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Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA

ICSC Centro Nazionale di Ricerca in HPC Big Data and Quantum Computing

Emulating the interstellar medium chemistry with neural operators

a recap & update on the project:

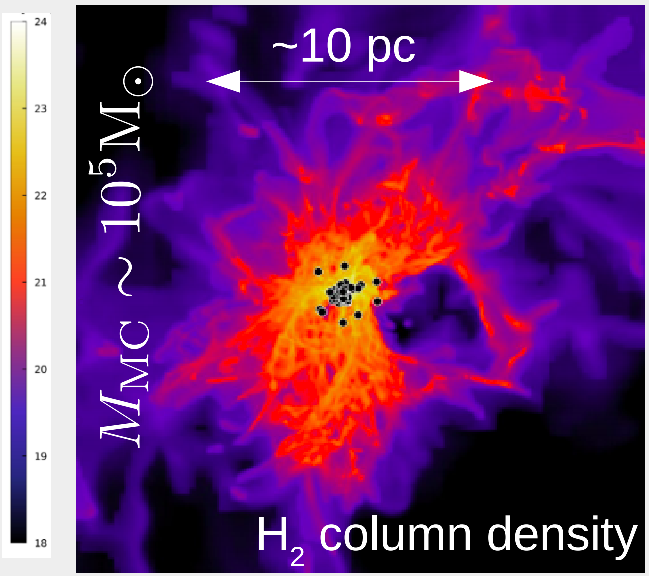
- why should we focus on the chemistry of the ISM?
- what are the problems for numerical solvers?
- which are the ways to speed-up our computations?

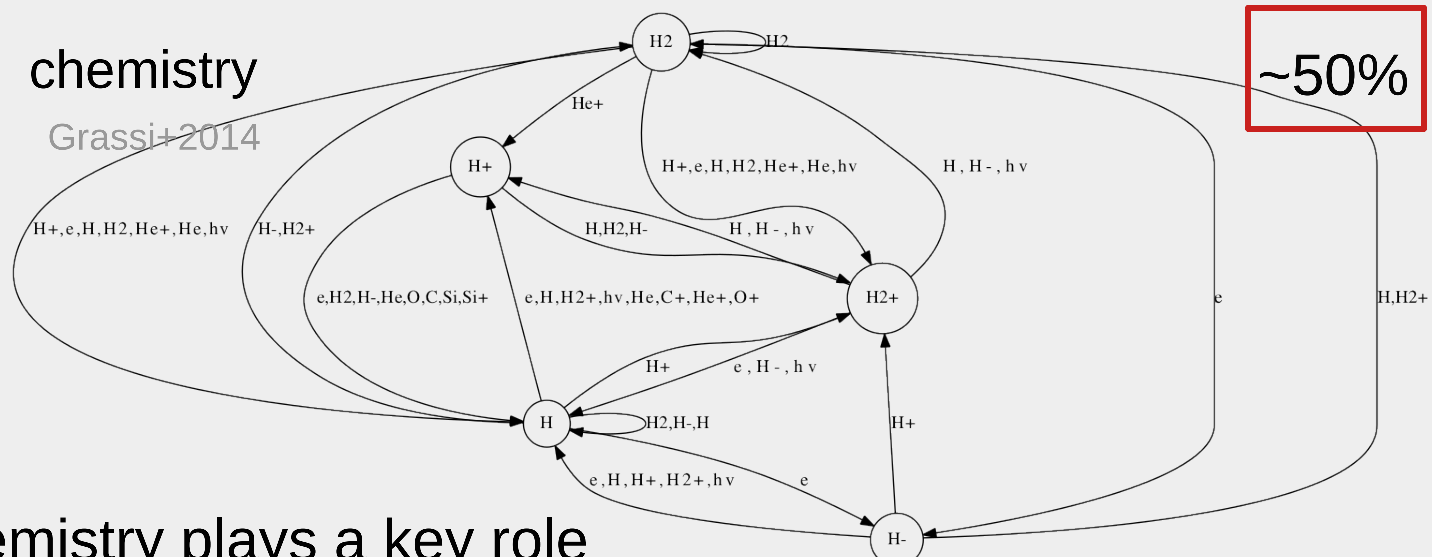
Andrea Pallottini

SCUOLA NORMALE SUPERIORE

Example: breakdown of a Molecular Cloud

Decataldo+2020



physical processes		CPU cost per step
(self)-gravity Guillet & Teyssier 2011	$\Delta\Phi = 4\pi G\rho$	~10%
hydro Teyssier 2002	$\dot{\mathcal{U}} + \nabla\mathcal{F} = \mathcal{S}$	~15%
radiation Roshadal+2015	$\dot{I}_\nu/c + \hat{n}\vec{\nabla} I_\nu = j_\nu - k_\nu I_\nu$	~20%
chemistry Grassi+2014		$\boxed{\text{~50\%}}$

- about 900-60 mpc spatial resolution
- about 10^9 finite (AMR) elements
- about 0.4 MCPUhr for 3 Myr evolution

non-equilibrium ISM chemistry plays a key role in astrophysical and cosmological studies for galactic environments see Pallottini+2017

Solving the chemistry in the InterStellar Medium

$$\begin{cases} \dot{n}_k = \underbrace{\boxed{A_k^{ij}(T) n_j n_i}}_{\text{2-body reactions}} + \underbrace{\boxed{B_k^i(I_\nu) n_i}}_{\text{photo-chemistry/CR}} \equiv M_k^i n_i \\ \dot{T} = \underbrace{\boxed{\Gamma(I_\nu) - \Lambda(n_k, T)}}_{\text{heating/cooling}} \end{cases}$$

Bovino+2015, Pallottini+2017, Decataldo+2020

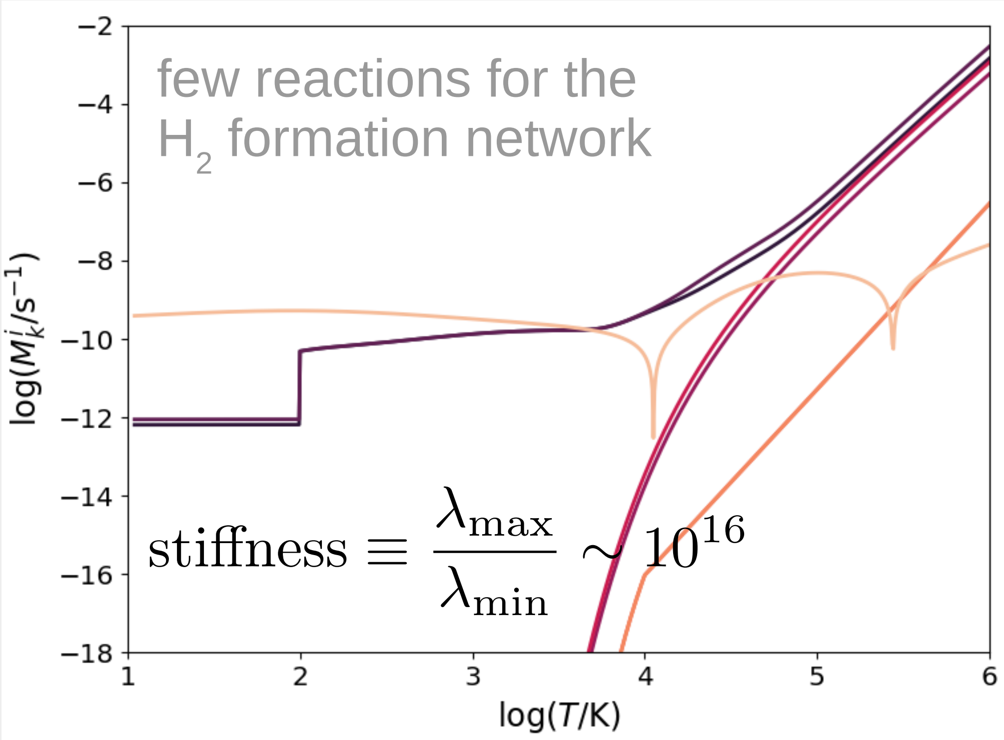
9 species (+T) and 52 reactions to follow up to H_2 formation

<u>robust implicit solvers are needed</u>

- CPU cost is high
- load balancing can be spoiled

can we use fast emulators instead?

Branca & Pallottini 2023



features of the numerical system:

- wide range of initial conditions: cold/warm neutral medium, molecular gas, hot ionized gas ...
- problem size increases superlinearly with number of chemical species
- non trivial dependencies with T
- incredibly stiff ODE system
- timescale are short wrt hydro, gravity, ...
- ...

Physics-Informed Neural Networks: a sketch

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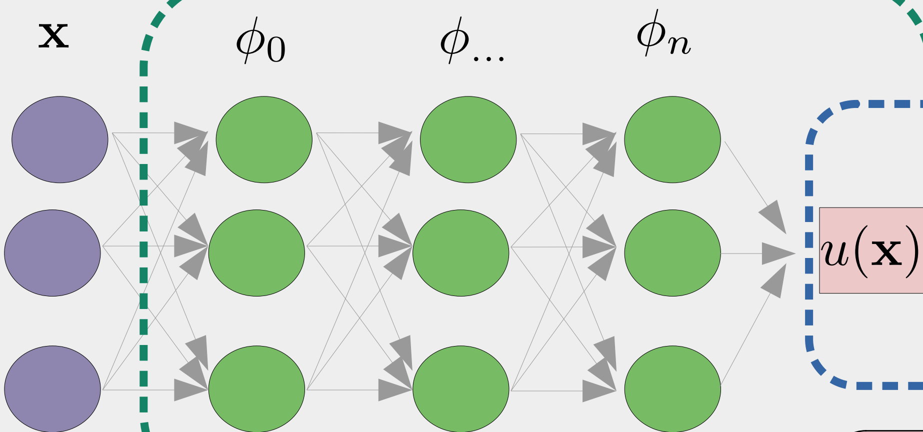
image for a simple feed-forward network,
actually we adopt Deep Galerkin layers (Sirignano & Spiliopoulos 2018)

also applicable to a PDE/BC
see Raissi+2019 for original formulation



problem to solve

$$\mathcal{D}(u(\mathbf{x})) = f(\mathbf{x}),\ \text{ODE}$$

$$\mathcal{B}(u(\mathbf{x})) = g(\mathbf{x}),\ \text{IC}$$

$$\begin{cases} \dot{\mathbf{x}} = M\mathbf{x} \\ \mathbf{x}(t=0) = \mathbf{x}_0 \\ \mathbf{x} = (n_i, T) \end{cases}$$

strategy: minimize the loss function
to approximate the ODE solution

$$\mathcal{L}(\theta^\star) < \epsilon \Rightarrow u_{NN}(\mathbf{x}, \theta^\star) \simeq u(\mathbf{x})$$

stochastic adaptive
gradient descent
(Kingma & Ba 2014)

loss function to train the NN

$$\mathcal{L}(\theta) = |\mathcal{D}(u_{NN}(\mathbf{x}, \theta)) - f(\mathbf{x})| + |\mathcal{B}(u_{NN}(\mathbf{x}, \theta)) - g(\mathbf{x})|$$

Physics-Informed
part of the NN

- NN built to be differentiable at machine precision
- evolution equations directly embedded in the loss

Performance of a PINN emulator

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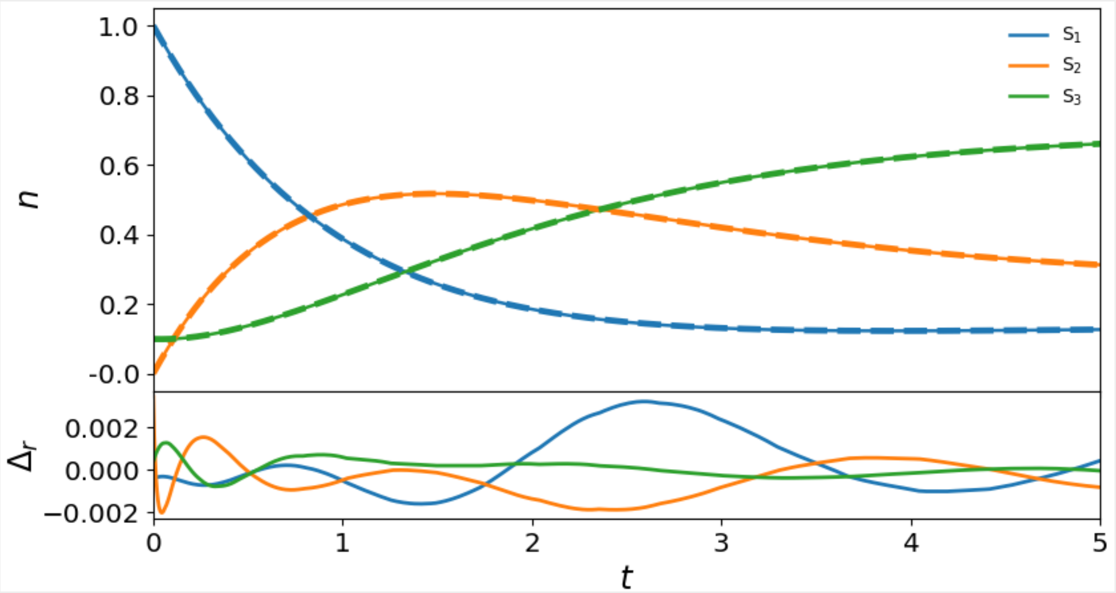
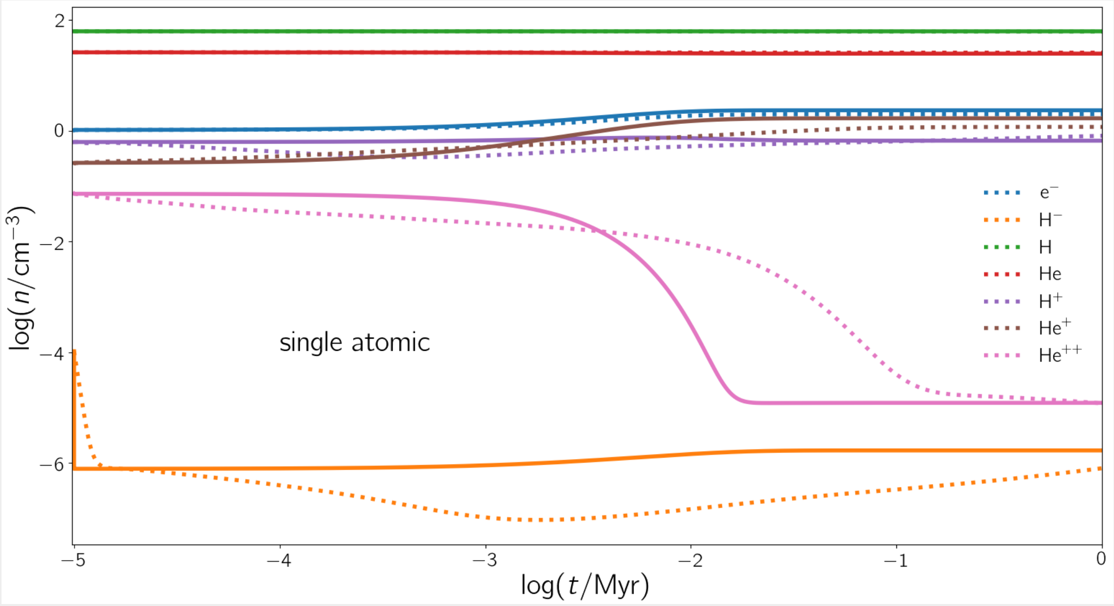
stiff ODE



ISM chemistry



performances similar to with Grassi+2022 and Holdship+2021, (for slightly different problems)

good effort, but likely too costly to reach the required precision

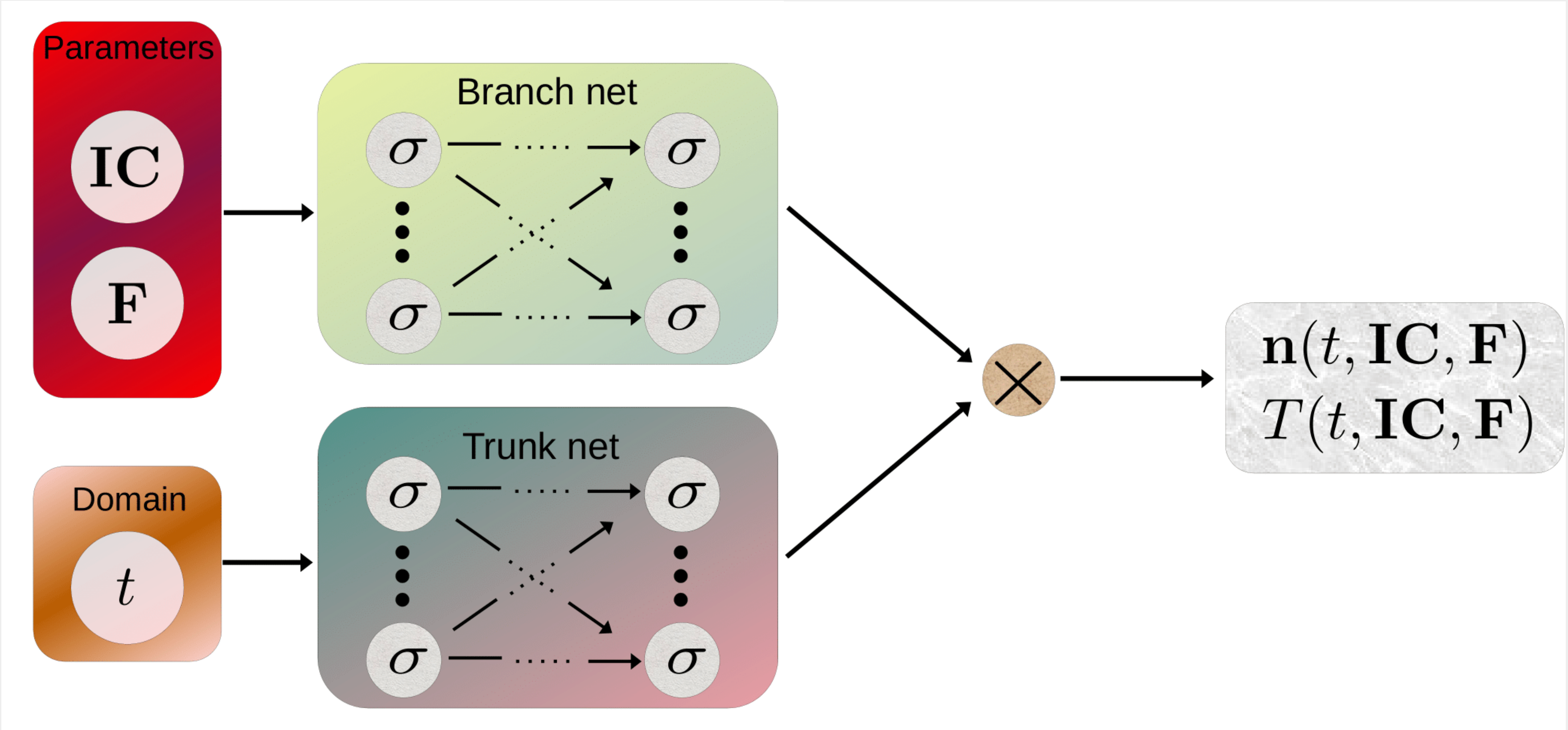
training set

$$\mathrm{T/K} \in [20, 10^{5.5}]$$
$$\mathrm{n/cm^{-3}} \in [10^{-2}, 10^{3}]$$
$$\mathrm{n}_k/\mathrm{n} \in [10^{-6}, 0.8]$$

relative error	$\simeq 0.1$
speed up	$\times 100$
training time	$\simeq 2k\,\mathrm{GPUhr}$

Changing gears: Deep Neural Operator

Branca & Pallottini submitted



main differences wrt the PINN model

- DeepONet is a implementation UAT for operators
- the emulator is data driven
- shape and intensity of the radiation Field can change

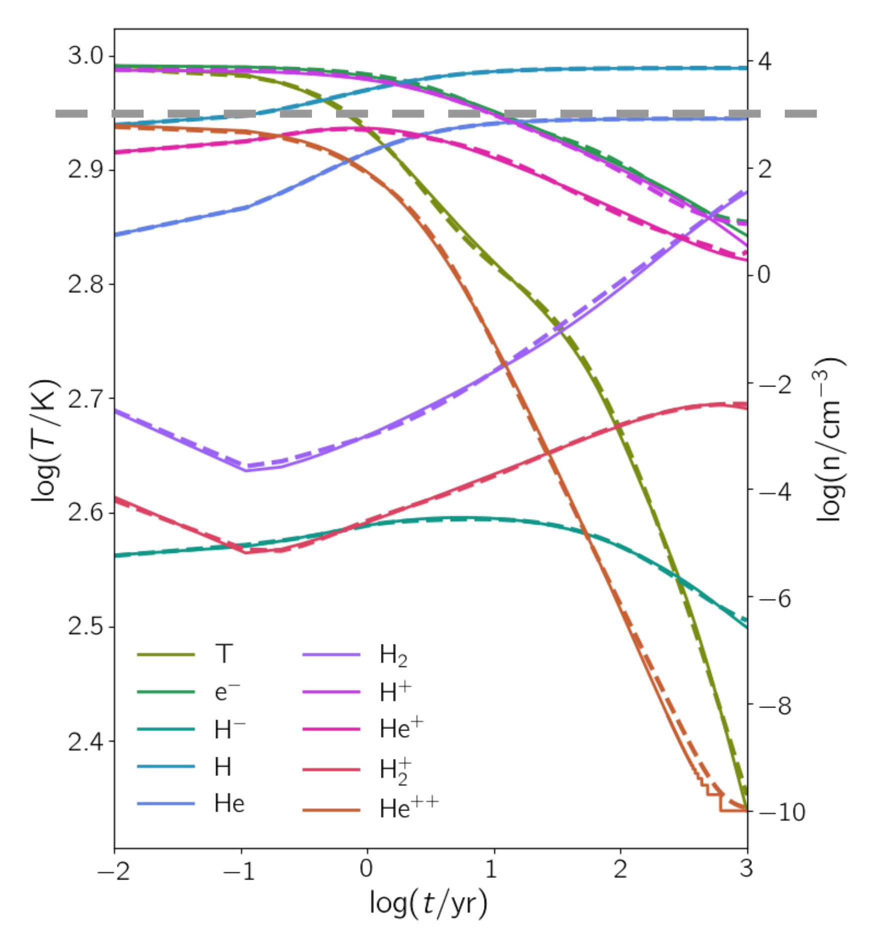
Lu+2021
Grassi+2014
10 energy bins

DeepONet: performance & validation

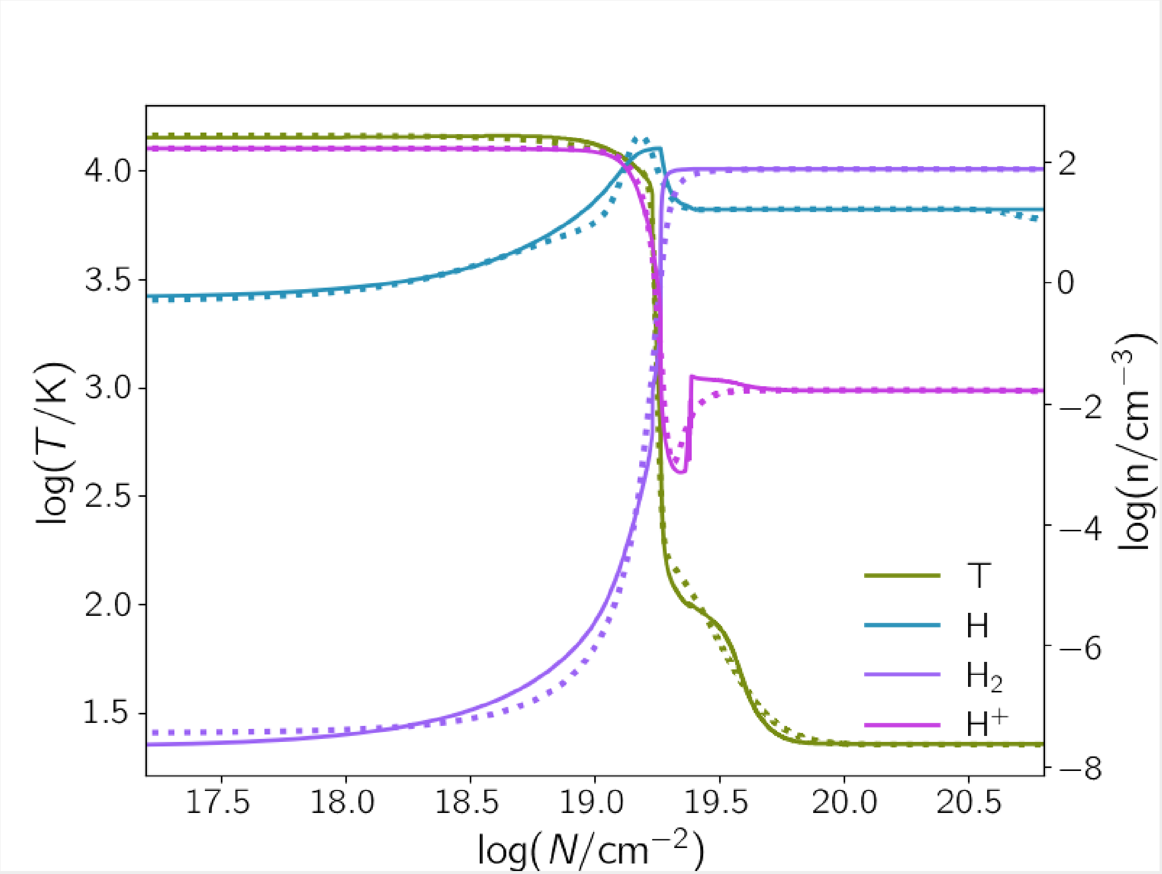
$$
\begin{aligned}
\text{relative error} &\quad \simeq 0.01 \\
\text{speed up} &\quad \times 128 \\
\text{training time} &\quad \simeq 40\,\mathrm{GPUhr}
\end{aligned}
$$

Branca & Pallottini submitted

i.e. 10x more precise at x40 less cost wrt the PINN, which did not allowed for a varying radiation field



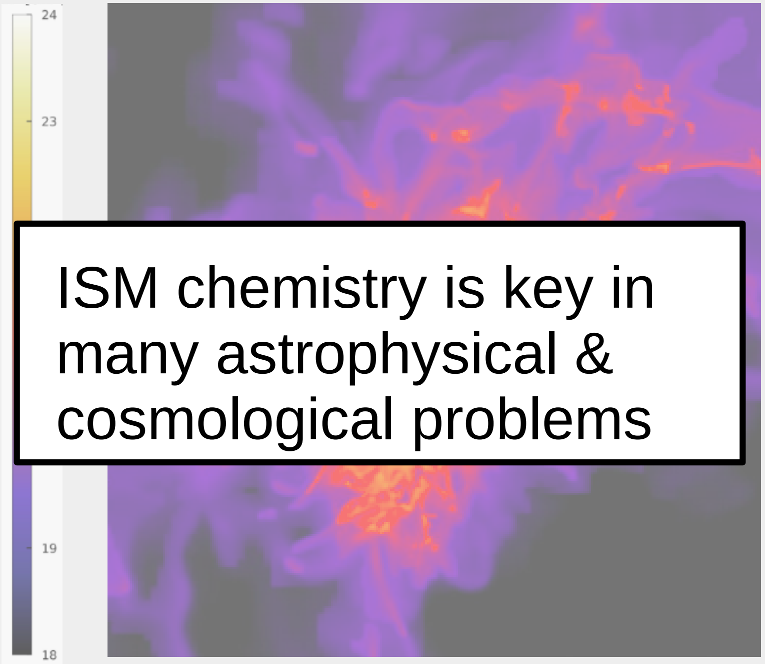
very adaptable: validation with PDR



— — — boundary of the training set

Conclusions:

Decataldo+2020



ISM chemistry is key in many astrophysical & cosmological problems

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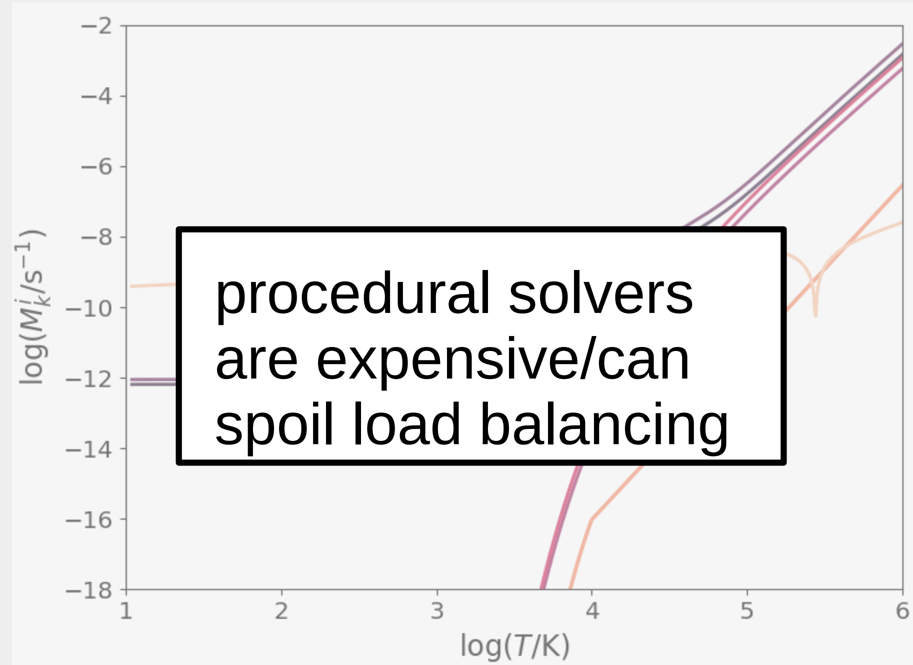

procedural solvers are expensive/can spoil load balancing

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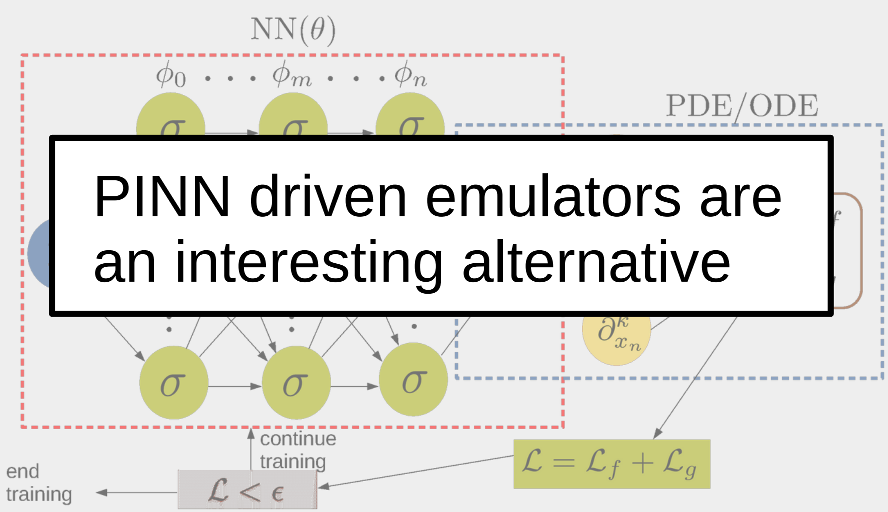
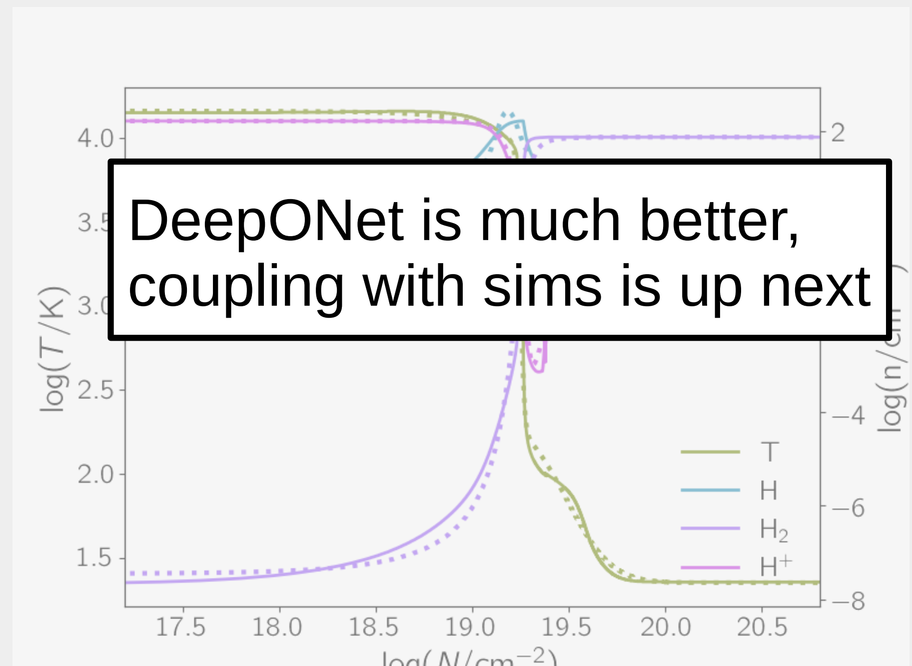


PINN driven emulators are an interesting alternative

✓KPI: paper submitted

Branca & Pallottini submitted



DeepONet is much better, coupling with sims is up next