Preview of molecular population models

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ADAS-EU
University of Strathclyde

ADAS-EU course – 26 – 30 Mars 2012

Outline

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- Molecules desorbed from the wall contribute to the neutral density and influence the divertor physics.
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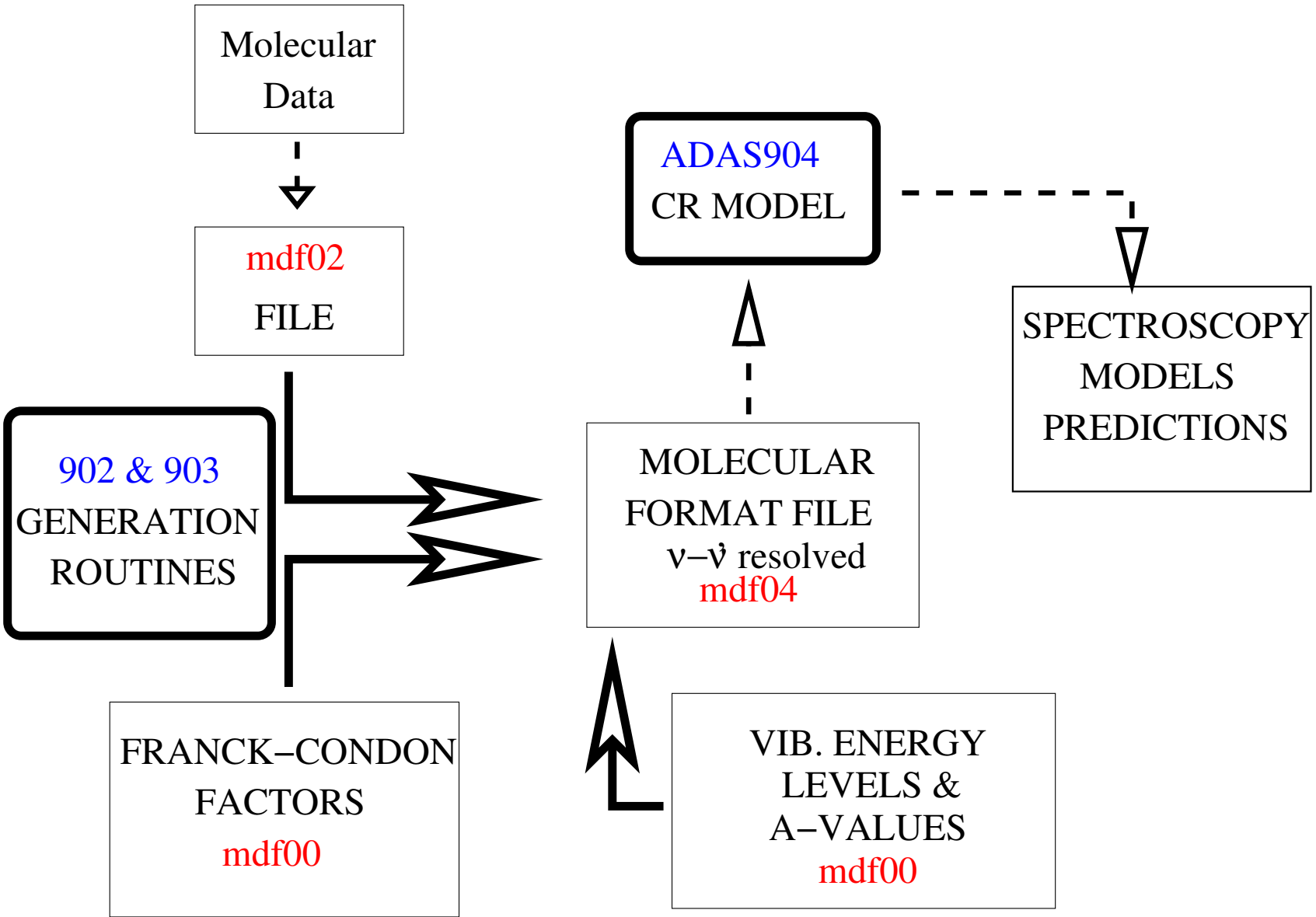
- We want to provide molecular data tools to use in plasma edge and divertor calculations and experiments.

Outline

ADAS900

ADAS-EU
ADAS for fusion in Europe



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Two resolution are accounted: vibrational and electronic.

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ADAS for fusion in Europe

mdf00 General information. Vibrational energies, Potential curves. FC factors. A-values.

mdf02 Cross sections and rates obtained from external sources or calculations.

mdf33/34 ADAS902 product. Rates (upsilons and $cm^3 s^{-1}$) obtained from maxwellian integratrion of *mdf02*.

mdf04/14 ADAS903 product. Maxwellian rates completed with EIQIP and EICIP to be used in population models.

mdf11 ADAS904 product. Molecular effective coefficients.

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MDF02: Compiling H_2 system

- **Excitation data** The avalaible data have been checked to be in good agreement with the fitting formulas.
- **Ionization data** Checked as well. Only ionization from ground state. Ionization from excited states can be achieved using IP models.
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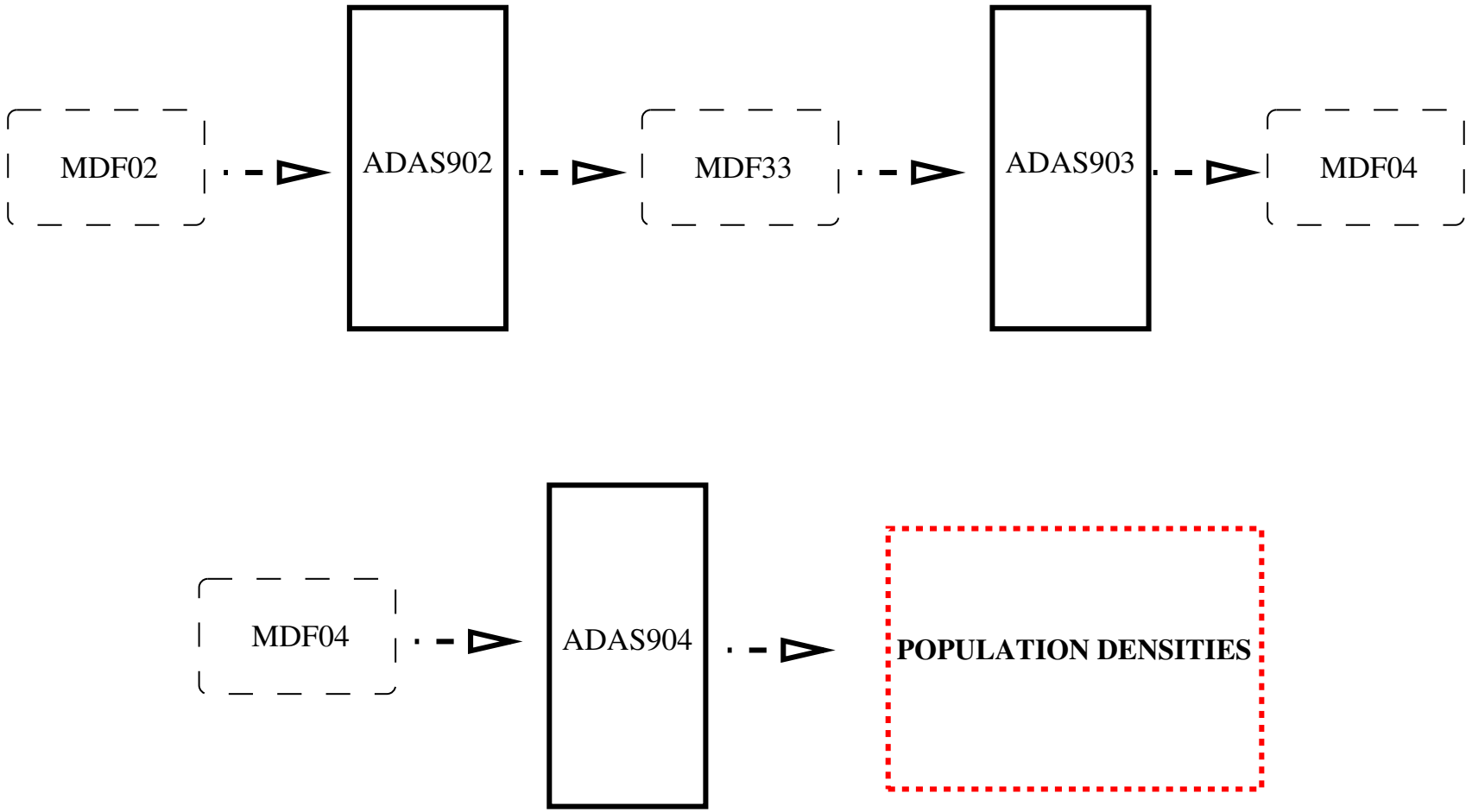

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- ADAS902 integrates, interpolates and extrapolates (if necessary) the **existing** cross sections and creates the maxwellian rate coefficients. Also create different resolution files.
- ADAS903 look for the gaps in the transitions matrix and calculate them by semi-classical Impact Parameter approach in the required resolution.
- ADAS904 calculates the molecular effective coefficients, write them in the various *mdf11* formats and invert the matrix to obtain the populations.
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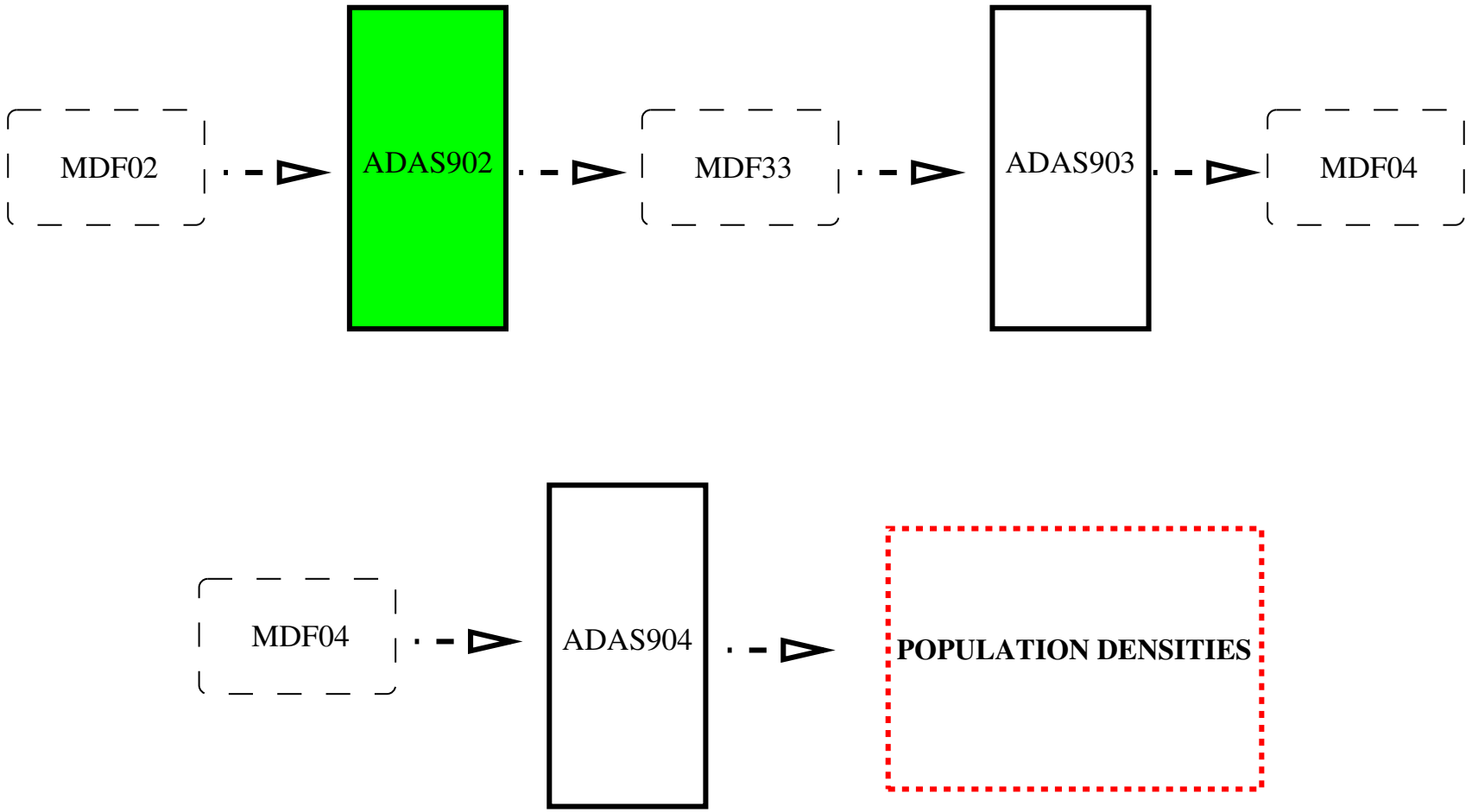
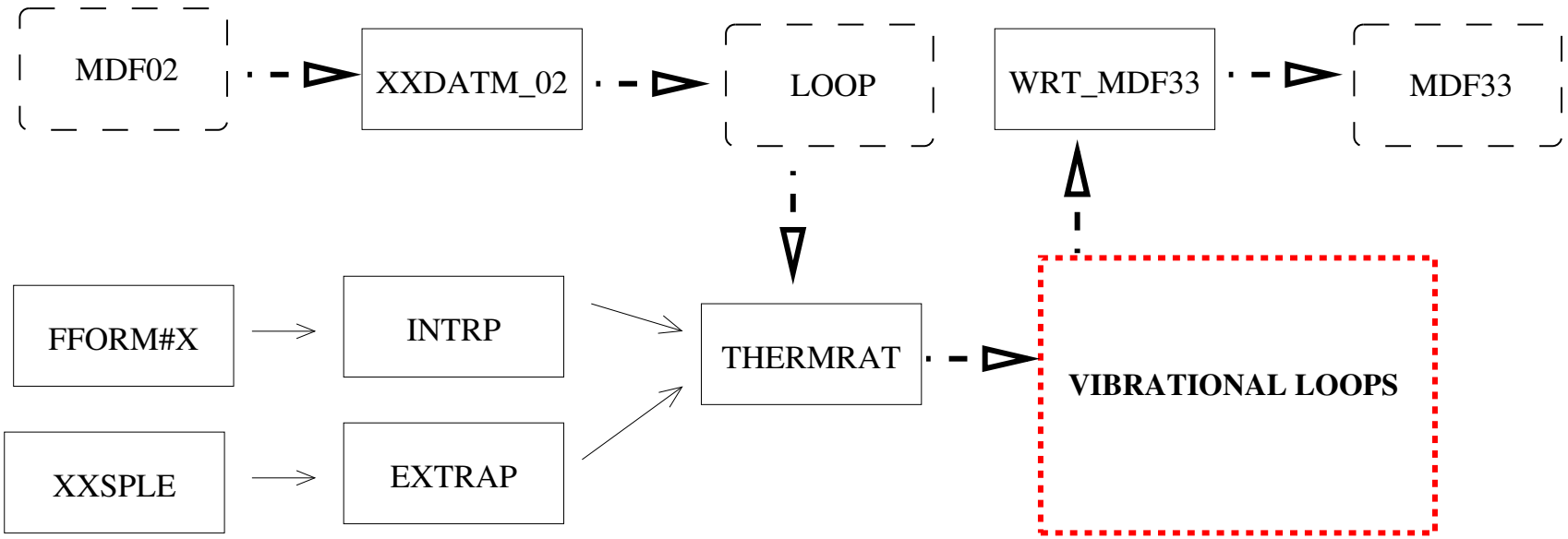


ADAS902: Interpolation and maxwellians



Interpolation & Extrapolation

If a fitting formula exist, this is chosen by default.

Extrapolation approaches:

- Bethe model for high energy ionization.
- Spline for high and low energies excitation.
- Overbarrier model for high energies CX.

Dissociation can come from excitation or ionization so the approaches above are taken.

The extrapolation models are normalized to the data to avoid peaks and steps.

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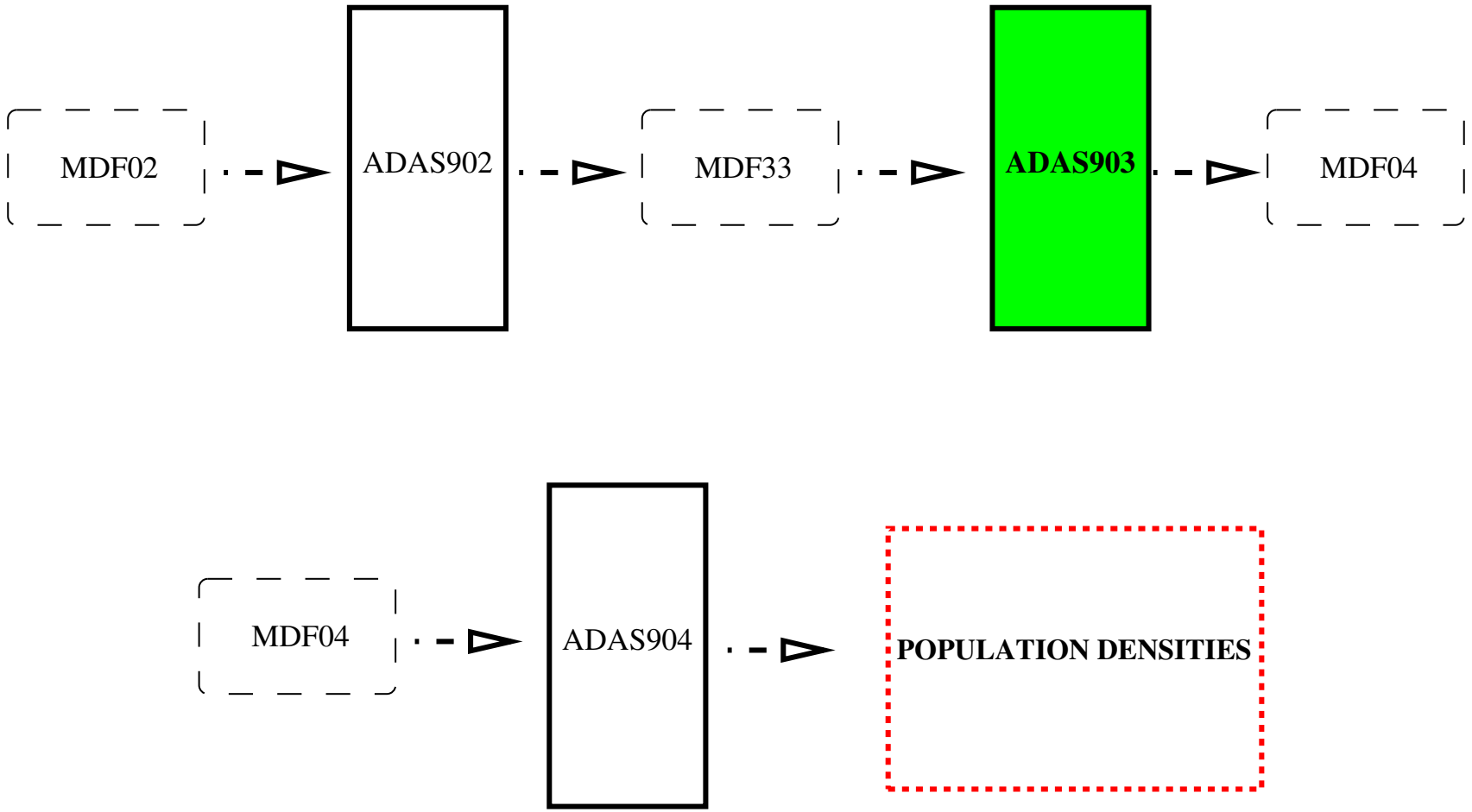

ADAS903: filling the matrix

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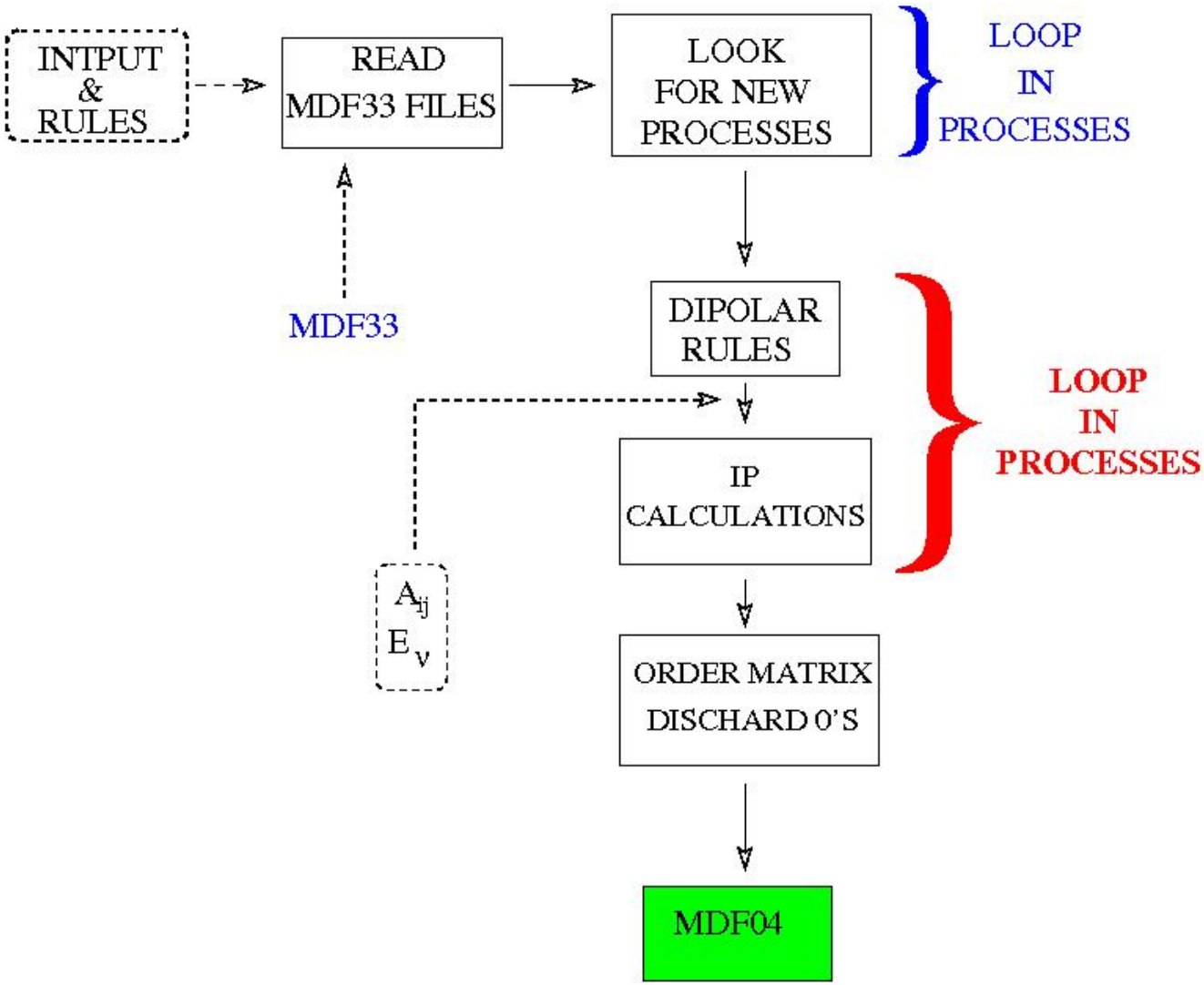

ADAS903 input file

- There is the possibility to put a lower limit in the rates to consider the transitions,
- Driver *input903.dat* must be created and dissociative states should be defined with rule “ED” (Excitation to dissociative).
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- ECIP (bound-free collisional IP) is used for ionization (dissociative and non-dissociative) and dissociative excitation.
- Calculation is performed over vibronic levels and summed.
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mdf04 are ascii and human readable. Not so funny though!

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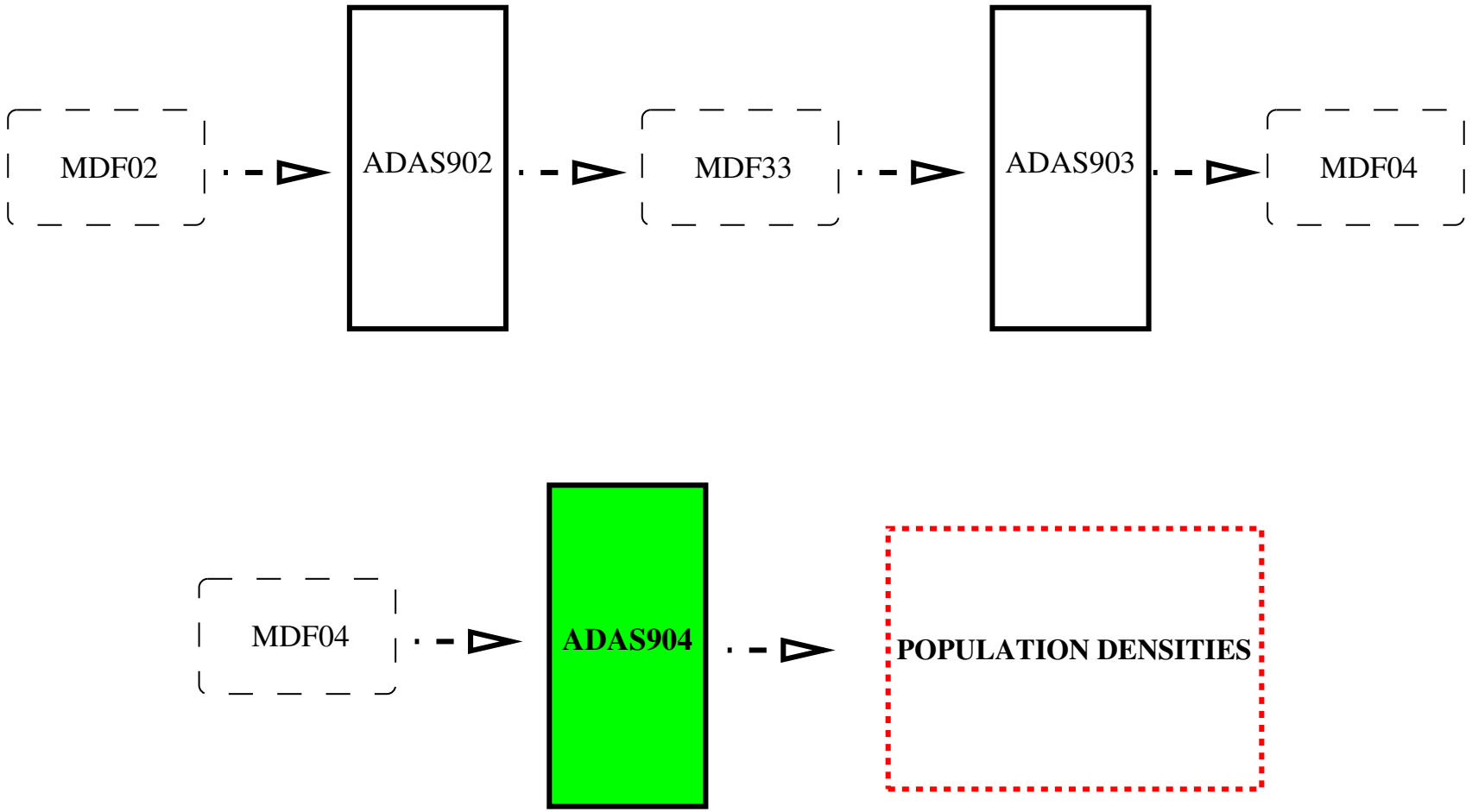

ADAS904: solving CR

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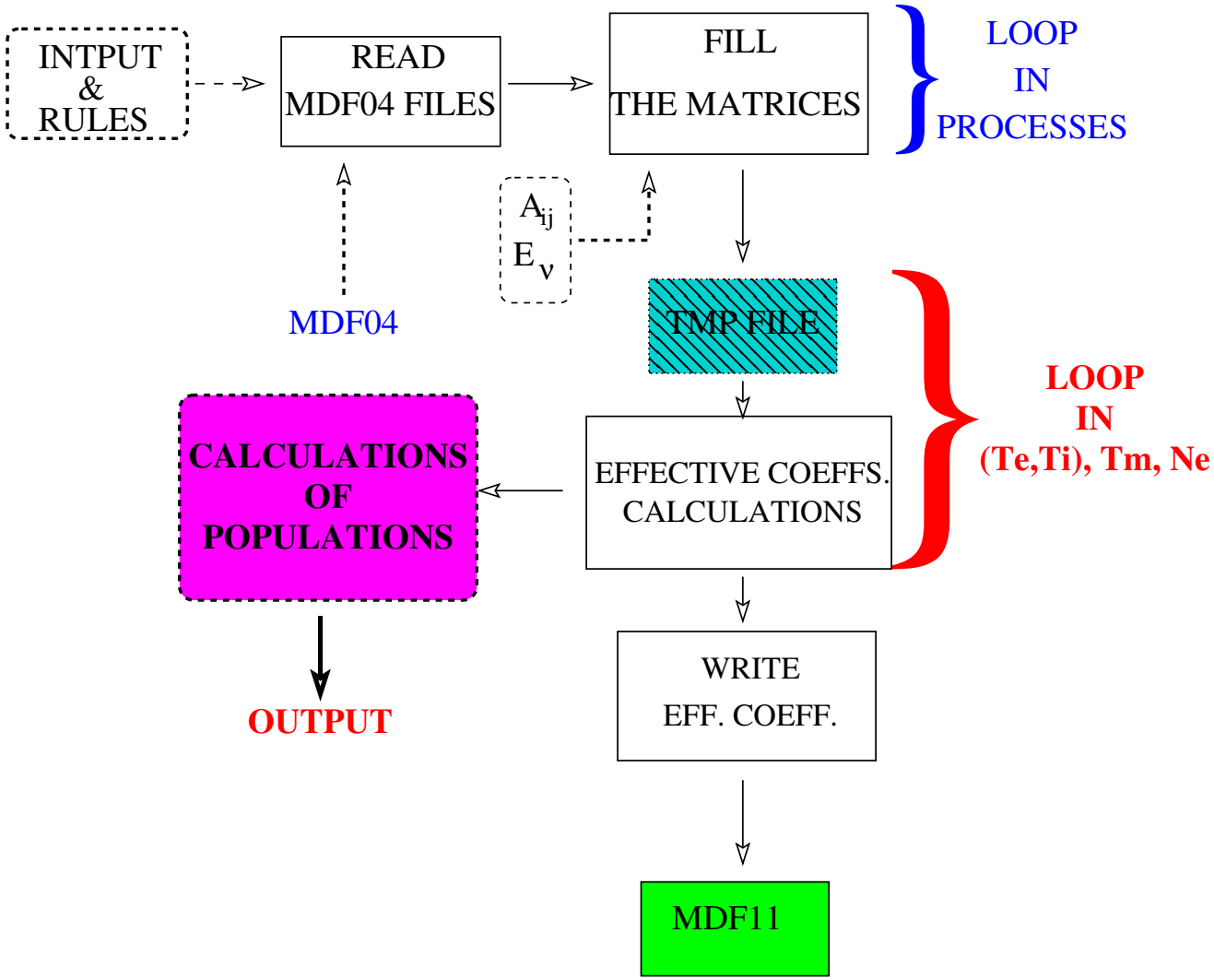

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- Dissociative processes are all that go to dissociation (diss. excitation, ionisation, CX, recombination . . .).
- Metastables are allways vibrationally resolved $\longrightarrow$ 150×150 maximum dimension of metastable matrix.
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ADAS904: The population model

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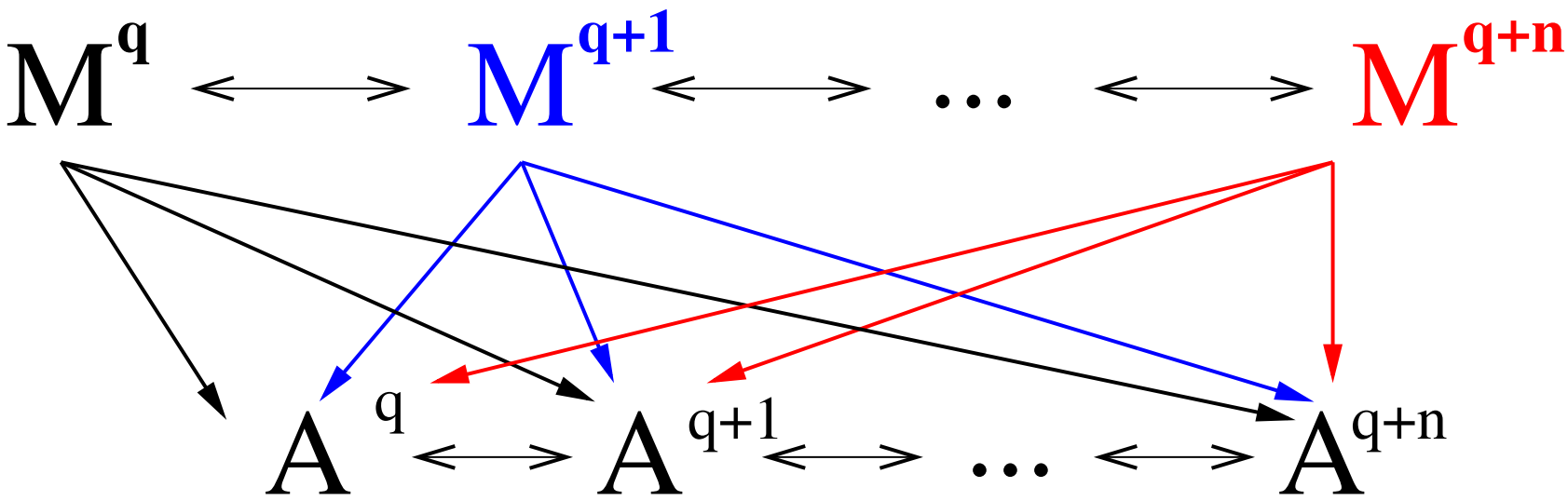
CR Equation

$$\begin{pmatrix} \frac{dN_X}{dt} \end{pmatrix} = \underbrace{\left(\begin{array}{c|c|c} H_2 & \sim 0 & 0 \\ \hline \neq 0 & H_2^+ & 0 \\ \hline \neq 0 & \neq 0 & H(n), H^+ \end{array}\right)}_{\begin{pmatrix} \cdots \\ \text{states} \\ \cdots \end{pmatrix}} \times \begin{pmatrix} N_X \end{pmatrix} - \begin{pmatrix} \Gamma_{in} \end{pmatrix}$$

Γ_{in} can correspond to the collisional terms from constant populations.

The population model



Non linear terms

Charge exchange is creating non linear terms to be sum to the background populations of neutrals and protons.

$$H_2 + H^+ \Longleftrightarrow H_2^+ + H$$

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$$0 \equiv \frac{dN_H^{(1)}}{dt} = \mathcal{C}_{HH} N_H^{(1)} - N_H^{(0)} \mathcal{C}_{HH} - Q^{\mathrm{ICX}} N_{H_2^+} N_H^{(0)} + Q^{\mathrm{CX}} N_{H^+}^{(0)} N_{H_2}$$

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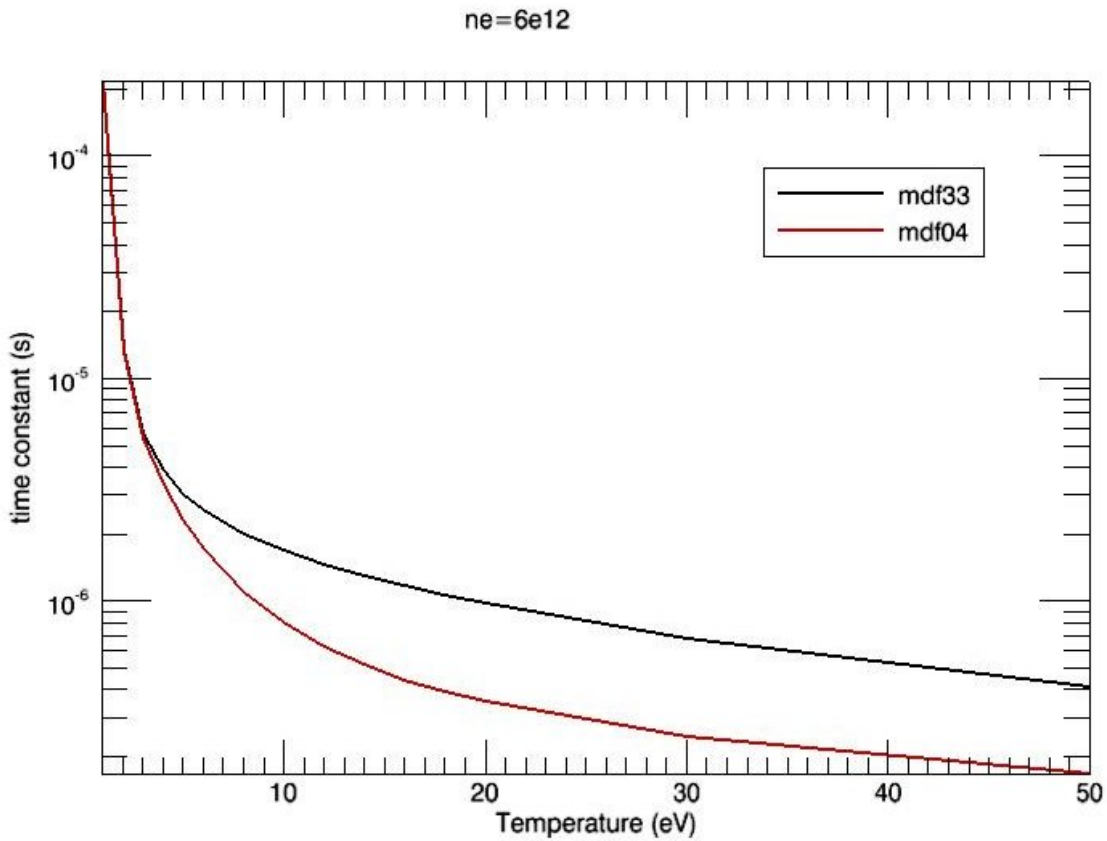

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2. Optimization and extension of data base for Hydrogen
3. Implementation in ADAS and IDL
4. Interaction to cover the experimental needs.
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