Disequilibrium chemistry of exoplanet atmospheres in the JWST era.
An opportunity for Machine Learning.

Keywords

Exoplanet atmospheres, chemical kinetics, photochemistry, numerical methods.

Project description

The James Webb Space Telescope (JWST) is changing our understanding of exoplanets. In particular, the observations made during its first year of operation are offering unprecedented insights into the composition, dynamics and energetics of a broad range of exoplanet atmospheres. Given the complexity of atmospheric phenomena, the data will be scrutinized with the aid of sophisticated models for many years to come. The ARIEL space mission, to be launched in 2029 to survey ~1,000 warm and hot exoplanets, will contribute in due course to the ongoing revolution of our understanding of exoplanet atmospheres.

The term *disequilibrium* has emerged as a keyword in the frontier investigation of exoplanet atmospheres. Indeed, a main finding of the first JWST spectrum of an exoplanet[1] – the hot Saturn WASP-39b – is the occurrence of SO_2 in its atmosphere in abundances unexplained by equilibrium chemistry. Modeling atmospheres in disequilibrium is both complex and computationally expensive as it requires solving hundreds of chemical reactions and transport processes that occur at the microscopic scales yet are connected with the macroscopic properties of the gas. Importantly, there is a true need to consider such processes for the correct interpretation of the salient features of the spectra obtained by the new generation of space telescopes.

The present project is concerned with the modelling of disequilibrium chemistry in exoplanet atmospheres and its goal is twofold.

The first goal is to investigate the implications of disequilibrium chemistry in the atmospheres of JWST targets for which transmission spectra exist. The list of such targets and published spectra is rapidly expanding. Dr. García Muñoz has participated in some of those works [ERS23,ES23] and is co-proposer of other JWST proposals for GO Cycle 3 that, if successful, will secure further observations of exoplanet atmospheres. The proposed work will benefit from an in-house photochemical model [GM07] that includes the relevant processes for neutral-ion photochemistry. The PhD candidate will tune the chemical network to the needs of the problem, exploring possible deficiencies in our knowledge of the chemical kinetics. We will use the software PUMPKIN [MA14] to identify the chemical pathways that control the simulated compositions. We will turn this knowledge into recommendations about chemical reactions that should be better quantified in laboratory experiments or through computational chemistry calculations.

The second goal of the project is about speeding up the photochemical model using techniques of Machine Learning (ML). Specifically, we will use ML techniques to construct *emulators* of the photochemical model that predict the chemical composition of the atmosphere at a reduced computational cost. ML-based emulators digest the information contained in a set of training photochemical model calculations (for example, those produced in the first part of this project)

[1] https://www.jwst.fr/2022/12/wasp-39b-webb-revele-latmosphere-dune-exoplanete-comme-jamais-auparavant/

and infer the input-output relations with which new outputs can be predicted. We will use the ML-based emulator to produce recommendations for atmospheric retrieval models that operate on the observed spectra and constrain from them the atmospheric composition of exoplanets. ML-based emulators are at the cutting-edge of techniques that are being used in the modelling of complex chemical systems and remote sensing applications [SM22,WA22]. Our project will contribute to the exploration of these techniques on new fronts.

Bibliography

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Timeliness, skills acquired & team

The PhD topic is timely as there is a clear need for the interpretation of the exoplanet spectra being measured by JWST and, further into the future, by ARIEL. The project will help train the PhD candidate in the complex physics and chemistry of planetary atmospheres, and the relevant numerical methods, and in techniques of Machine Learning. There will be many opportunities for interacting with other groups at the (inter-)national level through e.g. the ARIEL Consortium.

The PhD candidate will be supervised by Dr. García Muñoz, at CEA Paris-Saclay. The project takes place at the Laboratoire Dynamique des Etoiles, des Exoplanètes et de leur Environment (LDE3/DAp), which is composed of experts in astrophysical fluid dynamics and exoplanets involved in the JWST, ARIEL and PLATO missions. To go beyond:

http://irfu.cea.fr/dap/LDEE/index.php (http://irfu.cea.fr/dap/LDEE/index.php)
https://antoniogarciamunoz.wordpress.com/

Candidate profile

The candidate must have a Masters in Astrophysics or a related field (e.g. Applied Mathematics or Engineering) and a strong interest in theoretical/numerical work and in the comparison of observations with model simulations. In particular, the candidate must:

- be proficient in scientific programming (one of fortran, C, C++).
- be proficient in numerical simulations of physical systems.
- have some knowledge of or the interest to learn about chemical kinetics.
- have some knowledge of or the interest to learn about Machine Learning techniques.
- be willing to learn about exoplanet atmospheres.