Appendix A – Case Studies

A1. Galaxy simulations and the links to observations and physics

Cosmological, hydrodynamical simulations model the evolution of a representative part of the universe. Starting shortly after the big bang from initial conditions inferred from observations of the cosmic microwave background and large-scale structure, they model the growth of structure and naturally form galaxies in the process.

Virtual observations of cosmological simulations are used to test theoretical scenarios, measure physical parameters, guide the interpretation of observations, develop and test data analysis techniques, design observing campaigns, and evaluate the implications of trade-offs in the design of instrumentation. Furthermore, visuals of the virtual universe are frequently used in education and public outreach.

Due to the need to model both small and large length and time scales, cosmological simulations are extremely challenging. They require state-of-the-art computational methods, use tens of millions of core hours on supercomputers, and produce petabytes of data. The astrophysics modules need to capture diverse astrophysical processes including radiative processes, star formation, stellar evolution, black holes, and winds driven by stars and active galactic nuclei. The initial conditions depend on the physics of the very early universe and the growth of structure depends on the nature of dark matter and dark energy. Hence, the field of cosmological simulations is interdisciplinary, sitting at the intersection of astronomy, physics and computer science.

Successful simulations are in great demand. A good example are the EAGLE simulations, which were developed by an international team led by Leiden that included Leiden PhD students and postdocs as well as researchers in the UK, Belgium, Germany, Spain, Canada and the USA. The simulations are publicly available and have been used by astronomers from all NOVA and NWO institutes in research papers, grant applications, observing proposals, education and outreach. EAGLE has already resulted in many hundreds of papers, including the most cited paper in all of astronomy published in 2015 (Schaye et al. 2015). In recognition of its ongoing impact, the EAGLE team was awarded the 2022 group achievement award from the Royal Astronomical Society.

Leiden University recognizes the strategic importance of the field of cosmological simulations. This is demonstrated by the recent hire of Matthieu Schaller on a faculty position jointly by the departments of physics and astronomy, as well as by the provision of structural funding by Leiden Observatory for a software engineer for cosmological simulations.

After years of development, two Leiden-led international teams are close to finishing new simulation projects that use new open source code SWIFT developed by the teams. These projects improve on EAGLE in different ways.

FLAMINGO simulates much larger volumes, includes a sophisticated treatment of neutrinos, used machine learning to calibrate subgrid parameters, and compares different cosmological scenarios. The runs were recently completed, including one with a record number of resolution elements. FLAMINGO will be particularly useful for cosmology. Indeed, surveys like the ones planned with ESA's soon to be launched Euclid satellite cannot fulfil their science objectives without predictions from cosmological simulations like FLAMINGO.

The COLIBRE simulations include much more astrophysical processes, such as molecules, dust, and a varying radiation field, and use higher resolution. COLIBRE test runs produce populations of galaxies of unprecedented realism and are currently being scaled up towards the final production runs. COLIBRE will be particularly useful for studies of galaxy formation and evolution.

A large fraction of the extragalactic community has benefitted from the EAGLE simulations and will also benefit from these upcoming simulations. The Leiden groups working on high-redshift galaxies, galaxy and AGN evolution, clusters of galaxies, gravitational lensing, gravitational waves, and users of facilities such as ALMA, JWST, Euclid, the ELT, and Athena can for example all take advantage of the availability of state-of-the-art models.

A2. Astrochemistry: from Lab to JWST

The Universe is littered with the debris of dead and dying stars. This debris includes large quantities of micron and sub-micron sized dust grains and over the last decades it has become more and more clear that these act as extra-terrestrial surfaces on which new molecules, small and tall, can form. The involved processes span millions of years along different stages of star and planet formation. Large molecular clouds start collapsing under their own gravitational weight, forming denser and colder cores, in which interstellar gas particles start accreting on dust particles, forming icy monolayers and providing the chemical ingredients from which other species can form upon impacting atoms, electrons, cosmic particles or upon irradiation with UV photons from the interstellar radiation field. Ultimately, this chemically enriched material is the starting point from which planetary systems form. With the recent launch of the James Webb Space Telescope (JWST) astronomers are now able to obtain an unprecedented view on the cosmochemical evolution of ices in space.

In the Laboratory for Astrophysics (LfA Prof. Harold Linnartz) five experimental setups are fully dedicated to study the involved solid state astrochemical processes. Two setups focus on providing high resolution infrared spectra and optical constants that are needed to interpret JWST observations. “Which molecules are frozen out in dark interstellar clouds, prestellar cores and protoplanetary disks? How are these ice spatially distributed and what are their column densities and abundances?” For this ices are spectroscopically characterized with high precision for different mixing rates, at different temperatures and ice morphologies, e.g. by varying the level of ice porosity. Absorption cross sections are determined that allow to calculate how much JWST time is needed for a positive identification. All data are stored in world’s largest database for inter- and circumstellar ices ,LIDA, the Leiden Ice Database for Ice (https://icedb.strw.leidenuniv.nl/) that also provides tools to fit and simulate interstellar spectra. The other three setups focus on the “Why?” Why do we see specific molecules in the birthplaces of new stars and planets, e.g., what are the chemical processes at play that result in their formation. Specifically we look into the interaction of ice and particles, such as free atoms that dominate reactions on ice surfaces in dark interstellar clouds, or the interaction of ice and light, e.g. around a young stellar object. In this way we have been able to show how water forms in space, as well as larger prebiotic species, such as small sugars (i.e. glycerol) and amino acids (glycine). Understanding the reaction pathways and their rates allows us to predict which molecules form in space. UV photodesorption (the light induced evaporation of an ice) and ice photochemistry ultimately determine the chemical composition of planets around new stars: accurate reaction rates are a prerequisite to link astronomical observations to the outcome of astrochemical modelling.

The ultrahigh vacuum and cryogenic ice setups in the LfA are equipped with special UV lamps, simulating the interstellar radiation field, and atomic beam lines allowing to produce clean H, D, O, N, and C-depositions in ices. Sensitive diagnostic physical chemical diagnostic tools, such as Fourier Transform Infrared reflection absorption spectroscopy (FTIR RAIRS), Temperature Programmed Desorption Quadrupole Mass Spectrometry (TPD QMS) and Laser Desorption Post Ionization Mass Spectrometry (LD-PIMS) are used to record data. These find their way to astronomical applications through LfA involvement in a large number of JWST projects, such as the Early Release Science program (ICE AGE - http://jwst-iceage.org/), in which the LfA coordinates the laboratory actions, JOYS, a GTO JWST program focusing on ices towards high mass stars and INTERCAT (the center for Interstellar Catalysis - https://phys.au.dk/intercat) that looks into the interaction of surfaces and ices. The latter is important to characterise processes that take place or are determined by the chemical composition and structure of an interstellar ice grain. Furthermore, the LfA is involved in gas phase surveys, typically with ALMA and IRAM-30m based programs, that investigate the amount of chemical complexity in the gas phase in regions that are also observe by JWST. This allows us to understand how species once formed in the solid state are transferred into the gas phase, through photo-desorption or reactive desorption, i.e. following a local hot spot where excess energy is generated by a surface reaction.

The LfA is fully embedded within Leiden Observatory and as such one of the few large laboratories fully dedicated to astrochemistry and embedded in a large academic observatory. In recent years a number of developments have strengthened its position: the recent hires on a permanent position of Dr. KoJu Chuang (LfA) and Dr. Melissa McClure (PI ICE AGE) as well as close links to the Leiden Institute of Chemistry through a part-time position of Dr. Thanja Lamberts (TC) to put a theoretical chemical base under processes measured experimentally.

A3. Exoplanets: theory, observations and instrument development

Over the last decade, Leiden Observatory has transformed into a major hub for exoplanet studies. The seven permanent members of staff who now have exoplanets as their main research subject, together with the several dozen in-house postdoctoral researchers and PhD students, provide a vibrant community with close links to the lively astrochemistry and planet formation groups.

Research at Leiden Observatory covers many aspects of exoplanets. New insights on the internal structure of Solar System planets such as Jupiter (NASA Juno mission) are used to constrain those of extrasolar gas giants, shining light on how they could have formed. Star-planet interactions driven by stellar winds and intense radiation are linked to significant atmospheric losses of particularly close-in planets, while the first detections of coherent low-frequency radio emission from red dwarf systems with LOFAR point to magnetic star-planet interactions. An exciting new direction that in the future is expected to lead to the first planet magnetic field estimates.

Discoveries of new exoplanetary systems and their subsequent characterization go hand in hand, using state-of-the-art instrumentation such as SPHERE, MUSE, and CRIRES+ at ESO's Very Large Telescope (VLT). Novel observational strategies and data analysis techniques have resulted in groundbreaking findings, such as the first accreting multi proto-planet system and the first multi-planet system around a young sunlike star – both recent Leiden-led studies. Leiden is also well known for its pioneering work on ground-based high-dispersion spectroscopy to characterise exoplanet atmospheres, such as the presence and abundance of atomic, ionic, and molecular species, temperature structure, circulation patterns, winds, and planet spin rotation. This has recently also resulted in the first isotopic measurements – an exciting new avenue of study. Leiden astronomers are also actively working on JWST studies, particularly in providing theoretical studies for gas giants and the latest predictions for strongly irradiated lava worlds.

Instrumentation development is another important pillar of Leiden exoplanet research, and vital for the future directions in this field. This involves development studies of polarimetric instruments, integral-field spectrographs, coronagraphy, and wavefront-sensing algorithms. Particularly successful and unique in the world is vector-Apodizing Phase Plate coronagraphy based on liquid-crystal technology – now installed on most large telescopes, including the recently commissioned ERIS instrument on the VLT.

With NOVA leading the construction of METIS, one of the three first-generation instruments for the Extremely Large Telescope, a great future for exoplanet research is cemented. Its unique capacity of high-contrast coronagraphic imaging at mid-infrared wavelengths is combined with high-dispersion spectroscopy – ideal for exoplanet atmospheric studies such as of the potentially Earth-like planet Proxima Centauri b. In the next decade, much of the instrumentation development studies at Leiden Observatory will be focused on the ultimate ELT exoplanet imager EPICS (a.k.a. PCS). Within our lifetimes, we can study planets that will be much like Earth, investigate their atmospheric constituencies and constrain their climates. Are circumstances such that life could have developed? Any sign of biological activity? We live in exciting times!

A4. IAU100 — 100 Years Under One Sky

In 2019, the International Astronomical Union (IAU) celebrated its 100th anniversary and organised a year-long celebration to increase awareness of a century of astronomical discoveries as well as what astronomy has brought to society. The central hub that implemented and coordinated the IAU100 project was the Astronomy & Society group of Leiden Observatory (Leiden University). The Astronomy & Society group is a Research & Development Lab that designs, implements and evaluates public engagement with astronomy activities at the local, national, and European level. Some of these projects include the global programmes like Universe Awareness[2], Space Awareness[3], spaceEU, International Day of Light[4] and the IAU European Regional Office of Astronomy for Development[5]. Most of the research findings of these projects have been summarised in the Annual Reviews' article: Astronomers Engaging with the Education Ecosystem: A Best-Evidence Synthesis by Pompea, S. & Russo, P. (2020)

IAU100 was implemented under the central theme "Under One Sky" and showcases how astronomy can be used as a tool for communication, education, development and diplomacy. The Dutch Astronomy Council was one of the IAU100 sponsors. A small IAU100 team effectively developed and implemented various innovative astronomy communication initiatives to engage the public. As a result, at least five million people worldwide celebrated the astronomical breakthroughs that have shaped science, technology and culture over the last century while looking ahead to what awaits us in the future. In addition, IAU100 fostered opportunities and resources for amateur and professional astronomers, educators, communicators, scientists, organisations, and institutions.

Eleven total global IAU100 initiatives were implemented between January 2019 and February 2020. These initiatives were facilitated with limited resources, with each global project driven by a single part-time person effectively coordinating a global national node network that spanned 124 countries to lead IAU100's activities locally and regionally. Through this network, IAU100 found creative and effective means of disseminating astronomy in an accessible way for the public around the world, reaching the general public and children of all ages. Low-budget astronomy outreach and education resources were made available for event organisers for each of the global projects. For example, an innovative exhibition, Above and Beyond: Making Sense of the Universe, was displayed in over 75 countries. This exhibition summarises the past 100 years of astronomical discoveries, and all the content and designs are available under an open-source licence which enabled the international community to translate and localise it. A Dutch version featured at the Old Observatory in Leiden attracted 15 000 visitors.

By implementing astronomy communication initiatives on local, regional and global scales, IAU100 demonstrated the power and inspiration of astronomy to bring people together, regardless of background. In total, IAU100 had over 5000 registered activities in 143 countries, and facilitated the direct involvement of an estimated 5 to 10 million people. The impacts of IAU100 also go far beyond the celebration of the 100th anniversary of the IAU. It has cemented an active framework of national coordinators and event organisers who will continue to disseminate the values, goals, and resources of IAU100 for years to come.

More information: https://www.iau-100.org/

IAU100 Final Report: https://iau.org/news/announcements/detail/ann20019/

[2] https://www.unawe.org/

[3] http://www.space-awareness.org/en/

[4] https://www.lightday.org/

[5] https://astro4dev.eu/

A5. ALMA and Allegro

As the ALMA Regional Center node in the Netherlands, Allegro provides support for ALMA users in the Netherlands. Allegro also develops methods and tools that enhance the science capabilities of ALMA. Allegro is hosted by Leiden Observatory and receives funding from NWO. Allegro supports the ALMA use of both staff and students at the Dutch astronomical institutes, ranging from answering questions about proposing or archive mining to in-depth problem solving and advanced data processing. Over the past 5 years, Allegro has played a significant role in projects involving Leiden astronomers.

Contact Scientist support of the REBELS Large Program – Each successful ALMA proposal is assigned a Contact Scientist (CS) who acts as a liaison between the PI and ALMA, and Allegro provides CSs for projects led by the Netherlands. Each cycle, ALMA awards a small number of Large Programs that exceed 50 hours of observing time and that have a unique legacy value. In Cycle 7 (2019), Bouwens was awarded a 69-hr Large Program, REBELS, which aimed at detecting the star-forming gas reservoir in a carefully selected sample of 40 high redshift galaxies. Allegro provided extensive support for REBELS, helping prepare, organise, and implement optimization of the observing program through many Change Requests submitted to ALMA. This optimization was needed because of continuous updates to redshift estimates from other telescopes and affected the selection of the most promising targets and frequency ranges. Without careful management of the Change Requests, the high detection rate of REBELS (tripling the number of detections) would not have been achieved. Allegro will also assist REBELS in making the final data products publicly available.

ALMA Science Archive mining support – The ALMA Science Data Archive contains a rich collection of publicly accessible data, which is being mined by an increasing number of studies. Using the ALMA archive, Leiden PhD student Stapper extracted a volume limited sample of observations of planet-forming disks around Herbig Ae/Be stars (~1.5-8 Solar mass). At a 33% completeness level, this represents the first systematic and homogeneous study of the disk masses and size around this population of young stars. This study relied heavily on the archive mining tool ALMINER that was developed at Allegro, and that provides a python-based interface to search and filter the ALMA data archive. In addition, Allegro provided the computational and data storage resources necessary to process the wealth of data that was retrieved.

Massively parallel ALMA data processing – Some ALMA projects are so massive that manual processing of the data becomes infeasible. One such project is the SODA survey of Leiden PhD student van Terwisga. This project contains imaging of 800 (!) fields in the Orion star forming region. Using containerized processing at the SURFsara facility, Allegro developed massively parallel processing of this data set, ultimately allowing imaging of the 800 fields in just 30 minutes of wall-clock time. This containerized ALMA data processing is generally available for Allegro users and is currently implemented for the processing of the data of two Large Programs with NL involvement.

Imaging the Supermassive Black Holes in M87 and the Milky Way galaxies – One of the highest profile astronomical results from the past years is the imaging of the shadows of the black holes in the Milky Way and M87, by the Event Horizon Telescope consortium including ALMA. Allegro played a pivotal role in enabling these observations, through the Project Manager roles of Tilanus and the involvement of Impellizzeri and Goddi in the observations and data processing. Specifically, the ALMA data processing Quality Control procedures for VLBI data were developed by Goddi at Allegro. The streamlined QA2 processing and packaging forms a *crucial* step in the data flow before correlation can happen. Without these procedures developed at Allegro, EHT cannot operate as efficiently as it does.

Enabling calibration of high-frequencies at ALMA – A final, technical example of how Allegro contributes to the overall ALMA operations, is given by the work of Maud who, while at Allegro, started the investigation of transferring phase corrections from a (lower) frequency to a (higher) frequency. At these higher frequencies (>600 GHz), suitable phase calibrators become rare, and band-to-band phase transfer is essential. Maud's work included both the proof of principle at the telescope and the development of solid operational procedures that are now part of the standard observational protocol at ALMA.