Constraining Uncertainties in Cosmic Rays Chemical Modeling

(using interpretable machine learning)

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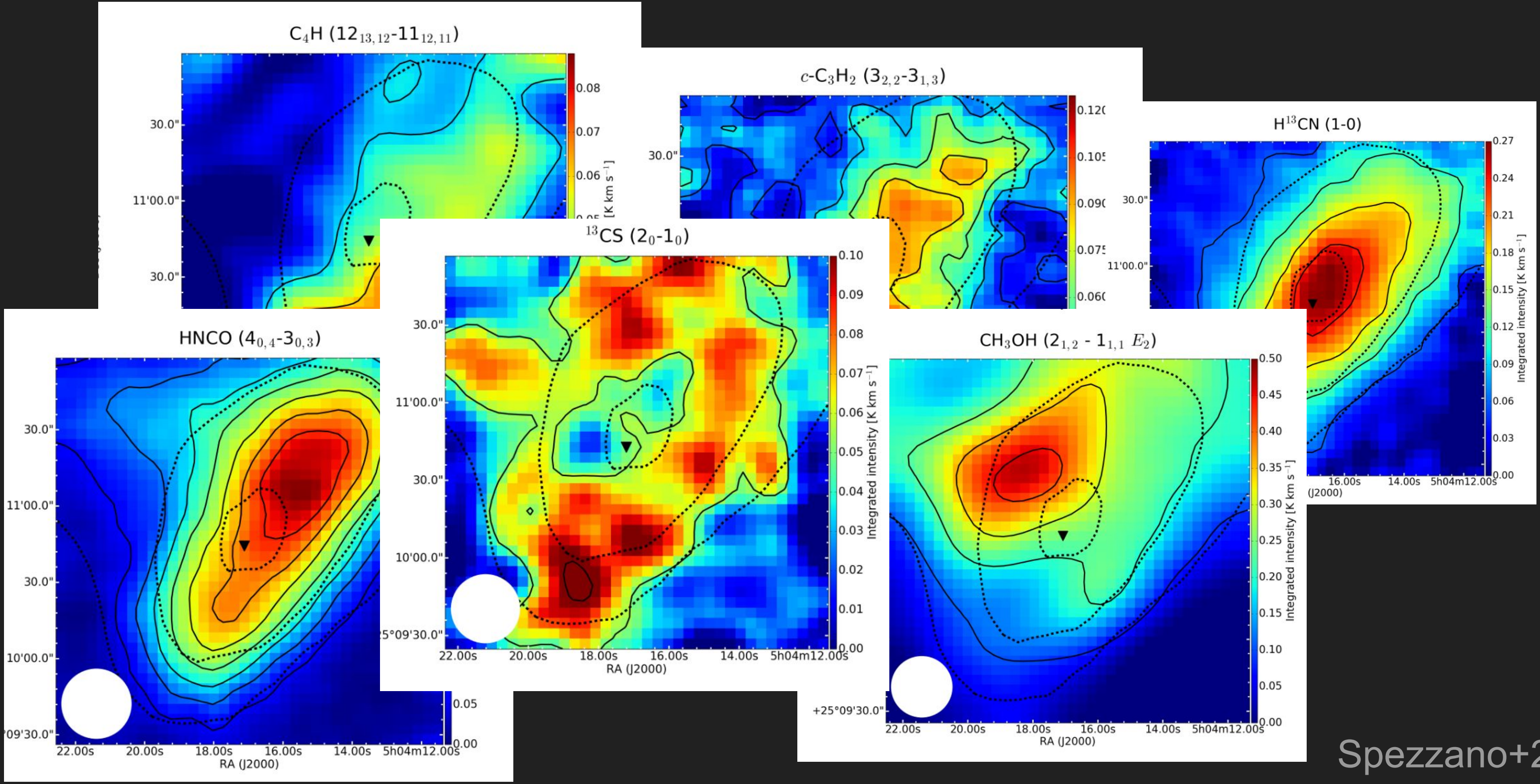
Motivations

Cosmic rays are important

See e.g. Everyone in This Conference

Prestellar Cores



Spezzano+2017

The Plan: From models to “observations” (and back)

Randomize

Parameters

Zoo Models

“Indirect” observation

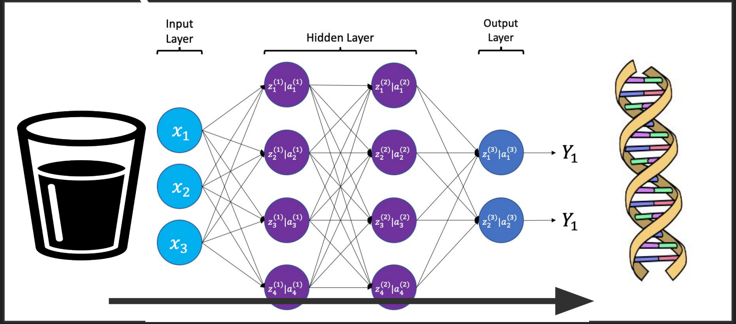
?

- Can we reconstruct information?
- Do we know where information resides?

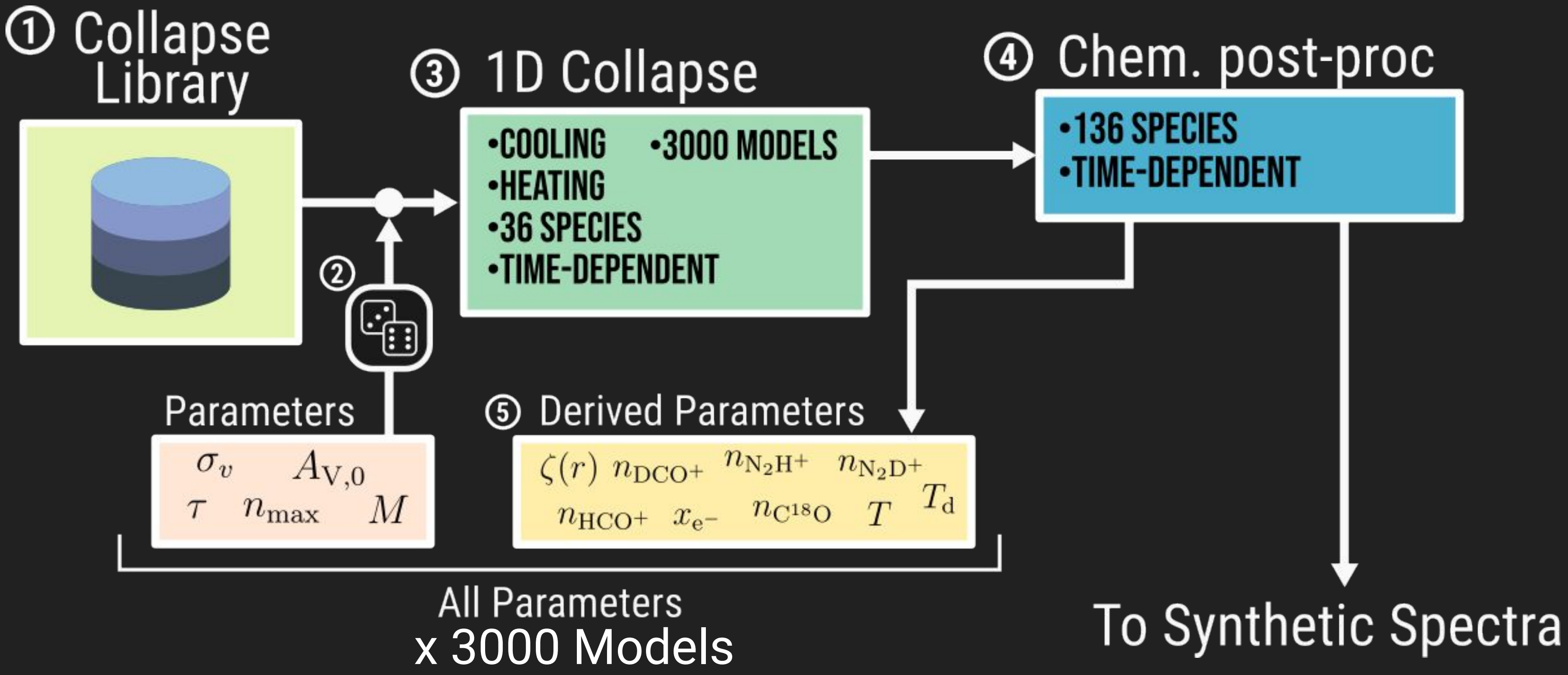
See e.g. Gratier+21, Heyl+23, Shimajiri+23, Behrens+24, Einig+24, Diop+24

Outline

- Model generation
- Synthetic observations
- Machine learning emulation
- Sensitivity analysis



Model Generation

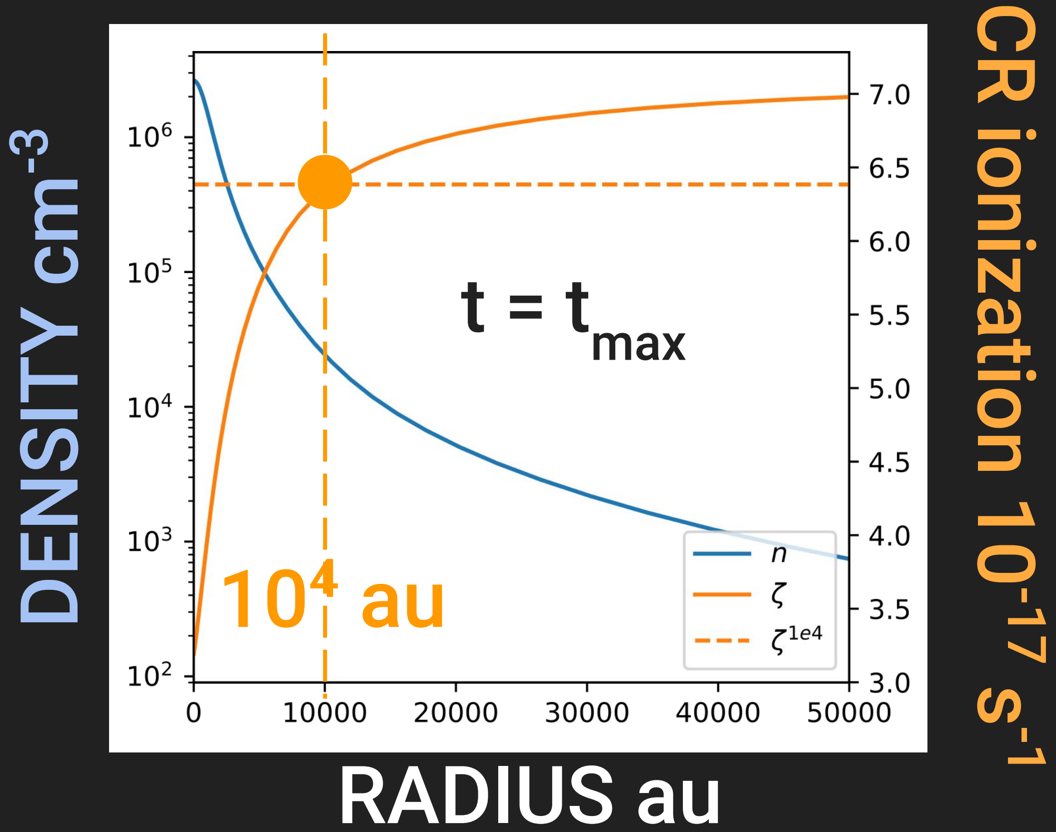


Hydro: Vaytet+18 | Networks: Glover+*, Bovino+20 | Solver: Grassi+14

A Model Example (1 out of 3000)

σ_v $A_{\mathrm{V},0}$

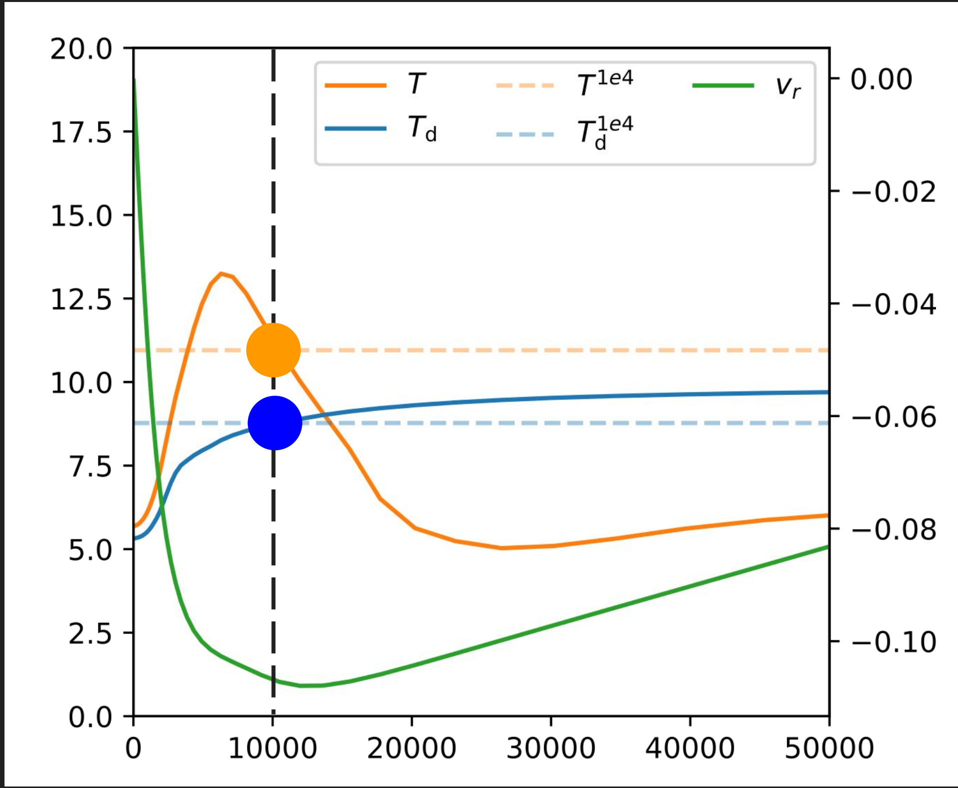
τ $n_{\max}$ M



See e.g. Keto+08, Sipila+22, Jensen+23

Temperature and Velocity Profiles

T_{gas} (K) and T_{dust} (K)



VELOCITY km s^{-1}

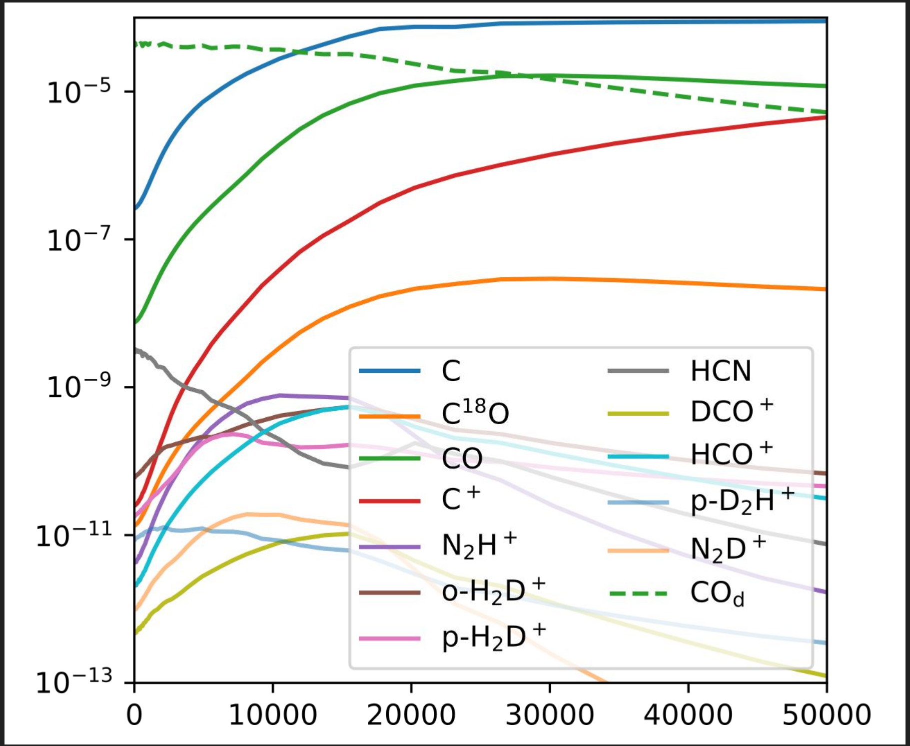
RADIUS au

time-dependent
36 species
275 reactions
cooling+heating

See e.g. Keto+08, Sipila+22, Jensen+23

Post-processing Additional Chemistry

FRACTIONAL ABUNDANCE



RADIUS au

time-dependent
136 species
4470 reactions

See e.g. Keto+08, Sipila+22, Jensen+23

Parameters

σ_v $A_{\mathrm{V},0}$ τ $n_{\max}$ M

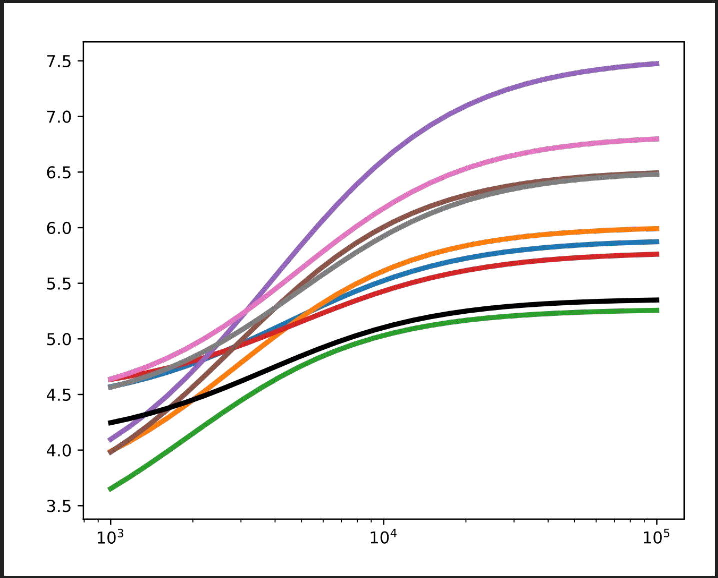
⑤ Derived Parameters

$\zeta(r)$ $n_{\mathrm{DCO^+}}$ $n_{\mathrm{N_2H^+}}$ $n_{\mathrm{N_2D^+}}$ T_{d} $n_{\mathrm{HCO^+}}$ $x_{\mathrm{e^-}}$ $n_{\mathrm{C^{18}O}}$ T

All Parameters

x 3000 Models

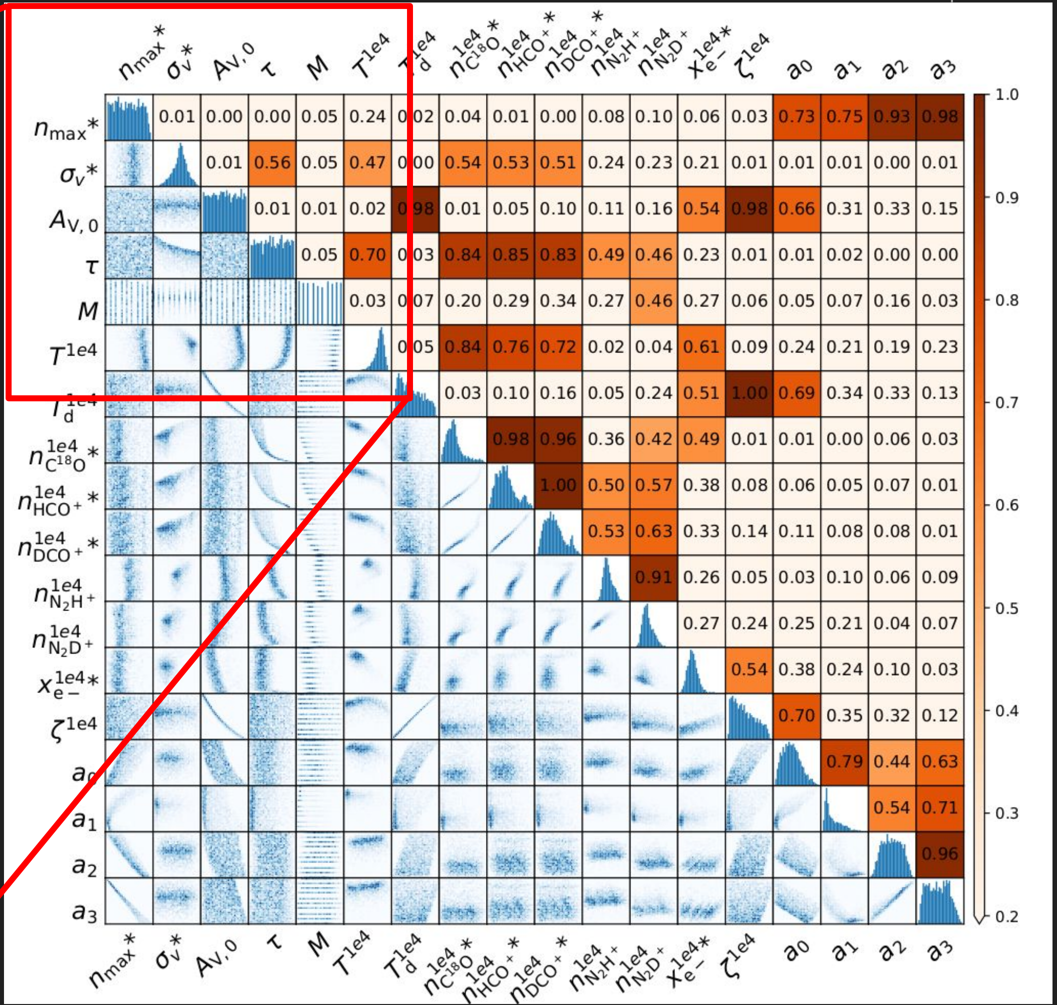
CR ionization 10^{-17} s^{-1}

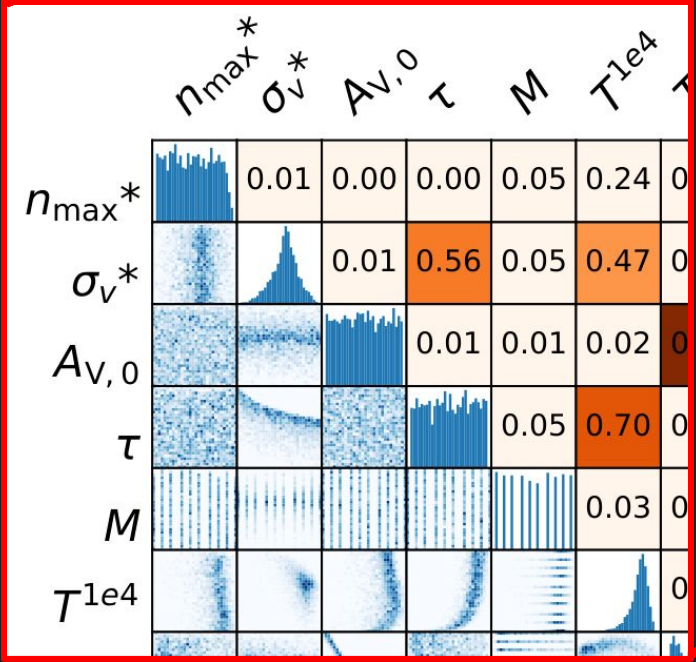


RADIUS au

$$\zeta(r) = \frac{a_0}{1 + \exp[a_1(r - a_2)]} + a_3$$

Parameters Correlation





Synthetic Observations

From Models

6

LOC
by Mika Juvela

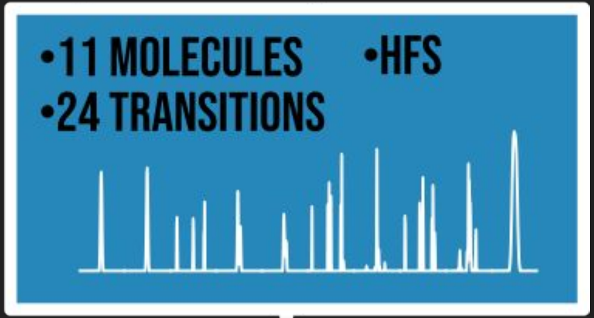
NLTE Radiative Transfer

T(r), v(r), x(r)

7

Beam Convolution

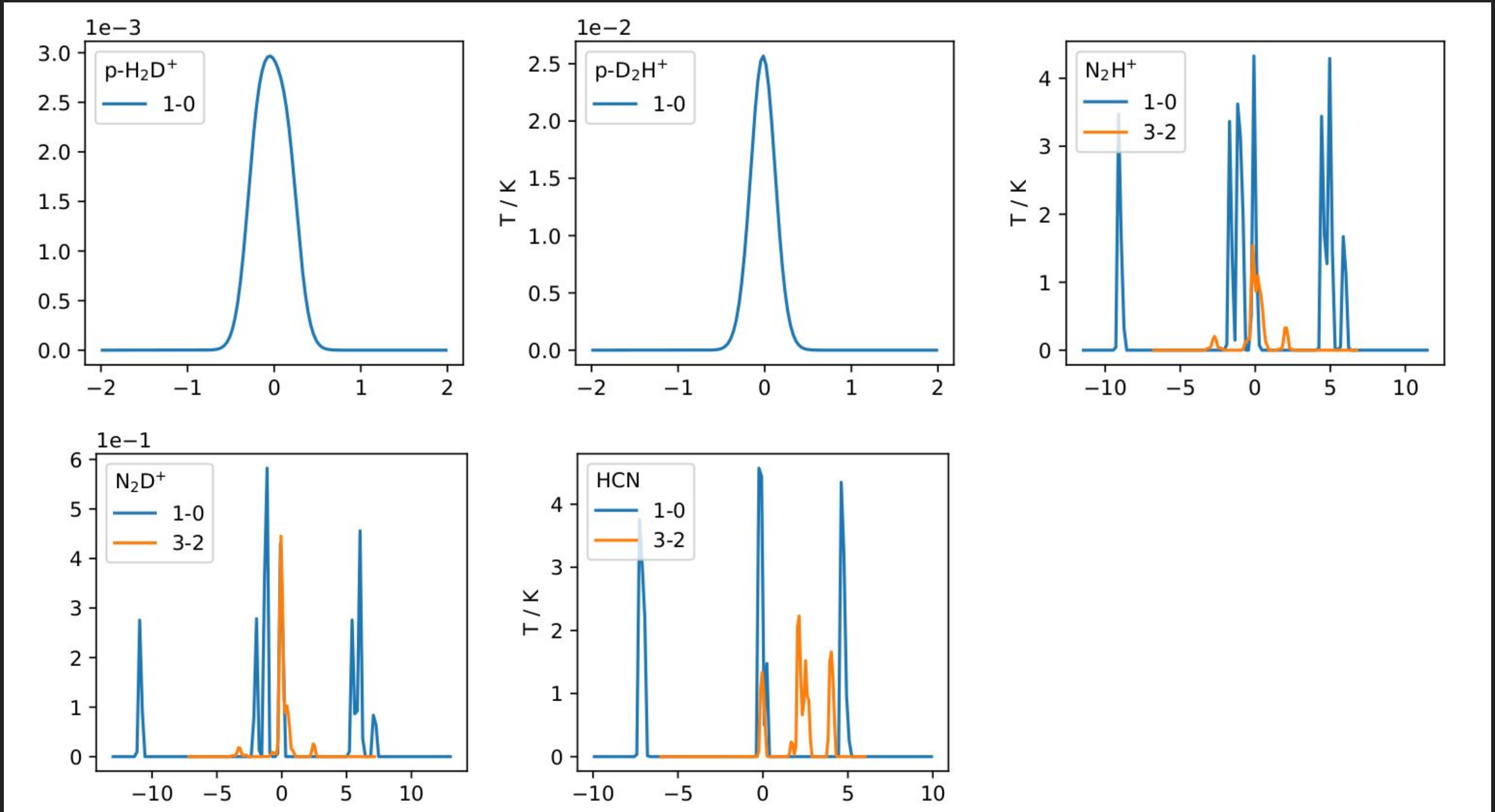
8 Synth. Spectra



To Emulation

See Juvela 1997, 2020

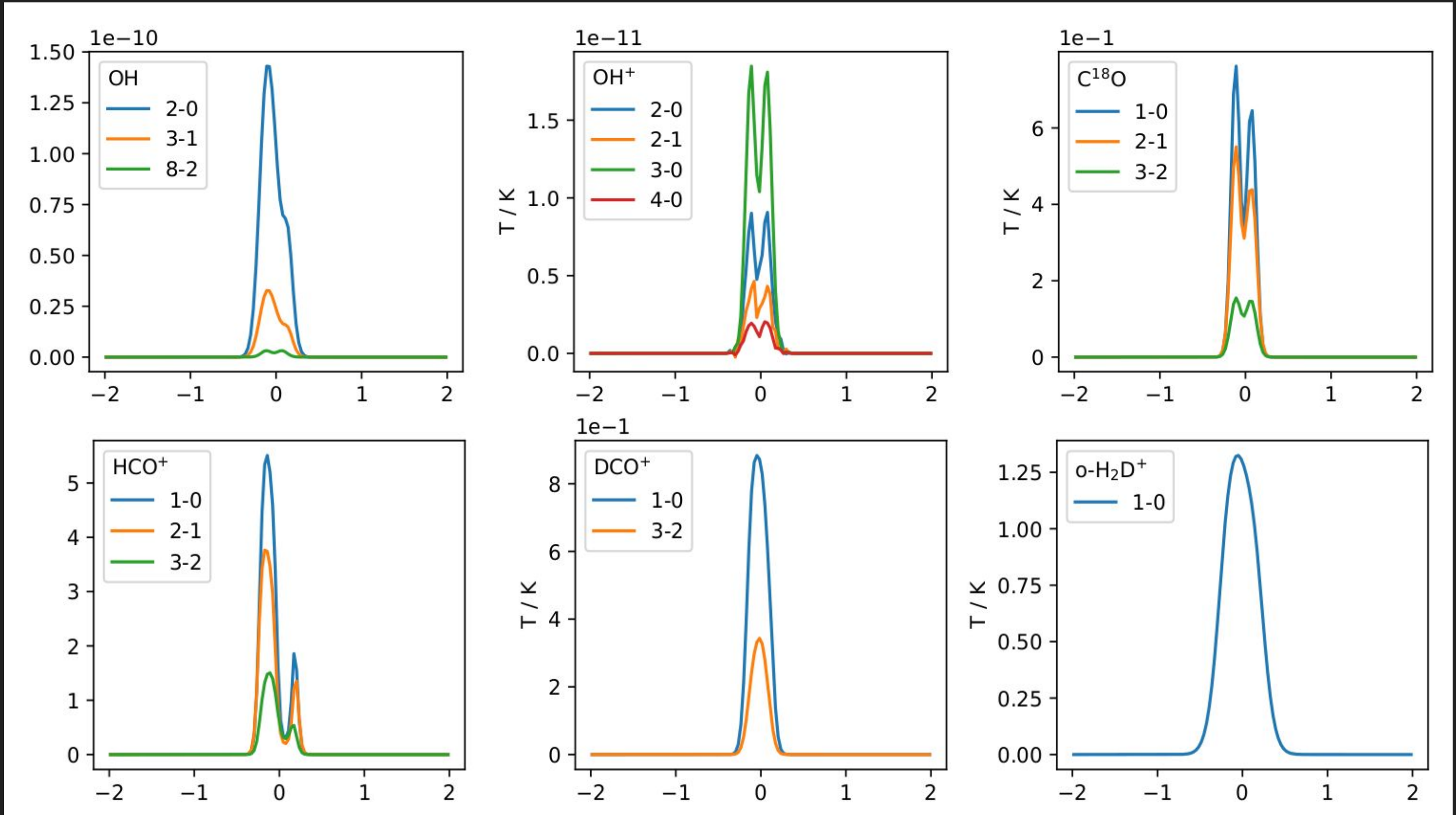
Temperature K



Velocity km s^{-1}

x 3000 Models

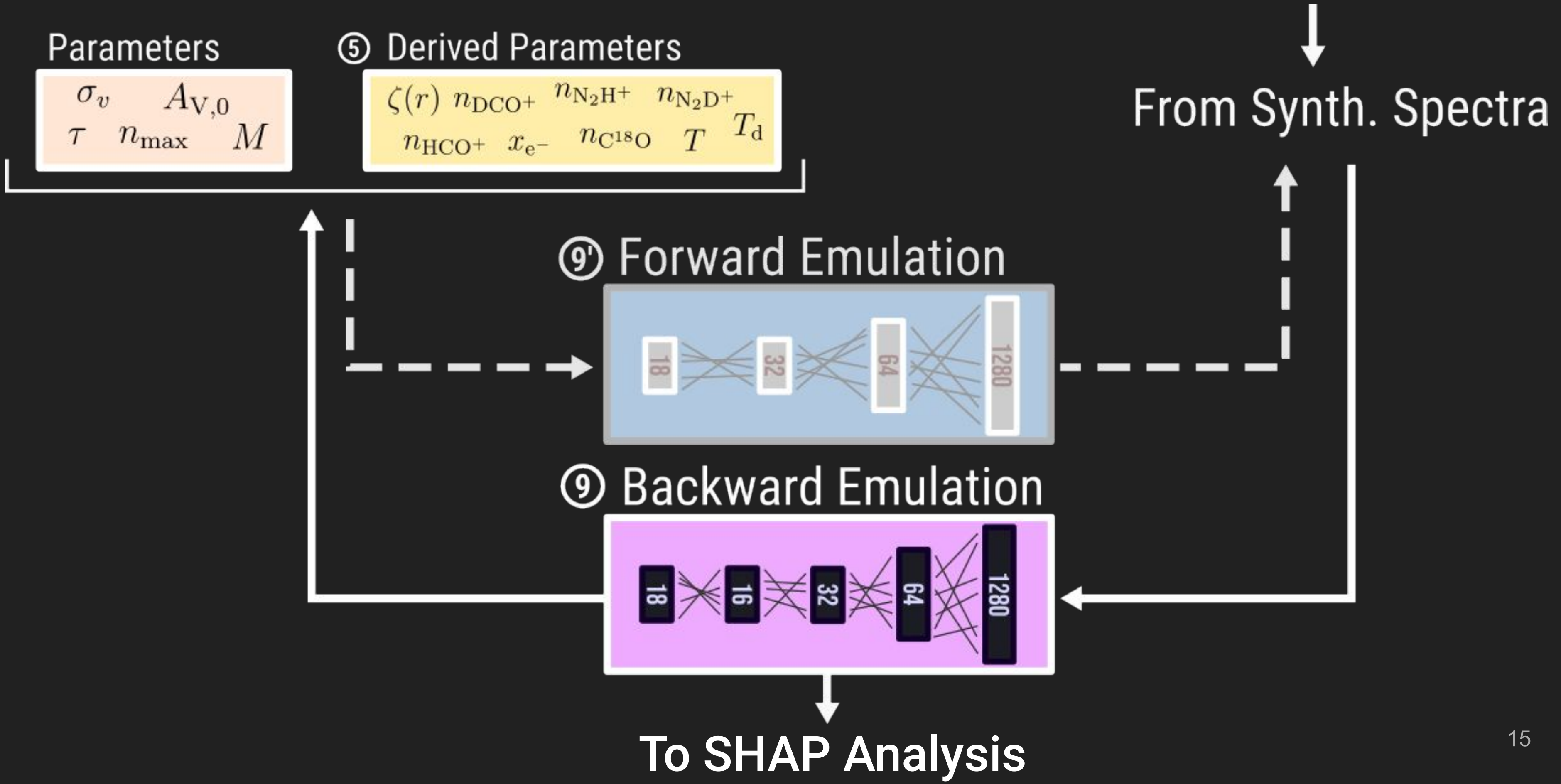
Temperature K



Velocity km s^{-1}

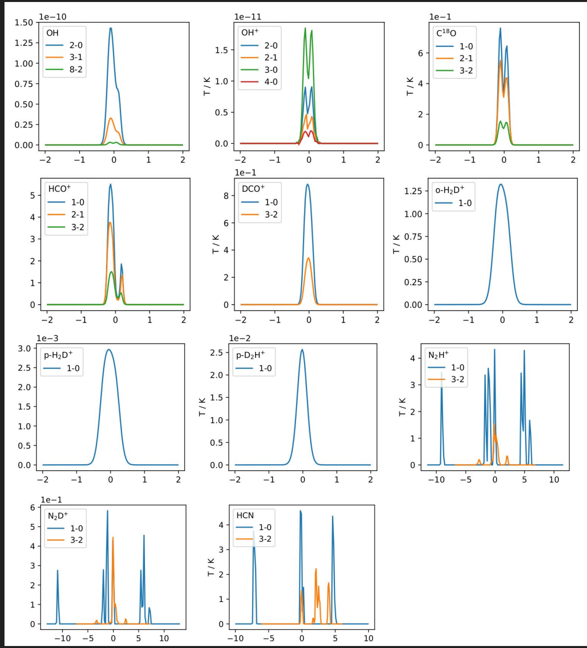
x 3000 Models

Emulation



Parameters
σ_v $A_{V,0}$ τ n_{max} M
⑤ Derived Parameters
$\zeta(r)$ n_{DCO^+} $n_{N_2H^+}$ $n_{N_2D^+}$ T_d n_{HCO^+} x_{e^-} $n_{C^{18}O}$ T
From Synth. Spectra
⑨' Forward Emulation
18
32
64
1280
⑨ Backward Emulation
18
16
32
64
1280
To SHAP Analysis

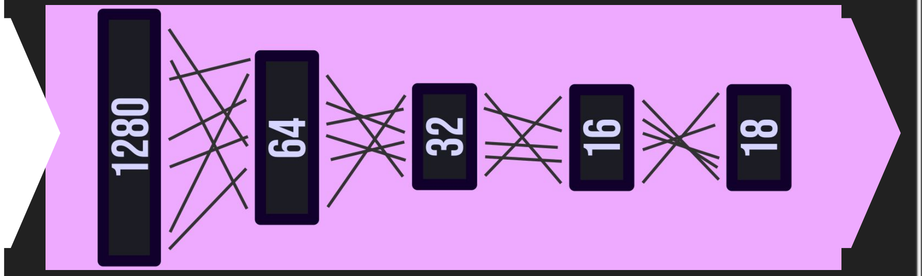
Emulator for the Inverse Problem



1280 v channels

Noise ~10 mK

Neural Network

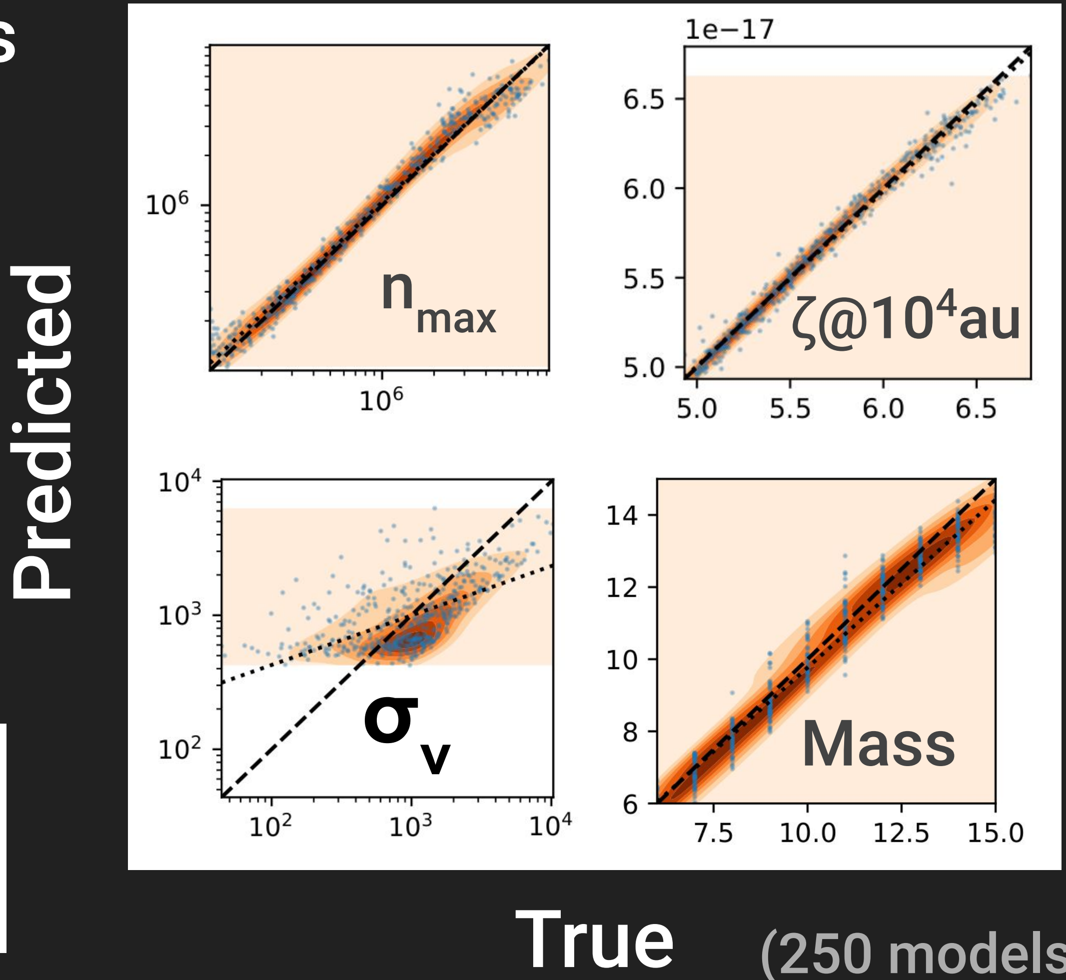


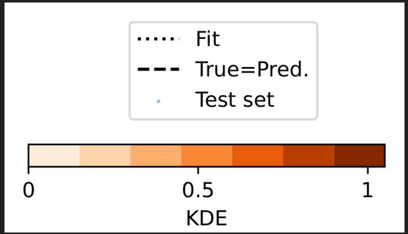
Fully-connected, ReLU, Adam, RMSE loss, Pytorch

18 parameters

see Grassi+11, Holdship+21, Grassi+22, Smirnov-Pinchukov+22, Palud+23, Heyl+23 Sulzer+23, Asensio Ramos+24, Branca+24, Maes+24

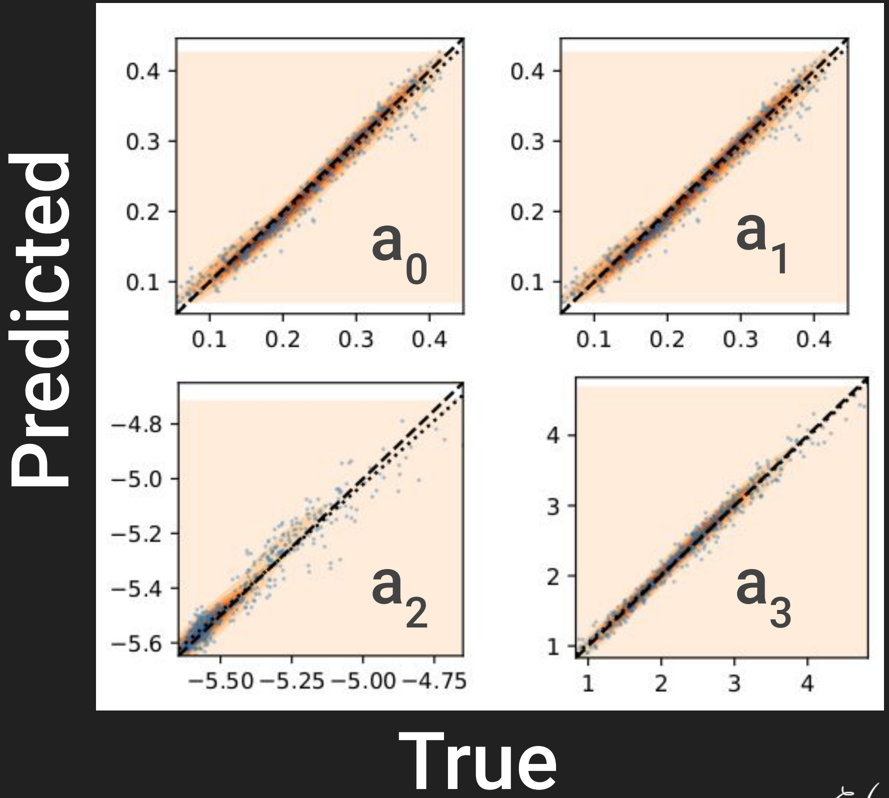
NN Predictions

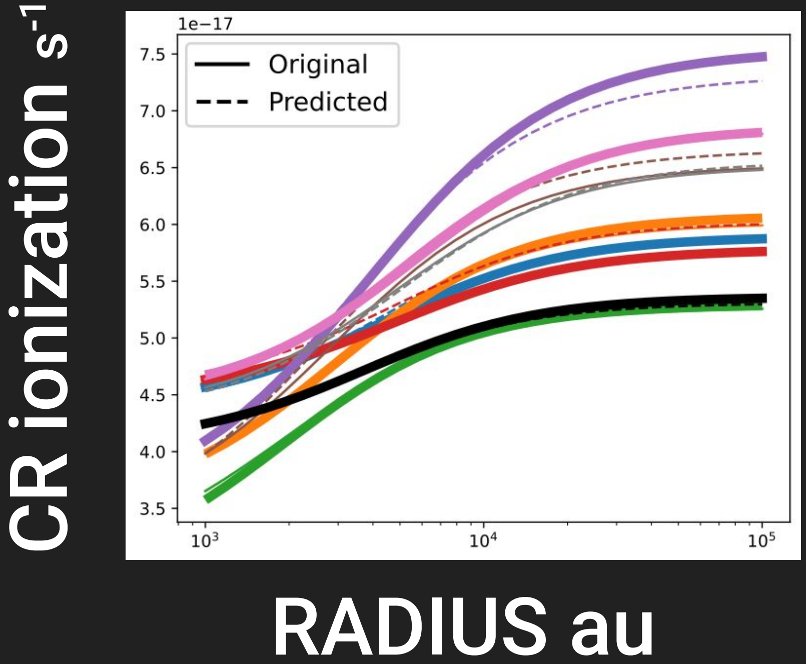




(250 models in test set)

NN Predictions





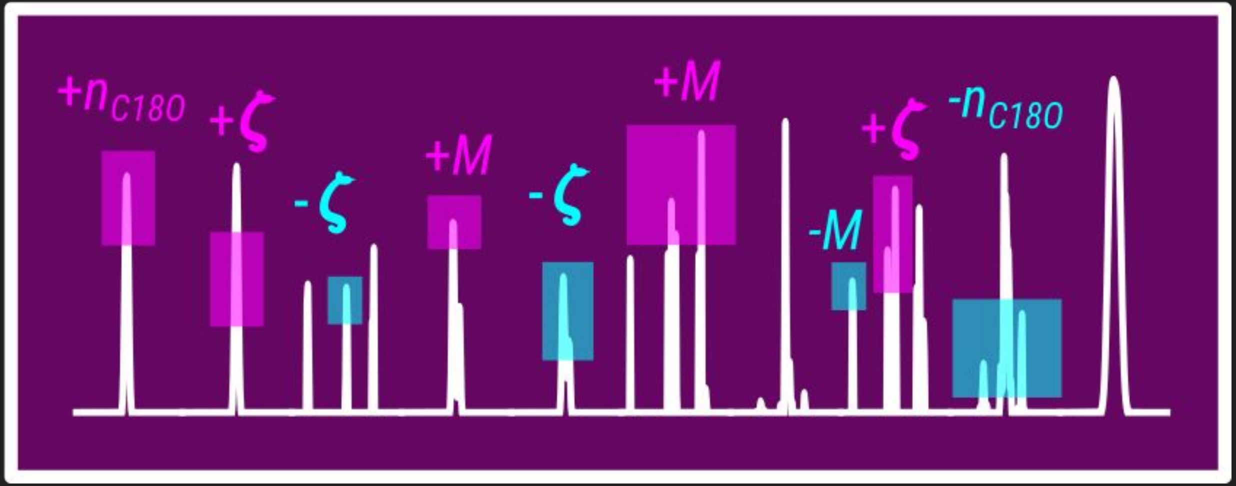
$$\zeta(r) = \frac{a_0}{1 + \exp[a_1(r - a_2)]} + a_3$$

(250 models in test set)

Interpretable Machine Learning

From Emulation (Fast and Differentiable!)

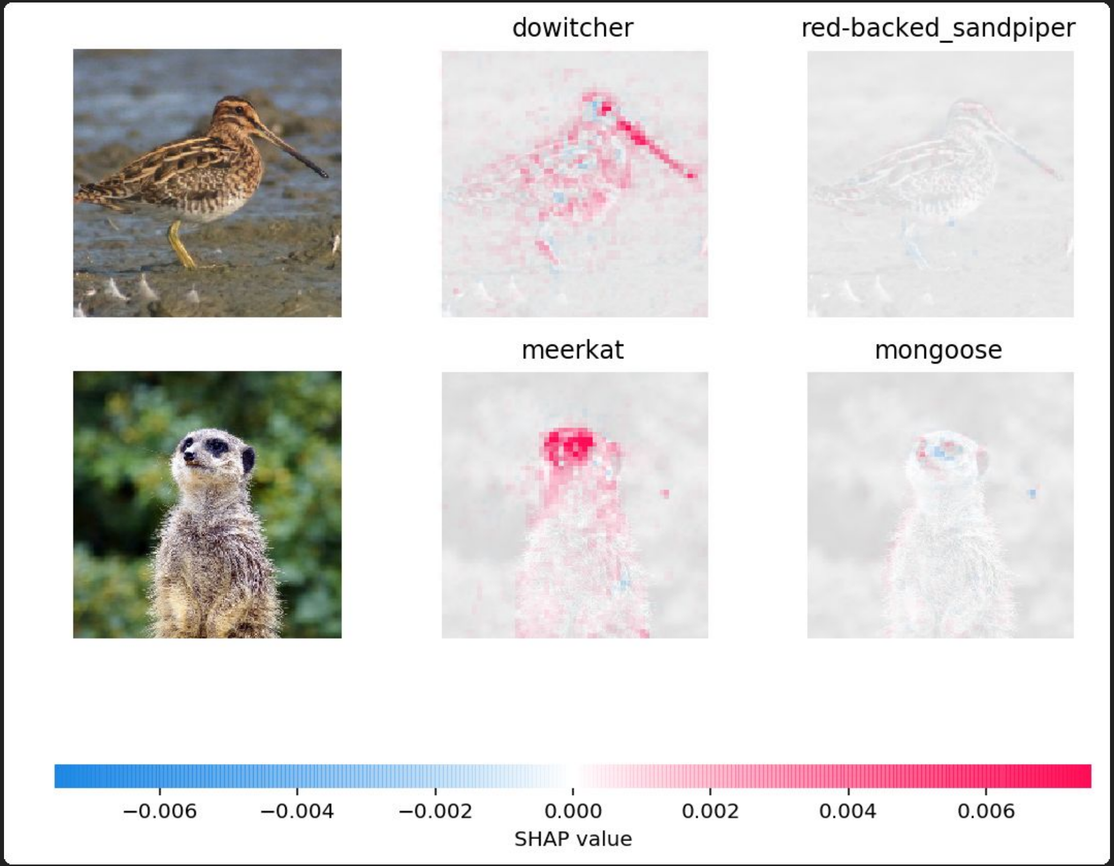
⑩ SHAP Analysis



Where the information resides?

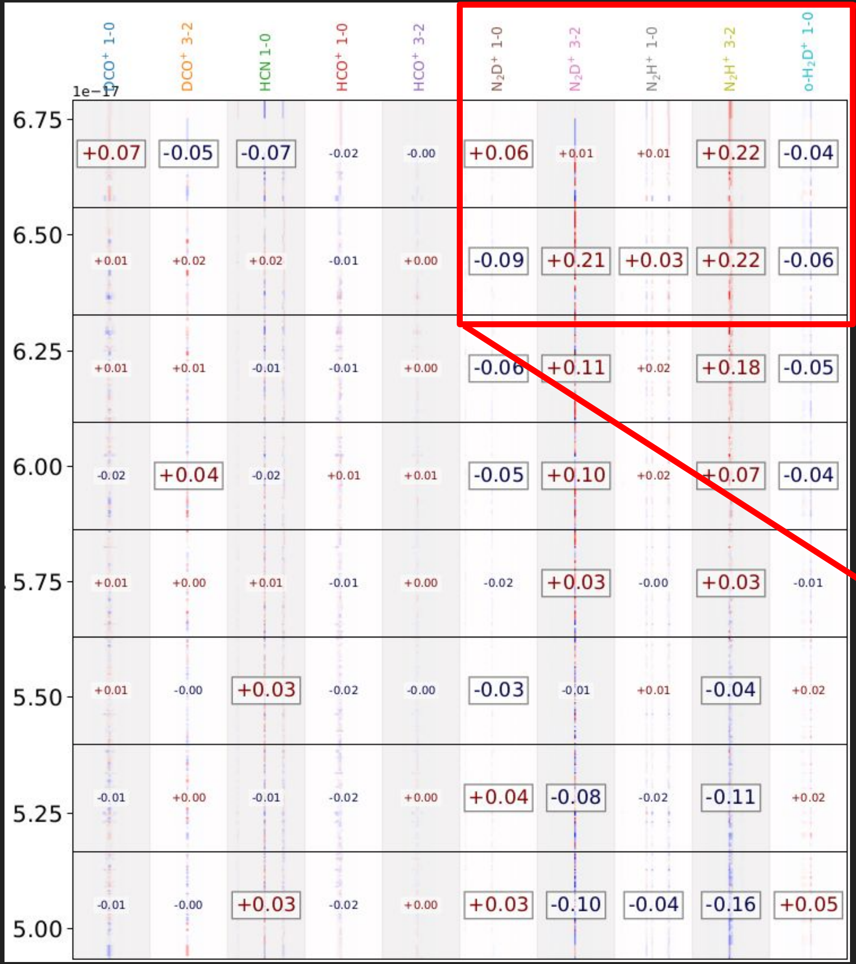
SHAP

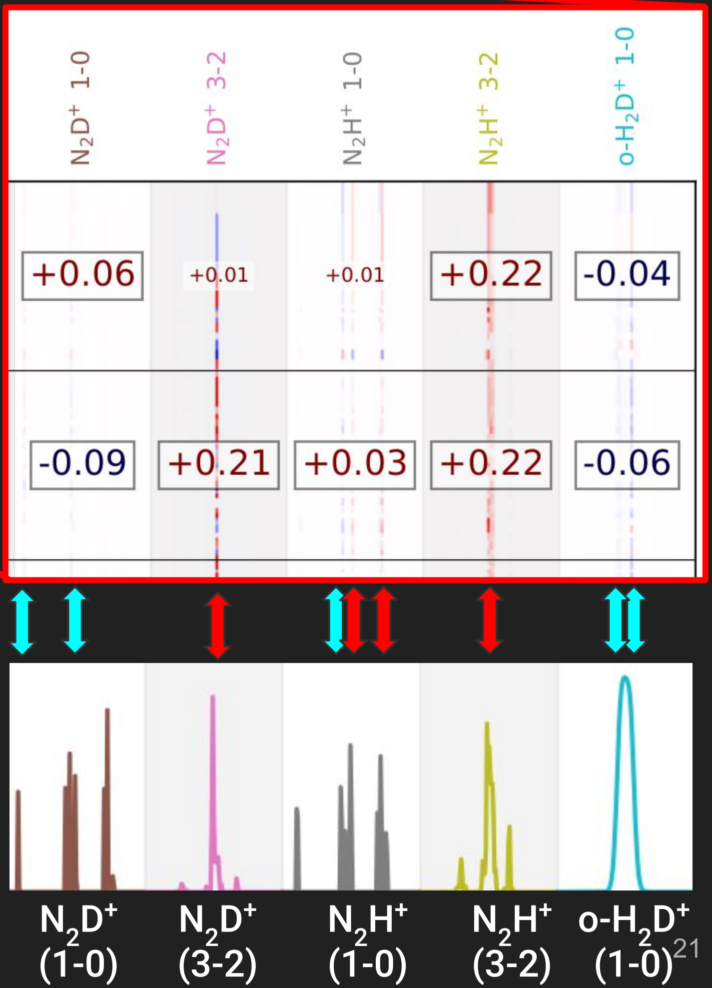
SHapley
Additive
ex**P**lanations



See Lundberg+2017,
Shrikumar+2017,
Heyl+23

CR ionization s^{-1}
ζ@10^4au

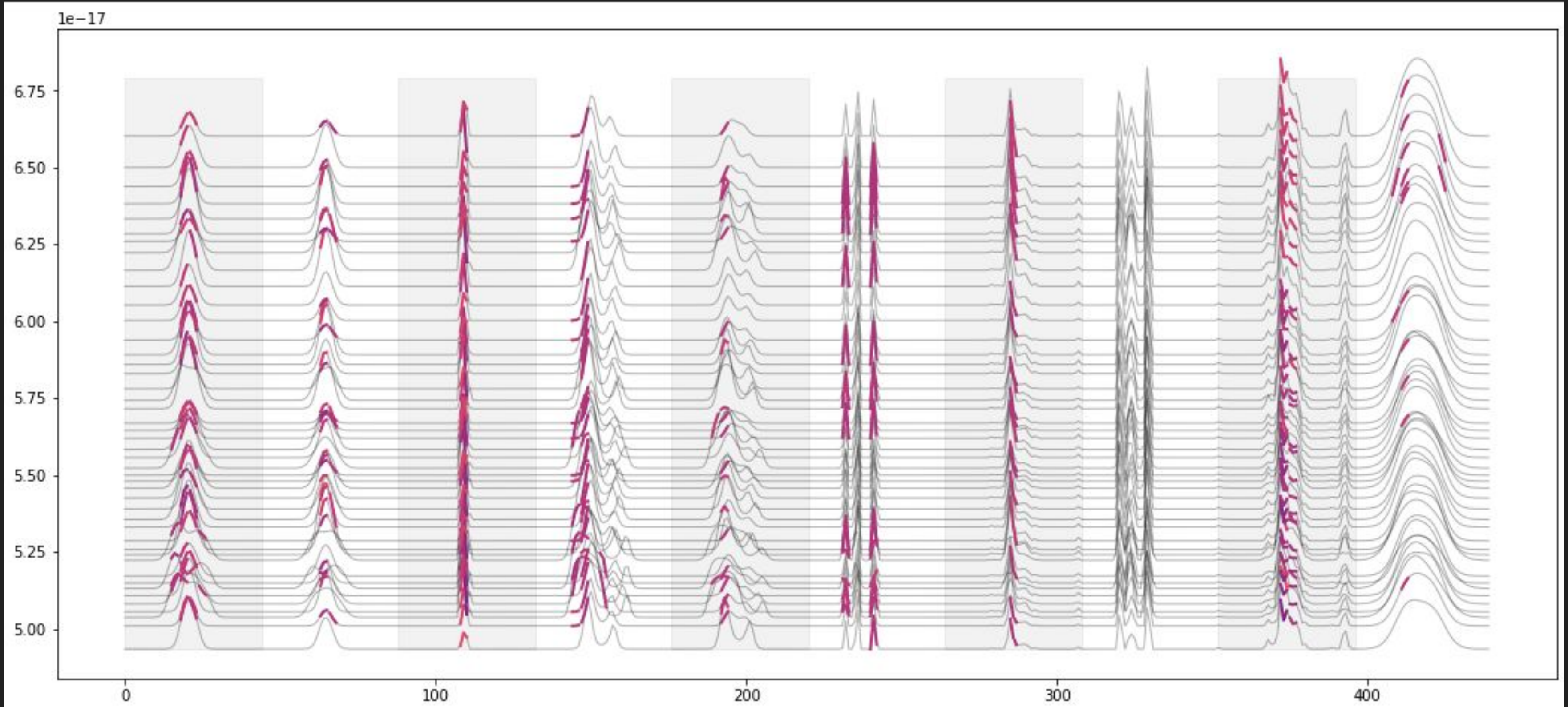




Velocity channels

(250 models in test set)

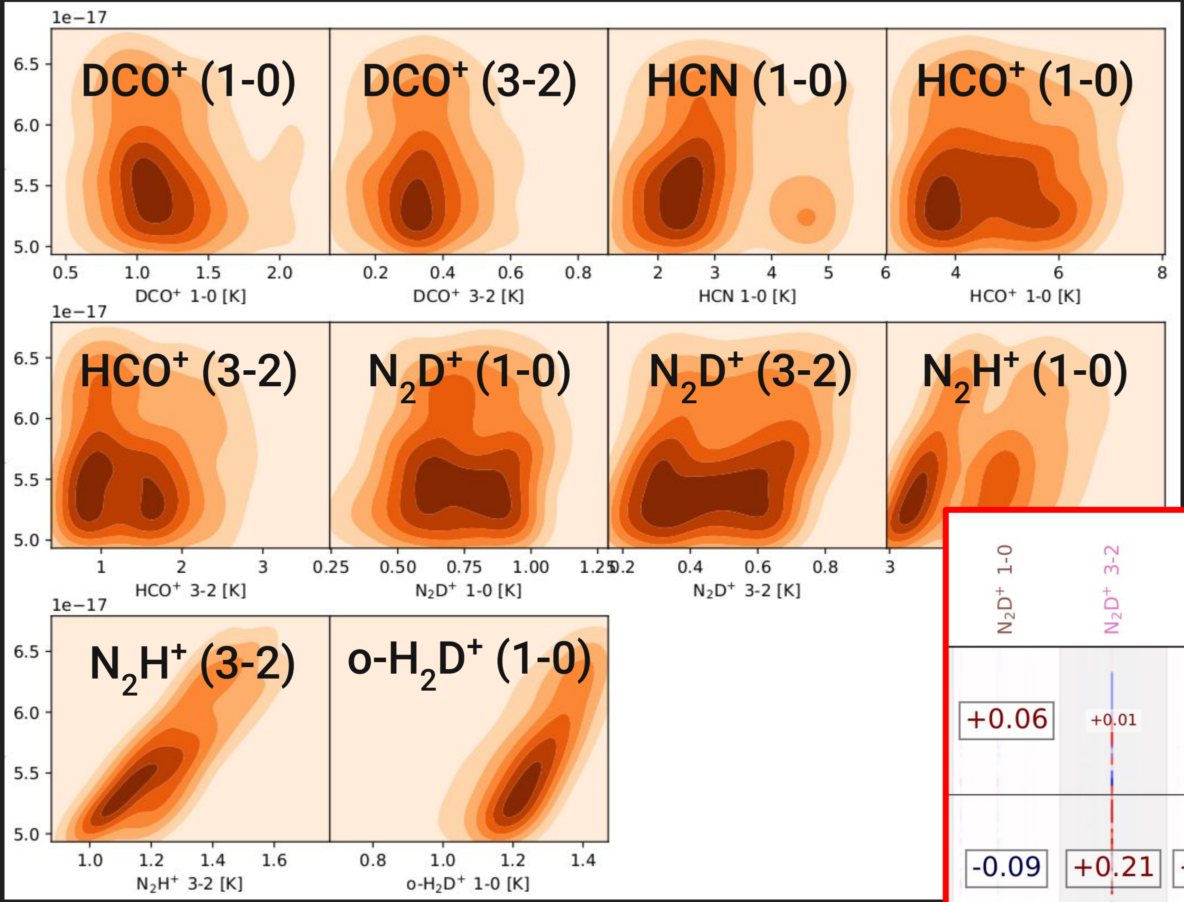
Known pleasure

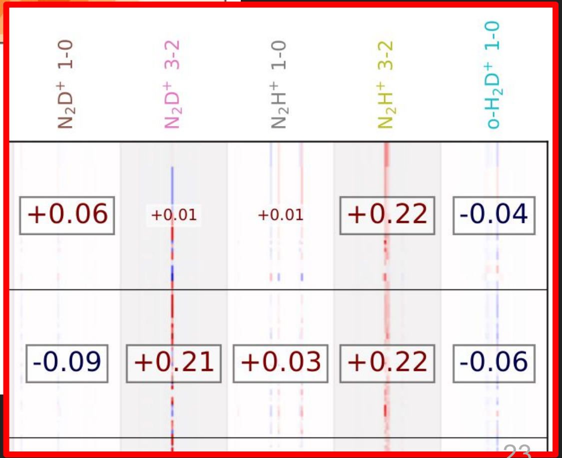


CR ionization s^{-1}

Velocity channels

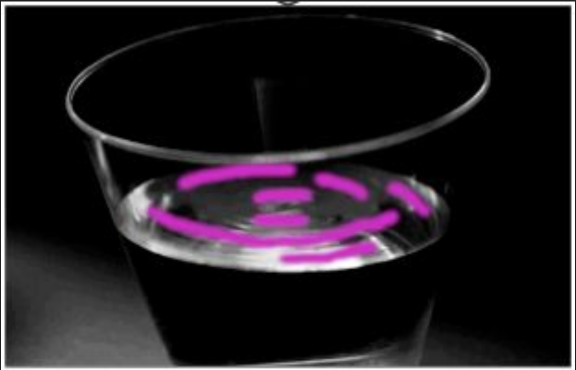
CR ionization s^{-1}
ζ@10^{4}au





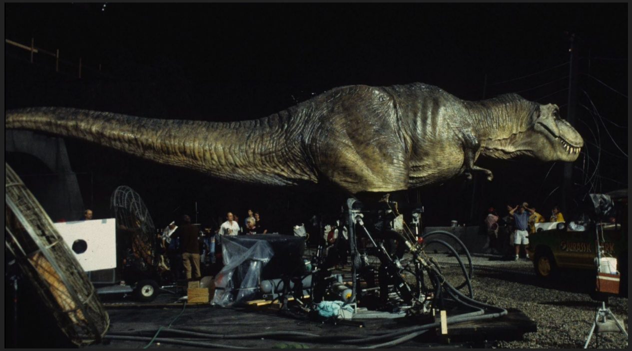
Max emission

Conclusions



- We developed a pipeline to generate synth. spectra
- Backward emulation is possible via neural networks
- SHAP allows to analyse where the information resides
- Can we reconstruct information? **YES**
- Do we know where information resides? **YES**

But…



- "All models are wrong, some are useful" (G. Box)
- Our models are limited (e.g., 1D, no MHD, i.c., …)
- Chemical network are limited (species, rates, …)
- Application to real spectra produces hallucinations
- What is missing in the models?
- Use SHAP to determine models uncertainties