates in ERO data for PSI

W sputtering with B admix (SDTrimSP)

H.Kumpulainen, PSI-2025





A. Mutzke et al. SDTrimSP Version 6.00, IPP-Report 2019-02

Recent Be CAPS data (MolDyn)

N.F.Mofrad, J.Romazanov, et al.
JNM 609 (2025) 155758

Summary of 2026 TSVV-K contribution form FZJ:

ModCR (standalone) development – A&M data, surface data

- *Provide molecular reactions based on PLOUTOS files, test the H2 model (F.Cianfrani, 2022/3)*
- *Consider development of W-B-D(H,T) – if extra resources are available. Data producers are working on the basic data for B molecules, but not all fundamental data is good available yet.*
- *Provide new data for surface processes.*
- *IAEA: continue work on the data policy document, participation in CRP on molecules etc.*

Code development - ModCR

- *Implement ODE solution using various routines (Sundials, CVODE, …), test convergence, achieve good match with LTE, validate with experiments at PSI-2 (and Magnum-PSI?..)*
- *Go on with merging of ModCR and ColRad functionality where possible, start implementing build-in into EIRNE use of ModCR.*
- *Provide sensitivity checks and other functionality similar to PLOUTOS (HydKin) Solver.*

ACHs and infrastructure

- *Provide SimDB server and portfolio of simulation cases (with KUL and others)*
- *Continue coordination of ACH support to TSVV-K.*
- *Work on coding practices (incl. tested with ModCR), CI cases and versioning of EIRENE and ModCR*

Thanks for the attention!

PLOUTOS 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)*

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

ModCR interaction with EIRENE and other tools