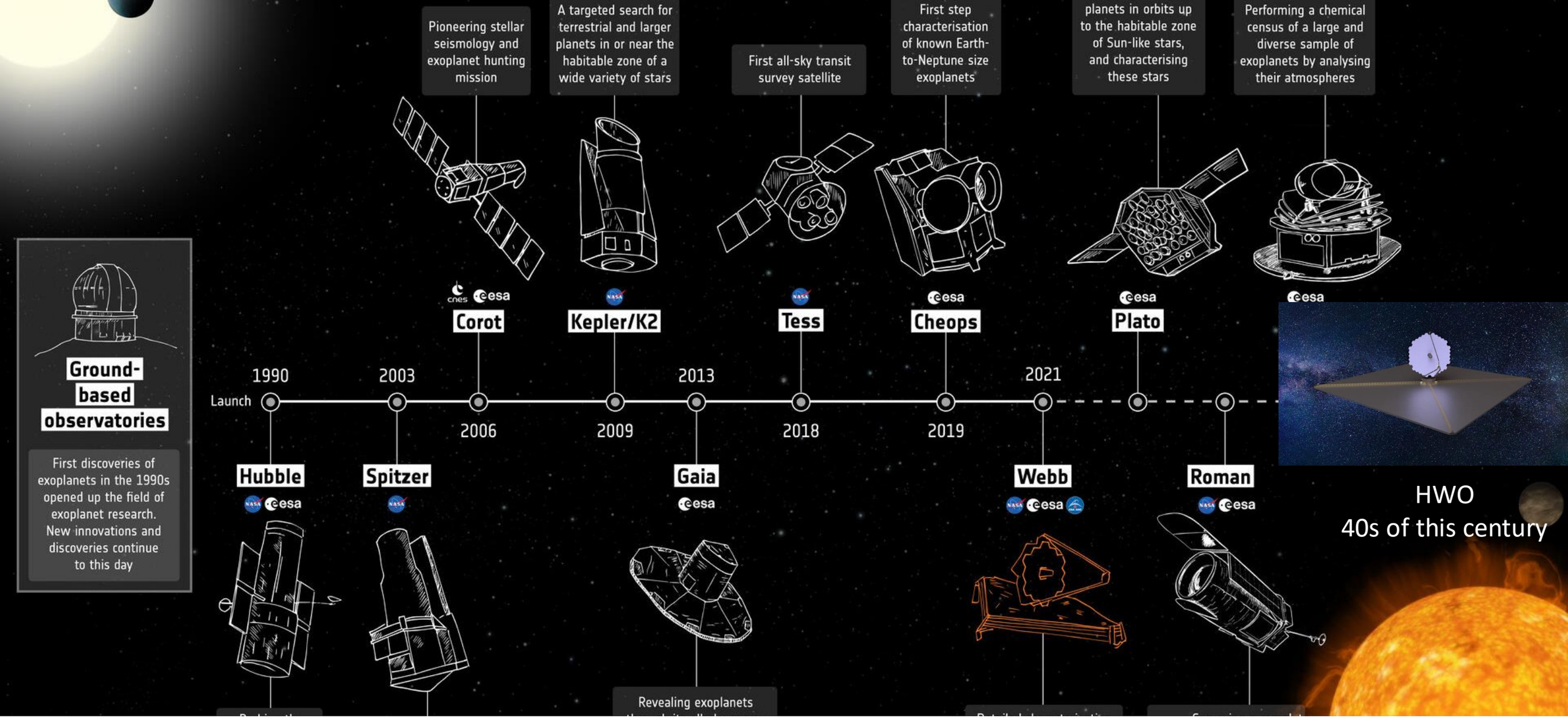
Atmospheric Retrievals

from machine learning to quantum technologies

Shaping the Italian Contribution to HWO
Rome 11/07/2025

Tiziano Zingales

General Introduction



The Golden Age of Exoplanets

As of today we know 7549 exoplanets / 5174 planetary systems / 1050 multiple planets systems

Atmospheric modelling

$$\mu \frac{dI_\lambda(\tau,\mu)}{d\tau} = I_\lambda(\tau,\mu) - B_\lambda(T)$$

$$I_\lambda(\tau=0) = B_\lambda(T_s)e^{-\tau_s} + \int_{\tau_s}^{0} B_\lambda(\tau)\frac{\partial T_\lambda(\tau)}{\partial \tau}d\tau$$

$$F_P/F_* = \frac{I_\lambda(\tau=0,\mu=1)}{I_*} \times \left(\frac{R_P}{R_*}\right)^2$$

$$T^4(\tau) = \frac{3T_{int}^4}{4}\left(\frac{2}{3}+\tau\right) + \frac{3T_{irr}^4}{4}\xi_{\gamma_1}(\tau)$$

$$\tau_{\lambda,m}(z) = 2\int_0^{l(z)} \varsigma_m(\lambda)\chi_m(z)\rho_N(z)\mathrm{d}l$$

$$I_\lambda(z) = I_\lambda(0)e^{-\tau_\lambda(z)}$$

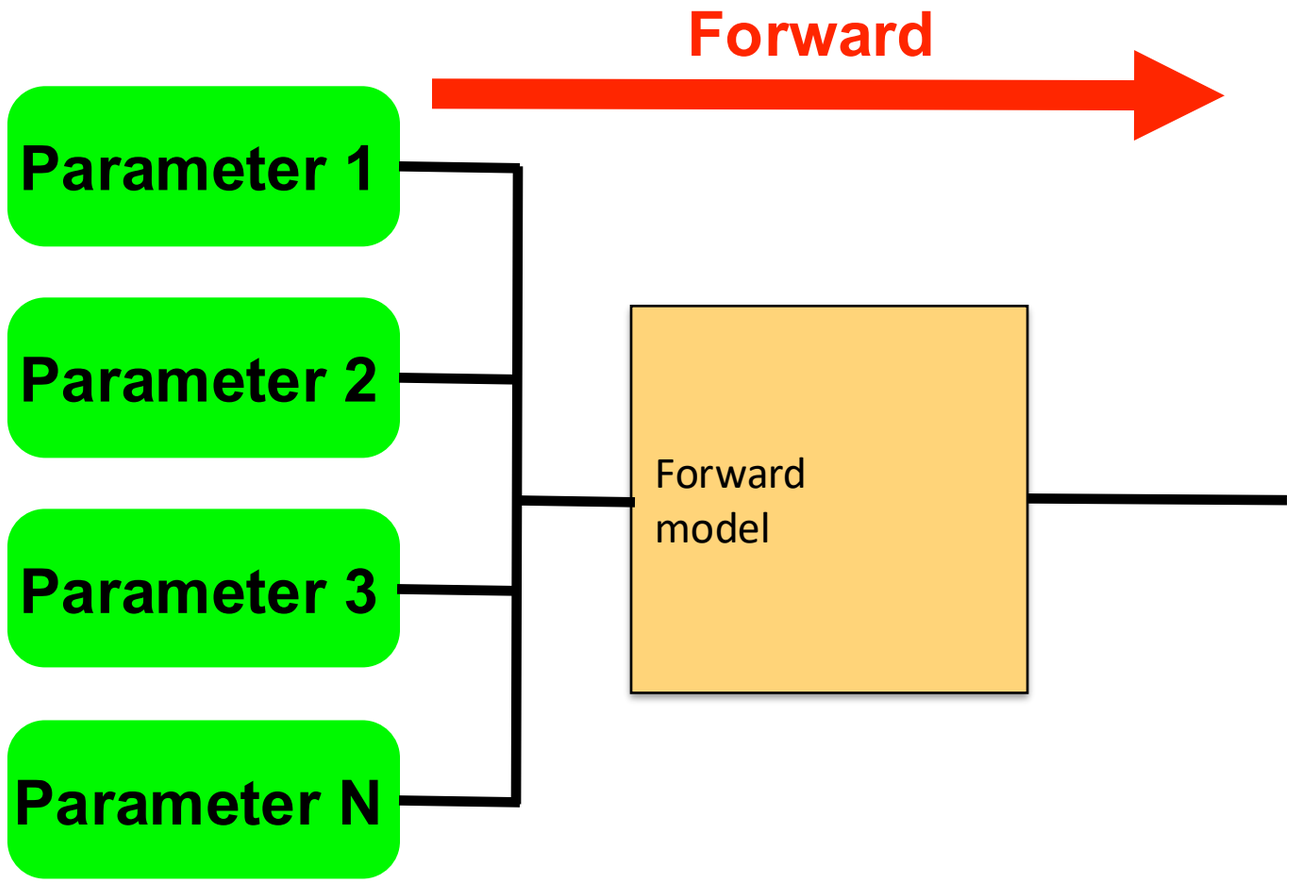
$$\alpha_\lambda = 2\int_0^{z_{max}} (R_p+z)(1-e^{-\tau_\lambda(z)})\mathrm{d}z$$

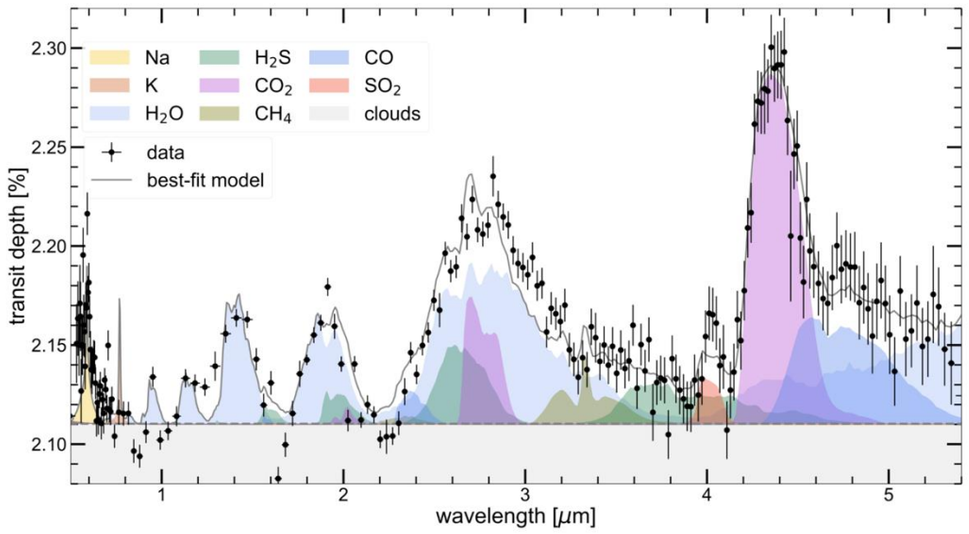
$$\delta_\lambda = \frac{R_p^2+\alpha_\lambda}{R_*^2}$$

What is an atmospheric retrieval?

The forward modelling takes atmospheric parameters, through an atmospheric model to produce a spectrum. Often the fit to the data is assessed ‘by hand’

Inverse retrievals reverse this process and we try to derive the parameters of the model from the data. Usually models are simpler but the statistical fit can be better constrained





Z. Rustamkulov et al 2022

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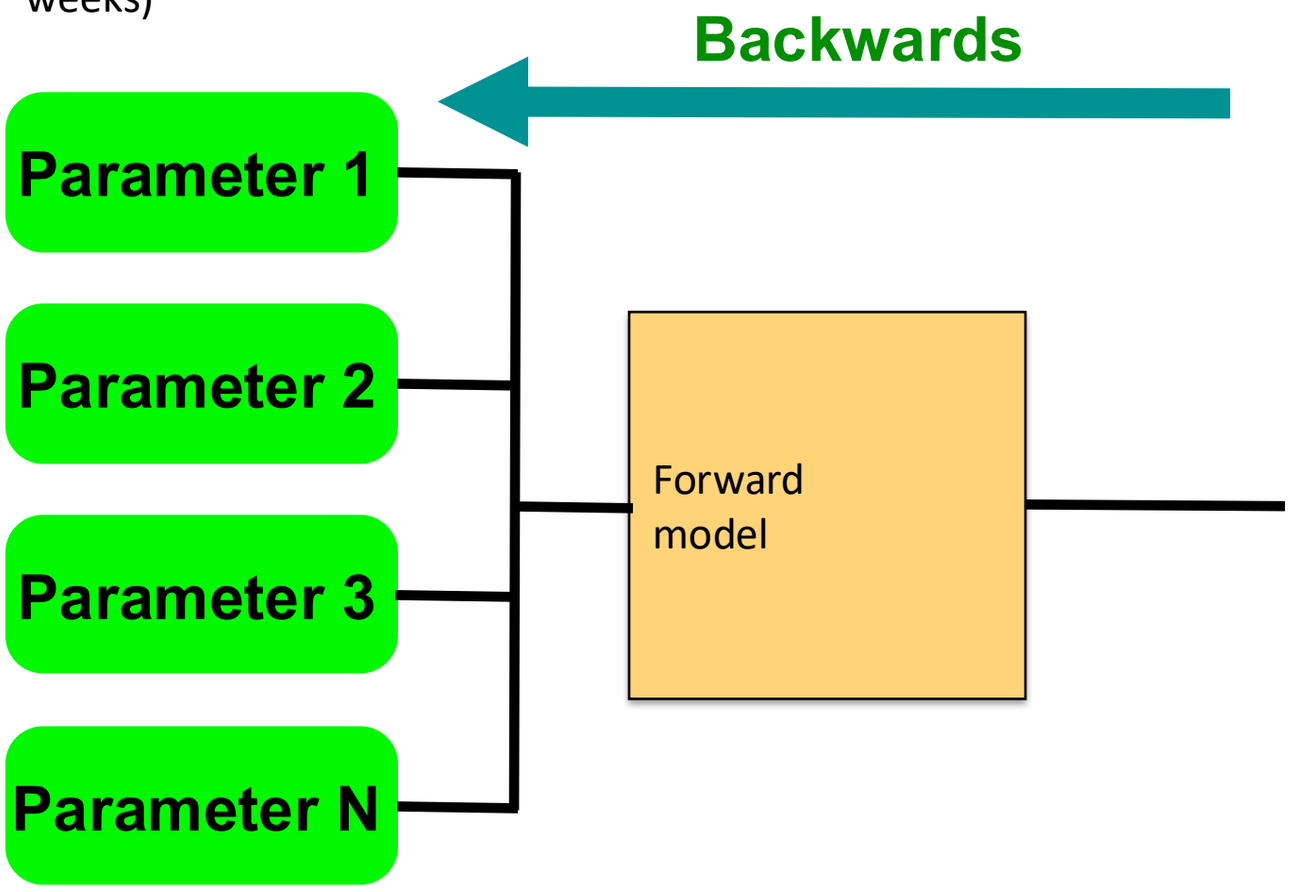
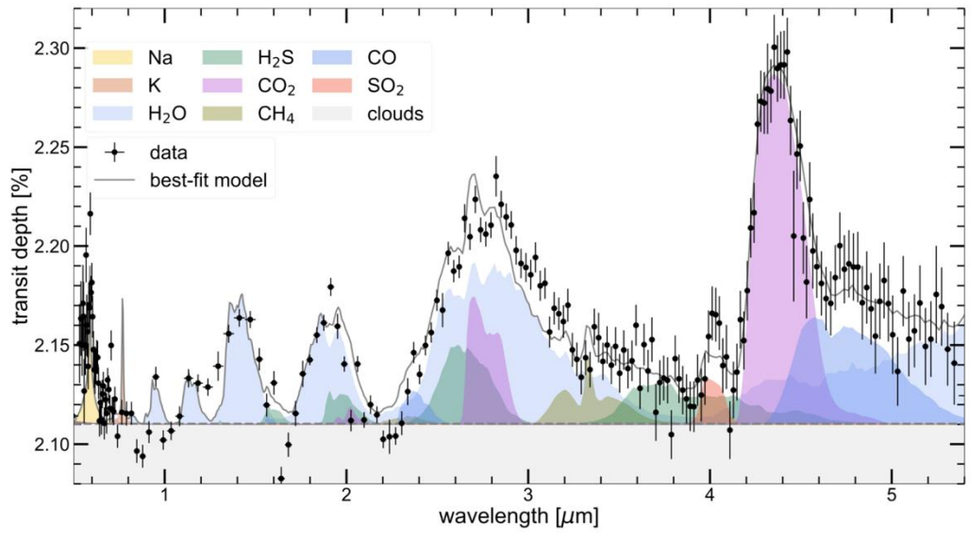
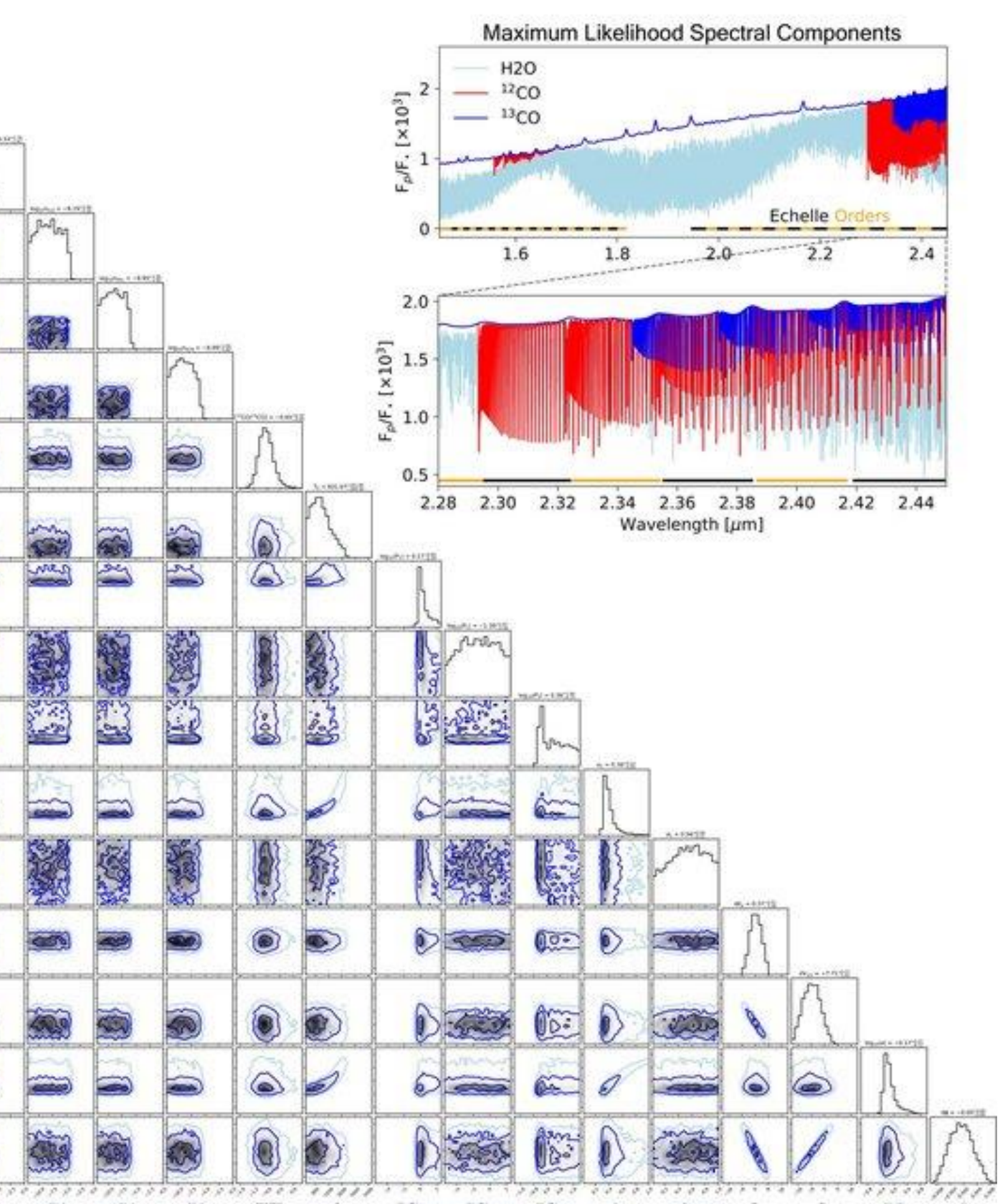
Bayesian frameworks represent the best approach, many codes exist to solve this problem, but we need to simplify (sometimes too much the model assumptions to make it converge in a reasonable amount of time, in minutes, days or weeks)





Z. Rustamkulov et al 2022



Atmospheric retrievals

- Computationally Intensive
- Forces us to simple models

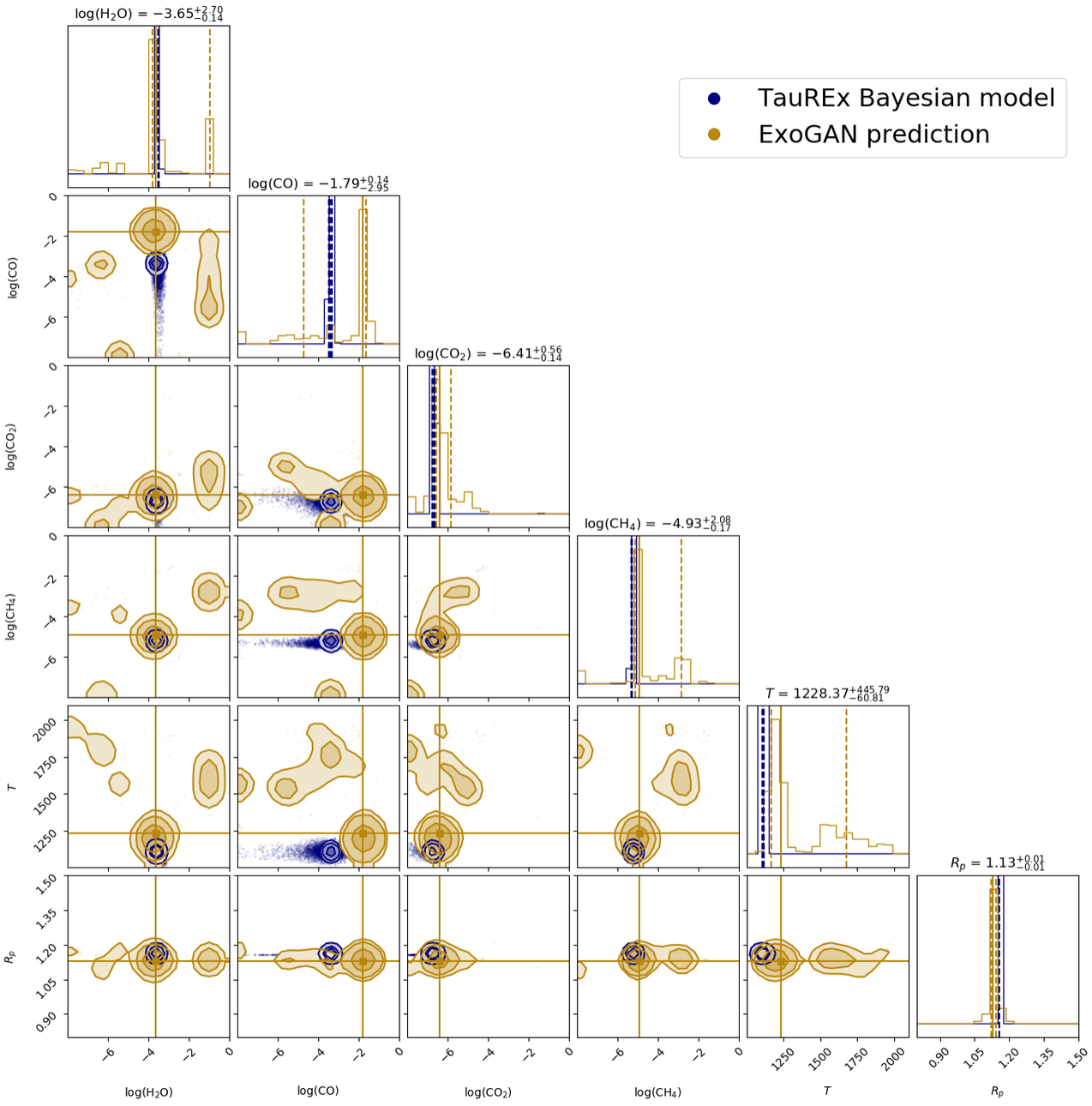
Machine Learning found its way

Find hidden pattern in huge astronomical data (images, time series, signal processing);

Speed-up computation time (Bayesian frameworks);

Mitigate the complexity of physics models (i.e. atmospheric models)

Generative AI for atmospheric Learning



The Astronomical Journal, 156:268 (14pp), 2018 December https://doi.org/10.3847/1538-3881/aae77c

ExoGAN: Retrieving Exoplanetary Atmospheres Using Deep Convolutional Generative Adversarial Networks

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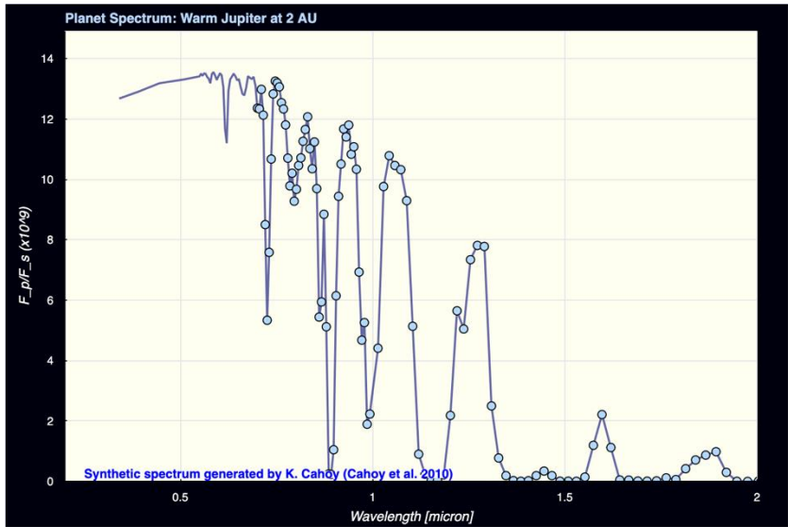
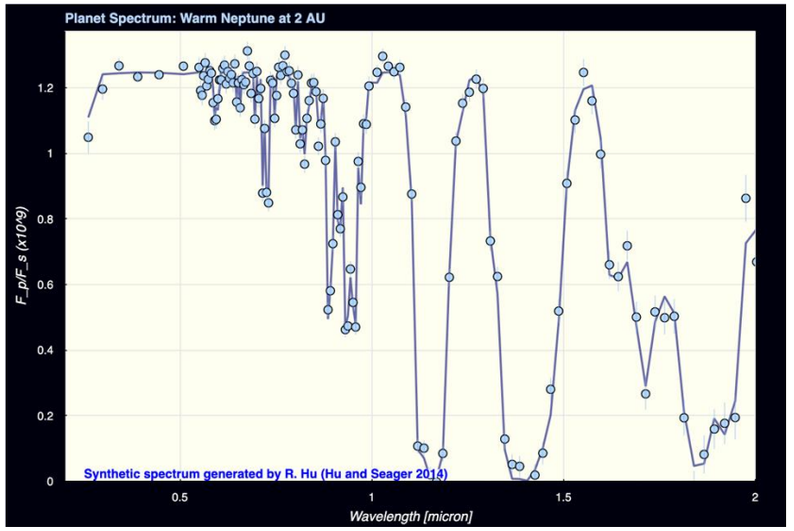
Abstract

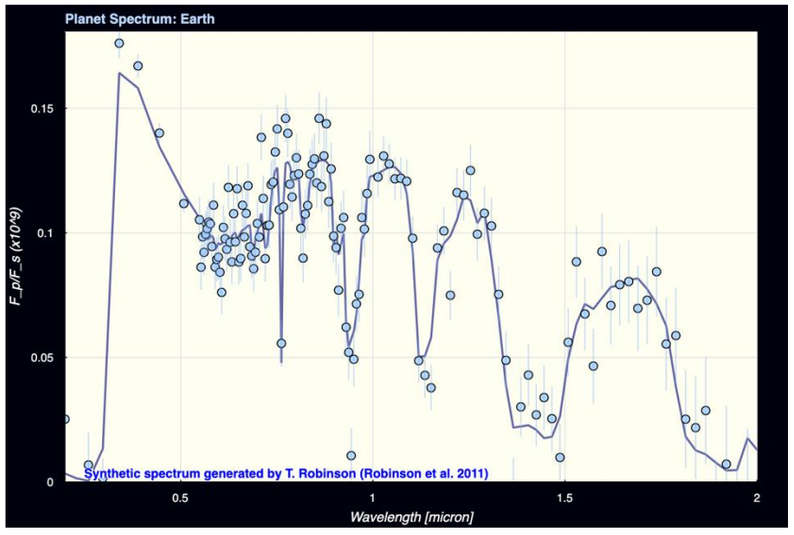
Atmospheric retrievals on exoplanets usually involve computationally intensive Bayesian sampling methods. Large parameter spaces and increasingly complex atmospheric models create a computational bottleneck forcing a trade-off between statistical sampling accuracy and model complexity. It is especially true for upcoming *JWST* and ARIEL observations. We introduce ExoGAN, the Exoplanet Generative Adversarial Network, a new deep-learning algorithm able to recognize molecular features, atmospheric trace-gas abundances, and planetary parameters using unsupervised learning. Once trained, ExoGAN is widely applicable to a large number of instruments and planetary types. The ExoGAN retrievals constitute a significant speed improvement over traditional retrievals and can be used either as a final atmospheric analysis or provide prior constraints to subsequent retrieval.

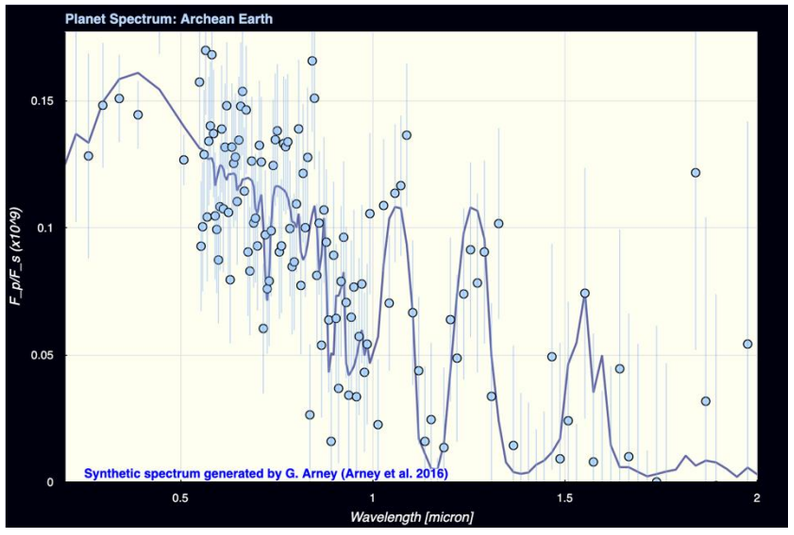
Key words: methods: statistical – planets and satellites: atmospheres – radiative transfer – techniques: spectroscopic

Direct imaging spectra with HWO





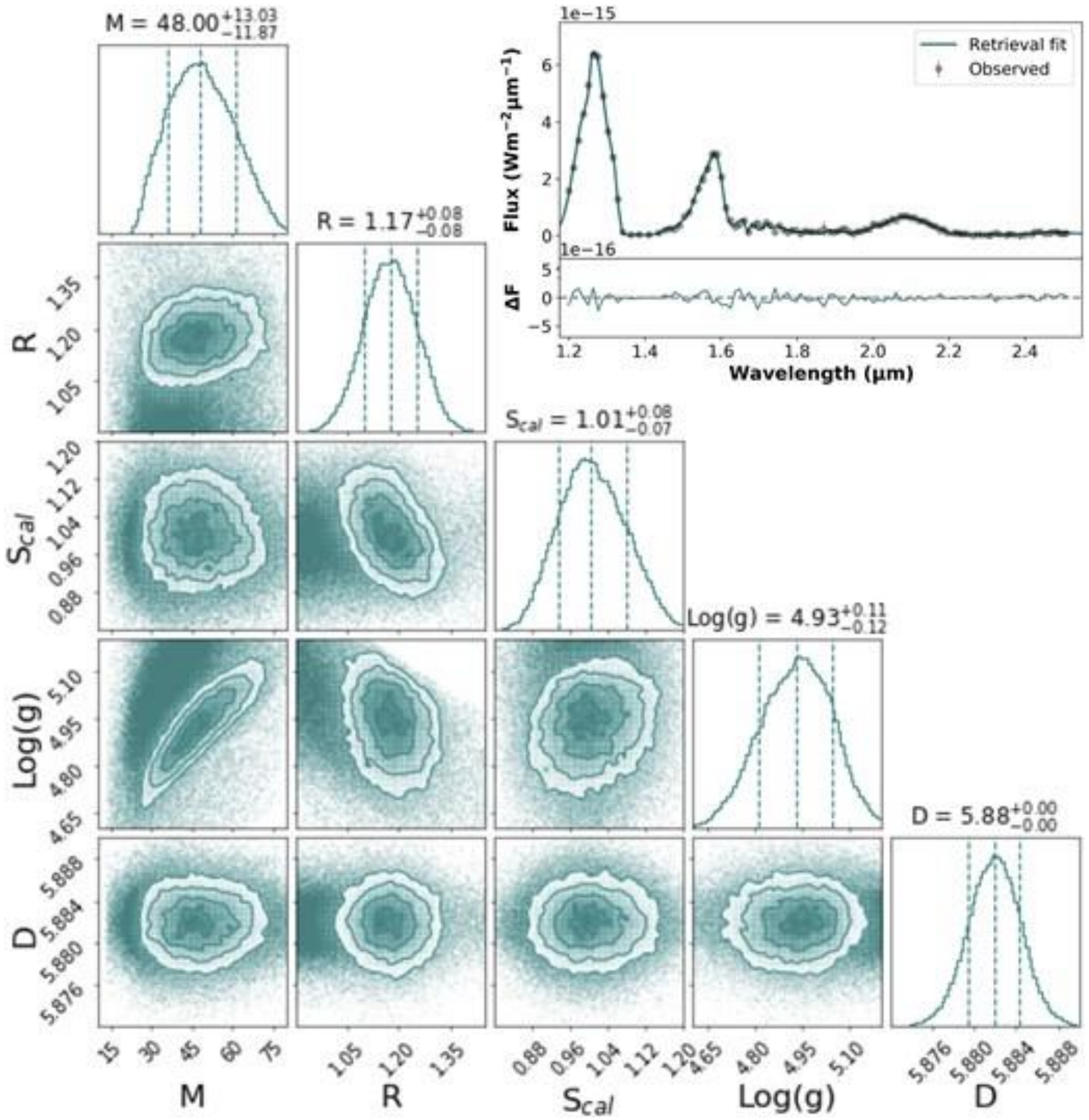




https://hwo.stsci.edu/coron_model

Retrievals with Direct Imaging

- Classical retrievals already available (Whiteford et al 2023);
- Preparation of a Direct Imaging dataset to train our ML tools;
- Extend retrieval tools to classic hardware (CPU/GPU/TPU)



GJ 570D bulk parameter posterior probability distributions for the spectral fit of the 1.2–2.5 μm data used (Whiteford et al 2023)

Towards the future

Machine Learning found its way

Find hidden pattern in huge astronomical data (images, time series, signal processing);

Speed-up computation time (Bayesian frameworks);

Mitigate the complexity of physics models (i.e. atmospheric models)

Quantum Alternatives

Find hidden pattern in huge astronomical data

Quantum Machine Learning

Speed-up computation time

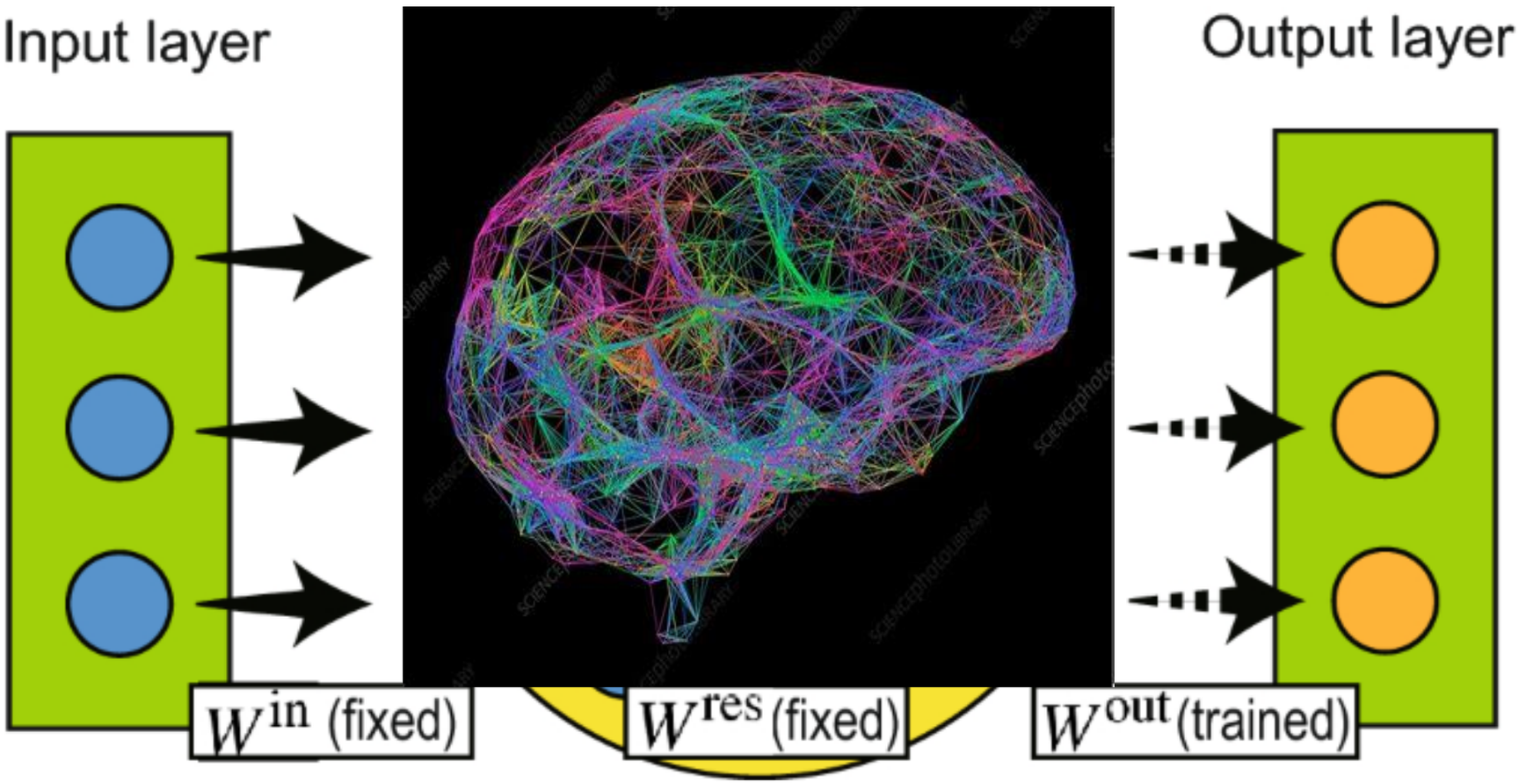
Quantum Optimisation

Solve the complexity of physics models

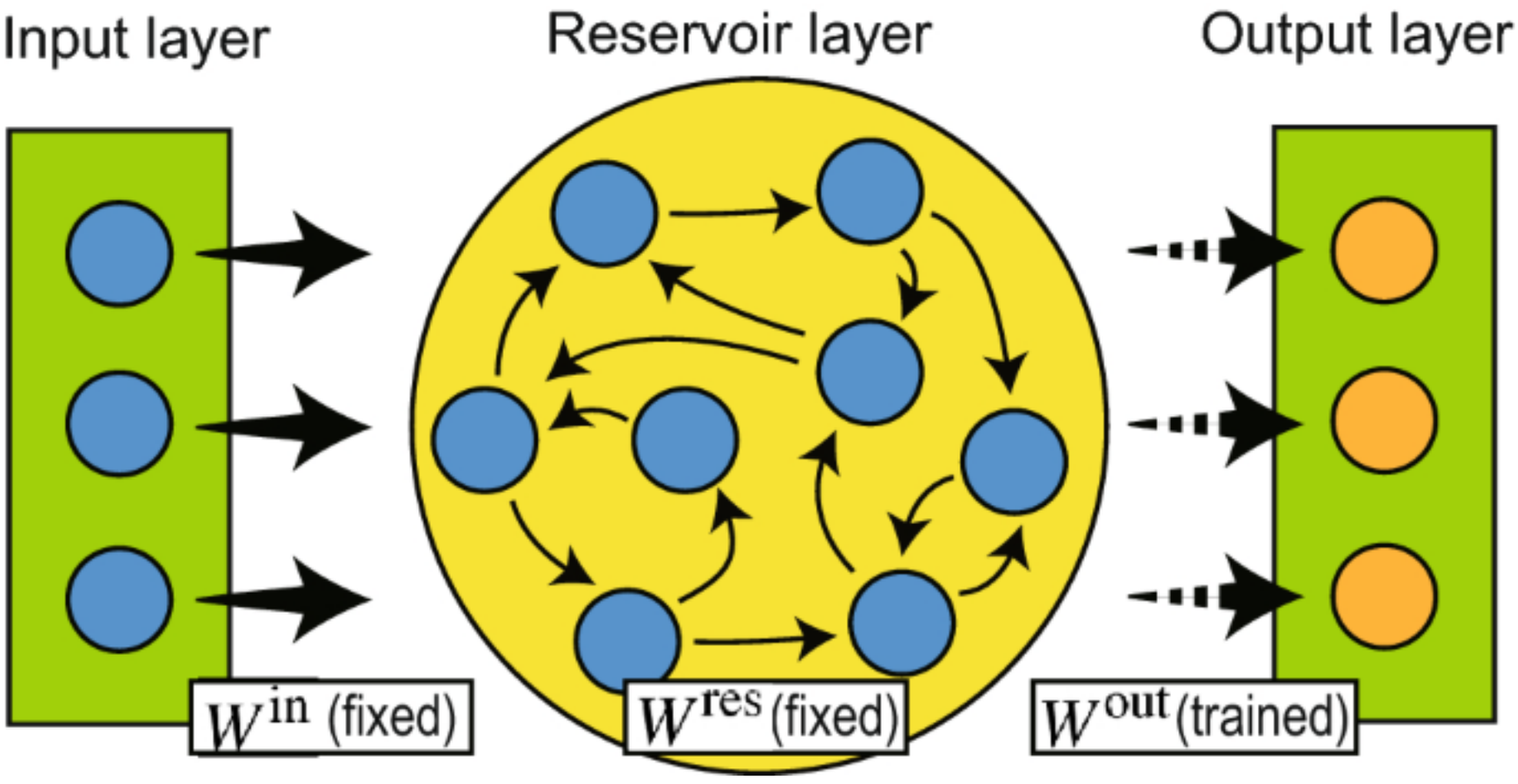
Quantum Simulation

Extreme Learning Machines

A few approximative concepts

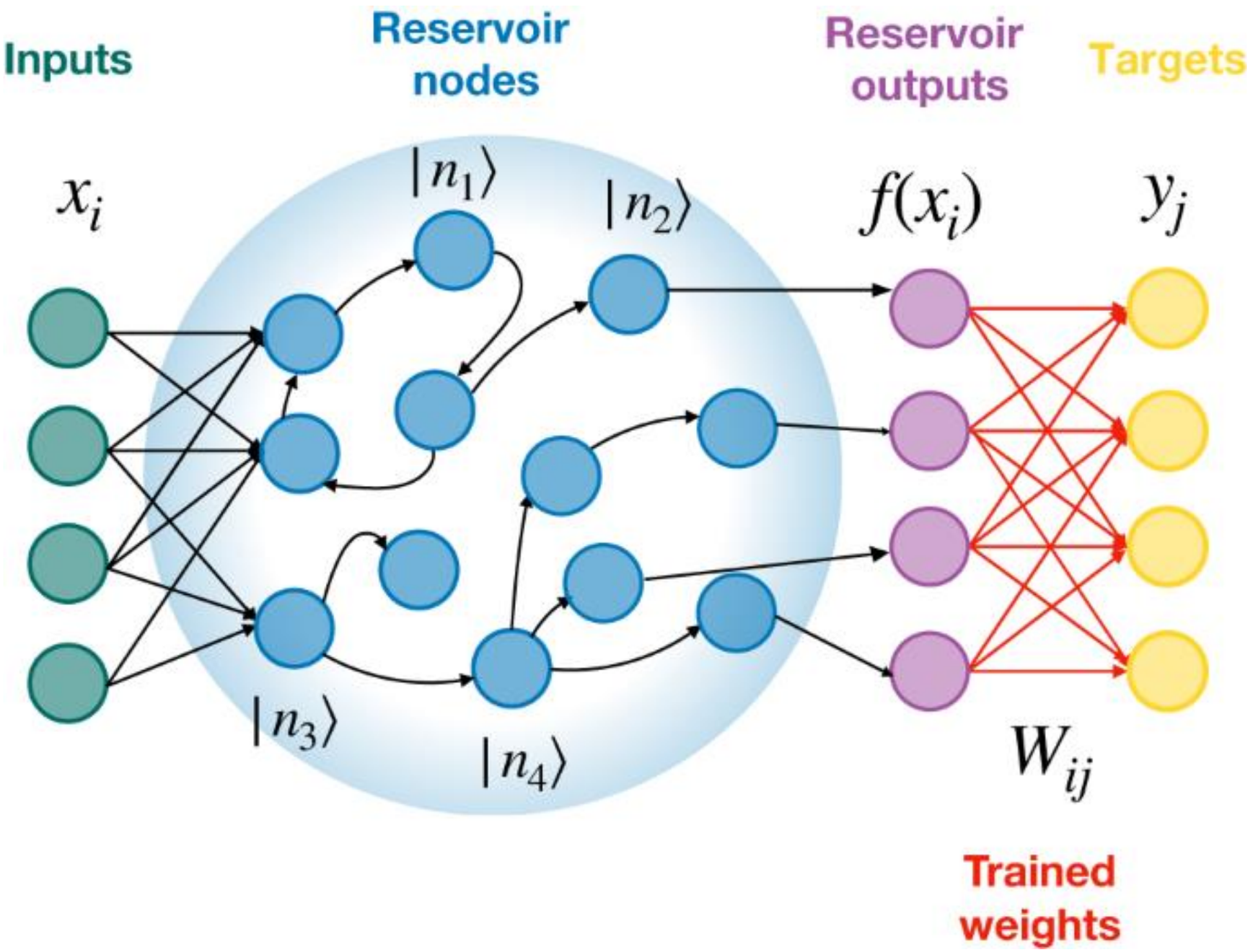


Reservoir Computing



Sakemi et al 2020

Quantum Reservoirs



Dudas et al, 2023

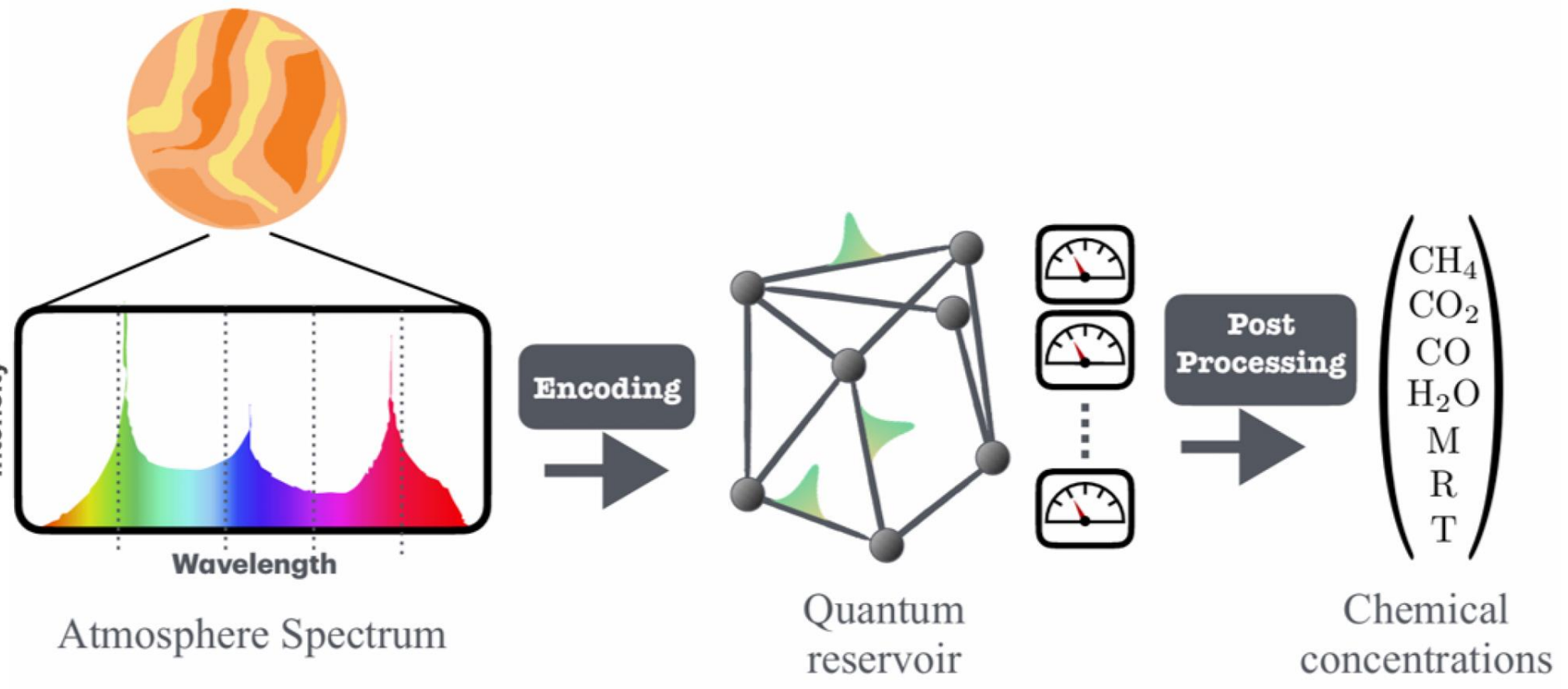
Why using (q)ELMs

Fast training due to the only need to solve a linear regression problem

Possibility to use real hardware instead of neural networks as reservoir

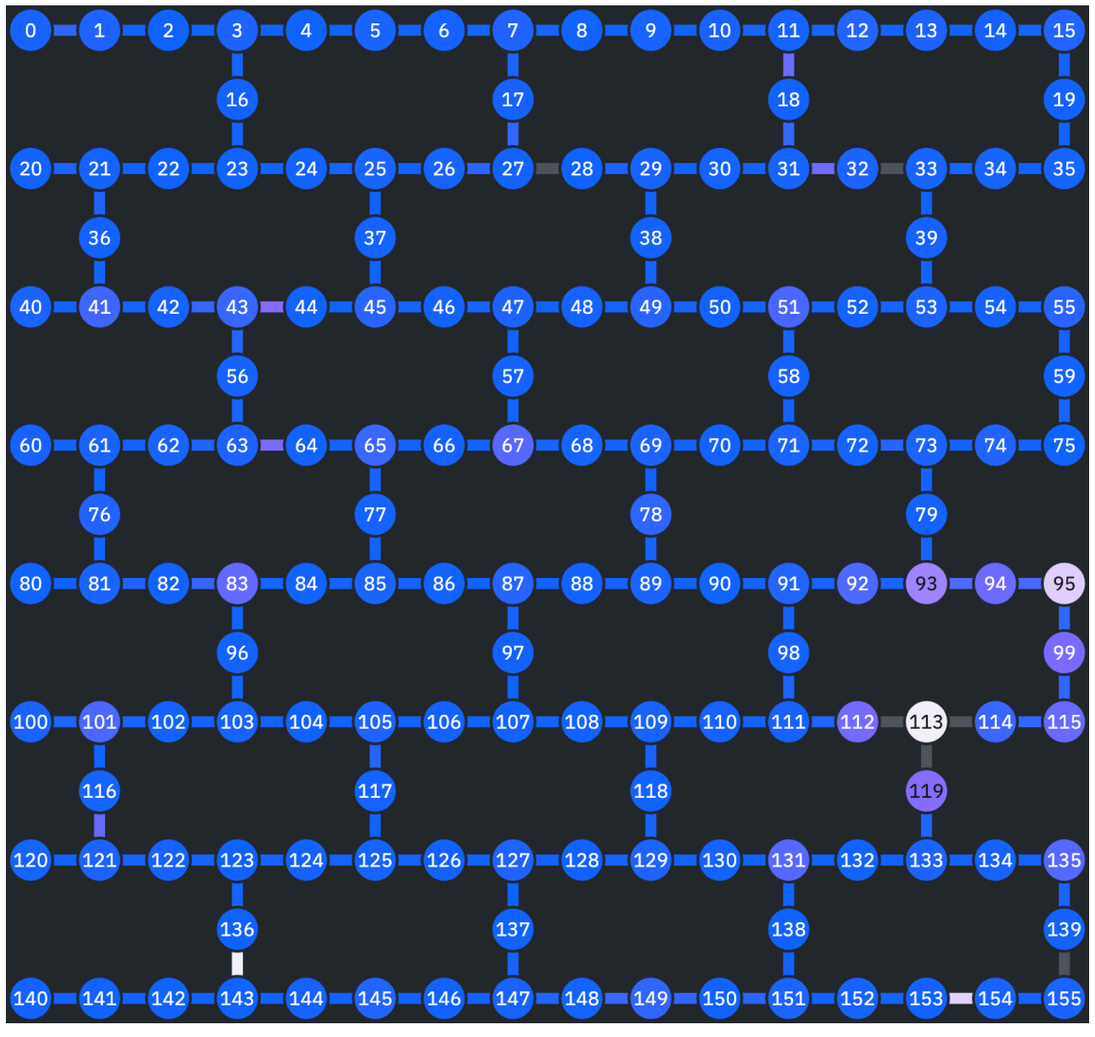
Tanaka, G. et al. Recent advances in physical reservoir computing: A review. Neural Networks 115, 100 – 123 (2019). URL https://www.sciencedirect.com/science/article/pii/S0893608019300784

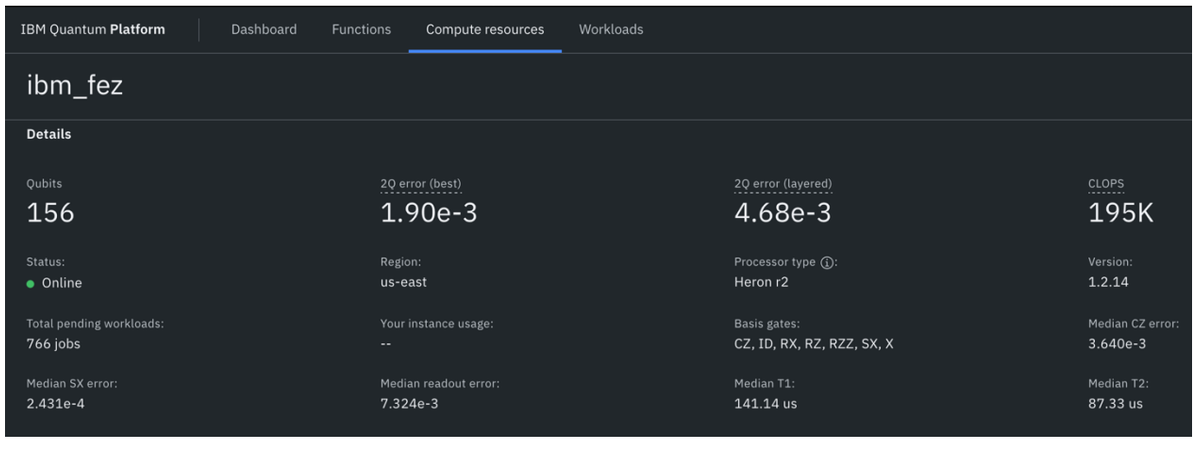
Atmospheric QELM



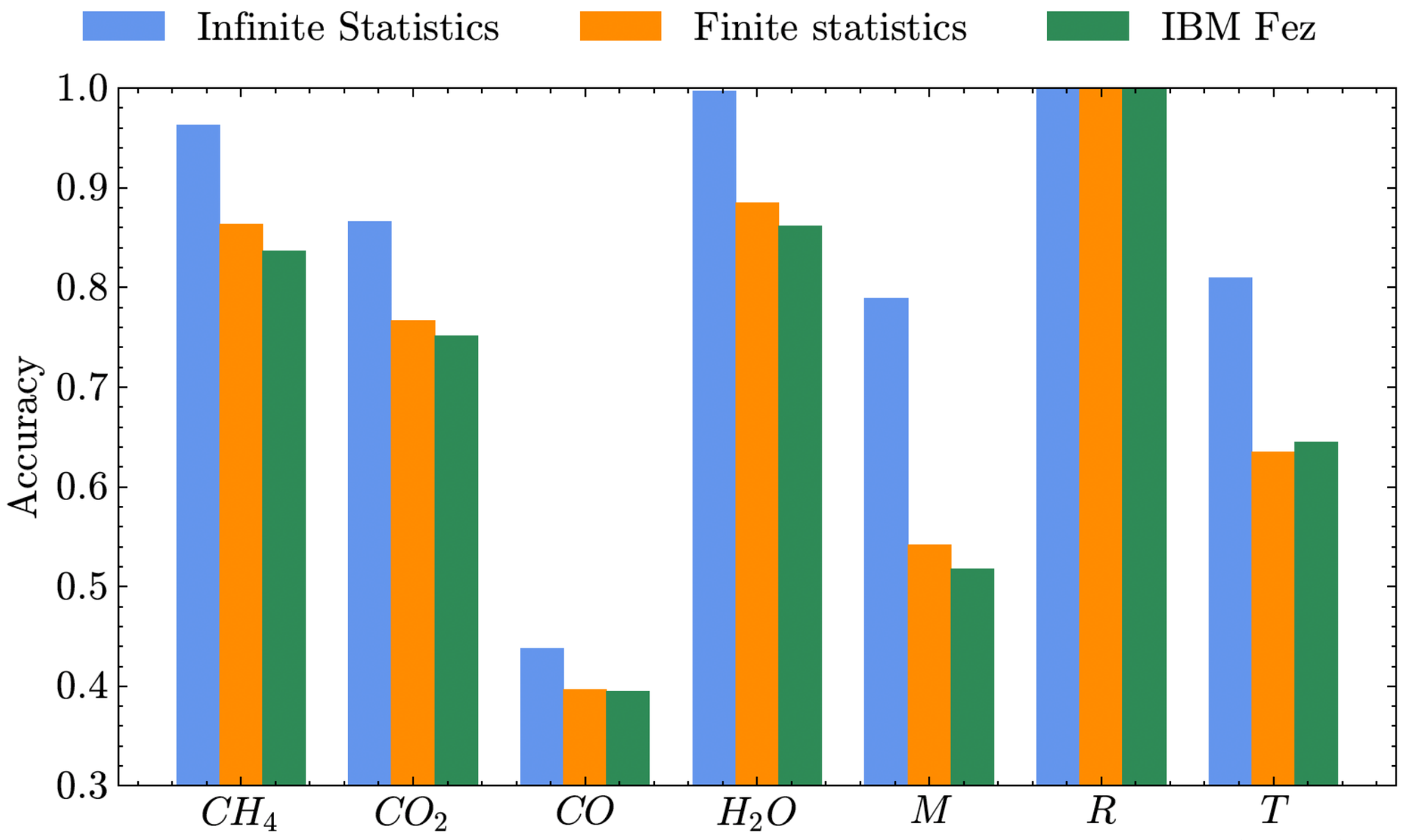
Vetrano et al, submitted

The Hardware





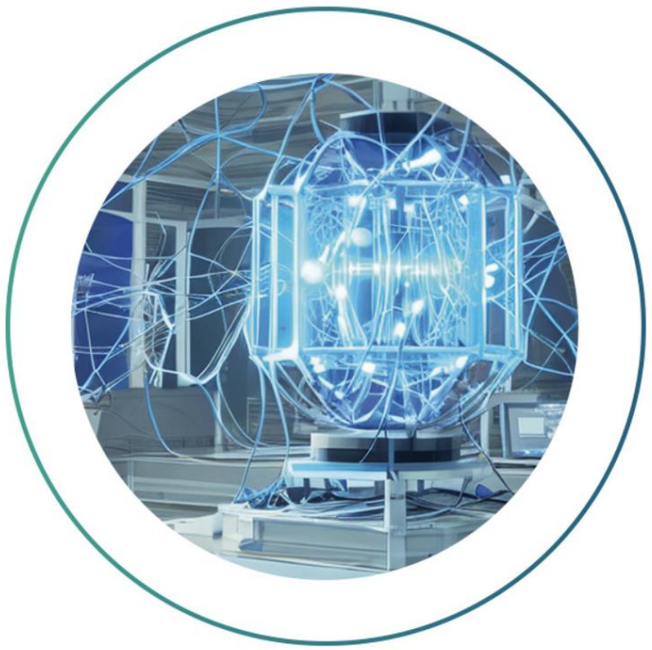
Results



Vetrano et al, submitted

The distribution of parameters is either a solution by itself or can be used as informative prior to a Bayesian framework

Quantum Computing and Simulation Center



About

We plan to develop a general-purpose quantum computer at the Department of Physics and Astronomy of the University of Padua and together with local, national and international actors, to create around it a competence center to guide and nurture the development and the inclusion of quantum technologies in the Italian academic and business environment.

VIEW MORE ›

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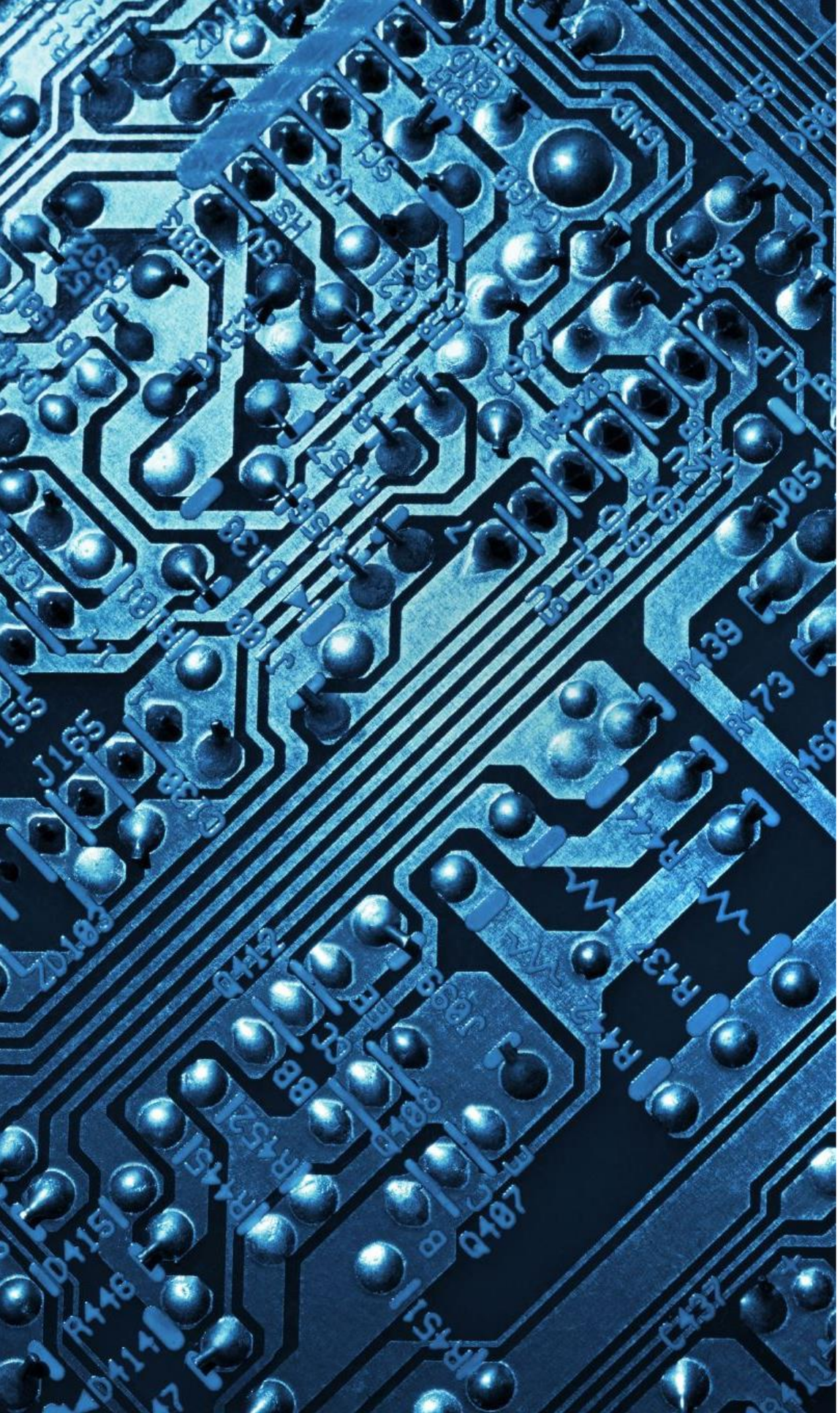

Conclusion

- Technology and software advancement must go together;
- ML offers a possibility to optimise the scientific outcome;
- Quantum Technologies may be a game changer in the 40s;
- A (q)ML Task force within HWO could work on dataset and algorithmicand model improvement.

Let’s Stay in Touch

contact: tiziano.zingales@unipd.it