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Report on the ESO Workshop

Atmospheres, Atmospheres! Do I look like I care about atmospheres?

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The discovery rate of exoplanets has been such that we have now moved from a simple detection regime to one in which planets can be characterised. Alongside precise determinations of planetary radii and bulk compositions, the properties of their atmospheres are now being revealed. This provides a powerful window onto the formation history of planetary systems, the composition of the initial protoplanetary disc in which planets form, and the locations of planet formation. Moreover, this allows us to study various chemical and thermodynamical processes in the upper atmosphere, as well as to probe planetary interiors. ESO recently organised an online workshop on these topics, with some quite unique aspects: it addressed results from transmission and emission spectroscopy from the ground in the study of exo-atmospheres; it looked at synergies with studies of giant planets in the Solar System; it provided two days of hands-on activities to prepare the future generation; and it included invited talks by the most promising young scientists working in this field.

Transiting exoplanets, that is, those passing across the disc of their host stars, present an unrivalled opportunity to study and characterise the physical properties of exoplanets and in particular of their atmospheres. The atmospheric metallicity, temperature structure, cloud properties, and dynamics can be revealed by studying either spectroscopic imprints in starlight traversing an exoplanet's upper atmosphere — a technique known as transmission spectroscopy — or the light emitted from the planet's dayside — emission spectroscopy. A whole host of ions, atoms and molecules have been detected through a variety of, often complementary, techniques, such as differential spectrophotometry using low- to mid-resolution spectroscopy, and high-resolution spectroscopic techniques, including the use of cross correlation. These detections serve as unique and strong diagnostics of chemical and dynamical processes in the exo-atmospheres.

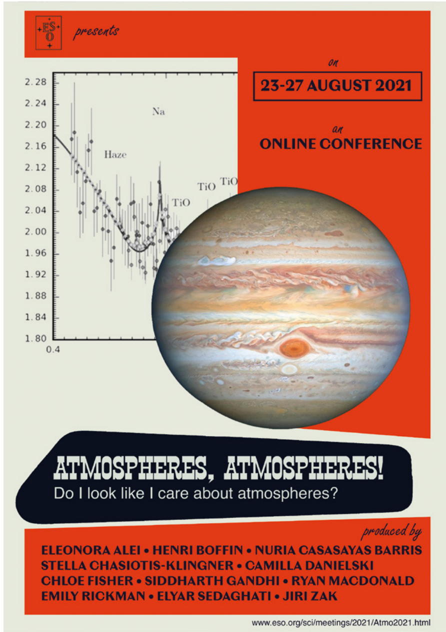

Figure 1. Conference poster. Jupiter image credit: NASA, ESA, A. Simon (Goddard Space Flight Center) and M. H. Wong (University of California, Berkeley) and the OPAL-Team.

A unique conference

Even if the pioneering work on exoplanet atmospheres was done with the Hubble Space Telescope, and much hope is now placed on the James Webb Space Telescope (JWST), most results have come from ground-based facilities, with ESO instruments — mostly the FOcal Reducer and low-dispersion Spectrograph 2 (FORS2), the Ultraviolet and Visual Echelle Spectrograph (UVES), the CRyogenic high resolution InfraRed Echelle Spectrograph (CRIRES), the High Accuracy Radial velocity Planet Searcher (HARPS), and the Echelle SPectrograph for Rocky Exoplanet and Stable Spectroscopic Observations (ESPRESSO) — playing a central role. Soon the upgraded CRIRES (CRIRES+) and the Near InfraRed Planet Searcher (NIRPS) will also be major tools for such studies. Elsewhere, instruments such as the Inamori-Magellan Areal Camera and Spectrograph (IMACS), the Calar Alto high-Resolution search for M dwarfs with Exoearths with Near-infrared and optical Echelle Spectrographs (CARMENES) instrument, and the OSIRIS integral field spectrograph, to name but a few, have also contributed to the field. Additionally, ground-based observations of exoplanetary atmospheres, especially those at visible and near-infrared wavelengths, will be essential in anchoring retrieval models by lifting degeneracies for JWST spectra, since the latter will not have coverage in those bands. Furthermore, ground-based, high-resolution observations will provide atmospheric details inaccessible to the spectral resolution of JWST.

This ESO conference accordingly brought together the communities working theoretically and observationally on understanding exoplanet atmospheres, with an emphasis on using ground-based facilities. It also tried to include those working on the atmospheres of close-in exoplanets and those studying the atmospheres of giant planets in our Solar System, to compare methodologies and see where synergies exist or could be made. The workshop had the further goal of preparing the next generation of astronomers to embark on this exciting and essential area of astrophysics, which is technically very challenging. Another key aspect of this workshop is that it was organised mostly by scientists at an early stage of their career — the only exception being the first author of this report. Similarly, preference was given to inviting young and brilliant speakers, providing them with a chance to shine in the complicated times we currently live in. The conference took place on the Zoom platform and used Slack for discussions, the exchange of files, and social interactions.

Hands-on session

The first two days of the workshop were devoted to a series of hands-on lectures, providing young astronomers with intensive training in how to extract observational data that are useful for exoplanet studies and how to interpret them, using sophisticated theoretical models and advanced methods such as machine learning. To ensure sufficient interaction between the participants and the lecturers, the number of participants in these lectures was limited to 30 — a selection therefore had to be made. The selection was based on the status of the participants, with preference given to early PhD students, and on a short motivation letter they had to write. For the benefit of those who weren't selected, however, and of those who would like to learn these techniques in future, all sessions were recorded and the videos posted on YouTube and linked from the programme page[1]. The material necessary to do the exercises, including the python notebooks, is provided on GitHub, and linked from the programme page[1]. During the lectures themselves, the material was provided to the participants via Google Colab notebooks, making it easier to run the codes without the hassle of installing various items of software.

There were seven hands-on sessions, covering many aspects of the study of exoplanet atmospheres. These were given mostly by members of the organising committee. First, Elyar Sedaghati showed how to remove the signature of Earth's atmosphere from spectra, using the ESO package Molecfit. This is the crucial final step in the data reduction, before one can start to apply specific techniques. Emily Rickman and Elyar then explained how to obtain useful data for atmosphere characterisation from spectrophotometric and direct-imaging observations. The next two lectures were dedicated to one of the most successful techniques used, namely narrow-band transmission spectroscopy using high-resolution spectra. Núria Casasayas-Barris and Julia Seidel demonstrated the general features of this technique and the caveats to be aware of, while Matteo Brogi and Jens Hoeijmakers explained in more detail how to use the cross-correlation method. The following day was devoted to the interpretation of observations. Chloe Fisher and Siddharth Gandhi led a hands-on session on how to interpret the cross-correlation maps, while Eleonora Alei and Evert Nasedkin showed how to use the petitRADTRANS code to perform low- and high-resolution forward models. This also included introducing a retrieval routine that is now part of the suite. Finally, Ryan MacDonald and Natasha Batalha gave the participants an overview of how theoretical atmospheric models are derived and their inputs and limitations.

These lectures were a clear success as evidenced by the feedback provided by the participants, most of whom can be seen in Figure 2. When asked to provide

Figure 2. Most of the participants in the hands-on lectures.

a score between 0 and 10 to rate the general content of the sessions, the average was 8.7, while the ease of the combined use of Zoom/Slack/Google Colab was also deemed excellent. All participants praised the quality of the lecturers.

From the Solar System to exoplanets

The last three days were dedicated to a conference, open to all and free to attend. Besides nine invited review talks, the conference included 19 contributed talks. The first invited talk was by Julia Seidel who gave a summary of what had been discussed during the hands-on sessions. She walked us through the most common complications when building a transmission spectrum and highlighted the most important results of recent years in the realm of narrow-band transmission spectroscopy using high-dispersion spectra, with a focus on the different spectrographs that are capable of this, whether currently or in the future.

Following this, Henrik Melin brought us back to our own neighbourhood, the Solar System, and presented what we currently know about the upper atmospheres of Uranus and Neptune. These two ice giants in our Solar System are excellent analogues for a vast number of exoplanets in the Universe, and their relative proximity to the Earth allows us to perform detailed observations of their atmospheres. One can, for example, study aurorae on these planets, which are capable of injecting large amounts of energy into their upper atmospheres. Observations over almost 30 years of the molecular ion H_3^+ have revealed that the upper atmosphere of Uranus is subject to long-term cooling. The situation of Neptune is even more surprising, as H_3^+ remains undetected in its atmosphere, the upper limit of its ionospheric density being much lower than predicted by models.

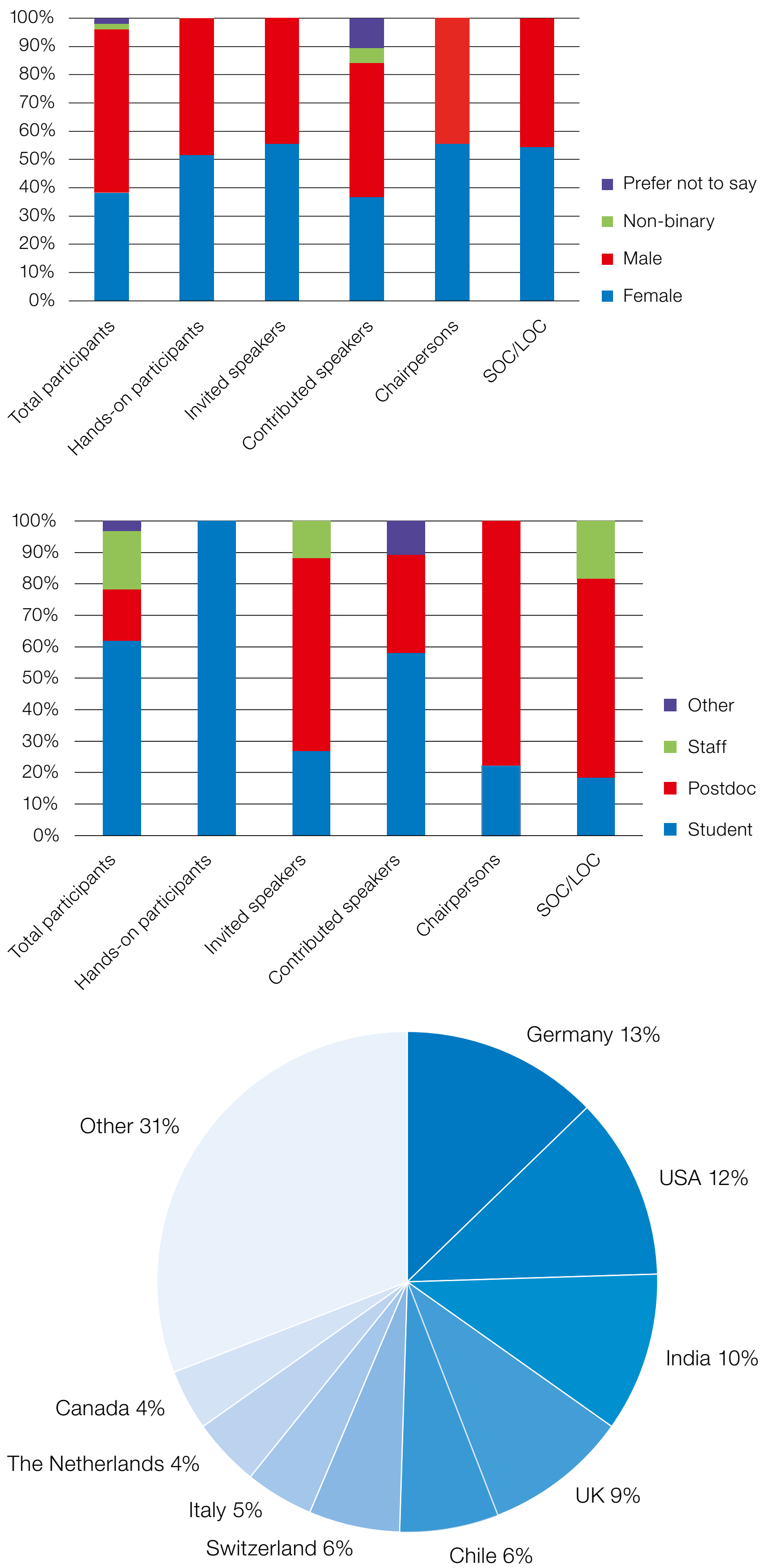

Figure 3. Charts depicting the distributions of gender (top) and career stage (middle) of the participants in the workshop, where we note that the categories shown may not accurately reflect the complex reality. The bottom panel shows the distribution of the registered participants according to their country of residence.

Molecules, molecules...

Molecules in the atmospheres of exoplanets was the topic of the talk by Katy Chubb, who showed how determining molecular spectra at the high temperatures of transiting exoplanets (typically up to 1000–2000 K) is challenging. Ambitious and demanding projects such as ExoMol and HITEMP have been set up in recent years to provide such spectra in the form of molecular line lists, whose computations can sometimes take years, particularly for molecules with more atoms/electrons. These line lists then need to be converted to pressure- and temperature-dependent spectra to be used in retrieval codes for atmospheric characterisation.

Focusing on a subset of these molecules, Aurora Kesseli described how metal hydrides (FeH, CaH, MgH etc.) and metal oxides (TiO, VO etc.) are likely to be important sources of opacity at visible wavelengths in hot and ultra-hot Jupiters and can also cause the temperature inversions that we see in some ultra-hot Jupiters. However, conclusively detecting any of these species has proven extremely challenging and more work is needed to obtain high-resolution line lists of these molecules. If such species can be unambiguously discovered in exoplanets, it will help us understand dayside to nightside temperature contrasts, cold-traps and more, and they could then be used as probes of exoplanet properties like metallicity, weather, and magnetism.

The detection of such molecules is best done with high-resolution cross-correlation techniques, which were reviewed by Matteo Brogi. Spectroscopy at very high resolution ($R > 25\,000$) with telescopes on the ground couples the ability to resolve the dense forest of molecular lines with sensitivity to the changing planet's orbital motion, and it extracts information from spectra via cross-correlation with models. While the cross-correlation method has shown enormous potential to recognise molecular species, exploring families of models and retrieving information about abundances and temperature have proven more challenging, and working solutions have only emerged in the last two years. Matteo also highlighted the complementarity between space- and ground-based observatories, which we are just starting to exploit and which will be fully realised when coupling the JWST to ESO's Extremely Large Telescope.

The following day, Neale Gibson provided convincing evidence that while the "classical" cross-correlation approach is efficient at finding atomic and molecular species, it is quite limited in its inability to recover quantitative information on the atmosphere, such as abundances and temperature profiles; nor can it place statistically robust uncertainties on the quantities it can measure. Recent pioneering efforts have therefore sought to develop likelihood "mappings" from the cross-correlation function, that can be used to directly compare model fits to high-resolution data sets, thereby solving these issues. Such frameworks can be based on a simple Gaussian likelihood, remarkably similar to the techniques that have been applied to transit light curves for over a decade. However, this only works if one can filter out the stellar and telluric lines from the data without losing the signal from the underlying exoplanet. Luckily, Neale showed that much progress has been made on these fronts.

Mornings and evenings

The above methods aim at understanding the atmospheres of exoplanets and inferring more information about the planets themselves. However, as Néstor Espinoza highlighted, care must be taken in the interpretation. During transit, stellar light gets filtered through the terminator region of an exoplanet, allowing us to peek into its atmospheric structure and composition. Because of its complex 3D nature, however, this region is most likely not homogeneous. Hot, highly irradiated and tidally-locked giant planets in particular have been predicted to have different properties around their morning (i.e., night-to-day) and evening (i.e., day-to-night) terminators, implying that they might have distinct temperature, pressure and thus compositional profiles that would give rise to different spectra on each side of a terminator. This can nevertheless be used to our advantage, as constraining those differences might give precious insights into circulation patterns and compositional stratification that might prove to be fundamental for our understanding of not only the weather patterns in the planets under study, but also of planetary formation signatures which might only be possible to extract once these features are well understood. Néstor reviewed the state-of-the-art models predicting this effect and the prospects for their observational detection, with a special focus on the role that high- and low-resolution ground-based spectrographs could have on the quest to constrain the mornings and evenings on these distant worlds.

Many of the results depend on how well we can model the spectra of planets. This topic, applied also to brown dwarfs, was reviewed by Theodora Karalidi, who showed how we are living in an era where developments in atmospheric models are data-driven. She gave an overview of the intricacies of modelling brown dwarf and exoplanet spectra and how observations have informed our models, and how high-resolution model spectra will help us constrain the 3D structure of brown dwarf and exoplanet atmospheres.

The goal is to gather information on the formation and evolution of exoplanets, and particularly hot Jupiters. This was the subject of the talk by Rebekah Dawson, who started by emphasising how hot Jupiters — the first exoplanets to be discovered around main sequence stars — astonished us with their close-in orbits. They are a prime example of how exoplanets have challenged our textbook, Solar-System-inspired story of how planetary systems form and evolve. More than twenty-five years after the discovery of the first hot Jupiter, there is still no consensus on their predominant origin channel. Three classes of hot Jupiter creation hypotheses have been proposed: *in-situ* formation, disc migration, and high-eccentricity tidal migration. Although no channel alone satisfactorily explains all the evidence, progress is now being made, in particular thanks to the study of atmospheres.

Looking forward

This unique set of review talks was complemented by highly interesting contributions, covering topics such as computing atmospheric models, retrieving atmospheric compositions, and identifying surface features. We don’t have space to review all these here, but almost all the presentations have been recorded: copies of the slides and links of the videos are available on the conference’s programme webpage[1]. Most slides were also included on Zenodo, allowing them to have a DOI and to be recorded in the ADS.

There is no doubt that the conference highlighted how dynamic the field of atmospheric studies of exoplanets is, a field in which many young scientists are playing a key role. Understanding the processes requires the use of many sophisticated techniques, whether to compute theoretical spectra or to analyse and interpret the data, including the use of machine learning. Things are evolving at an amazing pace, and we hope that with the material provided, even more young astronomers will be encouraged to embark on these amazing studies.

Demographics

In setting up the programme, the Science Organising Committee (SOC) decided to depart from usual practice and to give preference to young scientists who have already demonstrated remarkable achievements in their areas. The quality of the lectures and presentations witnesses that this approach paid off. Thus, most of the lecturers and invited speakers were at the postdoctoral or assistant professor level, with some of them also still about to finish their PhD. It was a further choice of the SOC not to have posters in this conference.

The selection of invited speakers was made to ensure gender and country balance, while the selection of contributed talks was done blindly by the SOC, who were only given the abstracts. This led to 39% of the contributed talks being given by women, higher than the 30% ratio of the submitted abstracts. A large fraction of the contributed talks were given by PhD students.

We had a total of 208 registered participants, even though during the workshop the number of live participants was always around 100–120. This is likely due to the fact that participants came from four continents and 35 countries in total. Live participation was therefore not always easy, given the difference in time zones. However, as most of the lectures and presentations were recorded, and the discussion took place on Slack, we are confident that all registered participants had the opportunity to enjoy the talks and ask questions if necessary.

The distribution of the participants, speakers, and session chairs according to gender, career stage, and countries is shown in Figure 3. A post-conference survey was conducted amongst the participants, which revealed that a large majority were very satisfied with the workshop — the final average rating of the quality of the talks was 9.1 — and that many wished to repeat this conference soon!

Acknowledgements

Many thanks go to all the lecturers and invited speakers for the quality of their presentations. It is a pleasure to thank the ESO librarians for their help with putting the slides of the talks on Zenodo. The title of the workshop is based on a line by Arletty in the 1938 French movie Hôtel du Nord by Marcel Carné. The workshop poster was made by N. Boffin.

Links

[1] Workshop programme webpage: https://www.eso.org/sci/meetings/2021/Atmo2021/program.html

P. Horálek/ESO

Located high on the top of a Chilean mountain, ESO’s Paranal Observatory benefits from stunning vistas of the surrounding Atacama Desert and — more importantly! — clear and beautiful skies. This photograph of the site shows an especially colourful scene, as the setting Sun paints the sky with beautiful hues of pink, orange, purple, blue, and yellow.