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

GUIBRUSH®: Where We Are and Where We're Headed

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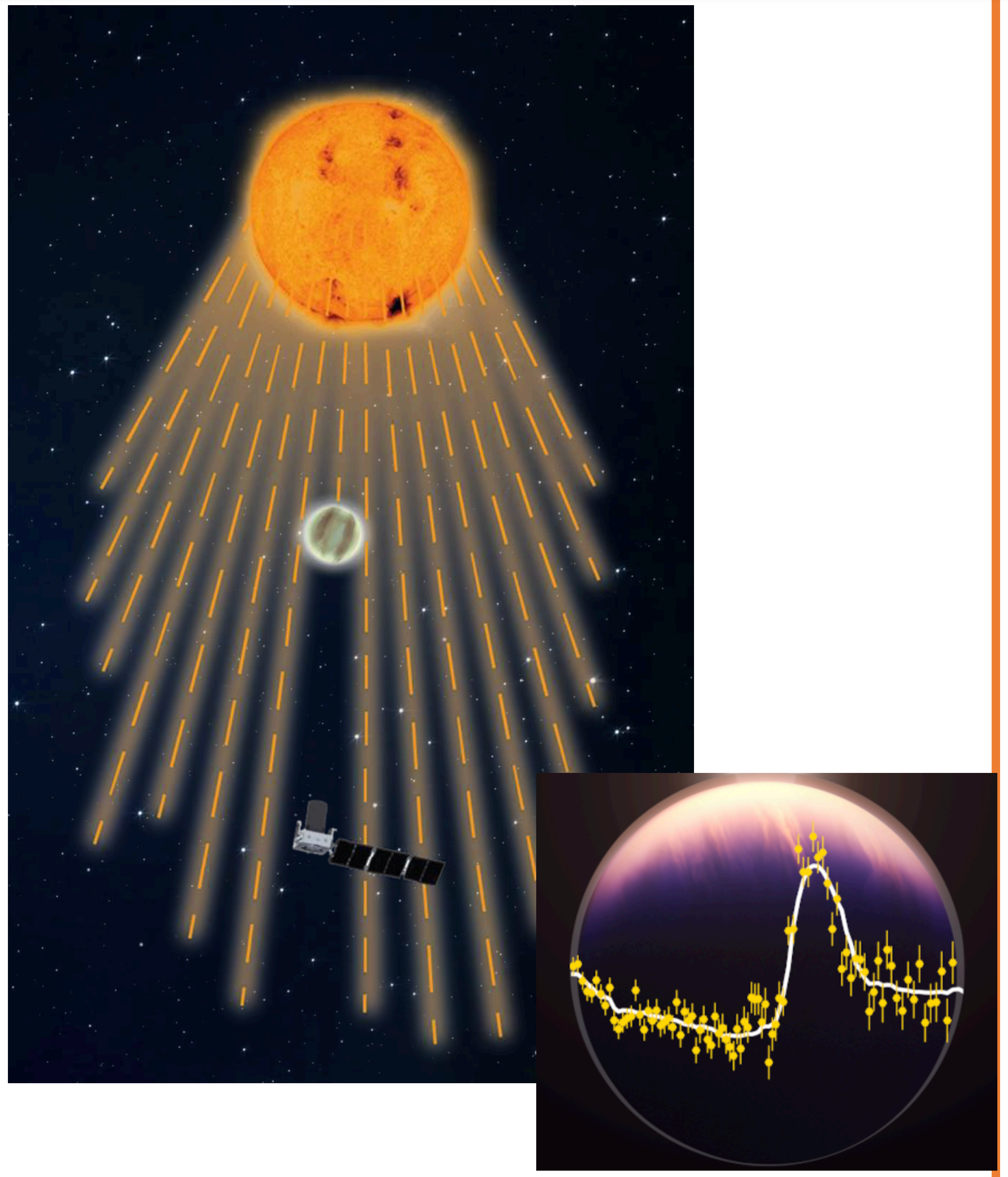
Scientific Rationale

EXOPLANETARY ATMOSPHERES

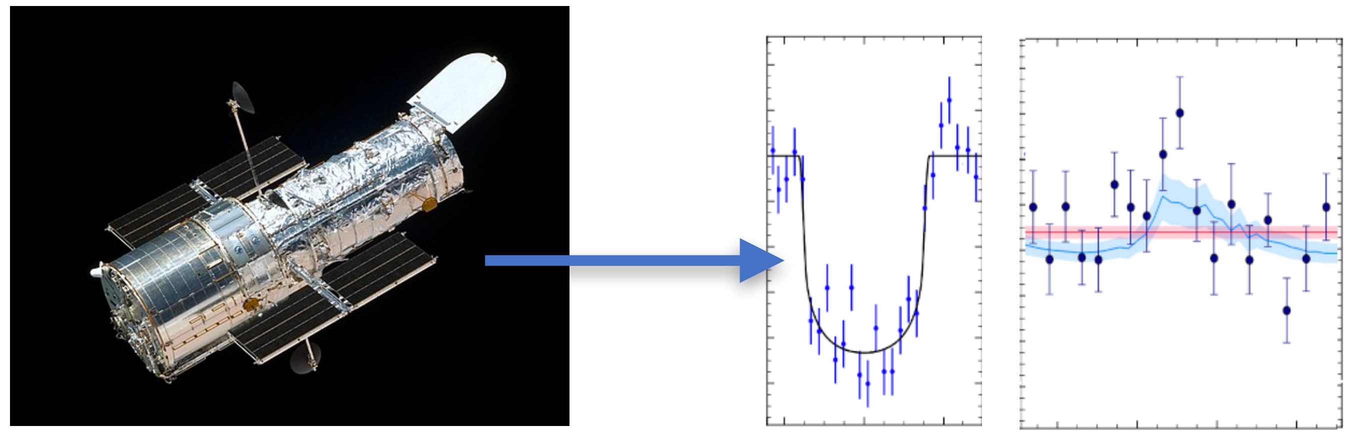
- A planet's spectrum holds clues to its formation and migration history

Transiting planets represent a gold booty to perform atmospheric studies.



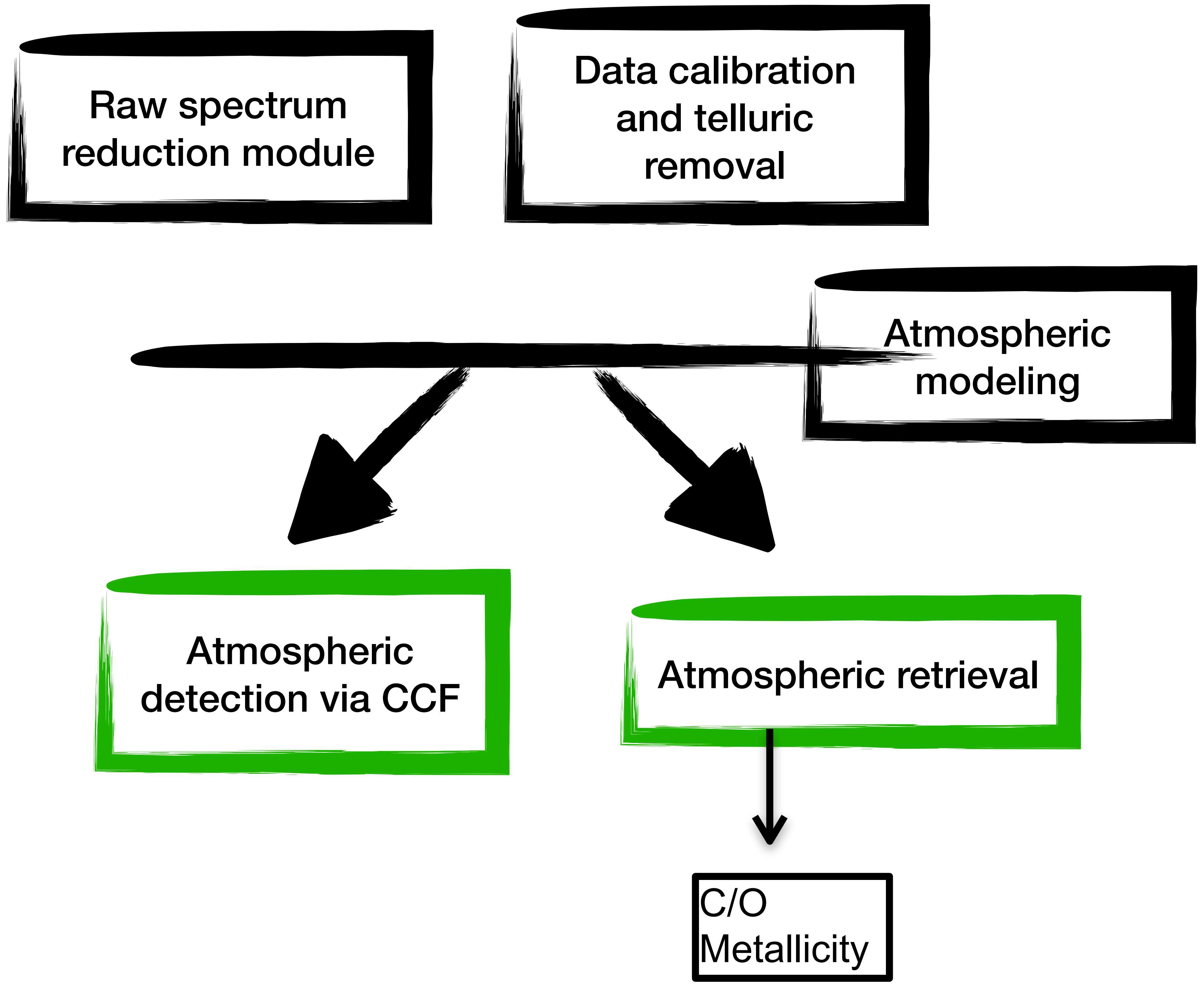
How do we probe exoplanetary atmospheres?

Space-borne Low-Resolution Spectroscopy



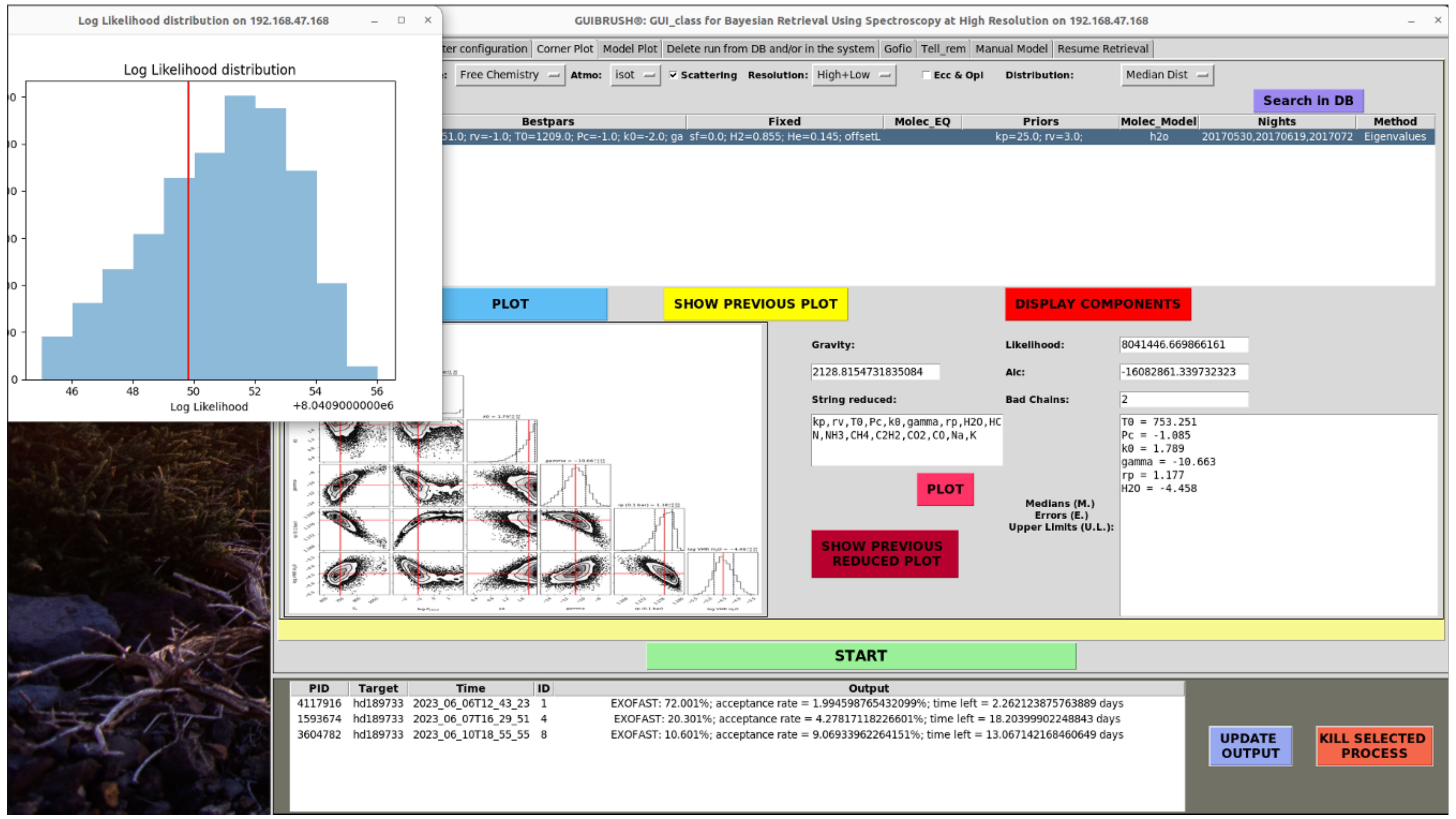
Ground-based High-Resolution Spectroscopy (R>20 000)

GUIBRUSH®:
Is a user friendly workspace to study and characterize exoplanetary atmospheres



Technical Objectives, Methodologies and Solutions

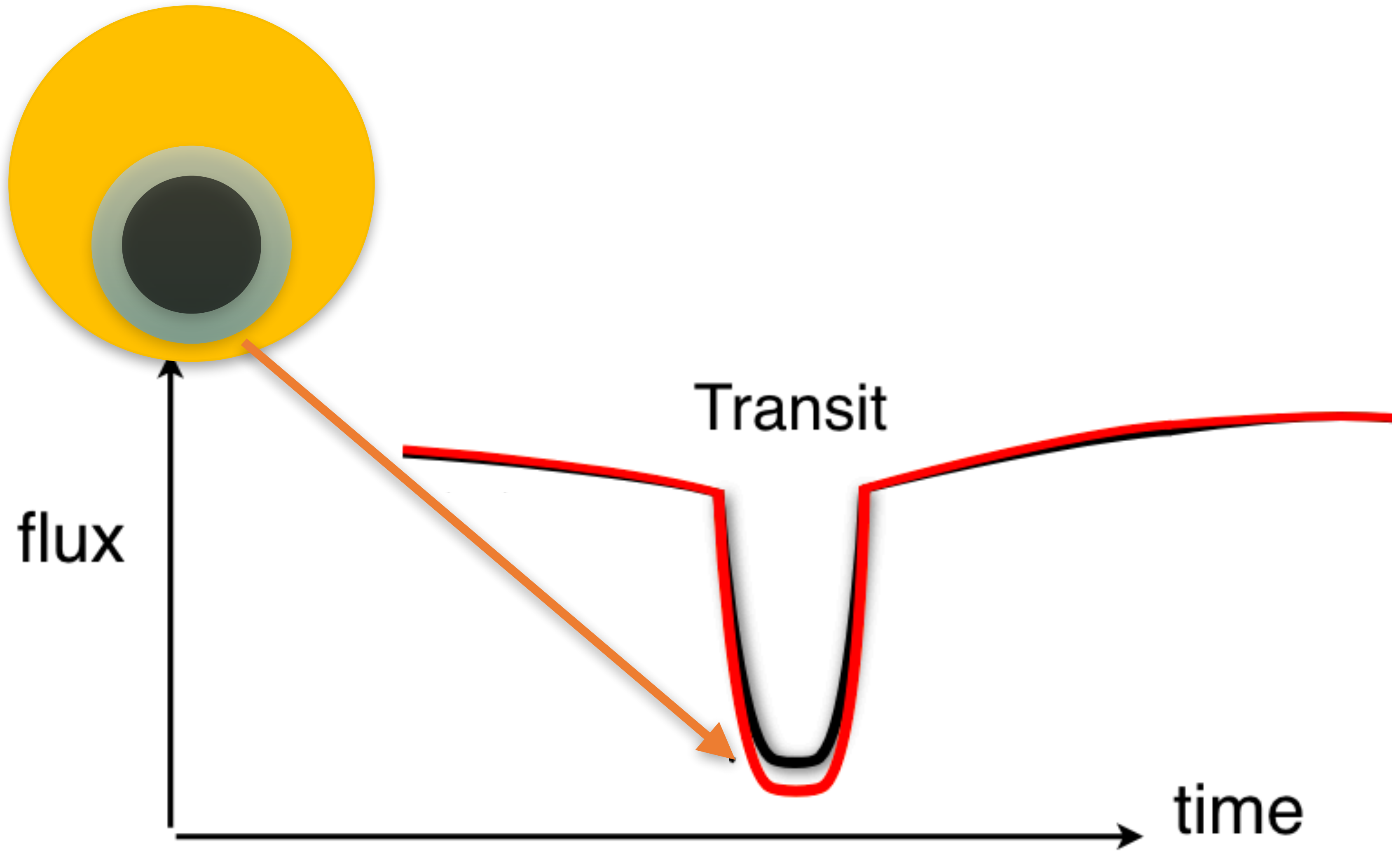
- **The Code: GUIBRUSH®** is coded in Python > 3.8 and makes use of the Bayesian differential evolution Markov chain Monte Carlo (DE-MCMC) technique to explore the parameter space and derive the posterior distributions of the free parameters such as the abundances of the probed chemical species.



- 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 bought another server with CPU + GPU Nvidia (16 k€) thanks to an INAF minigrant (PI: Giacobbe, 11 k€) + overhead CN-HPC Spoke 3 (2.5 k€) + overhead PRIN MUR 2022 ESPLORA (PI: A. S. Bonomo, 2.5 k€).

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

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

$$\tau(\nu) = \int e(\nu)\mathrm{d}s,$$

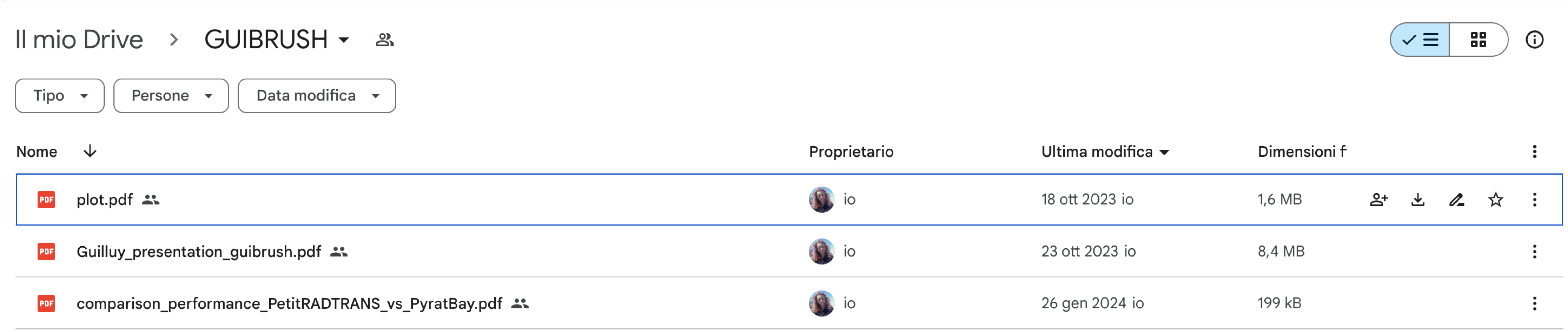
OPTICAL DEPTH:
how opaque the atmosphere is across a given path ds

- **Goal**: reduce the computation time of a single atmospheric model by at least a factor of 10, that is about or less than 1 s.

Timescale, Milestones and KPIs

Milestone	Target	KPIs	Date
M6	Translation of the differential evolution Markov chain Monte Carlo (DE-MCMC) Bayesian code from IDL to Python > 3.8 and parallelization of the DE-MCMC code with the Multiprocessing Python library (process class)	code available at https://www.ict.inaf.it/gitlab/paolo.giacobbe/giano-b (private gitlab repository); plot of the DE-MCMC posterior distributions of the free parameters obtained after a GUIBRUSH-R analysis for a typical hot Jupiter exoplanet (plot.pdf at https://drive.google.com/drive/folders/1uPRI3zgJqUNDUYHafKRmCd3HLH26HePQ?usp=sharing); presentation made by G. Guilluy at the Spoke 3 Technical Meeting in Trieste, 9-11 October 2023, (Guilluy_presentation_guibrush.pdf at https://drive.google.com/drive/folders/1uPRI3zgJqUNDUYHafKRmCd3HLH26HePQ?usp=sharing)	August 2023

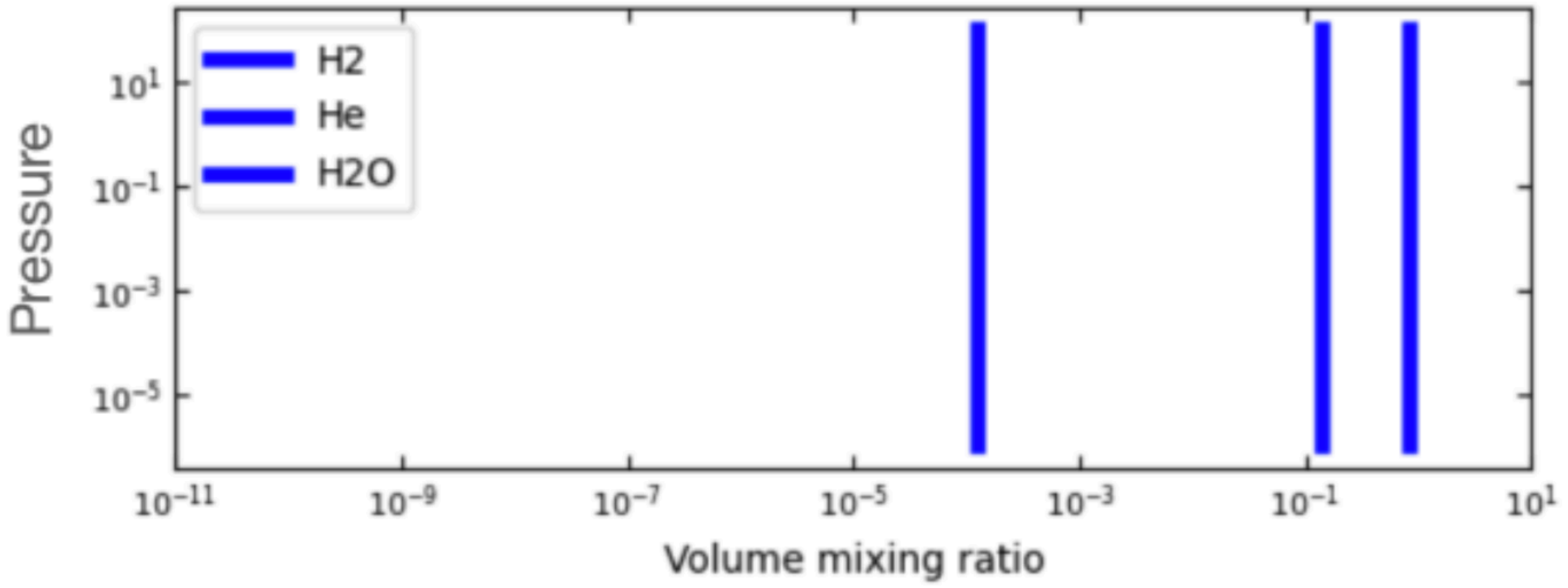
Decrease in computing time by a factor of 15



Timescale, Milestones and KPIs

Milestone	Target	KPIs	Date
M7	Decision on which radiative transfer code to use	internal report available at https://drive.google.com/drive/folders/1uPRI3zgJqUNDUYHafKRmCd3HLH26HePQ?usp=sharing (file comparison_performance_PetitRADTRAI	Dec 2023

We generated a transmission spectrum for an atmosphere composed of H_2O, H_2 and He with both PYRATBAY and PetitRADTRANS. The investigated atoms and molecule have a uniform distribution at different pressures (atmospheric layers) with fixed volume mixing ratio. We simulated 100 atmospheric layers with a pressure between 10^{-6} — 10^{+2} bar



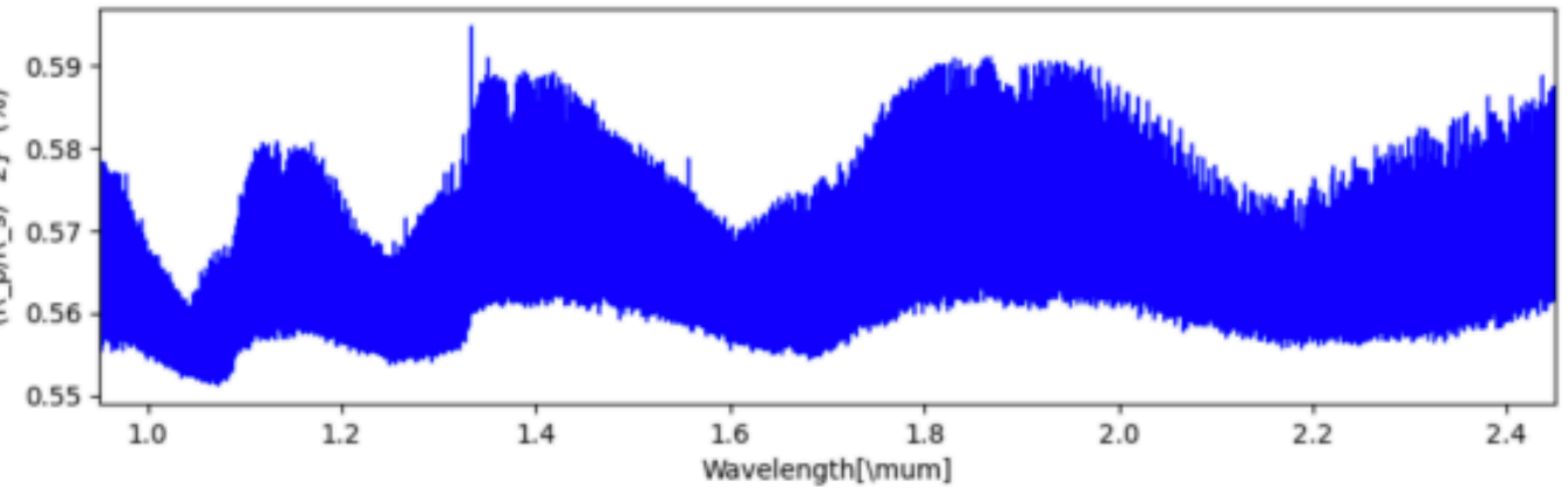


Figure 2, Transmission spectrum as a function of wavelength

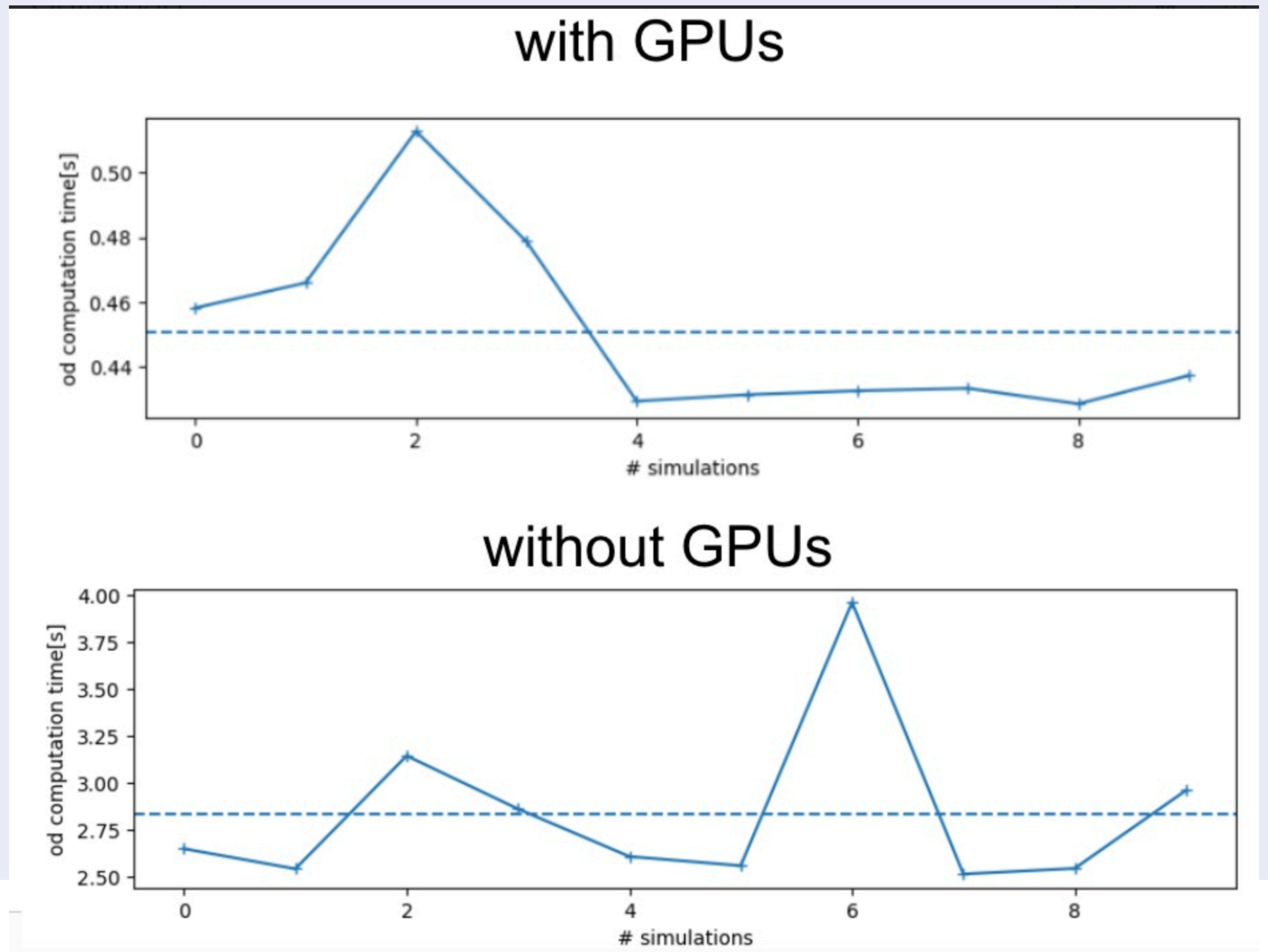
- We computed the opacity for H_2O from the HITEMP linelist at a resolution of R=250,000. We used a wavelength range [0.95-2.45] µm, which is the same range of the GIANO-B spectrograph at the Telescopio Nazionale Galileo (La Palma island).

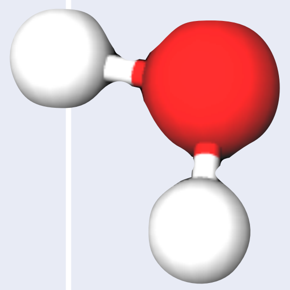
FINAL RESULT=> PetitRADTRANS takes: 2.630 s, while PYRATBAY takes: 2.405 s.

We thus decided to use the RADIATIVE TRANSFER CODE implemented in PYRATBAY, as it is a bit faster and the developer of the code is a close collaborator.

Timescale, Milestones and KPIs

Milestone	Target	KPIs	Date
M8	-Implementation of the GPU porting of the radiative transport code PyratBay (Cubillos & Blecic 2021), specifically of the subroutine performing the calculation of the optical depth integral, with PyCUDA. -We conducted several tests for an atmospheric synthetic model with only water vapor over a spectral range of 1 micron (0.95-1.95 micron) using the NVIDIA Tesla T4 GPU of Google Colab	internal report available at https://drive.google.com/drive/folders/1uPRI3zgJqUNDUYHafKRmCd3HLH26HePQ?usp=sharing	June 2024





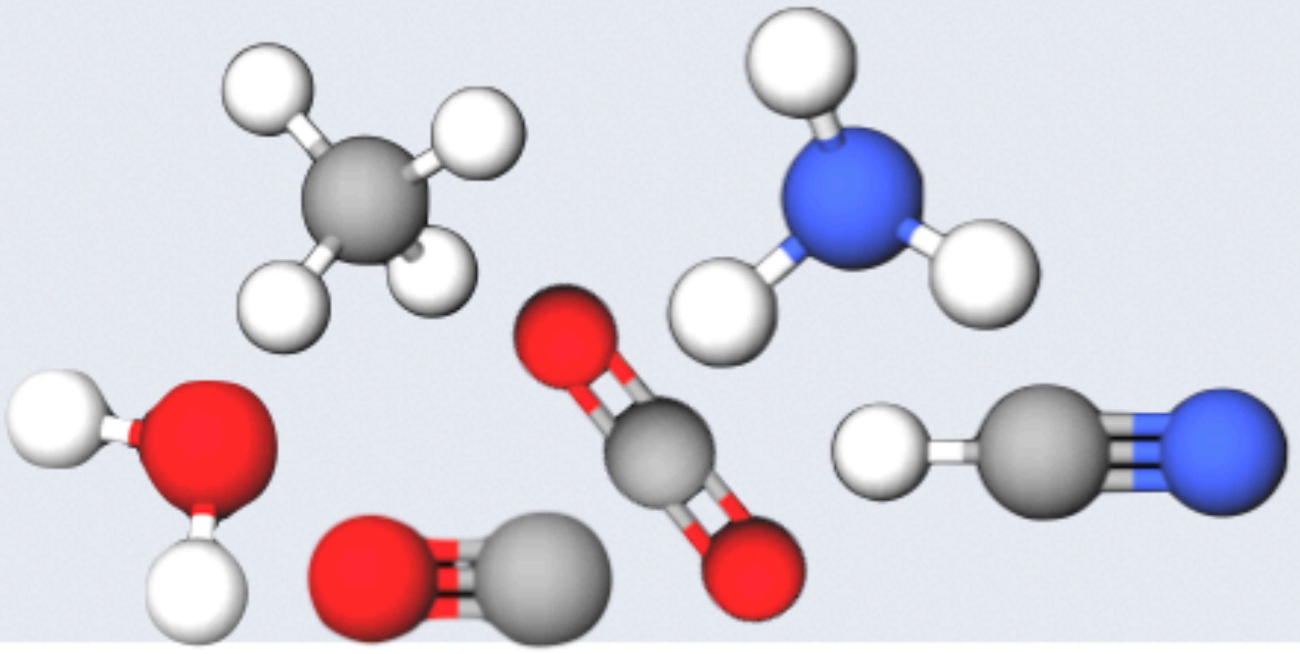
We achieved a gain in time by approximately a factor of 6.

-> We needed to carry out further tests for a model with more molecules (> 5) on a larger spectral range by using computational resources other than Google Colab, which is limited both in the available run-time and RAM.

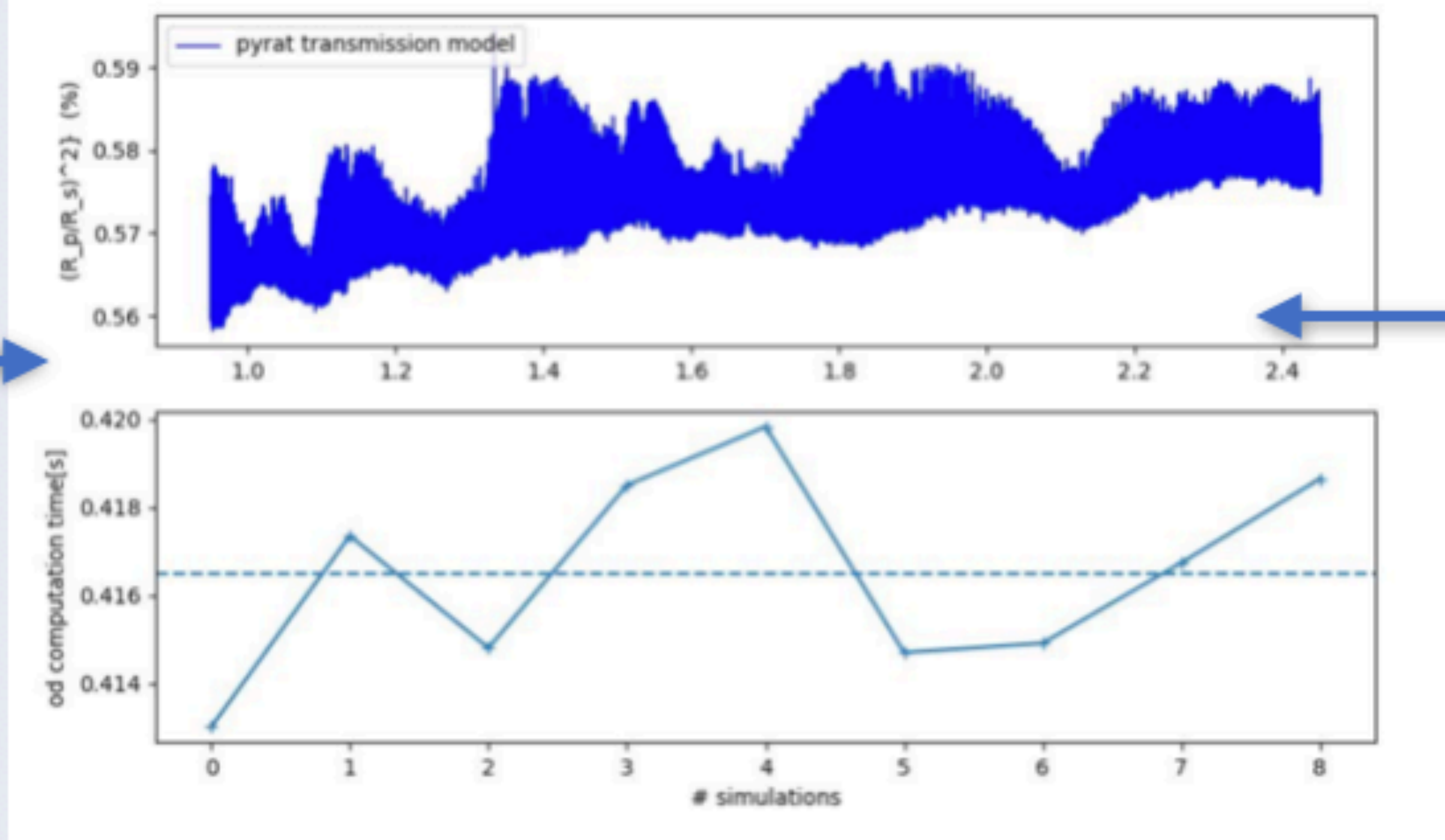
Timescale, Milestones and KPIs

- We requested computational resources from Leonardo

Milestone	Target	KPIs	Date
M9	Implementation in GUIBRUSH® of the sequential version of PyratBay (Cubillos & Blecic 2021) in place of PetitRADTRANS (Mollière 2019), Testing models with more molecules (> 5) over a larger spectral range.	internal report available at https://drive.google.com/drive/folders/1uPRI3zgJqUNDUYHafKRmCd3HLH26HePQ?usp=sharing	October 2024



Six molecules



All the GIANO-B range (0.95-2.45) micron

Timescale, Milestones and KPIs

- We requested computational resources from Leonardo

Milestone	Target	KPIs	Date
M10	-**Final optimisation of the GPU porting** of the radiative transfer module in PyratBay to further decrease the computation time in generating atmospheric models. Implementation of numerical integration (Gauss-Legendre) -**Identification of the new bottleneck**: the main bottleneck has been identified as the data transfer between CPU and GPU when performing the two different integrals in the Optical Depth Module and the Spectrum Module of the PyratBay code		May 2025

M10

FIRST STEP

1) OPTICAL DEPTH function

$$\tau(\nu) = \int e(\nu)\mathrm{d}s,$$

CPU

Input: Extinction coefficient

GPU

Output: od.depth (heavy)

CPU

⛔ copied from GPU to CPU

2) SPECTRUM function

$$\frac{\Delta F(\nu)}{F(\nu)}\bigg|_{transit} \equiv \frac{R_p^2}{R_s^2} = \frac{R_{top}^2 - 2\int_0^{R_{top}} e^{-\tau_\nu(b)}\,bdb}{R_s^2}$$

Input: od.depth (heavy)

GPU

Final Output: spectrum
→ Copied from GPU to CPU

CPU

🚨 Problem:
Two heavy data transfers of od.depth between GPU and CPU, causing inefficiency.

FINAL STEP

CPU

Input: Extinction coefficient

OPTICAL DEPTH function
➕
SPECTRUM function

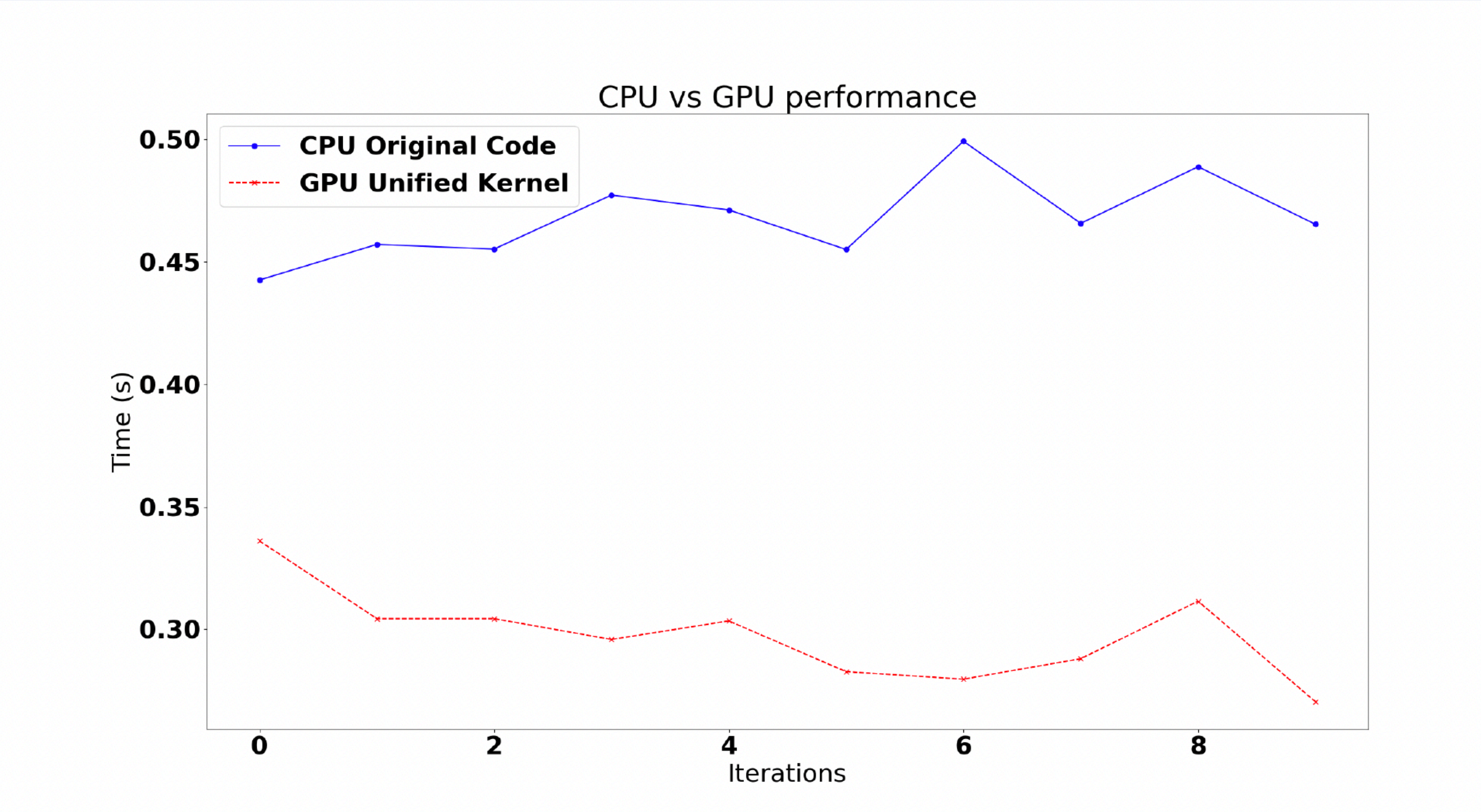
GPU

Final Output: spectrum

CPU

Timescale, Milestones and KPIs

- **We requested computational resources from Leonardo**

Milestone	Target	KPIs	Date
M10	**-Final optimisation of the GPU porting** of the radiative transfer module in PyratBay to further decrease the computation time in generating atmospheric models. Implementation of numerical integration (Gauss-Legendre) **-Identification of the new bottleneck**: the main bottleneck has been identified as the data transfer between CPU and GPU when performing the two different integrals in the Optical Depth Module and the Spectrum Module of the PyratBay code **-GPU Porting of the optical depth+spectrum integral calculation module**	GPU vs CPU performance  Figure: Plotting of ten executions of extinction, optical depth and spectrum with all the molecules (H_2, He, H_2O, CH_4, CO, NH_3, HCN, CO_2).	May 2025

Timescale, Milestones and KPIs

- We requested computational resources from Leonardo

<table>
<tr><th>Milestone</th><th>Target</th><th>KPIs</th><th>Date</th></tr>
<tr>
<td>M10</td>
<td>-Final optimisation of the GPU porting of the radiative transfer module in PyratBay to further decrease the computation time in generating atmospheric models. Implementation of numerical integration (Gauss-Legendre)

-Identification of the new bottleneck: the main bottleneck has been identified as the data transfer between CPU and GPU when performing the two different integrals in the Optical Depth Module and the Spectrum Module of the PyratBay code

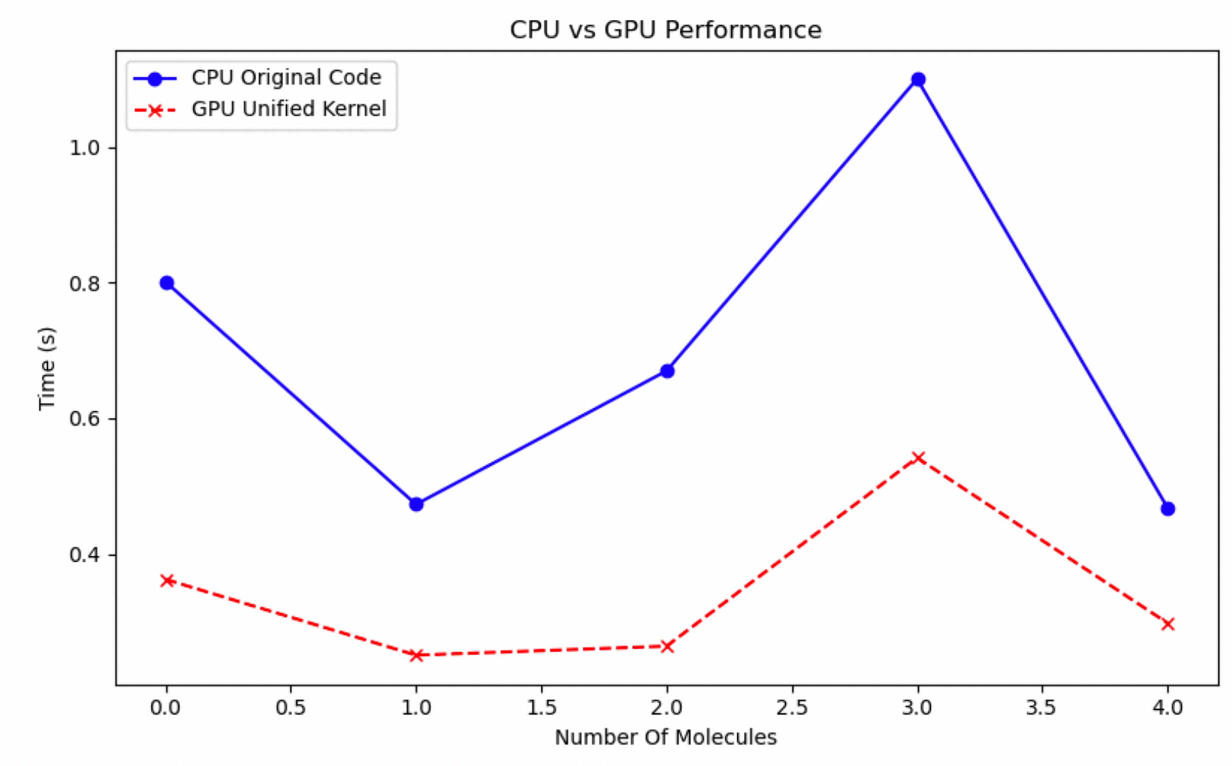
-GPU Porting of the optical depth+spectrum integral calculation module</td>
<td>Increasing #molecules


Figure: Execution of extinction, optical depth and spectrum with a different number of molecules each time. Check table 1 for the molecules used.</td>
<td>May 2025</td>
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Main results

- We **translated the DE-MCMC routines from IDL to Python and parallelized them with the Multiprocessing Python library** (process class), which has decreased the computation time approximately by a factor of 15;

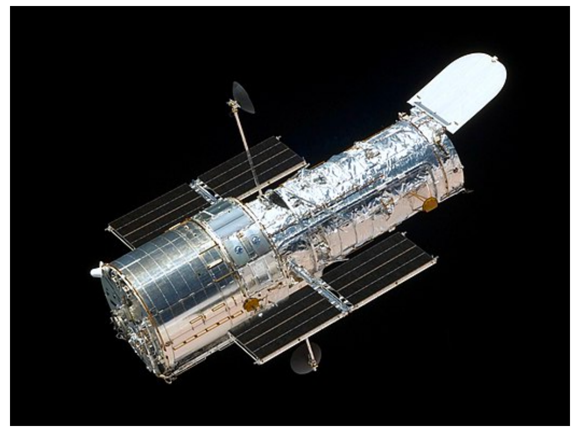
- We studied and got familiar with **radiative transfer codes PYRAT BAY** (Cubillos & Blecic 2021) and **petitRADTRANS** (Mollière 2019);

- We compared the performance of PYRAT BAY with that of petitRADTRANS;

- We completed the porting of the radiative-transfer module (optical depth+spectrum function) of **PYRAT BAY to GPU —> properly working code**

- **Final optimisation and finalization of the GPU porting** of the radiative transfer module in PyratBay (optical depth+spectrum function)

Final Steps



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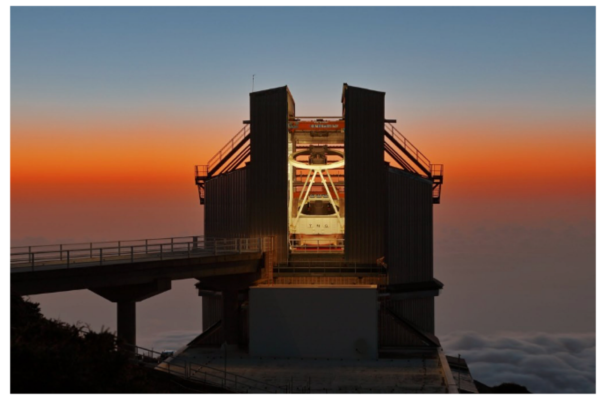

- Testing of the GUIBRUSH(R) code with the new GPU-ported version of PyratBay **on real low- (HST), high-resolution (GIANO-B@TNG) and the combination thereof of a couple of hot giant exoplanets**.

- **Posterior distributions of the molecular abundances and atmospheric parameters (e.g., Carbon-to-Oxygen ratio, metallicity, presence of clouds, temperature/pressure profile) obtained in the Bayesian DE-MCMC framework. Computation times of the analyses of the same targets performed with and without the GPU-ported version of PyratBay.**