Accelerating Physics-Based Simulations with AI models: Astrochemical use case

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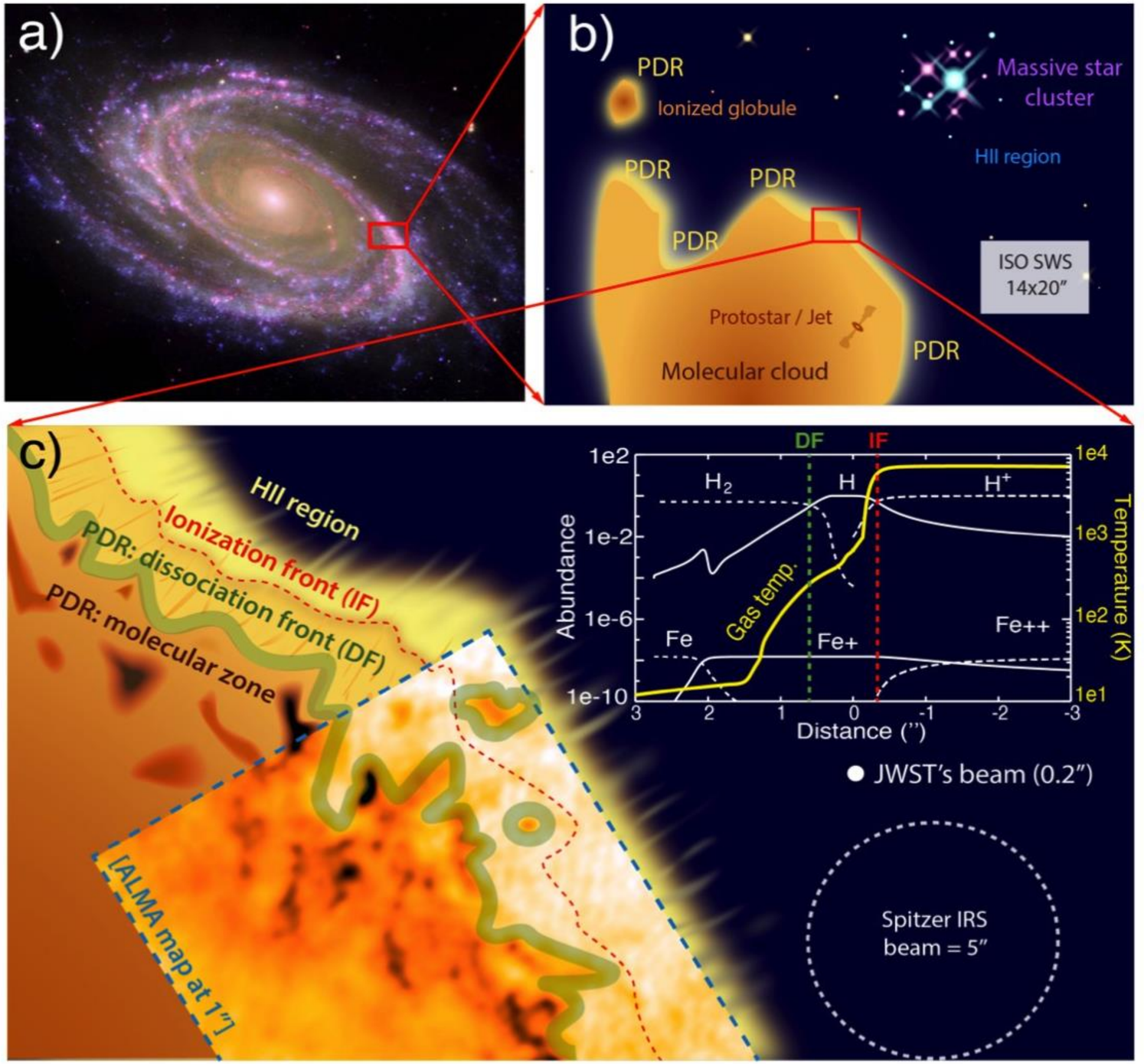
1. Scientific Motivation:
   towards Hydro-PDR simulations
2. 3D-PDR warm-start:
   Faster physical solutions through learned initialization
3. NeuralPDR+:
   Fast molecular abundance prediction

PDR:

Photo-Dissociation Region

or Photo-Dominated Region

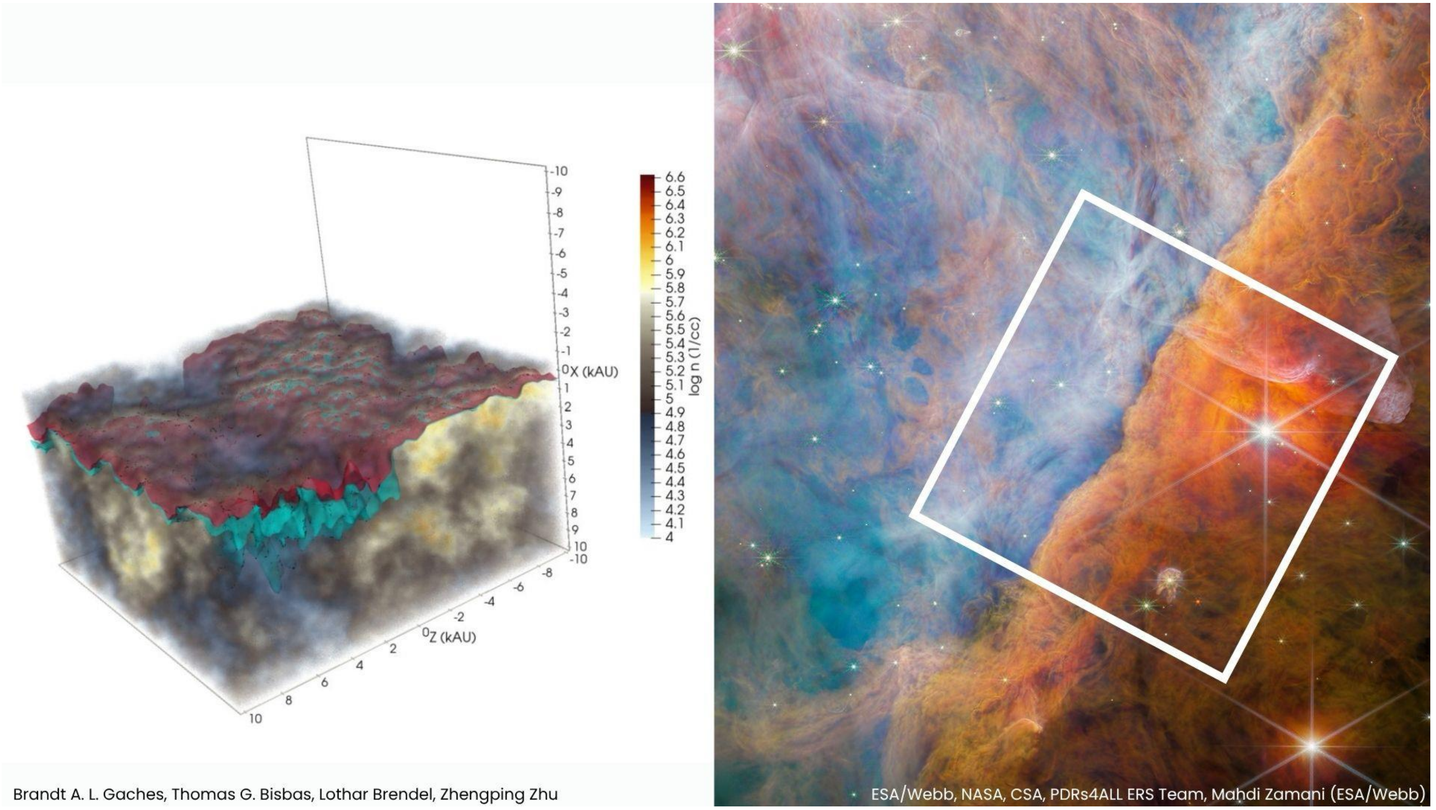
- Neutral ISM (Inter-Stellar Medium)
- FUV dominates the heating and chemistry
- Atomic-to-molecular (HI-to-H2) transition
- C+ / C / CO cycle
- Emission of [CII], [CI], [OI], CO lines



3D-PDR help addressing: How cloud structure shapes chemistry and observable emission?

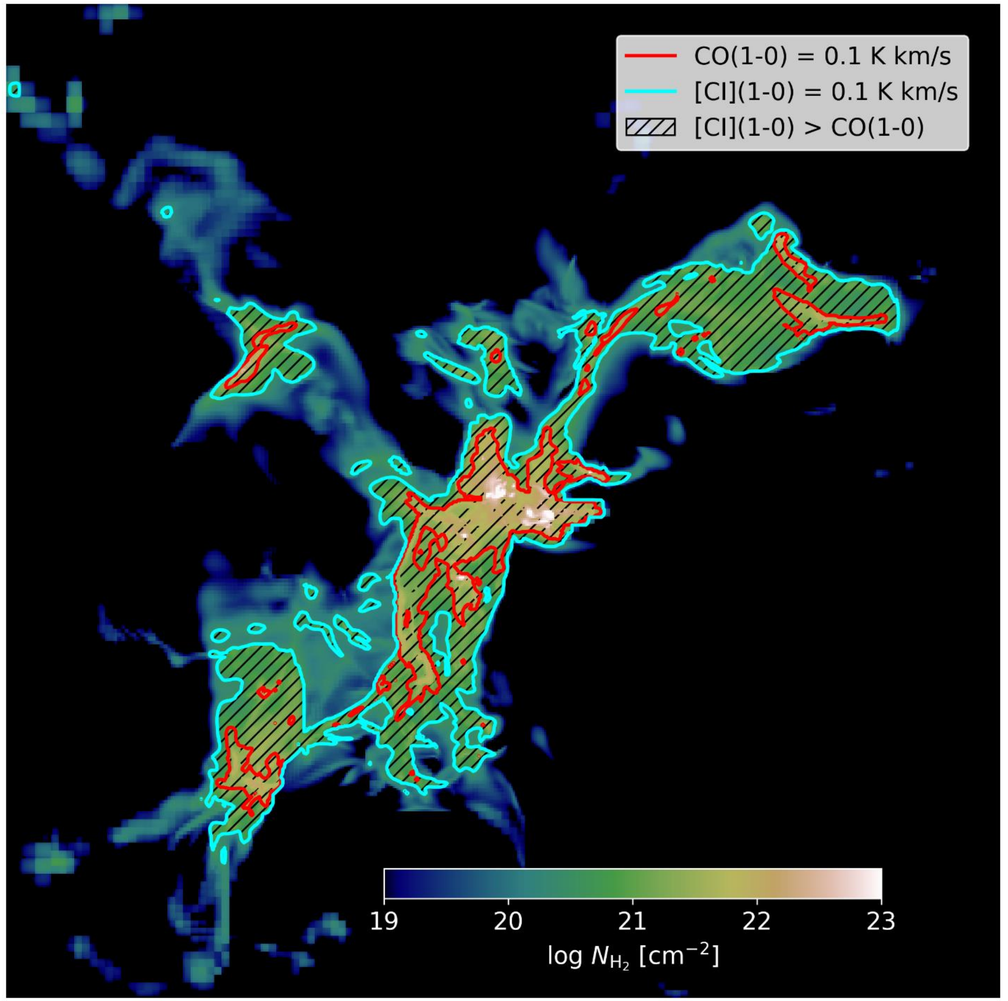
The uneven structure of stellar nurseries creates shadows that alter their chemistry and influence the infrared emission observed by the *James Webb Space Telescope*

latest work using 3D-PDR (Gaches, Bisbas, Brendel & Zhu, A&A 2026)



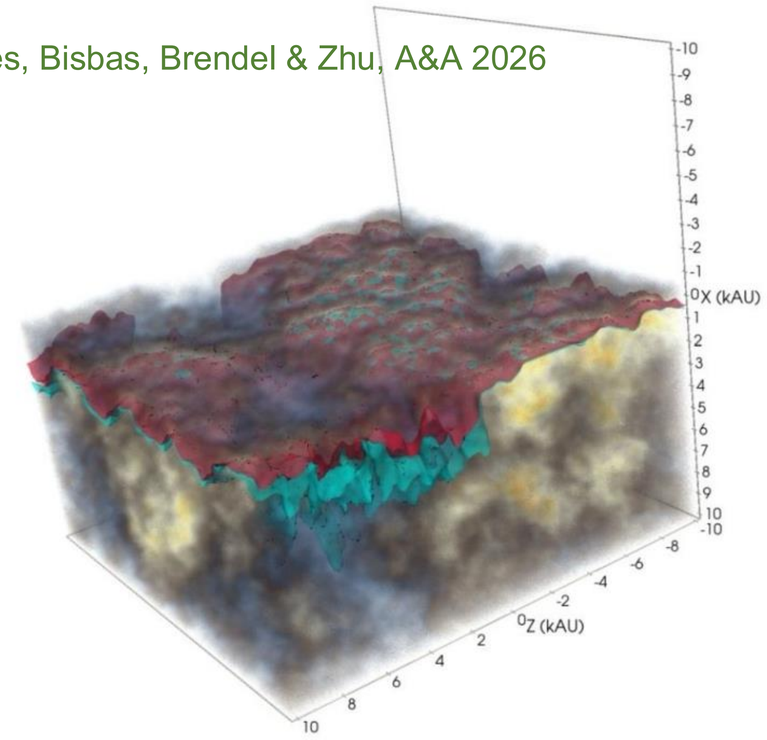
In certain regions, Atomic carbon dominates the carbon-species in molecular gas, where CO is not a good H2 tracer (CO-Dark).

Zhu, Bisbas, Tang et al. MNRAS 2026

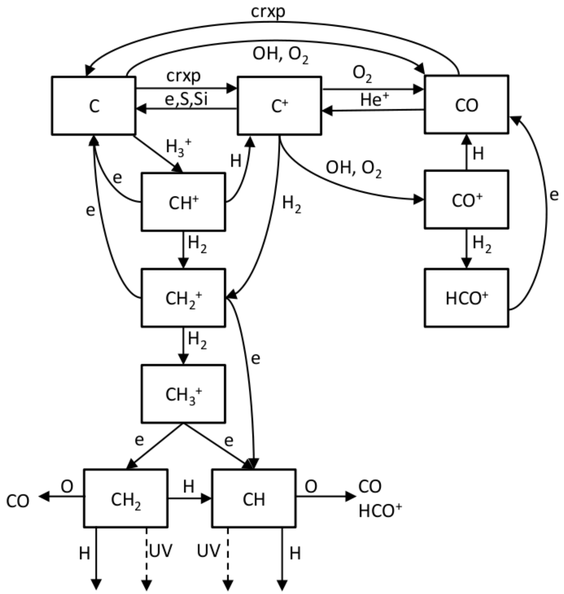


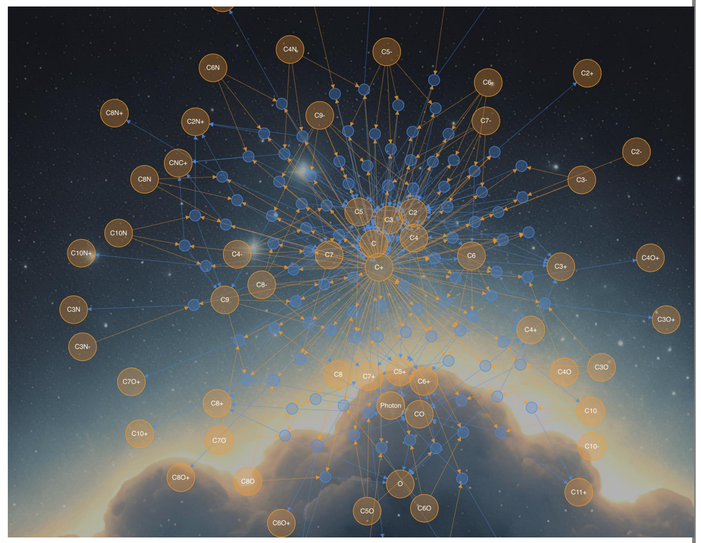
ISM/PDR model: Numerical Simulation

Gaches, Bisbas, Brendel & Zhu, A&A 2026



Chemical Network





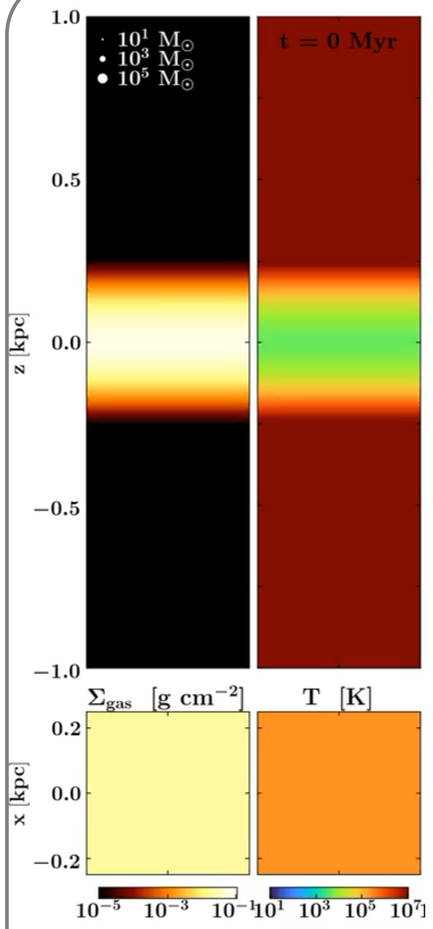
Bialy & Sternberg 2015

Not to be confused with:

AI model & Neural Network

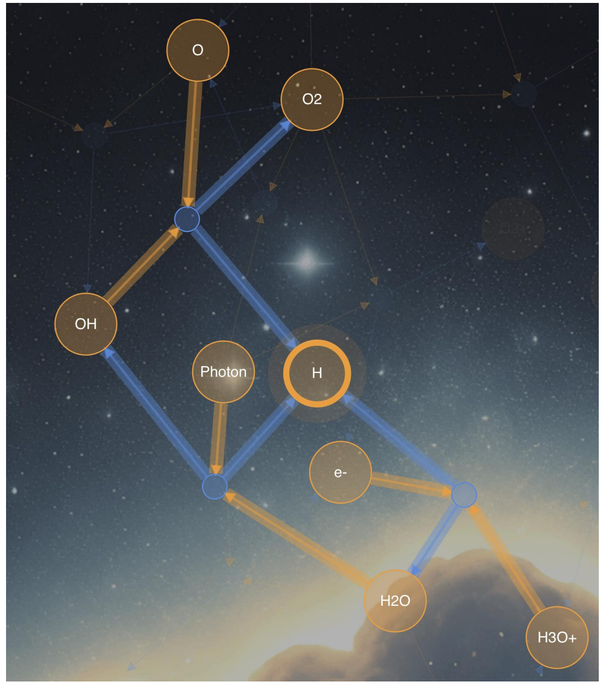
Numerical Challenges:

Detailed on-the-fly chemistry remains expensive in hydrodynamical simulations



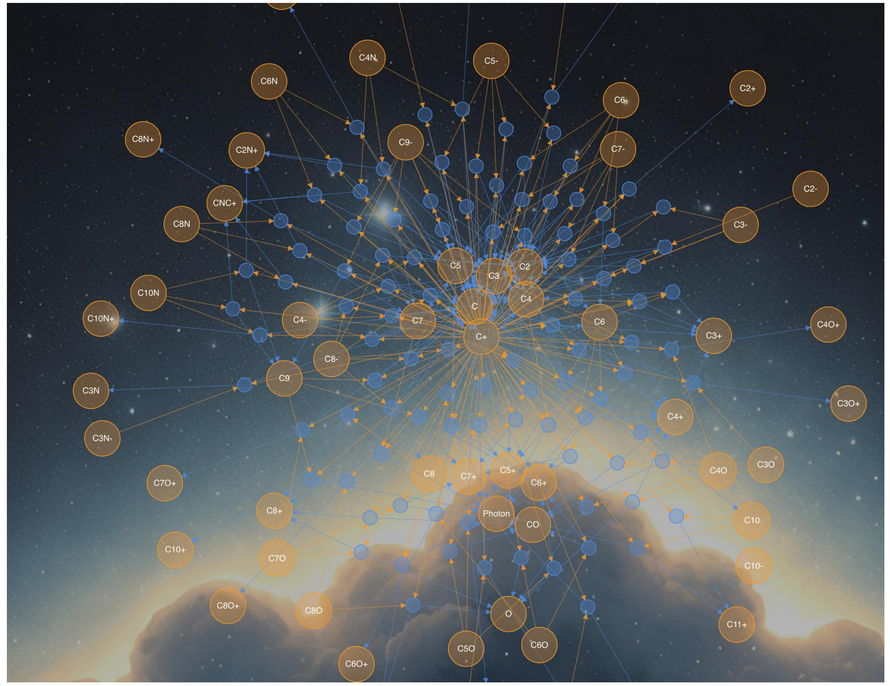
Rathjen et al. 2025

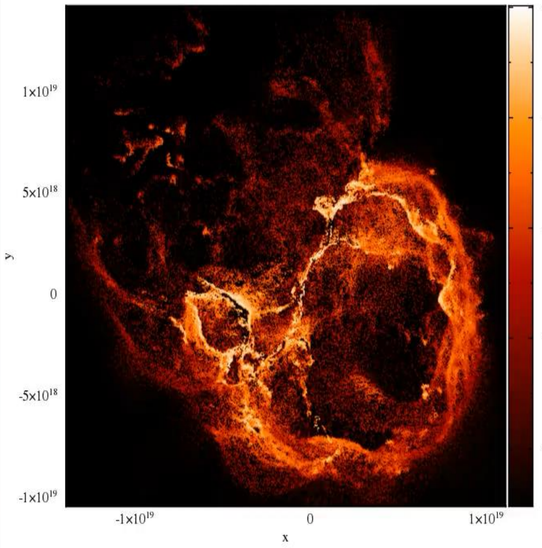
Simple Network



On-the-fly

Detailed Network





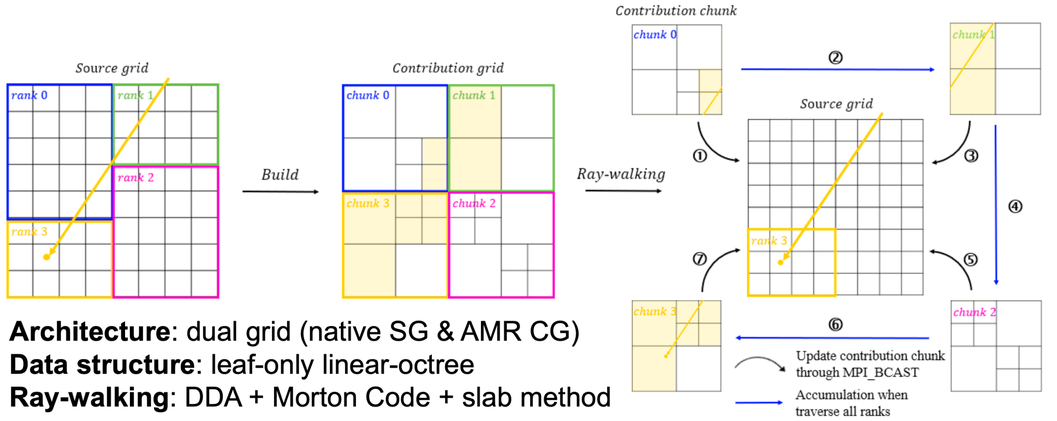
Computationally costly

Previous advances:

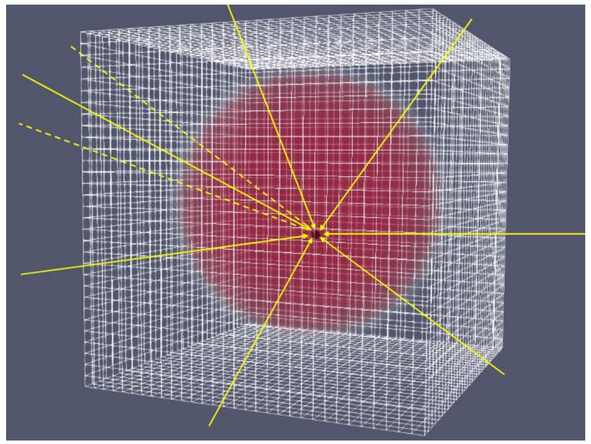
We have optimized 3D-PDR and generated unprecedented $\mathbf{512^3}$-cell simulation with:

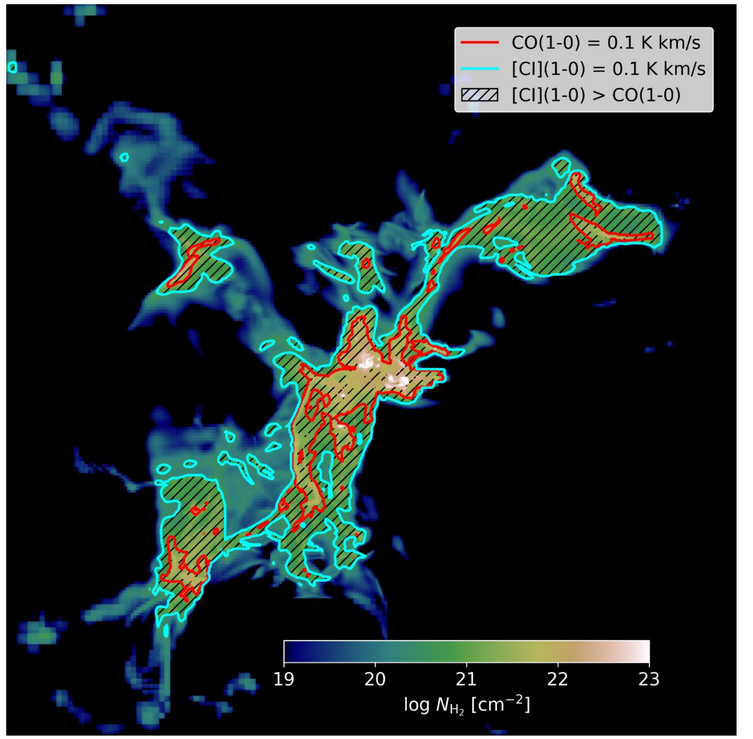
1. RAYTHEIA: a new grid-based ray-tracing (**100x faster)** approach (Zhu, et al. MNRAS 2026)

2. **MPI** parallelization on ZJLab's HPC



Architecture: dual grid (native SG & AMR CG)
Data structure: leaf-only linear-octree
Ray-walking: DDA + Morton Code + slab method





The next opportunity:

Scientifically guided agentic AI helps us develop and test new acceleration strategies—including neural-network warm starts.

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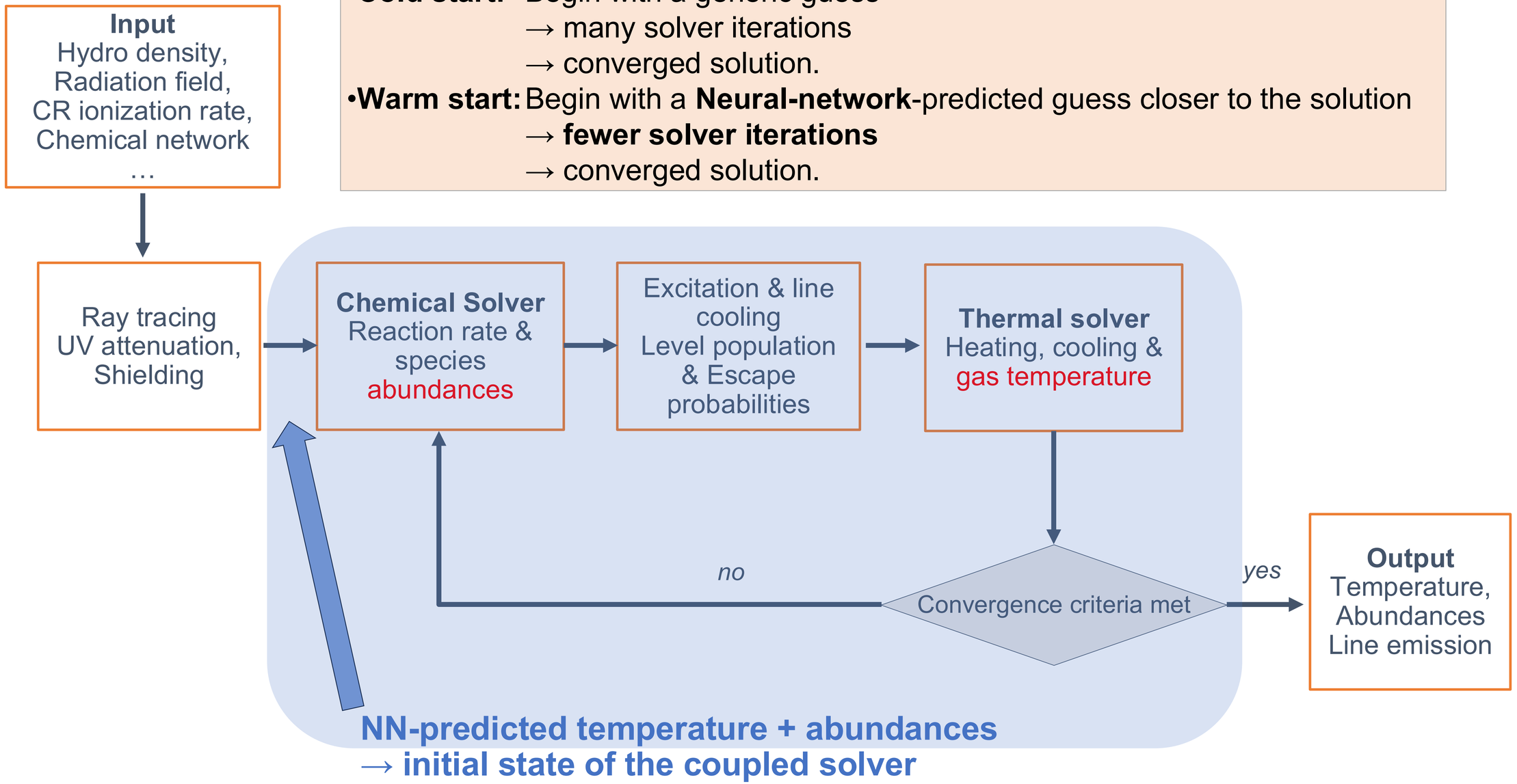
Warm-Start: Expensive iterations can be avoided with a Neural-network model

- **Cold start:** Begin with a generic guess
  → many solver iterations
  → converged solution.
- **Warm start:** Begin with a **Neural-network**-predicted guess closer to the solution
  → **fewer solver iterations**
  → converged solution.



Method and Model details

Cloud conditions
→ Small MLP neural network → Temperature + abundances
→ 3D-PDR refinement

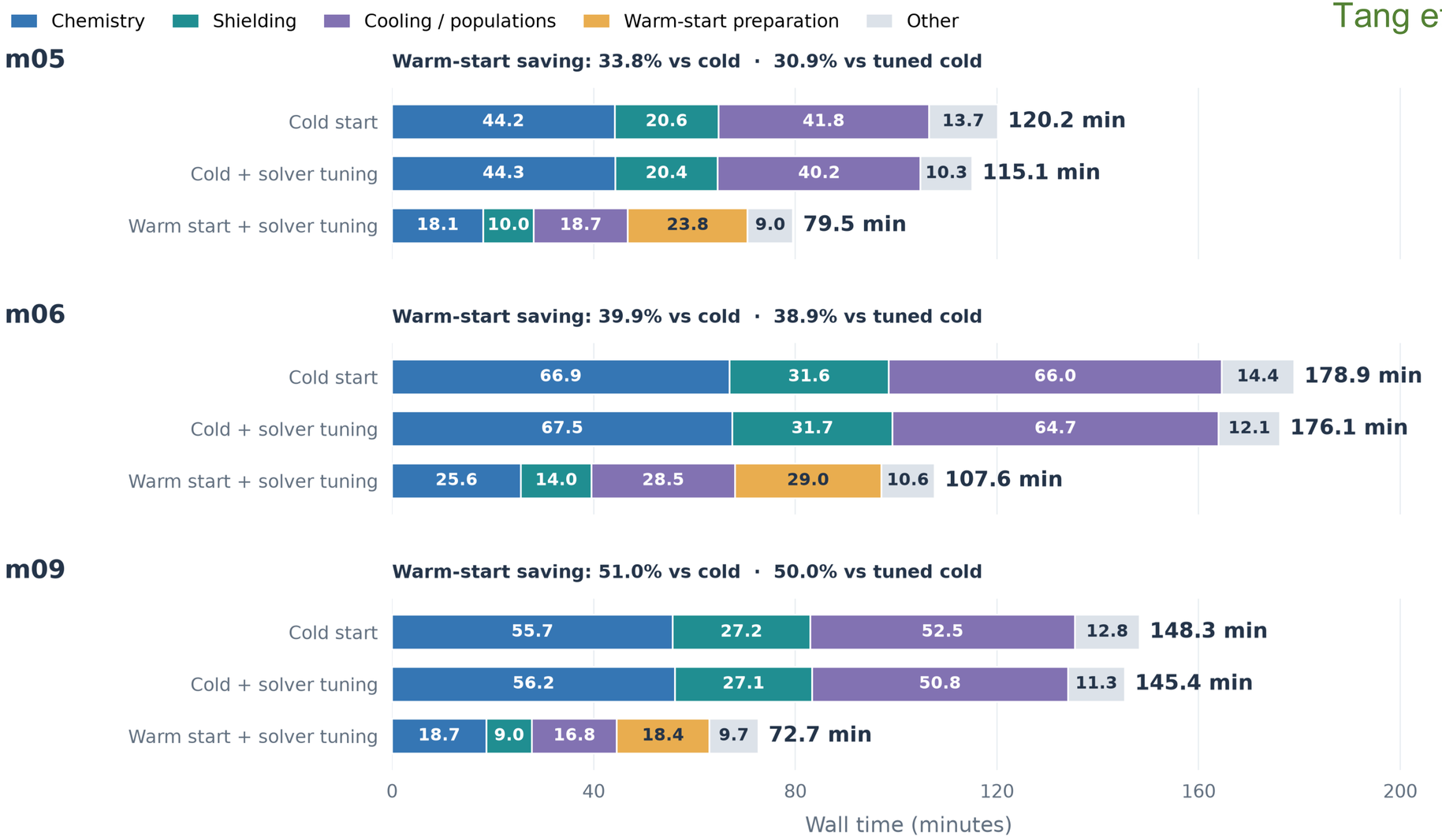
Physical model	3D-PDR: **33 species, 331 reactions**, coupled chemistry, cooling and thermal balance
Training data	**16 simulations on a 128^3 cloud**, varying UV radiation and cosmic-ray ionization; split by simulation: **8 training / 3 validation / 3 test / 2 held-out**
Neural network	**14 physical inputs → 3 hidden layers × 256 neurons (MLP)**; predicts an initial temperature and abundance state
Physics checks	Enforce elemental and charge constraints; reject unreliable predictions; then run the physical solver

Warm initialization reduces end-to-end time by 31%-50% with identical solver tuning

First result (CPU only) on 128^3 cubes, end-to-end time comparison

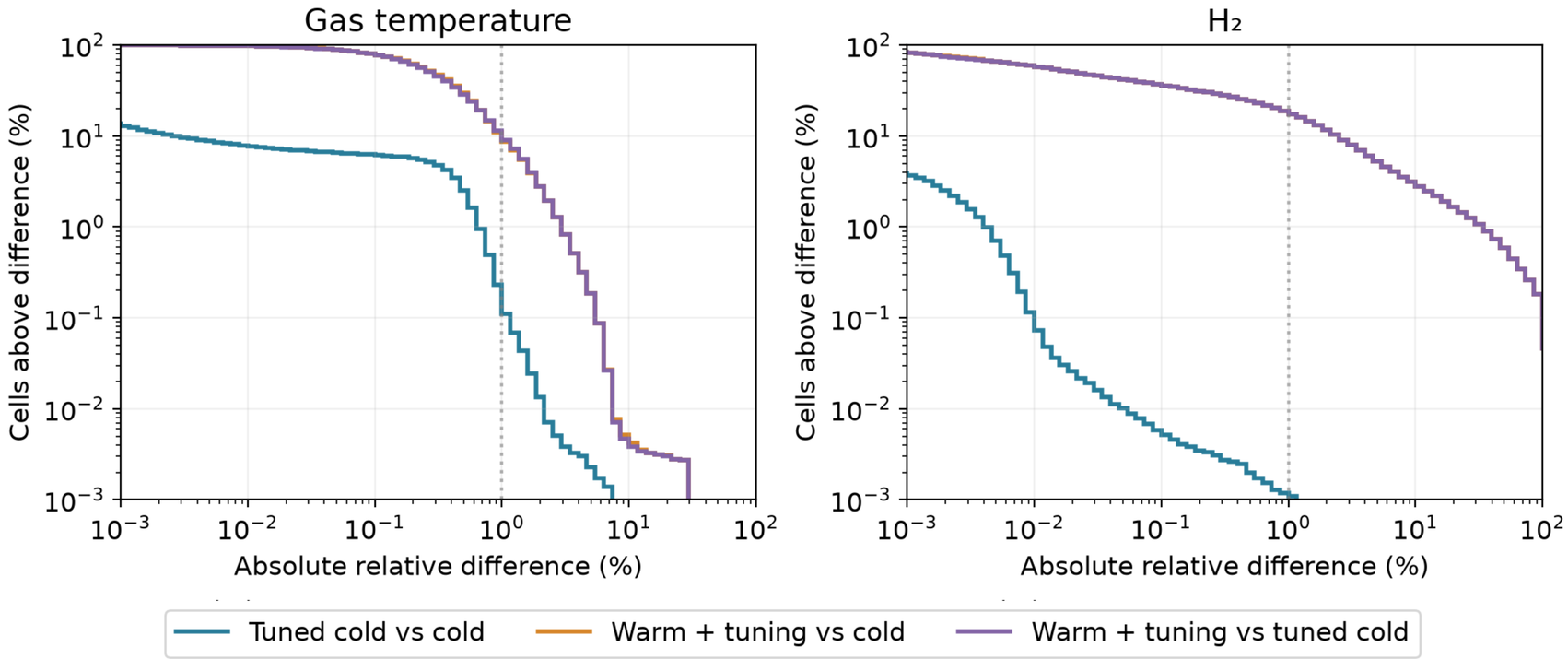
M05, M06, M09 are 3DPDR simulations on one cloud with different FUV & CRIR

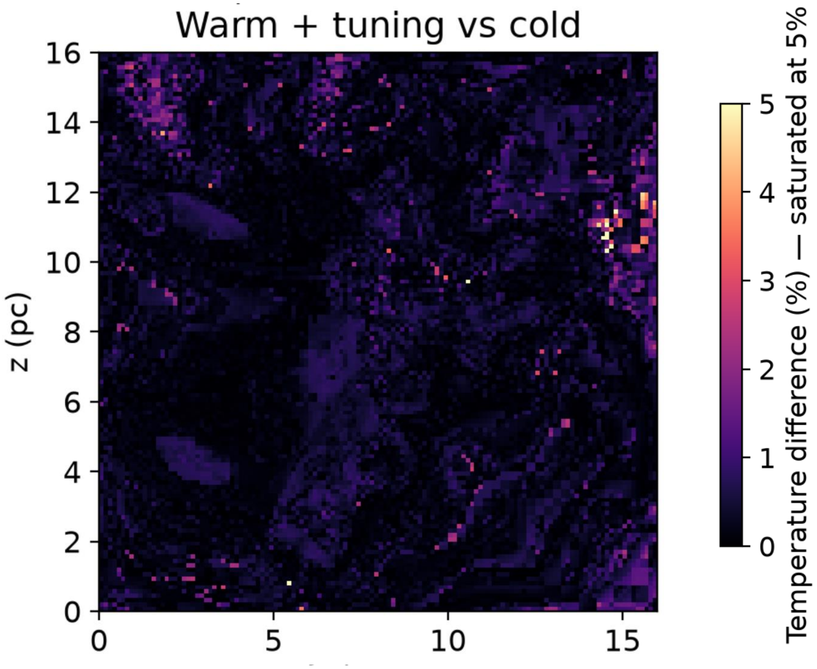
Tang et al. in prep



Validation on M05: close total cooling, but local differences remain – room to improve

- Total cooling difference: **0.037%**
- Temperature: **99% of cells differ by less than 2.73%**
- H_2 abundance: **95% differ by less than 4.92%; 99% by less than 31.1%**





Tang et al. in prep

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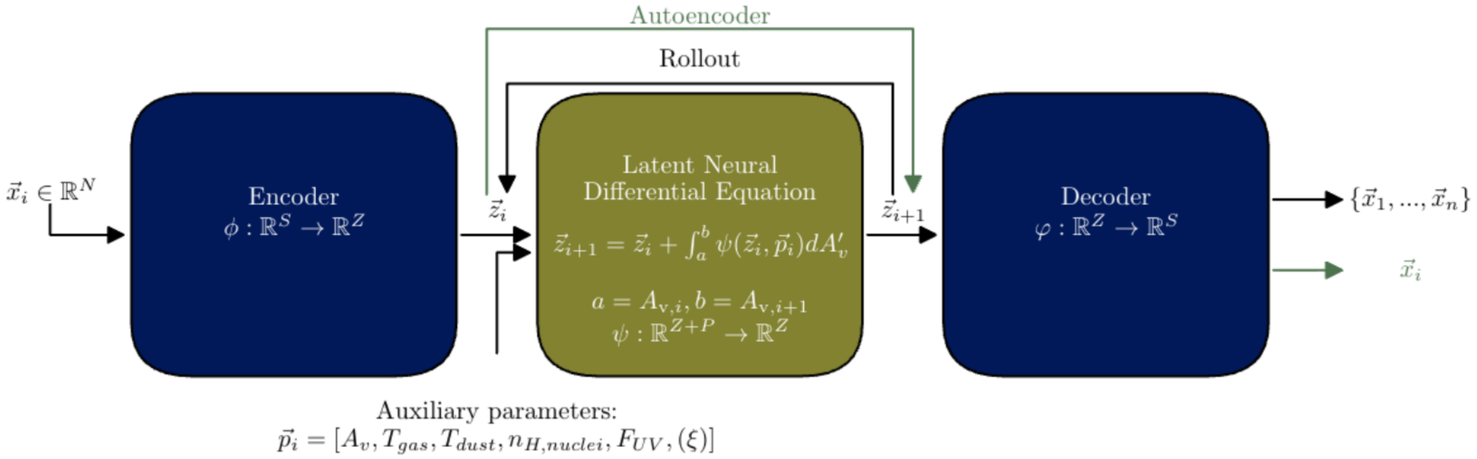
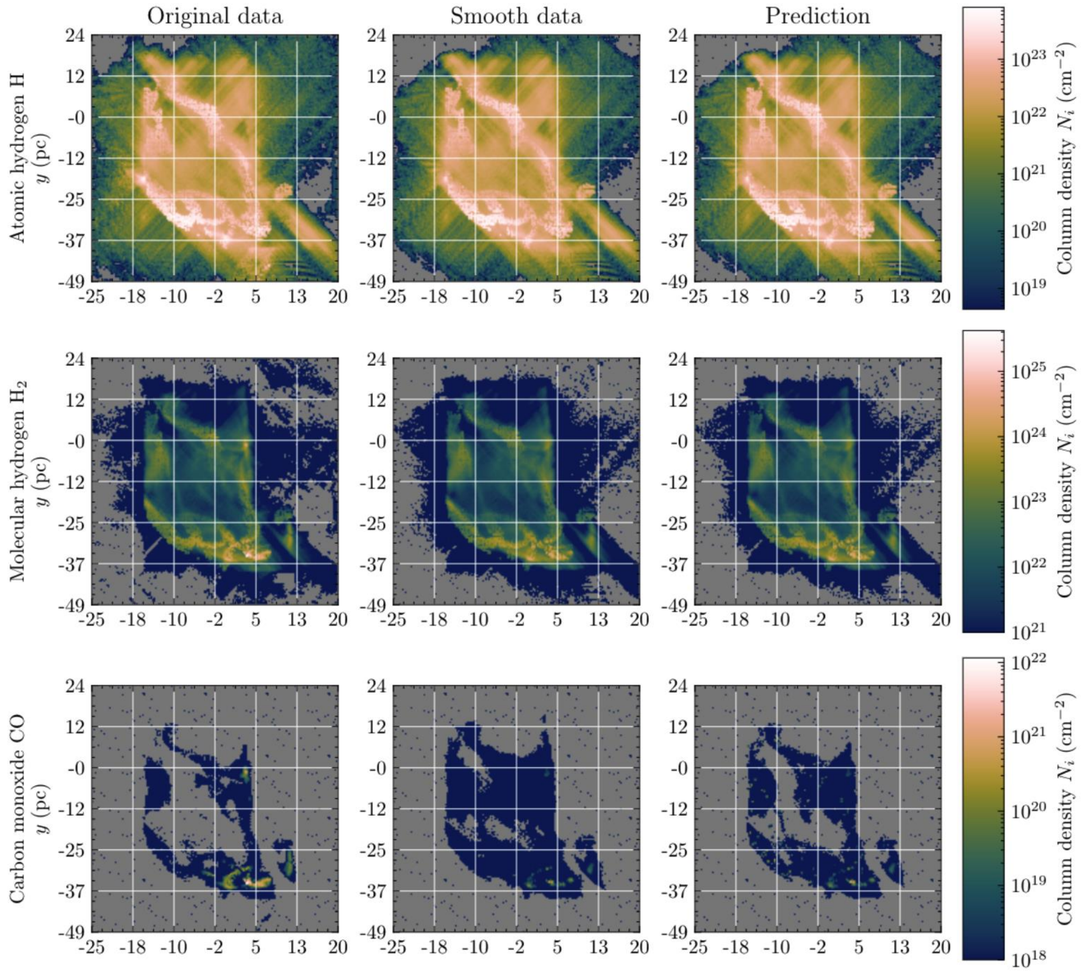
Two ways to accelerate:
1. help the solver, or
2. emulate its output.

NeuralPDR (Vermarien et al. NeurIPS 2024; Vermarien, Bisbas et al. 2025)

NeuralPDR uses neural ODEs to emulate abundance profiles, from which species column-density maps can be reconstructed.





Reproduces abundance profiles and enables reconstruction of species column-density maps at substantially lower computational cost.

NeuralPDR+ improves scientifically important predictions:

1. **Give core species higher weight**
   Prioritize errors in key species, including H, H_2, C, CO & C^+

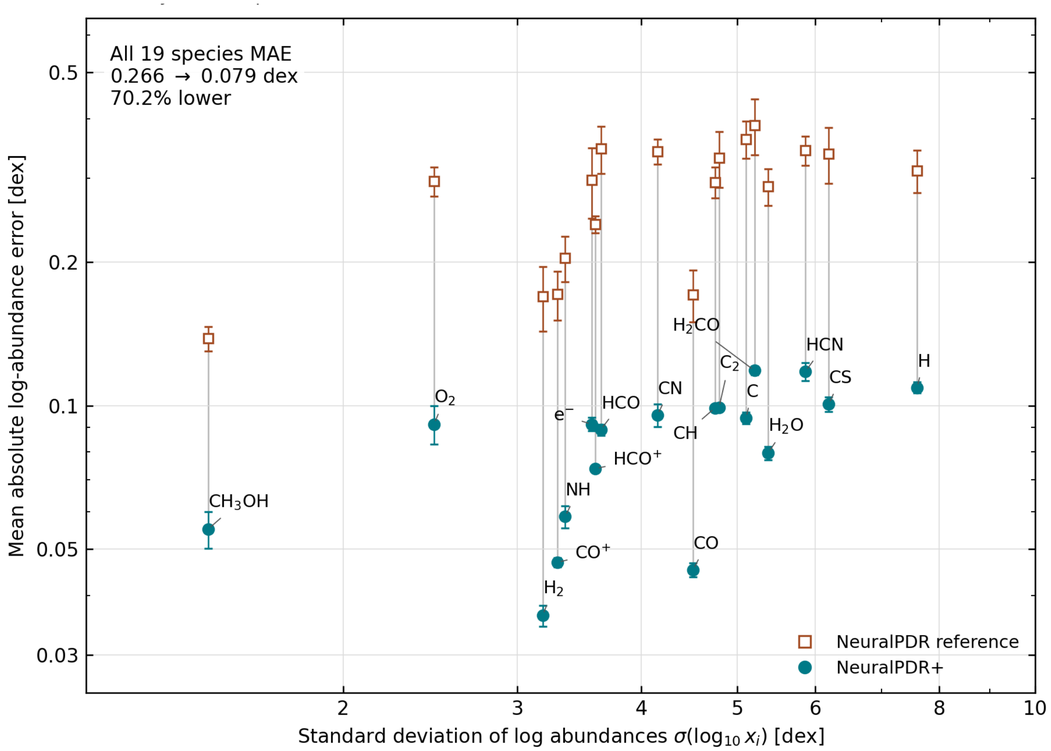
2. **Two-stage optimization**
   1) learn a useful representation of the chemical state;
   2) learn how it changes through the cloud.

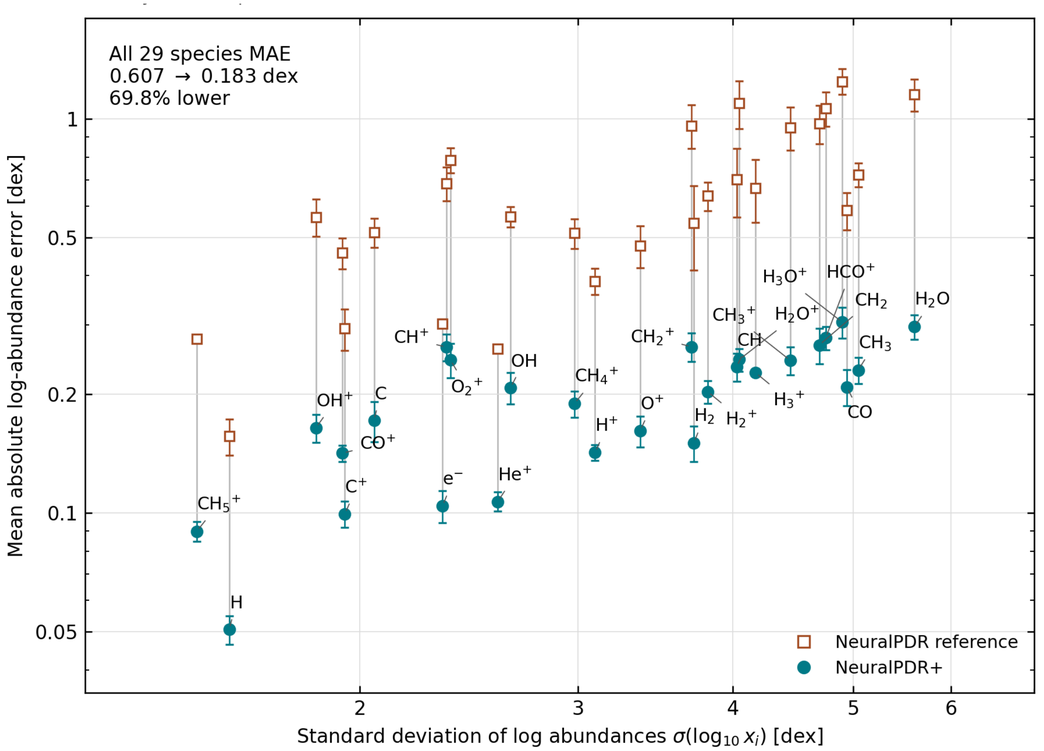
Main results:

≈70% lower mean absolute log-abundance error across species, compared to baseline;

26% lower error in **C+/C/CO-transition zone** abundance;

(Tang, Jiang et al. in prep)





Error bars: sample SD across three training seeds; species labels mark NeuralPDR+.

Exploratory development evidence

Takeaway messages

- Our ambition is to make 3D-PDR fit for next-generation hydro-chemical simulations;
- Warm-Start: uses AI to predict the initial state;
  keeping the physical solver in the loop;
  -- physically interpretable and directly verifiable;
- Early results of Warm-start reduces end-to-end time by 31%-50%;
- NeuralPDR+: an emulator of astrochemical abundances and column-densities.
- Domain knowledge and physical tests to guide AI and judge the results.

Thank you!