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Characterization of exoplanetary atmospheres with GUIBRUSH®

G. Guilluy, P. Giacobbe, A. S. Bonomo

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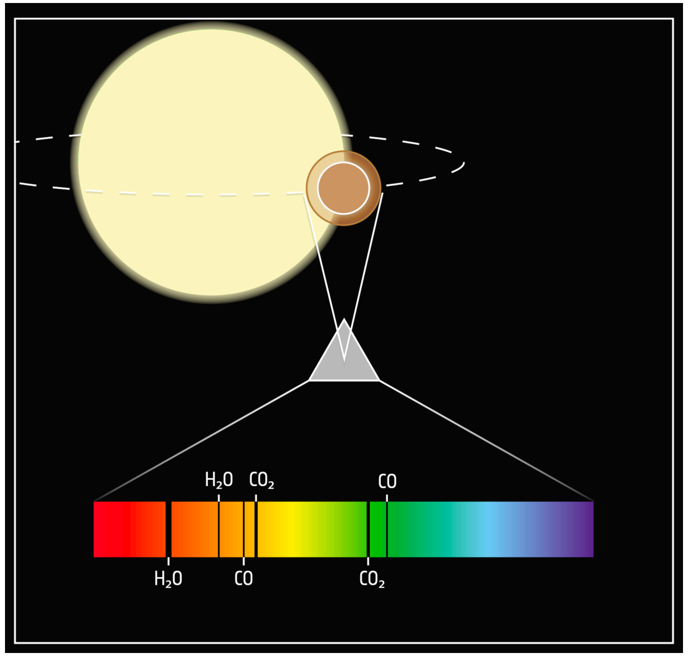
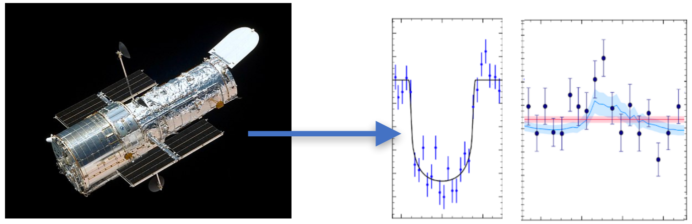
Scientific Rationale EXOPLANETARY ATMOSPHERES

- Encoded within a planet spectrum there is information about the *formation and migration history*.

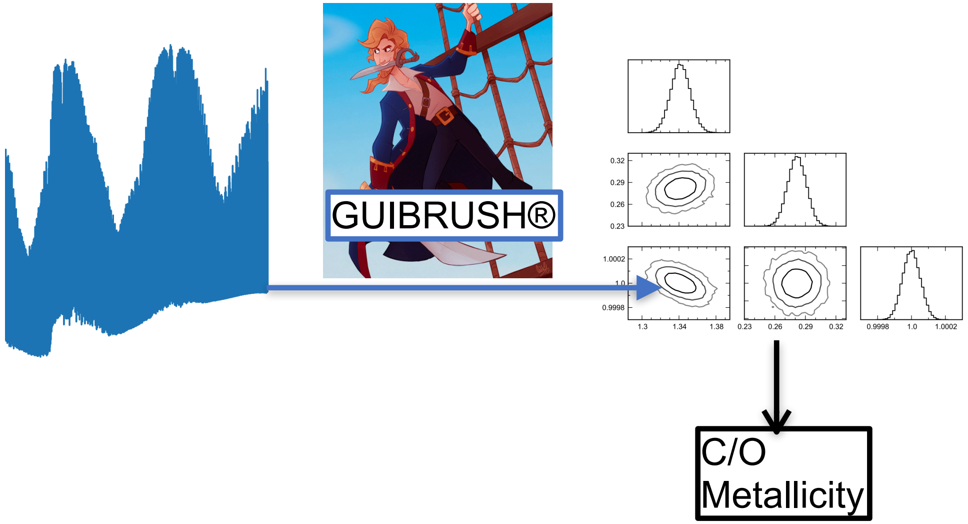
Transiting planets represent a gold booty to perform atmospheric studies.	How do we probe exoplanetary atmospheres?	GUIBRUSH®: A framework to determine the abundances of the detected species from transmission spectra



Space-borne Low-Resolution Spectroscopy



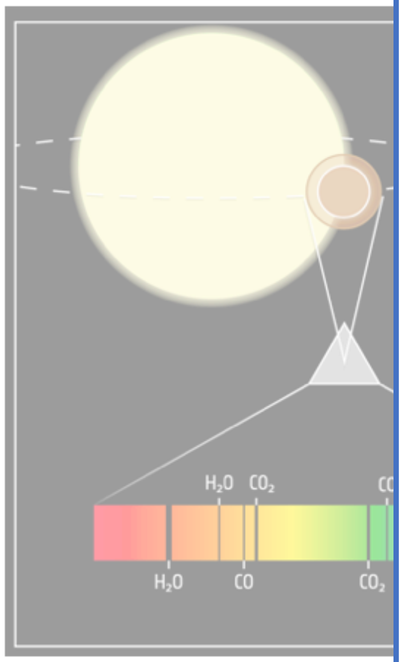
Ground-based High-Resolution Spectroscopy (R>20 000)



Scientific Rationale EXOPLANETARY ATMOSPHERES

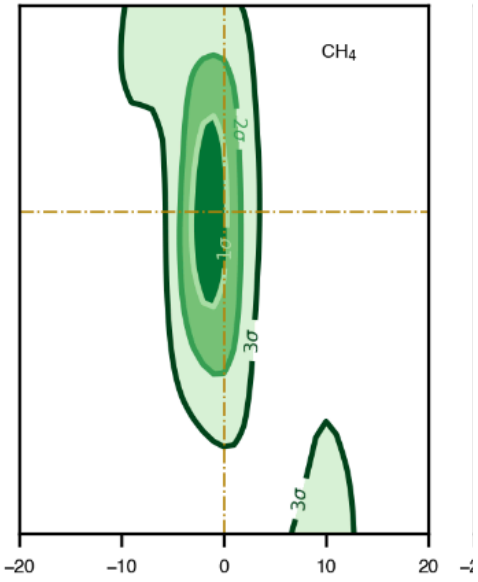
- Encoded within a planet spectrum there is information about the formation and migration history

Transiting planets r... booty to perform atm... ...ermine the abundances ...ransmission spectra



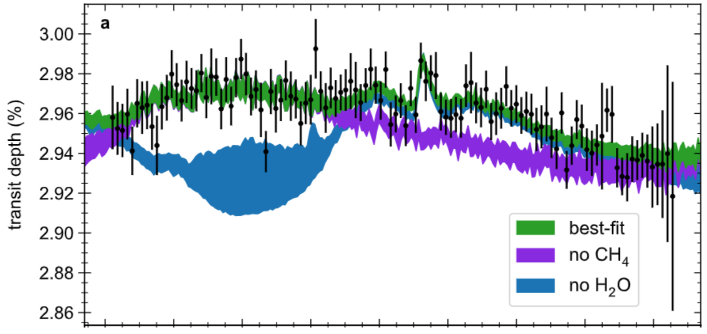
The future: HRS+LRS
An example WASP-80b

CH4 at HRS in transmission with GIANO-B

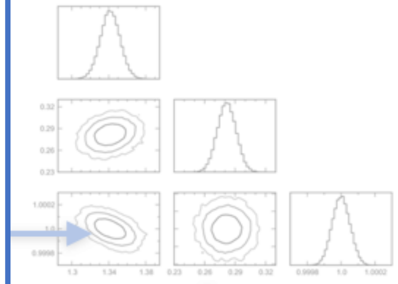


Carleo+2022

CH4 at LRS in transmission and emission with JWST's NIRCam



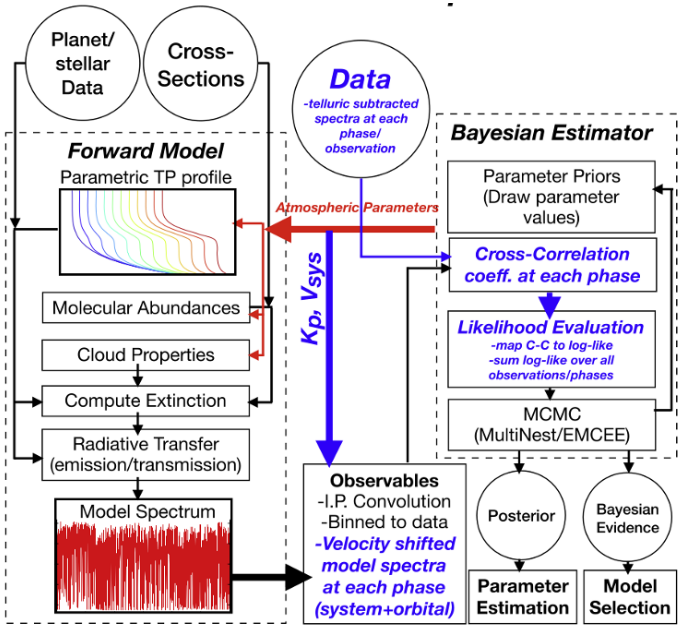
Bell+2023

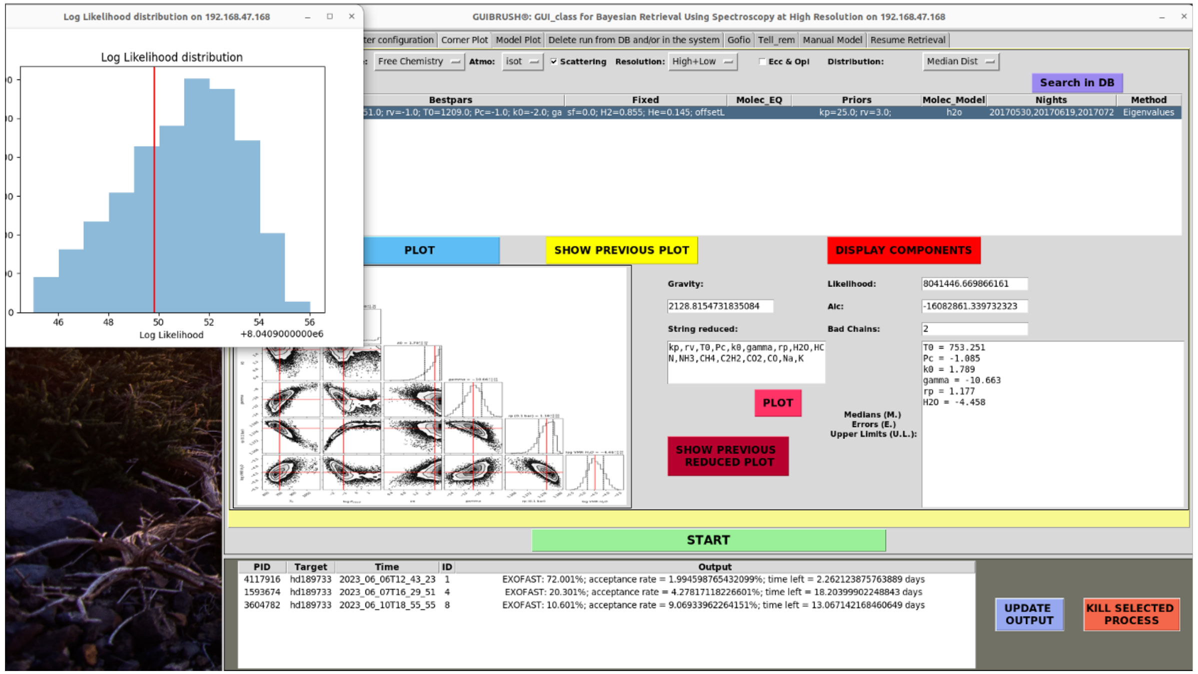


C/O
Metallicity

Technical Objectives, Methodologies and Solutions

- **The Code: GUIBRUSH®** is coded in Python > 3.8 and makes use of the Bayesian differential evolution Markov chain Monte Carlo (DE-MCMC) technique to explore the parameter space and derive the posterior distributions of the free parameters such as the abundances of the probed chemical species.

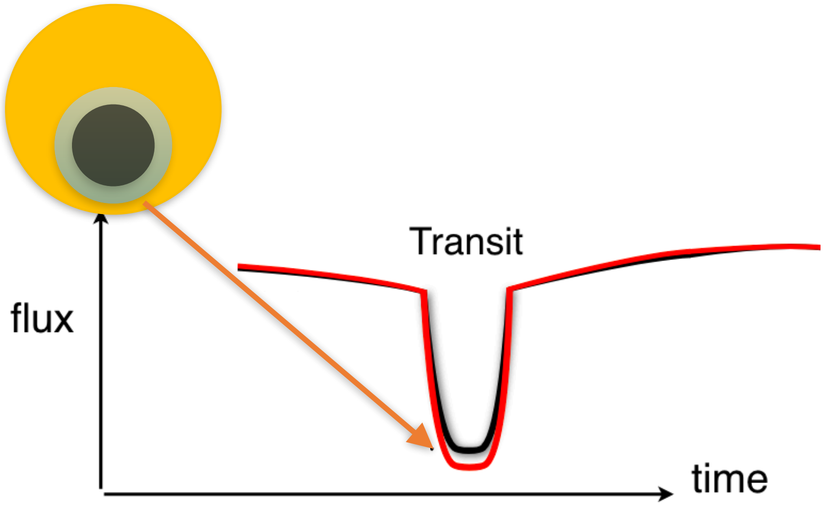




- GUIBRUSH® is currently run on the HPE Proliant DL560 Gen10 Server at INAF-Osservatorio Astrofisico di Torino, which was purchased with the PRIN-INAF 2019 project "HOT-ATMOS" (PI: A. S. Bonomo) and currently has 2 processors, 48 2.3Ghz cores and 256GB R AM; we will expand it to 6 processors, 144 cores, 750GB RAM in the next months thanks to an INAF minigrant (PI: P. Giacobbe).

Technical Objectives, Methodologies and Solutions

- The main <u>bottleneck</u> is due to the slowness of the radiative transfer code, which takes ~10 s to produce a single atmospheric model at each step of each DE-MCMC chain to be compared with the observed spectrum and thus compute the likelihood function. The currently employed radiative transfer code is the publicly available, open-source tool **petitRADTRANS** (Mollière 2019).



$$\text{Transit depth} = \frac{\Delta F_\lambda}{F_\lambda} = \frac{F_\lambda^{\text{out}} - F_\lambda^{\text{in}}}{F_\lambda^{\text{out}}}$$

RADIATIVE TRANSFER: $I_\lambda(\tau) = I_0 e^{-\tau_\lambda}$

$$\text{Transit depth} = \frac{1}{R_*^2}\left[R_{\text{top}}^2 - 2\int_0^{R_{\text{top}}} e^{-\tau_\lambda} b\,db\right]$$

- The <u>**goal**</u> would be to reduce the computation time of a single atmospheric model by at least a factor of 10, that is about or less than 1 s.

- A possible <u>**solution**</u> would be replace petitRADTRANS with **PYRAT BAY** (Cubillos & Blecic 202) "whose developers are our scientific collaborators" and parallelize it (still to understand how: CPU, GPU,…)

Timescale, Milestones and KPIs

March 2023
M1: **Parallelization of the DE-MCMC routines from IDL to Python with the Multiprocessing Python library** (process class)

February 2024
KPI1: implementation of Pyrat Bay in our code

August 2024
KPI2: tests on > 5 objects for which GIANO-B and JWST data are available
+ scientific results

End 2024
M2: **Parallelization of the radiative transfer code**

June 2024
KPI3: scalability of the process

August 2025
M3: **running GUIBRUSH® on larger (e.g., PNRR) HPC infrastructures**

->Times can vary depending on the work required for each step.

Accomplished Work, Results

- The work carried out since last September has consisted in **translating DE-MCMC routines from IDL to Python and parallelizing them with the Multiprocessing Python library** (process class), which has decreased the computation time approximately by a factor of 15

- We are getting familiar with the radiative transfer codes (i.e., PYRAT BAY and petitRADTRANS)

- We are studying a new open-source radiative transfer code **PYRAT BAY** (Cubillos & Blecic 2021), and comparing its performance with the currently used **petitRADTRANS** transfer code;

Next Steps and Expected Results (by next checkpoint: April 2024)

- **Replace the code petitRADTRANS with PYRAT BAY, if a significant gain in execution time is achieved**

- **Initial steps to parallelize the code**

GloriaGuilluy@INAF536.onmicrosoft.com

Nome utente *

GloriaGuilluy

@

Nome di dominio *

INAF536 .onmicrosoft.com

Salva

Password *

Siriotta1!

GloriaGuilluy@INAF536.onmicrosoft.com

Confermare password *

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