DARWEN: Data-Driven Algorithm for Reduction of Wide Exoplanetary Networks

An unbiased approach to accurately reduce chemical networks

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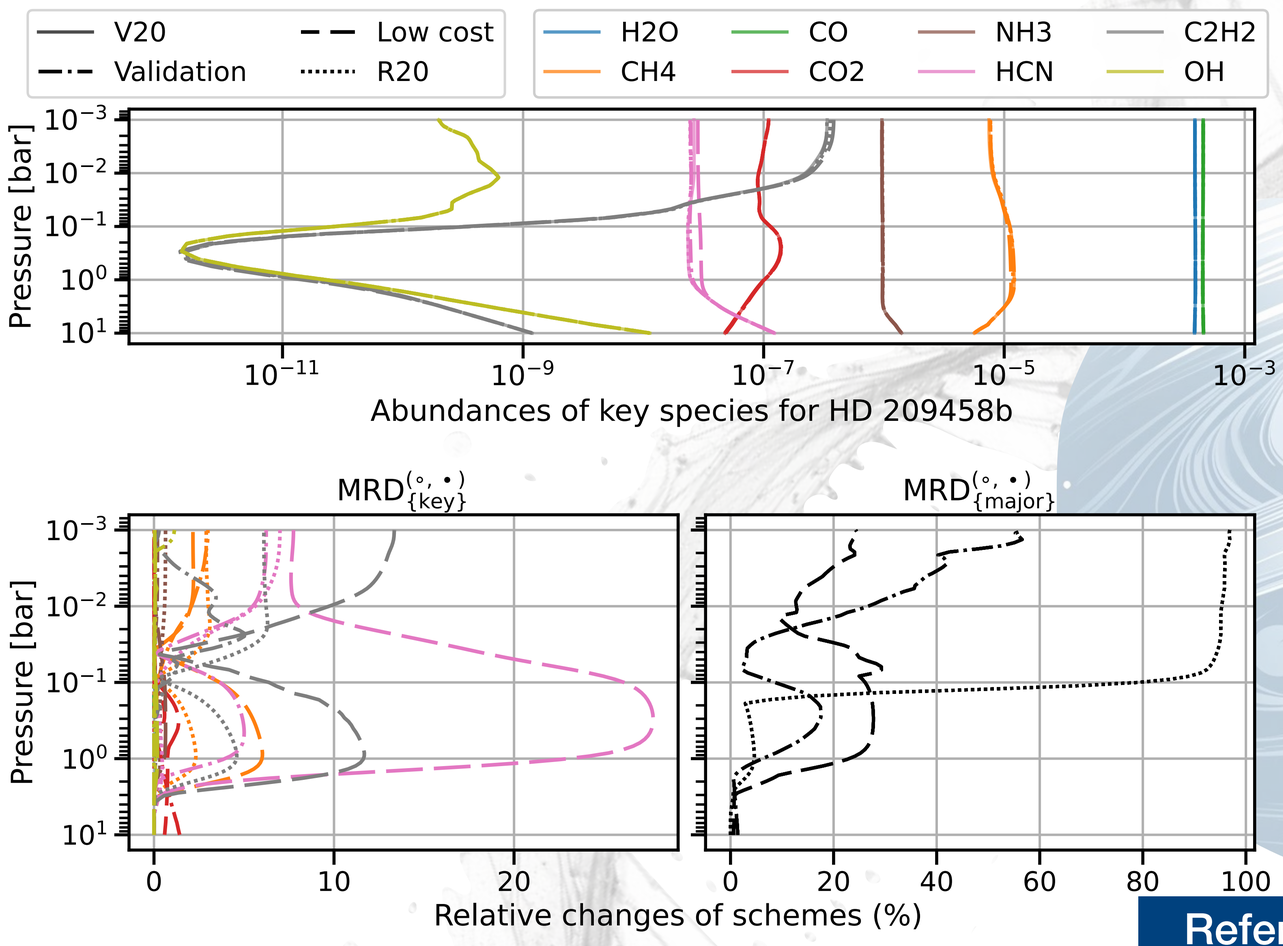
Introduction:

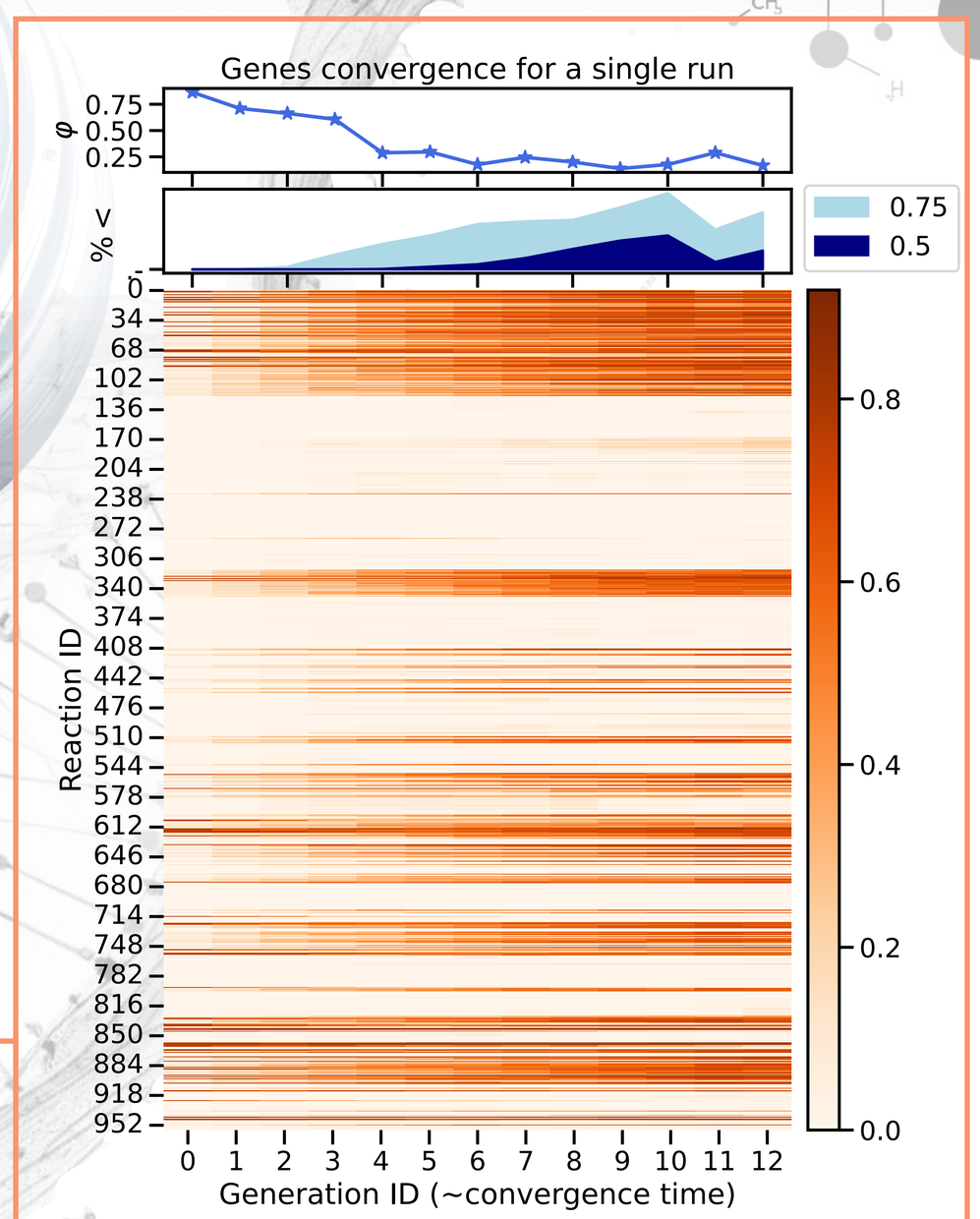
Advancements in exoplanet atmospheric modeling are crucial for interpreting observations from next-generation telescopes. Complex Global Circulation Models (GCMs) are often computationally expensive and limit chemical diversity. To address this, we introduce DARWEN, a genetic algorithm that reduces chemical networks efficiently, maintaining accuracy while enhancing computational efficiency.

Methodology:

Our method utilizes a 1D-model (Agúndez et al. 2014) and the full V20 network (Venot et al. 2020) for initial sensitivity analysis. We apply PCA to identify key reactions and species. DARWEN then optimizes the network by randomly generating and evaluating chemical schemes, progressing only the fittest to the next generation.



Abundances at each height and Maximum Relative Deviation (MRD) between full (•) and reduced schemes (∘); Validation, Low-cost and Venot et al. 2020 reduced (R20) scheme, for "key" molecules already found in exoplanets* and "major" species (molar fraction $> 10^{-20}$).



Example of one DARWEN's run:

Top: Minimum loss at each generation.

Middle: Percentage of the population below a certain loss.

Bottom: Average of the genes at each generation. Genes are binary (1 if the reaction is in the scheme, 0 otherwise). Averaging shows the prevalence of each reaction in the population.

Reference	Venot et al. 2020		Lira-Barria et al. (in prep)		
Scheme type	Full	Reduced	Validation	Low cost	Photo schemes
#reacs	1904	583	576	298	756
#species	107	44	47	32	48
MRD {key}	-	7%	**6%**	28%	16%
MRD {major}	-	97%	56%	29%	439%
Time	500s	26s	25s	**10s**	33s

Results:

DARWEN was used to reduce a full network for HD 209458b's atmosphere, focusing on different models:

Validation Schemes: Optimized for key molecular accuracies, achieving MRD as low as 0.06.

Low-Cost Schemes: Reduced computational times by over 2.5 times, maintaining high accuracy.

Photoschemes: Incorporated photochemical reactions for the first time, highlighting areas for future enhancement despite lower accuracy due to added complexity.

*Key molecules already observed in exoplanets: $\{key\} = \{H_2O, CO_2, CO, C_2H_2, OH, CH_4, NH_3\}$

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