Yacora status at Aalto

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Eirene-Yacora discussion sesh

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Remote connection

“H2VIBR-Yacora” inputs created for Eirene-Yacora comparison based on the instructions in the manual received

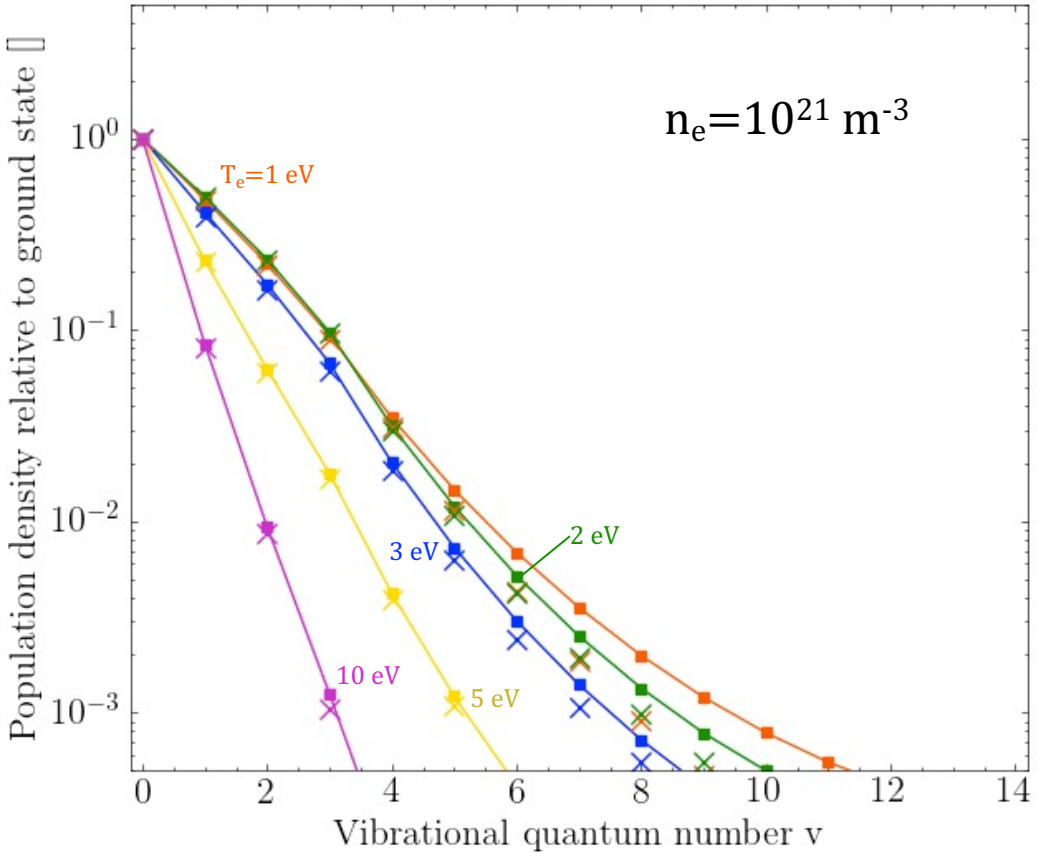
- Input creation routines were written for CRUMPET
  → Automated duplication of CRUMPET CR setups that can be supplied to Yacora

- The Yacora setup includes H2VIBR and AMJUEL rates
  – Special structure to account for the n_e-dependence of the AMJUEL rates

- H2VIBR-Yacora simulations were compared to Eirene simulations considering the same reactions

Vibrational distributions $\mathrm{P}(v)$ calculated using transport-free Eirene $\mathrm{H_2}(v)$ simulations match those predicted by Yacora

- The H2VIBR reactions were supplied to Yacora
- $\mathrm{T_e} < 1\ \mathrm{eV}$: recombination-dominated plasmas
- $\mathrm{T_e} \gtrsim 5\ \mathrm{eV}$: $\mathrm{n_{H2}} \rightarrow 0\ \mathrm{m^{-3}}$ and ionization-dominated plasmas
- No electronic transitions considered in the Eirene $\mathrm{H_2}(v)$ setup → $\mathrm{P(v)}$ density-independent



A set of “standard Yacora” simulations were run for the project by Dirk

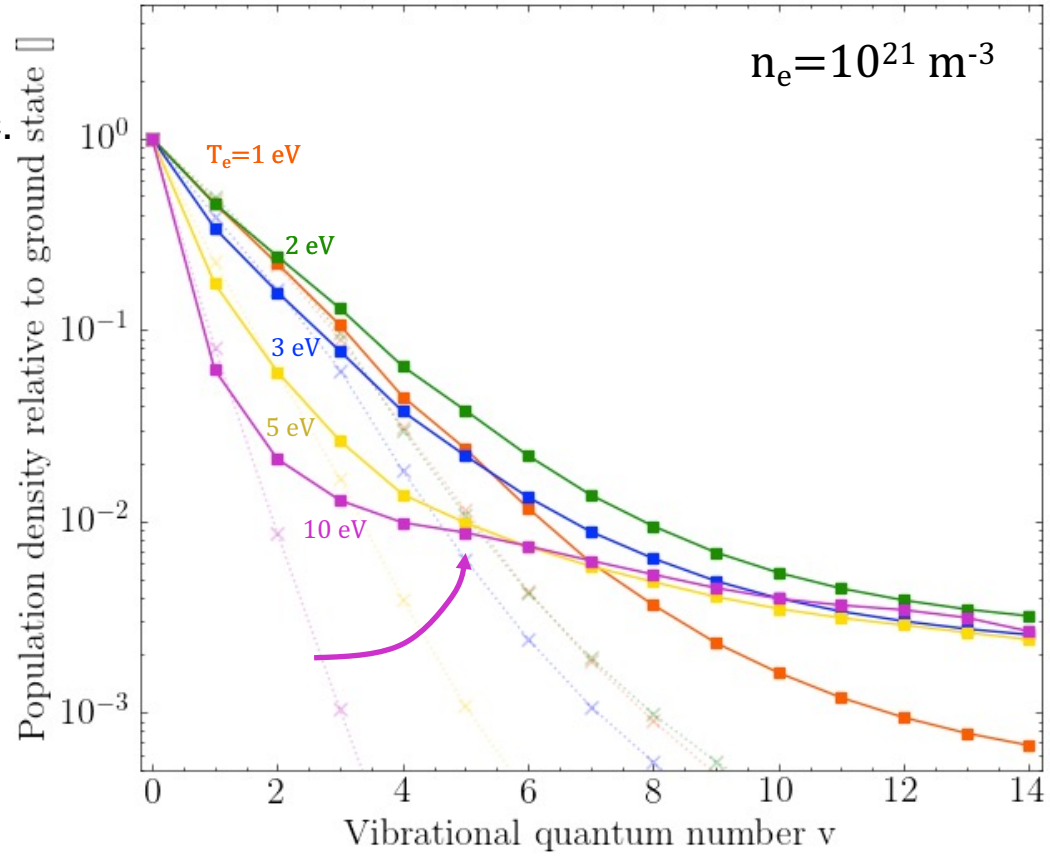
- Includes the standard Yacora reaction rates in the (presumably) IPP A&M database
- Considers all available reactions (redistribution via electronically excited states, off-diagonal vibrational transitions, quenching, etc)
- Used to evaluate the effect of additional CR processes on the vibrational distribution predicted by the H2VIBR rates

Re-distribution via electronically excited states shifts $P(v)$ to higher v, increasing the effective dissociation rate

- Full set of Yacora CR data used
  - Electronic transitions, full vibrational transition matrix, etc.
- Strong dependency of reaction rates on *v*

→ Even small shifts of P(*v*) may significantly impact the effective rates

→ <u>The Eirene $H_2(v)$ setup cannot capture all CR effects</u>

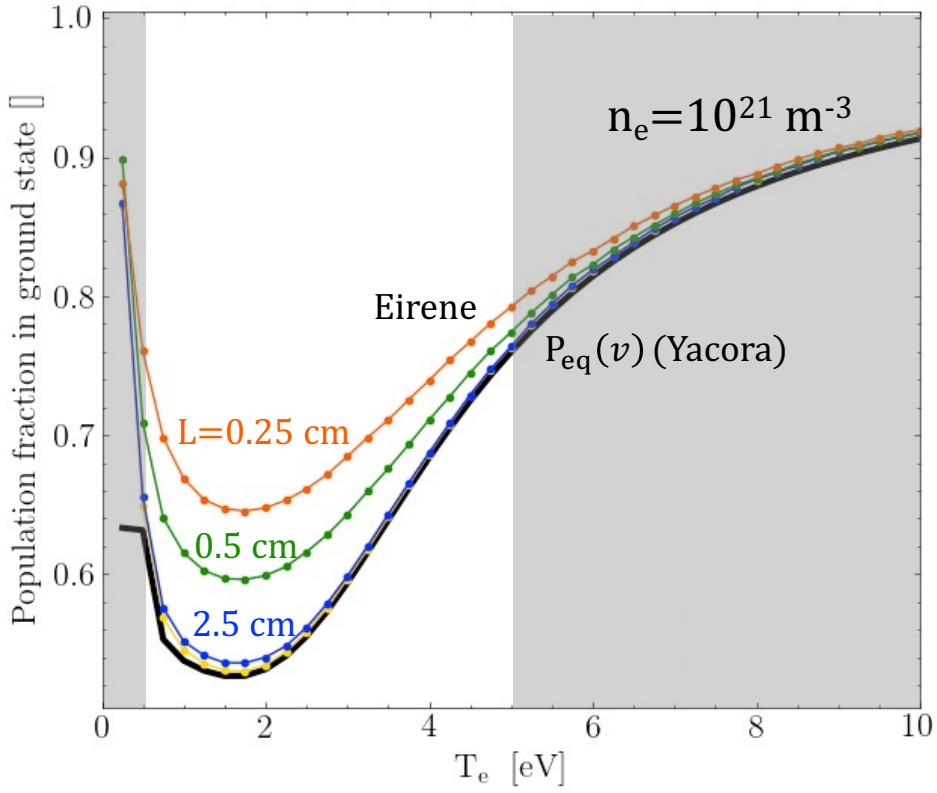


Yacora and Eirene were used to evaluate $\lambda_{mfp}^{P_{eq}(v)}$

n_e	10^{21} m^{-3}	10^{20} m^{-3}	10^{19} m^{-3}
$\lambda_{mfp}^{P_{eq}(v)}$	~2.5 cm	~10 cm	>10 cm

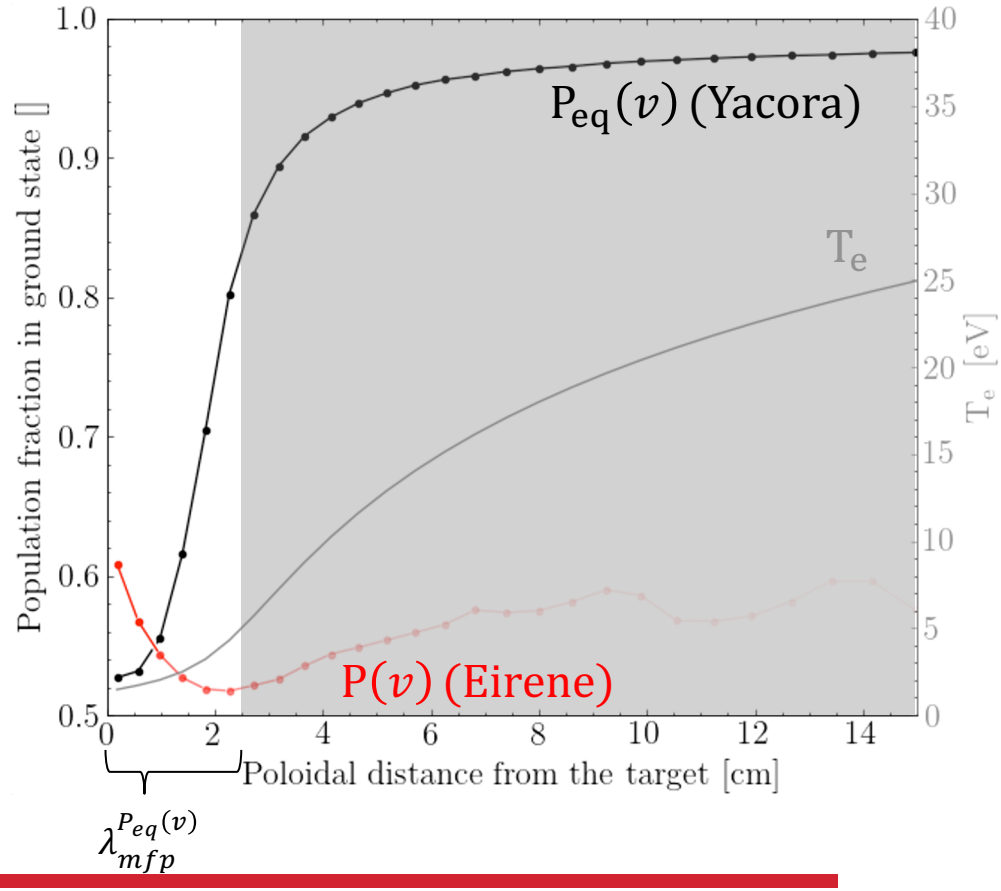
- If the domain size is shorter than $\lambda_{mfp}^{P_{eq}(v)}$ the molecule escapes before reaching $P_{eq}(v)$

→ Shifts P(v) to lower v

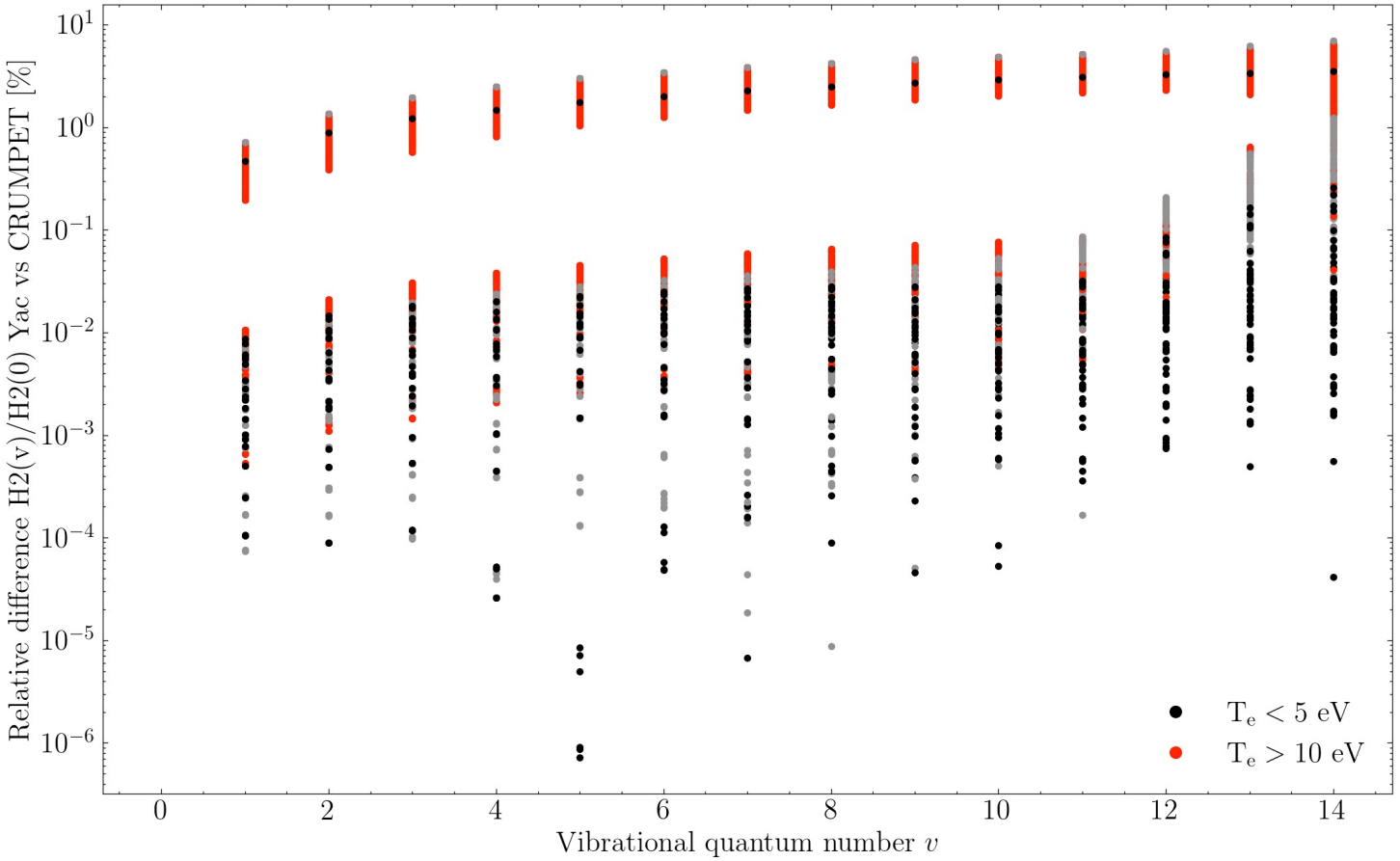


Yacora was used to assess the poloidal vibrational equilibrium distribution for a 1D flux tube

- Eirene simulations on a 1D flux tube do not achieve $\mathbf{P_{eq}}(v)$ due to the finite $\lambda_{mfp}^{P_{eq}(v)}$

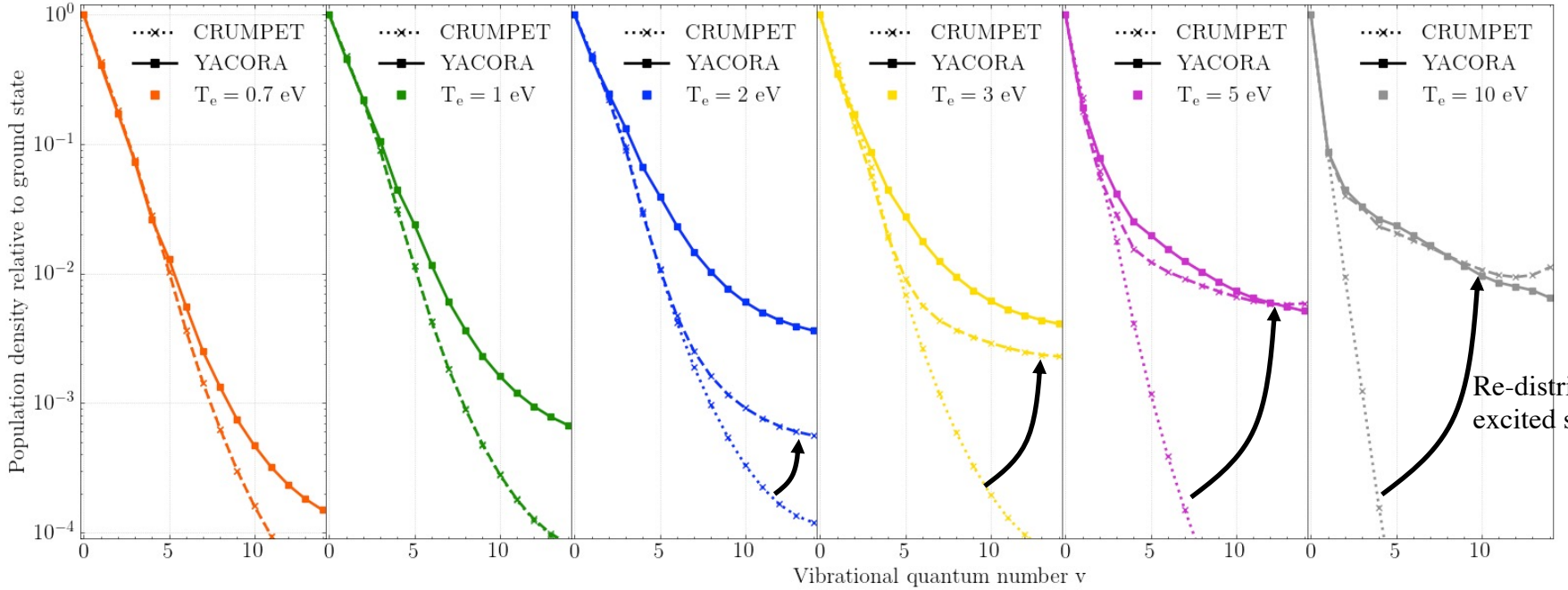


CRUMPET was benchmarked against Yacora using the H2VIBR-Yacora setup



- The codes agree within a few percent for v<11 and T_e<10 eV

CRUMPET simulations considering vibrationally resolved electronic states were compared to Yacora simulations



- CRUMPET-YACORA agreement is improved for T_e>1 eV when electronic excitation to n=3 are considered
- T_e<3 eV predictions unaffected ($\Delta E >> T_e$) → other processes not considered
  - Quenching, neutral-/heavy particle interactions
  - Absolute impact small?

Yacora is a flexible solver that is easily understood: scientifically relevant results in a few months

- Successfully created and evaluated a customized CR setup
  - Using the executable only→ Unix executable would be useful for future use
- The A&M database used by Yacora is a very valuable resource
- Scrping the surface: “advanced” options not yet explored
  - Neutral-neutral reactions
  - Diffusive transport approximation
  - H_2 velocity-dependent rates (?)
  - Photon transport (?)
  - Momentum and energy terms (?)
- Much more flexibility and insight compared to Yacora on the Web