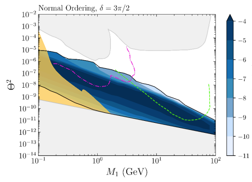
DEPARTMENT OF PHYSICS AND ASTRONOMY "AUGUSTO RIGHI"

ADVANCED SENSING LABORATORY



HIGH PERFORMANCE COMPUTING CLUSTER

ALMA MATER STUDIORUM UNIVERSITÀ DI BOLOGNA

OPH NEWSLETTER

FOCUS: The many scales of computational astrophysics and cosmology

The Universe is the largest object we can ever study in physics. Yet its evolution is dictated by the properties of the tiniest fundamental particles of nature. **In between these two extremes, a wide range of complex, interrelated phenomena cooperate to build up the structures that populate the cosmos as we observe it**, hosting stars, galaxies, planets, and – ultimately – us.

Understanding these different processes is a formidable challenge due to the complexity of the systems involved, and to their inherent multi-scale nature. **Computational methods are therefore an essential tool to tackle most of the current open questions in astrophysics and cosmology**.

The OPH computing cluster at DIFA is extensively employed by different research groups in the Astrophysics sector to investigate many of these intriguing phenomena, over a wide range of different scales.

On its largest scales **the Universe is governed by the laws of gravity and by the mysterious Dark Energy that is pushing its expansion to accelerate, while its structures are shaped by the properties of Dark Matter particles and neutrinos**. Investigating the interplay between possible hypotheses on the nature of the Dark Energy and different Dark Matter particle candidates requires simultaneously modeling their effects on the formation and evolution of cosmic structures, which can be fully captured only through large-volume sophisticated numerical simulations. The computational cosmology group at DIFA has been using the OPH parallel computing cluster to run and analyze cosmological simulations of a wide range of Dark Energy models, Modified Gravity theories, and Dark Matter candidates such as neutralinos, Ultra-

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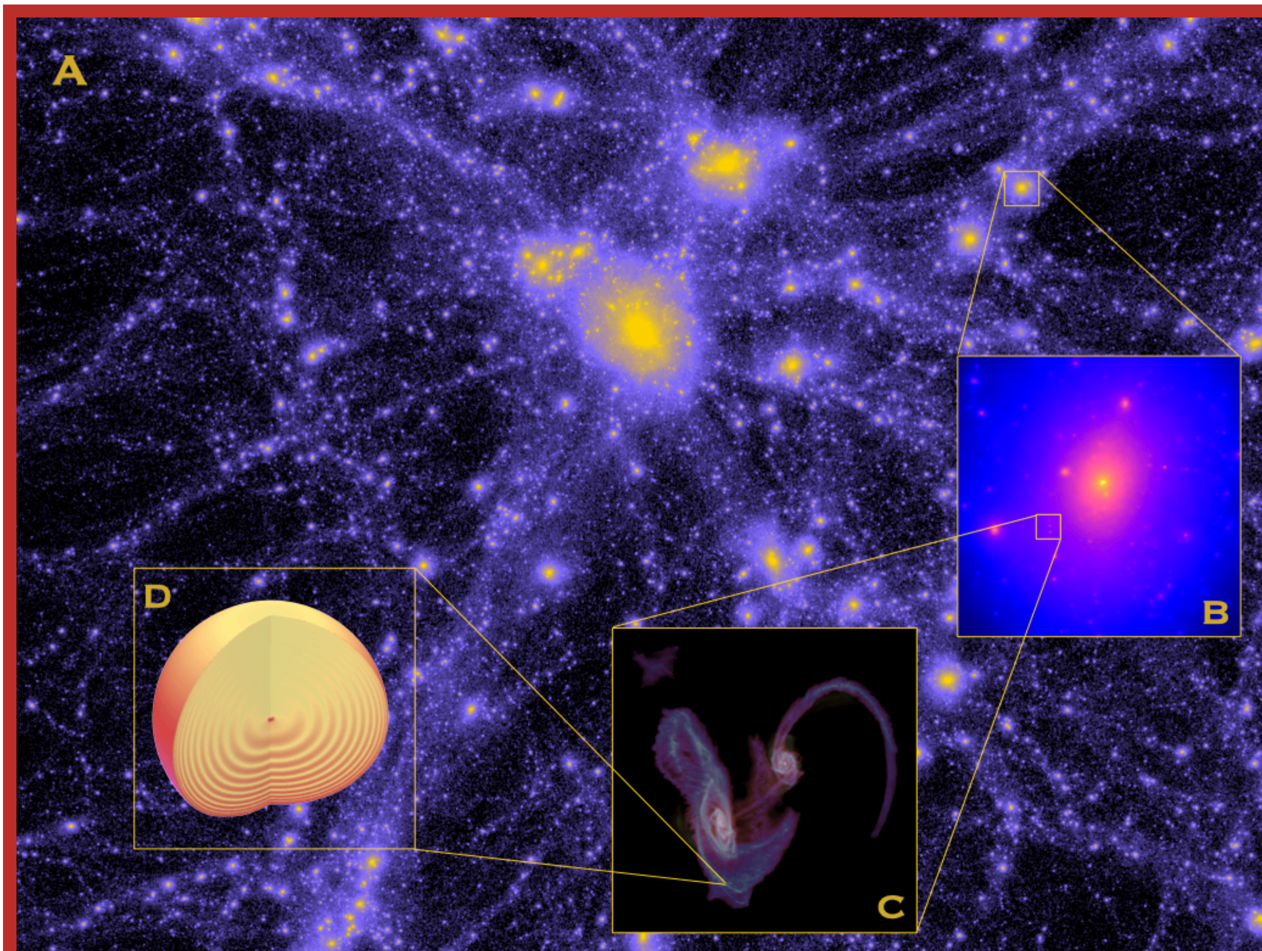
Light Axions, and massive neutrinos to produce mock universe observations of the so-called cosmic web: a backbone of Dark Matter filaments that cross each other in highly overdense regions corresponding to Dark Matter halos.

But what is Dark Matter? This is one of the most pressing questions facing physics and astronomy today. Experimental searches have so far not led to significant detections, and the parameter space of favored particle candidates corresponding to the so-called "cold" Dark Matter is increasingly tightly constrained. Astronomical observations have shown that "cold" Dark Matter successfully reproduces observed structures in the Universe on large scales, but discrepancies on the scales of galaxies or below still exist. These observations provide critical information to help direct future particle physics searches and in many cases, they provide the only robust, empirical constraints on the viable range of dark matter models. One of the most promising tools to investigate the nature of dark matter is gravitational lensing: similarly to the deflection caused by glass lenses, the image of a high-redshift galaxy is distorted and magnified by the presence of another galaxy along the line-of-sight and whose mass distorts space-time and acts



***A**: the cosmic web from a Dark Energy cosmological simulation (Baldi 2023 MNRAS 521)*

***B**: projected density of a simulated Dark Matter halo hosting an elliptical galaxy at its center (Despali et al. 2020, MNRAS 491)*

***C**: simulation of a merger of two spiral galaxies representative of the Andromeda-Milky Way system (Marinacci et al. 2019 MNRAS 489)*

***D**: Representation of a dipolar pulsation mode in a star with radius about 10 times the radius of the Sun*

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as a lens. This technique allows us to directly measure the total mass of objects, both dark and luminous, and thus put direct constraints on the dark matter distribution. But accurate predictions of the lensing signal for different Dark Matter particle candidates require detailed computer simulations of the formation of the gravitational lenses. By exploiting the OPH cluster at DIFA, it was possible to produce accurate hydrodynamical simulations including the physics of baryons and different Dark Matter models and to use them to study the galaxy properties and generate synthetic observations to be compared with real images of gravitational lenses.

Besides showing up as lenses deflecting the light of background galaxies, Dark Matter halos are also the cradle of star and galaxy formation processes, leading to the buildup of the large variety of galaxies we observe in the Universe. Numerical simulations play an essential role also in this context, allowing to gain a deeper theoretical understanding of the formation and evolution of galaxies. Modeling galaxy formation is an incredibly complex task due to the enormous range of spatial and temporal scales across which the key physical processes shaping galactic evolution operate. The computational galaxy formation and evolution group at DIFA has been using the OPH high performance computing resources to develop state-of-the-art models of galaxy formation physics that faithfully describe the multiphase nature of the interstellar medium and self-consistently include the effects of stellar feedback on galaxy evolution. These models have been employed to run advanced galaxy formation simulations investigating fundamental topics in the field, such as the gas cycle in star-forming galaxies, galaxy interactions and mergers, and the formation of Milky Way-like galaxies in a cosmological context.

Being systems of gravitationally bound stars, galaxies' formation is sensitive to the details of stellar evolution processes taking place at scales orders of magnitude smaller than the typical size of a galaxy.

Asteroseismology, i.e. the study of global, resonant oscillation modes in stars, has given us the ability to finally peer into the interiors of these otherwise opaque objects and to test our models of stellar structure and evolution. The ERC-funded asterochronometry group at DIFA has been intensively using the OPH cluster to generate model-predicted stellar structures and oscillation spectra which are then used, by comparison with observed pulsational frequencies, to infer precise and accurate stellar properties and to expose some of the shortcomings of our current understanding of stellar physics. Our efforts are currently focussing on pushing the limits of stellar age inference down to the 10% limit. This is key to provide the temporal resolution needed to reconstruct the assembly history of our Galaxy, and to place the Milky Way into the wider context of galaxy evolution, feeding this time information from the smallest scales of individual stars to the largest scales of galaxy populations sparkling throughout the Universe!

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Teaching and outreach

The 5th edition of the DIFA International Summer School on Physical Sensing and Processing

From 17 to 21 July 2023, the Aula Magna of the Department of Physics and Astronomy hosted the fifth edition of the Summer School on Physical Sensing and Processing (link).

OPH significantly contributed in financing and organizing the event, programmed within the Alma Strutture project by UNIBO. To promote international activities, the school featured 4 special talks by recognized experts from the university of Notre Dame (USA), Wollongong (Australia) and Europa Universität Flensburg (Germany).

The course was attended by 40 Master's and Ph.D. students in person and about 20 online auditors. A few international students from European and Asian universities were also present.

In addition to the featured special talks mentioned above, 11 lessons covering a broad research field were held in the morning sessions by external experts: Dr. Pietro Antonioli (INFN), prof. Franco Camera (University of Milan), Dr. Italo Foppiani (INAF), Dr. Jessie A. Posar (University of Sidney) and Stefano Toffanin (CNR); as well as colleagues from DIFA.

In the afternoon, 6 different project-oriented laboratory sessions (2-hour each) were carried out in group of ten students. These experimental activities represented the novelty of the 5th edition of the Summer School. The survey of student's opinion revealed that students had largely appreciated them.

In addition, the students in attendance participated in "Collaborative Work" activities, coordinated by a group of expert doctoral students or postdocs from DIFA. It gave the opportunity to the students to elaborate on the laboratory sessions, for instance to analyse the collected data. The students worked to prepare and present a short informative poster, addressed to school students and/or the public. A panel of professors awarded the best poster presentation with a special prize.

The pictures show two moments of the collaborative work. In the top panel a student (representing his working group) presents the poster on one topic studied during the laboratory session. In the bottom panel a group of students receive the best presentation award.

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Teaching and outreach

The 3rd edition of “ONSCI”: the DIFA summer school on science communication

The third edition of the “ONSCI – Officina di Narrazione della Scienza” summer school took place from 7 to 13 September, organized by the Department of Physics and Astronomy “A. Righi” of Bologna, supported by the OPH, the Collegio Superiore, the PNLS (National Scientific Degree Plan), the H2020 FEDORA project and the INFN and with the patronage of the Parliamone Ora association and the Italian Physics Society.

The school, traditionally designed for a variety of stake-holders (university students, professors, researchers, teachers, educators and communicators), hosted, as in previous editions, around 100 participants. ONSCI, in fact, provides essential communication tools in contexts such as seminars (both popular and specialist), educational activities (both formal and informal) and more generally for *public engagement with science* activities. With even greater urgency, who produces scientific knowledge is called to reflect in an ever more profound and articulated way on their communication practices in order to enrich and reshape increasingly congenial and fruitful relationships with society. ONSCI fully responds to this urgency.

In fact, for this third edition, the school proposed a stimulating interdisciplinary dialogue which consequently brought with it the study of different communicative, imaginative and narrative approaches. Speakers, as a matter of fact, were capable of interpreting science in its historical, epistemological/philosophical, methodological, socio-political dimensions.

After the introductory lecture about why we comunicate science by the scientific journalist and director of “Le Scienze”, the Italian edition of *Scientific American,* Marco Cattaneo which took place in the historical Specola building, there was a serie of talks, theoretical and as more practical testimonies, about the need to communicate science in society and about specific methods both in scientific research, in teaching and in the performing arts.

The school afternoons were dedicated to two workshops on storytelling production. The first, held by Andrea Brunello, physicist and playwright, focused on the production of very short and strategic speeches to keep the audience's attention high. The second, held by the research group in Physics Education and History with the collaboration of the scientific high school “A. Einstein” of Rimini brought to light innovative teaching paths in which the language of science and that of art were interconnected, creating unexpected synergies.

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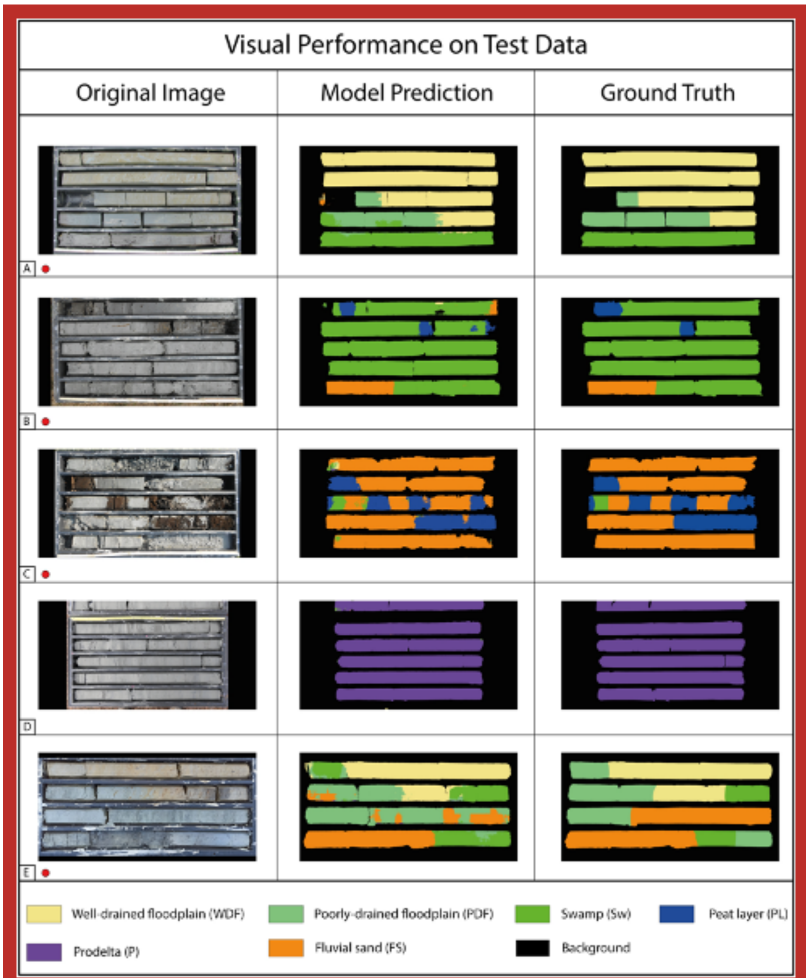
Publications related to OPH

Sediment core analysis using artificial intelligence

Subsurface modeling is crucial for a variety of environmental, societal, and economic challenges. However, the need for specific sedimentological skills in sediment core analysis may constitute a limitation. Methods based on Machine Learning and Deep Learning can play a central role in automatizing this time-consuming procedure. Nevertheless, automated approaches based on Artificial Intelligence are still lacking in subsurface geological sciences compared to other fields, partially due to the scarcity of publicly available labeled data. In this work, we manually annotated a large dataset of high-resolution digital images from continuous sediment cores of Holocene age that reflect a wide spectrum of continental to shallow-marine depositional environments. We then used the produced annotated data to train a Convolutional Neural Network, developing a novel deep-learning-based approach to perform automatic semantic segmentation directly on core images. Part of the model training was performed thanks to the computation capabilities of the OPH facility. To optimize the interpretation process and maximize scientific value, we used six sedimentary facies associations as target classes in lieu of ineffective classification methods based uniquely on lithology. The method was thoroughly tested with different standard metrics used in semantic segmentation tasks and obtained high segmentation performance for all the classes involved in the study. We propose an automated model that can rapidly characterize sediment cores, allowing immediate guidance for stratigraphic correlation and subsurface reconstructions. The heterogeneity and variety of the data used to train the model make the developed method suitable for real-case analyses performed directly on the field, making it a valuable tool for technical and scientific applications.



Visual performance of the model on five representative images of the test dataset. The original full-resolution digital images, the model produced segmentation masks, and the corresponding ground truths are shown in the left, central, and right columns, respectively. The red dots mark the images coming from the external set of sediment cores.

Reference

Di Martino A., Carlini G., Castellani G., Remondini D., Amorosi A. (2023). *Sediment core analysis using artificial intelligence*. Sci Rep **13**, 20409 (2023). https://doi.org/10.1038/s41598-023-47546-2

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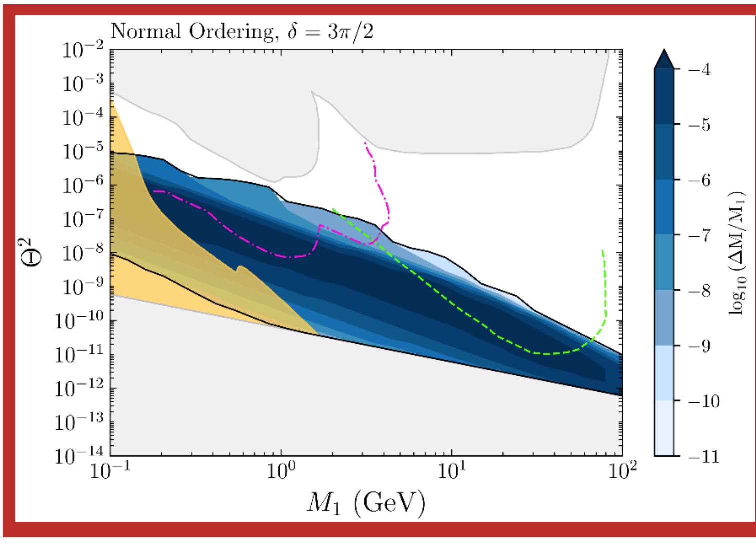
Publications related to OPH

The CP-violating Dirac phase behind the origin of the matter-antimatter asymmetry

The present observable Universe is predominantly made of matter and not antimatter. The asymmetry in baryons (protons and neutrons), also the Baryon Asymmetry of the Universe (BAU), can be parametrized by the difference between the number densities of baryons and antibaryons normalized to that of photons, η_B. The notable concordance between the measurements of the cosmic microwave background anisotropies and the abundances of light primordial elements, both agreeing on $\eta_B = 6.1 \cdot 10^{-10}$ [1, 2], represents a milestone of the Big Bang model.

A compelling mechanism is that of leptogenesis (LG) [3], consisting of an early generation of a lepton asymmetry, later converted into the present BAU by sphalerons. The simplest LG realization arises within the type-I seesaw extension of the Standard Model (SM), which also provides an explanation for the origin of the SM neutrinos' masses. In the type-I seesaw, the SM is augmented with right-handed sterile neutrinos, and a lepton asymmetry can be generated through processes involving the right-handed neutrinos, the Higgs boson and the left-handed leptons. In the case of two quasi-degenerate right-handed neutrinos, their oscillations during their out-of-equilibrium production are also crucial.

In [4], the authors made use of the Python package ULYSSES [5, 6] and the OPH High Performance Computing cluster "Matrix" to solve numerically the complicated sets of quantum density matrix equations relevant to LG. They demonstrated that LG via oscillations is feasible for accessible mass scales as low as 100 MeV with the requisite CP-violation provided uniquely by the Dirac phase (see figure). The Dirac phase regulates CP-violating effects in SM neutrino oscillation phenomena and will be measured experimentally with high precision in the coming years. It is quite remarkable that it might be the only responsible for the fundamental property of the Universe of preponderance of matter over antimatter, making the existence of life on Earth possible.



The parameter space of viable LG via oscillations with CP-violation solely from the Dirac phase δ. The plot is obtained for δ=3π/2 and in the case of a SM neutrino mass spectrumwith normal ordering. On the x and y axesare, respectively,the mass of the lightest right-handed neutrino and the total squared coupling to the SM. The shaded grey and yellow areasareexcluded, while the blue regionscorrespond to viable LGfor different mass splittings. The pink and green contours are sensitivity lines of future planned and proposed experiments [4].

References

[1] Aghanim N. et al. (2020). Astronomy & Astrophysics 641, A6. arXiv:1807.06209.
[2] Cooke R.J., Pettini M., Steidel C.C. (2018). The Astrophysical Journal 855, 102. arXiv:1710.11129.
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[4] Granelli A., Pascoli S., Petcov S.T. (2023). Physical Review D 108, L101302. arXiv: 2307.07476.
[5] Granelli A., Moffat K., Perez-Gonzalez Y.F., Schulz H., Turner J. (2021). Computer Physics Communications 262, 107813. arXiv:2007.09150.
[6] Granelli A., Leslie C., Perez-Gonzalez Y.F., Schulz H., Shuve B., Turner J., Walker R. (2023). Computer Physics Communications 291, 108834. arXiv:2301.05722.

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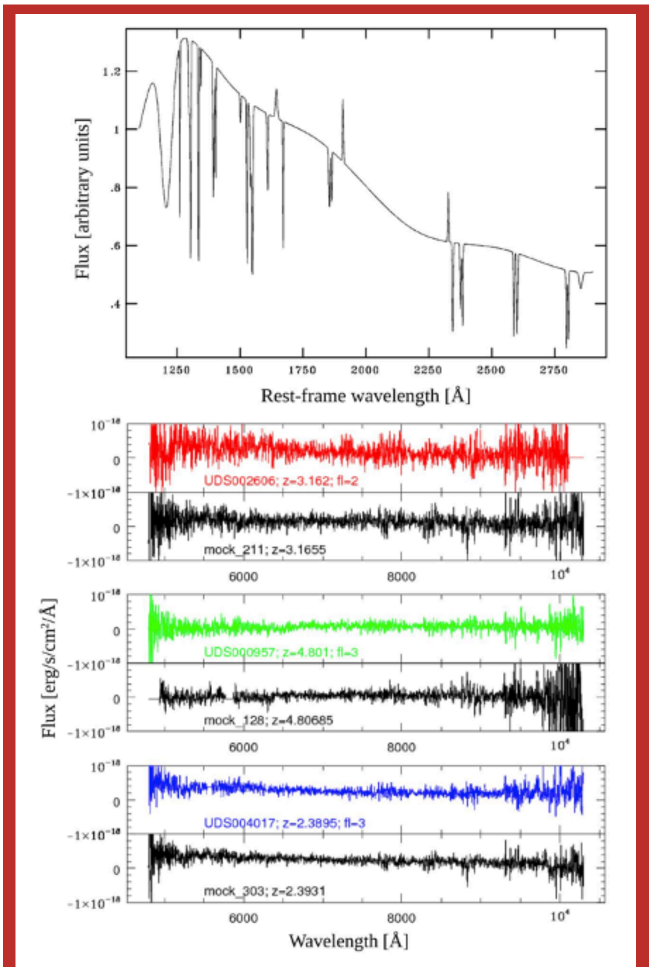
Publications related to OPH

A catalogue of spectroscopic features measurements from the VANDELS ESO public spectroscopic survey: enabling galaxy evolution studies at 2.5<z<5.5

VANDELS is an ESO public spectroscopic survey conducted with the VIMOS instrument at the Very Large Telescope (VLT), aimed at studying high-redshift galaxies in the CANDELS Chandra Deep-Field South (CDFS) and Ultra-Deep Survey (UDS) fields (McLure et al. 2018; Pentericci et al. 2018a). The survey targeted approximately 2100 sources. The focus of VANDELS was not just to obtain redshift information, but also to get high signal-to-noise ratio spectra to study galaxies' physical properties in detail.

This paper presents the release of the VANDELS spectroscopic measurements catalogues produced using the OPH cluster.

The spectroscopic features were measured using two methods: Gaussian fit and direct integration. The Gaussian fit measurements were performed with slinefit (Schreiber et al. 2018), an automated code that models the observed spectrum of a galaxy as a combination of a stellar continuum model and a set of emission and absorption lines, while the direct integration measurements were performed using pylick (Borghi et al. 2022), a flexible Python tool to measure spectral indices and associated uncertainties, which had been extensively tested using spectra and results from the LEGA-C survey (van der Wel et al. 2016; Straatman et al. 2018). To validate the performance of the slinefit code and calibrate its input parameters, we constructed a set of mock 1D spectra with realistic noise, as shown in the Figure. Results showed good agreement between measured spectral quantities and their input values. We further checked the accuracy of our catalogues by comparing subsets of measurements to previous results obtained with different codes and methods.



Construction of the 1D mock spectra for the slinefit code validation. Top: synthetic rest-frame template, normalised to unity at 1750Å. Bottom: comparison between three examples of mock 1D spectra and real VANDELS spectra; mock spectra are shown in black, while VANDELS spectra are colour-coded with respect to their depth: 20hrs of telescope time integration (red), 40hrs (green), and 80hrs (blue).

In total, we measured 40 individual lines with the Gaussian fit method, and 59 indices and breaks, three of which were firstly introduced in this work, with the direct integration method.

We also found that the error spectra included in the VANDELS data release (Garilli et al. 2021) underestimate the noise level when compared to the R.M.S. of the spectra and computed a correction that we provide as well.

The catalogues, which are available to the wider astrophysical community, will enable a large variety of galaxy evolution studies, in particular those related to the composition and properties of the interstellar medium.

Reference

Talia M. et al. (2023), Astronomy & Astrophysics, Volume 678, id.A25. arXiv:2309.14436

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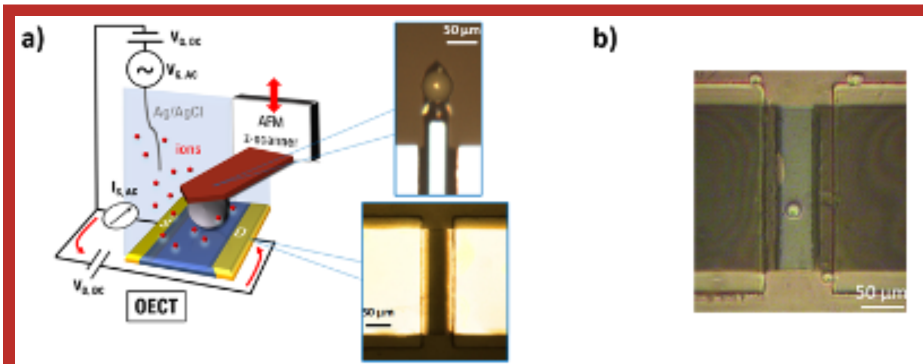
Publications related to OPH

Achieving single cell monitoring with highly sensitive, miniaturized biosensors

The realization of efficient biosensors able to monitor cell adhesion is a crucial task for the field of bioelectronics. Cell adhesion is an essential process in cell communication and regulation and becomes of fundamental importance in the development and maintenance of tissues. Organic electrochemical transistor (OECTs) based on the conducting polymer poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) are promising device architectures for this purpose due to their electrochemical transduction mechanisms and intrinsic amplification properties. The downscaling of the sensor dimensions opens the opportunity to translate cellular monitoring to the single-cell level. This ultimate sensor resolution is highly desired in biomedical research as the importance of single-cell phenotyping is increasingly recognized for the study of cell development and physiology, as well as for research on cellular pathologies such as cancer. Despite many promising results, a quantitative study which relates the OECT sensitivity to the device geometry and fundamental material properties is still lacking. Such a knowledge would be crucial for the rational optimization of cell biosensors able to tackle the limit of single cell resolution.

To overcome the issue, our research team from the OPH-lab introduced a model experiment on highly miniaturized OECT devices. As cellular *in-vitro* experiments are inherently difficult to control, we substitute the cell by a dielectric microparticle of similar dimensions. We control the position of the microparticle on top of the sensors with an atomic force microscope (AFM) and achieve highly reproducible measurements that enable to acquire the variation of the OECT sensor signal when the position of the microparticle is changed. The experimental setup is illustrated in Figure 1a, showing the microparticle attached to the bottom part of the AFM cantilever and precisely moved in close proximity to the micro-structured PEDOT:PSS channel of the OECT. Based on the data, we develop an analytical model that describes the device performances as a function of the device geometry and PEDOT:PSS materials properties. Relying on this model, we design an optimized sensor and demonstrate its efficiency by measuring the transients of single-cell adhesion and detachment in *in-vitro* experiments. An optical image acquired during the experiment, showing a single T98G cell placed on a OECT channel, is reported in Figure 1b. Noteworthy, we observe a significant gain reaching values of (20.2±0.9) dB for the transistor structure when compared to traditional microelectrode measurements, demonstrating the advantages arising from the OECT amplification in single cell sensing experiments. The novel OECT sensor achieving the reliable monitoring of single cell adhesion praves the way towards new biomedical experiments that elucidate the role of single cells in tumor formation or in regenerative processes such as wound healing.



a) Experimental set-up used for the model experiment. A microparticle simulating a single cell is attached to the bottom part of an AFM cantilever to control its position with respect to the active PEDOT:PSS channel (W × L = 200 × 50 µm) of an OECT device. The transistor output current is measured while changing the microparticle-channel distance. b) Optical microscope image showing a single T98G cell adhering on a PEDOT:PSS channel during the in-vitro experiment.

Link to the full paper
Link to Unibo Magazine

Reference

Bonafè F., Decataldo F., Zironi I., Remondini C., Cramer T., Fraboni B. (2022), *AC amplification gain in organic electrochemical transistors for impedance-based single cell sensors.* Nat Commun **13**, 5423 (2022). https://doi.org/10.1038/s41467-022-33094-2.

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Useful links

OPH website
Department of Physics and Astronomy "A. Righi"
INFN
CNAF
OPH Computing Cluster user guide
International Summer School on Physical Sensing and Processing
Astronomy Public Conferences

OPH Newsletter: previous issues

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#7 OPH_Newsletter_07_June 2023

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