PhD DAY

Insights from
Our Physics Doctoral Community

Dec 9th 2025

WORKSHOP AND POSTER SESSION

PhD DAY is a dedicated event showcasing the research carried out by students enrolled in the three Physics PhD programmes at DIFA. The day opens with an overview of the doctoral tracks presented by the programme coordinators, followed by a poster session in which PhD candidates present the progress of their work. The event provides a valuable opportunity for exchange, collaboration, and community building across the various areas of physics.

Scientific Committee: Silvana Di Sabatino, Laura Fabbri, Alessandro Gabrielli and Andrea Miglio.

AULA MAGNA

Complesso di Santa Lucia
Via de Chiari, 25/a - Bologna

FREE ENTRANCE

ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

DIPARTIMENTO
DI FISICA E ASTRONOMIA
"AUGUSTO RIGHI"

In collaborazione con

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ASTEROSEISMOLOGY

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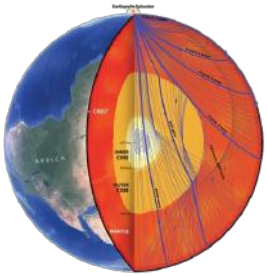
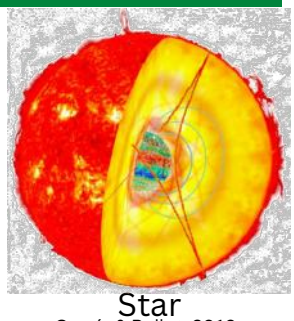
[2] INAF - Osservatorio di Astrofisica e Scienza dello Spazio di Bologna, via Gobetti 93/3, 40129, Bologna, Italy

Stellar evolution and stellar light are key to to both Galactic archaeology, exoplanetary study, and extragalactic research. However, constraining the stellar internal structure and evolution is challenging based on surface properties alone. In asteroseismology, we study stellar oscillations, which are detectable as variations in the light emitted at the surface of the star. These pulsations carry information on the internal structure with them to the surface.

JOURNEY TO THE CENTRE OF THE STAR



Earth
EarthScope Consortium



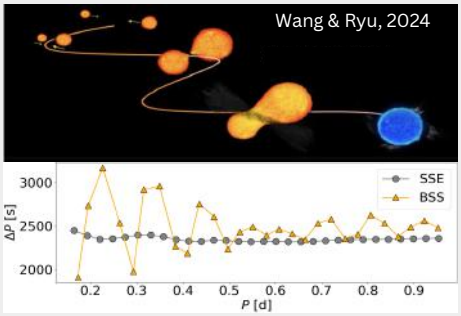
Star
García & Ballot, 2019

The study of pulsation frequencies allows us to dive into the deepest regions of the stars, expanding our knowledge about their interiors. In the same way we discovered the inside of the Earth through the propagation of seismic waves, with Asteroseismology we can get information about convective and radiative regions of the stars, as well as about internal rotation, chemical stratifications and magnetic activity. Seismology can therefore directly constrain model physics, infer global stellar parameters, or search for products of non-standard evolution.

BLUE STRAGGLERS PROBED WITH SEISMOLOGY

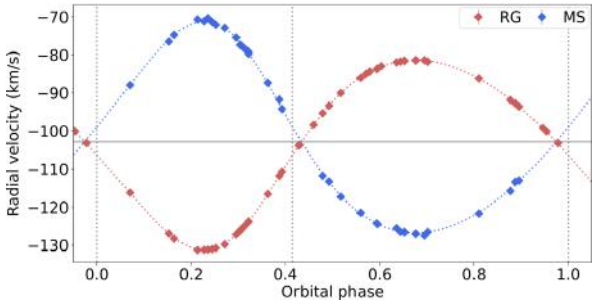
Blue straggler stars (BSSs) are objects which origin from mergers, collisions or mass transfer. Recently, we modelled BSSs formed through stellar collisions. We found that, while for single-stellar-evolution (SSE) objects the pulsation periods are uniformly spaced, in the case of the BSS the spacings between consecutive pulsation periods are not constant, but present periodic modulations. This is caused by a stratification in the chemical profile of the BSS, due to the collision event. This means that stars retain in their interior information on their dynamical past, and we can infer that through asteroseismology.

SCAN ME



L. Briganti et al., 2025, A&A accepted

THE ACCURACY OF ASTEROSEISMOLOGY



J. S. Thomsen, et al., 2025, A&A Vol 699

Asteroseismology constrain the internal structure, but seismic inferences of stellar parameters are inherently dependent on stellar evolution models. For Galactic archaeology, precise (<10%) seismic age measurements of old stars need verification. We studied KIC10001167, currently the only old eclipsing binary with precise seismic data. We mapped its binary orbital motion with radial velocities, and obtained a model independent mass of the oscillating star with <1% precision, verifying asteroseismic inferences for old stars to 1.5% in mass (6% in age).

SCAN ME

ASTERO CHRONOMETRY

Phd Day -2025

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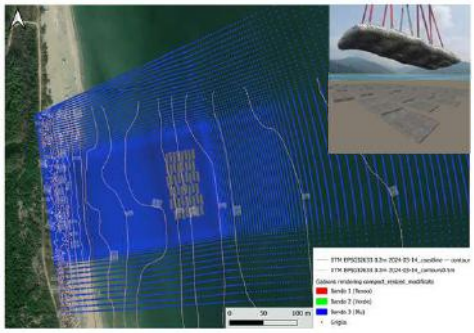
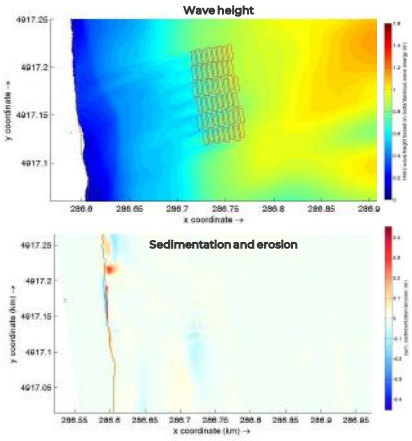
HYDRODYNAMIC STUDIES ON A RESTORED OYSTER REEF: METHODOLOGY AND PRELIMINARY RESULTS

DI ISABELLA CASADEI, Dipartimento di Ingegneria Civile, Chimica, Ambientale e dei Materiali - DICAM

THE REEF

The site is characterized by a sandy pristine beach exposed to several threats like coastal erosion, salt intrusion and flooding. For this reason, a type of protection has been chosen that meets the naturalness of the site. The submerged reef will be approximately 100 metres long and 50 metres wide, located approximately 120 metres from the shoreline. It consists of mattresses filled with basal limestone stones of small/medium size arranged close together and in a double layer. The height of the structure will be low: 60 cm in the central part and 30 cm at the edges.



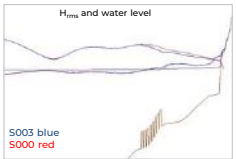


XBEACH

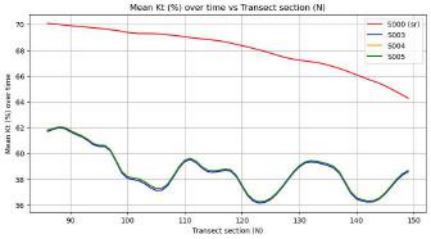
Hydrodynamic and morphodynamic effects of the reef are investigated through XBeach surfbeat, resolving both short-wave variations at the wave group scale and the long waves associated with them. Input files were created through the Delft3D suite: a 1.3 km × 500 m grid and the topobathymetry based on two surveys. Wave conditions were taken from the Nausicaa buoy under Bora and Sirocco storms. The study focuses on reducing wave attack, coastal erosion, and flooding, with emphasis on Kt reduction. A Manning sensitivity test was performed on two transects using 0.03, 0.04, and 0.05 $s/m^{1/3}$ in 1D and 2DH (single-wave and 3-hour storm) simulations.

RESULTS

Despite the reef's low height, hydrodynamic modelling shows the reduction of wave heights and the transmission coefficient, thereby achieving its objective of coastal protection. The model showed limited sensitivity to variations in Manning's coefficient. Morphologically, no erosion niches emerged, and the total eroded volume in simulation without reef is more than double that of the case with reef. Now we have a powerful and versatile tool that can support us in making predictions about future sea-level rise and the expected increase in extreme events.



Simulation	Global mean Kt
S000	68.07%
S003	58.53%
S004	58.62%
S005	58.62%



ABSTRACT

Numerical wave modelling of the wave propagation supported the design for a nature-based beach protection within a Nature 2000 site of the Po Delta Park, just north of the Bevano stream mouth (RA). The LIFE NatuReef project aims to restore the ancient oyster (*Ostrea edulis*) and sabellaria (*Sabellaria spinulosa*) reefs once present in the upper Adriatic Sea. The objective is twofold: the improvement of marine biodiversity and the natural coastal defence.

Intermittent Dynamics:

Structural properties, predictors and applications to the Earth system

ALMA MATER STUDIORUM UNIVERSITÀ DI BOLOGNA | DIPARTIMENTO DI FISICA E ASTRONOMIA "AUGUSTO RIGHI"

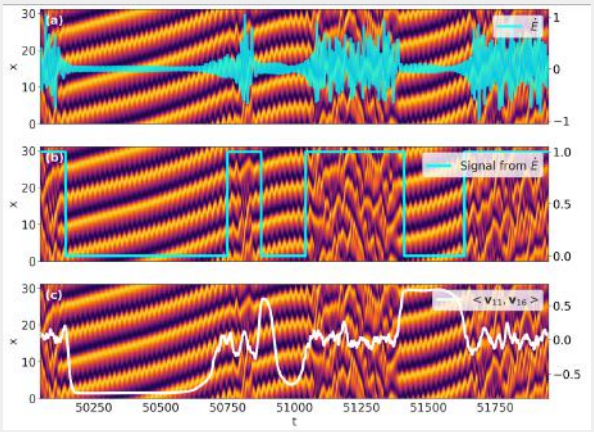
A. Barone [a], A. Carrassi [a], J. Demaeyer [b] & S. Vannitsem [b]

[a] DIFA – University of Bologna

[b] Royal Meteorological Institute of Belgium

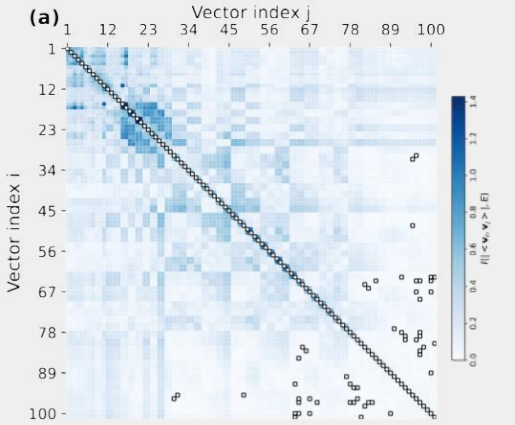
This research explores **intermittency** through two directions: first, we identify **Lyapunov-based indicators** that reveal **real-time predictors** of regime shifts in time series; second, we examine how intermittent signals form and propagate across **coupled fast–slow** components of the **Earth system.**

Predictors of intermittency*

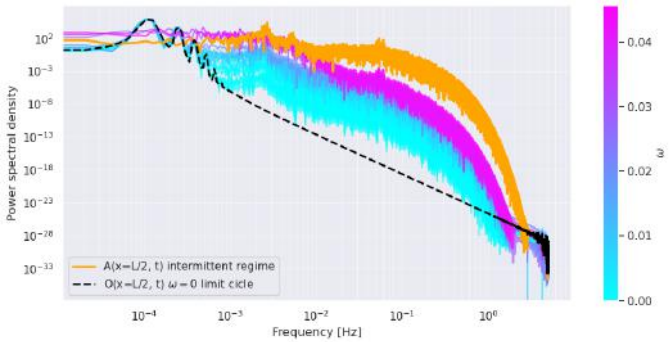


Lyapunov Exponents and **Covariant Lyapunov Vectors (CLVs)** reveal key **structural** features of intermittency across systems of different complexity. By tracking how selected CLVs align during the evolution, we identify combinations that act as reliable **real-time predictors** of regime shifts. This provides a genuinely **local perspective on intermittent dynamics**, moving beyond global statistics and enabling early **detection of transitions.**

We further show that the structure of the **tangent space** can guide the selection of a **reduced set of variables** that best capture the onset of intermittent events. This potentially allows us to define a **latent space** for machine-learning models trained to **classify and anticipate regime changes.** The approach opens the way to **automated prediction** tools capable of adapting to diverse mechanisms of intermittency.



Coupled systems



In this study, we analyze how a **fast intermittent system** can force a slow component in a stable quiet regime, such as a **slow limit cycle**. This fast–slow setup serves as a prototype of **Earth-system components** with strong scale separations, like **atmosphere–ocean**. We investigate how intermittent information transfers between the systems by examining mutual information between their **energies**, the fractal dimension of the involved **attractors**, and the **energy spectra** of fast and slow dynamics as key parameters vary.

*A. Barone, A. Carrassi, T. Savary, J. Demaeyer, S. Vannitsem; Structural origins and real-time predictors of intermittency. Chaos 1 October 2025; 35 (10): 103119. https://doi.org/10.1063/5.0287572

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A new window on the Ionosphere: A LOFAR perspective, from Geomagnetic Storms to Statistical Trends

BY REBECCA GHIDONI[1,2]

Supervisiors: Luca Spogli[2], Tiziano Maestri[1] **Co-supervisor:** Claudio Cesaroni[2]

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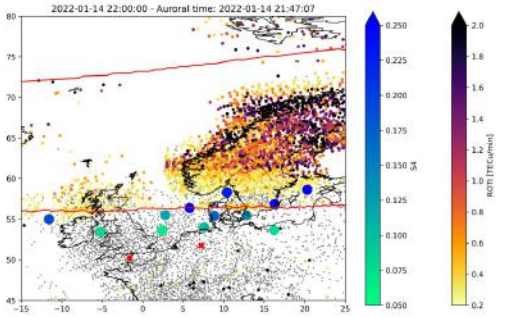
2) Istituto Nazionale di Geofisica e Vulcanologia, Via di Vigna Murata 605, 00143, Roma, Italy

January 2022 storm

This study successfully validated LOFAR's high-resolution capabilities by investigating the ionospheric response during the January 2022 geomagnetic storm. Comparing LOFAR-derived S4 scintillation index with GNSS-derived ROTI revealed a key mismatch in the sub-auroral region. LOFAR's fine time resolution allowed it to capture small-scale irregularities (<10 km), which were spatially and temporally averaged out by the comparatively coarser 30-second sampling and processing of GNSS data for ROTI. This established LOFAR's precision in probing a finer, kilometre-scale regime of plasma turbulence in the upper atmosphere.



All the results (and many more) are available in the paper

Figure 1. Map of the ionospheric irregularities measured around 22:00 UT of January 14 over the between 45° and 80° N and -15° and 25°E. The red lines represent the boundaries of the auroral oval. The ROTI data are represented in the yellow-black scale if over the threshold of 0.2 TECU/min or as simple grey dots if under it. The LOFAR S4 present a threshold of 0.05 and a green/blue gradient and red 'x'.

May 2024 Superstorm

This study showcased LOFAR's unique operational resilience during the May 2024 "Mother's Day" Superstorm, where it provided continuous, high-quality data when conventional instruments, such as the European ionosonde network, were rendered inoperable due to extreme absorption and G-conditions. A novel algorithm was developed and successfully applied to retrieve the time-resolved effective altitude of the irregularity layer. The results quantified a dramatic ionospheric uplift event, with the effective altitude reaching up to 1500 km and a high-speed plasma drifts reaching 800 m/s.

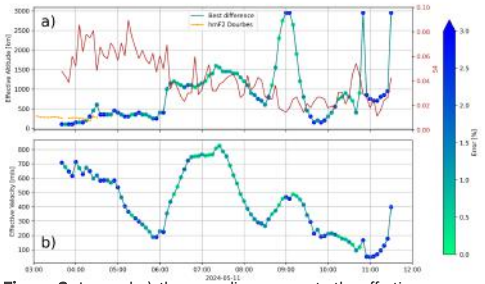


Figure 2. In panel a) the green line represents the effective altitude reconstructed by the comparison of the two algorithms. The colour of the scatter plots represents the relative percentage error between the two methods. The comparison is done with the velocities measured using the 140 MHz data. S4 values, measured at the same frequency, are shown as a red line. The yellow dots represent the altitude reconstructed by the Dourbes ionosonde. Panel b) shows the velocity obtained, by the cross-correlation method, measured at the effective altitude.

All the results (and many more) are available in the paper

Climatological Analysis

The climatological analysis of over 2400 hours of LOFAR observations established the fundamental and persistent characteristic of a magnetic field-alignment. The analysis revealed that only the structures with high temporal coherence (i.e., persistent and physically stable over 7 minutes) perfectly align with the predicted B × LoS$_{tg}$ direction. This demonstrated that the cross-correlation algorithm effectively isolates physically real, stable, field-aligned plasma structures from transient fluctuations or noise. Furthermore, the study determined that anomalous velocity measurements—not following the magnetic field—correlate with the presence of Sporadic-E layers, implying a failure of the thin-screen model.

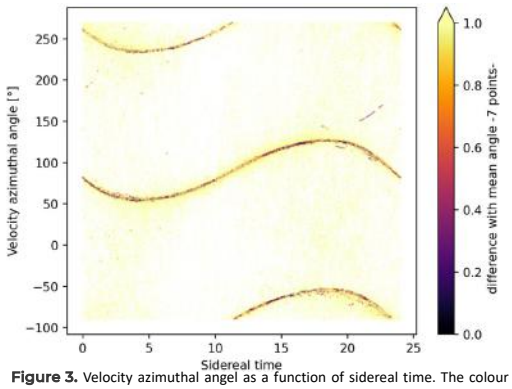


Figure 3. Velocity azimuthal angel as a function of sidereal time. The colour represents the difference of the direction of the major axis of the fitted gaussian with the angle obtained by the mean of the directions of the major axis obtained in the three minutes before and after, with darker shades representing smaller differences.

GENERAL INTRO

My work leverages the **Low Frequency ARray (LOFAR)** radio telescope for unprecedented ionospheric monitoring. The ionosphere, a highly dynamic plasma layer, disrupts trans-ionospheric radio signals, a key challenge for LOFAR astronomy. By turning this "noise" into a signal, the research aims to validate LOFAR's utility, apply it to extreme space weather events, and establish a long-term statistical understanding of plasma irregularities. The work combines LOFAR's high-resolution scintillation data with established systems like GNSS and ionosondes.

CONCLUSIONS & FUTURE WORK

The thesis successfully validates LOFAR as an indispensable tool, uniquely capable of probing the fine, kilometre-scale irregularity regime. Future work will refine the altitude retrieval algorithm (e.g., using phase spectrum methods) and apply it to the full dataset to model irregularity height. This advances understanding of multi-scale coupling.

ISTITUTO NAZIONALE DI GEOFISICA E VULCANOLOGIA

Satellite radiances assimilation to forecast severe convection in high-resolution regional models

Marcello Grenzi [1], Thomas Gastaldo [2,3], Virginia Poli [2,3], Chiara Marsigli [3], Carlo Cacciamani [2], Tijana Janjic [4], Alberto Carrassi [1]

[1] Department of Physics and Astronomy, University of Bologna, Italy [2] National Agency for Meteorology and Climatology ItaliaMeteo, Bologna, Italy [3] Arpae Emilia-Romagna, Bologna, Italy [4] Catholic University of Eichstätt-Ingolstadt, Ingolstadt, Germany

Assimilation of clear-sky and all-sky satellite radiances is crucial for Numerical Weather Predictions (NWP): large impact on forecast skill in global models. However, satellite data are under-used in Limited-Area Models (LAM) - **especially at microwaves.**

Can we exploit satellite radiances better in convective-scale data assimilation?

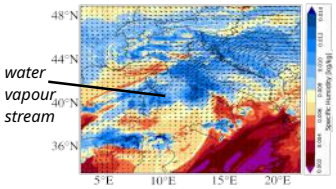
Joint assimilation of microwave and infrared data

Microwaves: low spatio-temporal resolution (polar satellites), good clouds penetration. **Infrared**: high spatio-temporal resolution (geostationary), no clouds penetration. **Complementary information** at different times and levels in the atmosphere.

Focusing on humidity-sensitive satellite channels

Humidity is undersampled in conventional data, but crucial for **convective systems** development (moisture convergence, CAPE).

METHODOLOGY



Control exp. forecast of specific humidity field at 850hPa (17UTC 15/09/2022), initialized at 00UTC

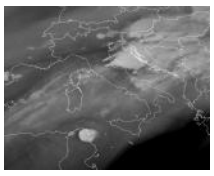


Image from SEVIRI instrument, water vapor channel at 6.2μm (15/09/2022 17UTC). Storm location in yellow.

Badly predicted by numerical models
(Grenzi, M., 2025, NCC)

ICON: ***ICOsahedral Non-hydrostatic model***
KENDA: *Kilometre-Scale Ensemble Data Assimilation* system, based on a Local Ensemble Transform Kalman Filter (**LETKF**)

- **2.2km res.** (convection-permitting), 65 vertical levels
- LETKF analysis every 1h (40 members), long forecasts every 3h
- **Severe convection case study**: Central Italy, 15/09/2022

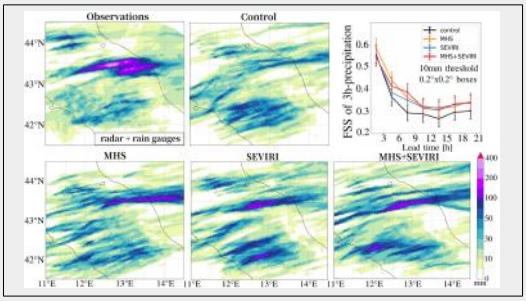
Observations	control	MHS	SEVIRI	MHS+SEVIRI
Conventional (SYNOP, AIREP, TEMP)	✓	✓	✓	✓
Radar volumes (reflectivity and radial winds)	✓	✓	✓	✓
Latent Heat Nudging (LHN)	✓	✓	✓	✓
Microwave Humidity Sounder (MHS) chan. 3, 4, 5 in *clear-sky* conditions	✗	✓	✗	✓
SEVIRI chan. 5, 6 in *all-sky* conditions	✗	✗	✓	✓

RESULTS: PRECIPITATION

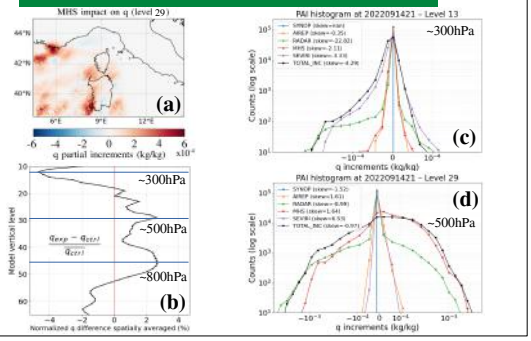
24h-rainfall: ICON forecasts compared with observations. Showing added value of satellite data assimilation, especially MHS+SEVIRI. Forecasts initialization time: 15/09/2022 00UTC

Upper right panel: **3h-rainfall** verification against radar adjusted data. **Fractions Skill Score (FSS)** as function of lead time. Statistics using all 40 forecasts in 5-days pediod. Higher is the better. Satellite radiances assimilation always improves compared to control run. MHS showing better performance compared to SEVIRI here.

Not shown here: verification of **surface and upper levels variables** (temperature and humidity) shows positive impact of radiances assimilation, with a good contribution of SEVIRI thanks to the high temporal frequency of data (every hour). MHS+SEVIRI the best one.



ANALYSIS INCREMENTS



How different observations contribute to the storm forecast? Use **Partial Analysis Increments (PAI)**: computes the relative analysis increment attributed to each observation, using the Kalman gain based on ensemble analysis perturbations.

Panel (a): relative increment of MHS on **specific humidity** (q) in mid-troposphere. Analysis of 21UTC 14/09 (last MHS passage over Italy before forecast initialization).

Panel (b): normalized q difference in the storm's forecast initial conditions (15/09 00UTC). MHS+SEVIRI compared to control. Average over the panel (a) area.

Panels (c, d): PAI histograms for q on two significant model levels. Skewness values shown. Total increment in black.

Microwave data provide the largest increments on humidity field in mid-low levels. SEVIRI in upper levels.

Contacts: marcello.grenzi3@unibo.it

TESTING ENSO DRIVEN OLR INTER-ANNUAL VARIABILITY OF CMIP6 MODELS WITH SPECTRAL SATELLITE OBSERVATIONS

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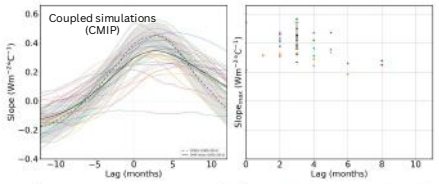
[1]CNR-ISAC, [2]Università di Bologna, [3]CNR-IFAC

This work focusses on the study of the Outgoing Longwave Radiation (OLR) at the top-of-atmosphere in the tropical oceans in relation to the El Niño - Southern Oscillation (ENSO). Studying the mechanisms behind the OLR response to natural variability is key to understand the evolution of the OLR in observations and climate models. In this context, spectral OLR offers a valuable insight into the physical processes shaping OLR variability.

How do well Climate models simulate ENSO?



Linear regressions have been performed between the **OLR anomalies from CMIP6 AMIP and CMIP simulations** and the **Niño 3.4 index**, which accounts for ENSO phase and magnitude, shifting the Niño 3.4 index time series of one month at a time from -12 to + 12 months:

- according to broadband OLR observations acquired by the Clouds and Earth Radiant Energy System (CERES) instrument, the **TOA OLR emission peaks two months after ENSO** activity
- the **magnitude** of the radiative response is reproduced quite well by CMIP models, while more spread is found in the corresponding **lag**
- AMIP models match the observed **lag**, but the **magnitude** is characterized by a great inter-model spread

What are the physical processes behind the spread?

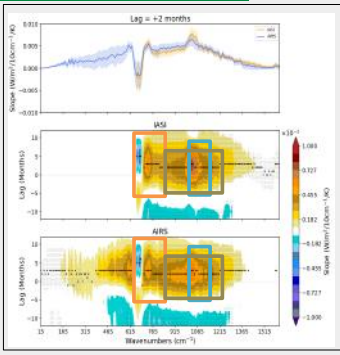
The contribution of spectral observations

Spectrally resolved OLR observations are used to highlight the physical processes behind models discrepancies.

The main advantages of the spectral dimension are:

- to isolate single contributions by examining different spectral regions
- to identify the atmospheric layers where the radiation originates

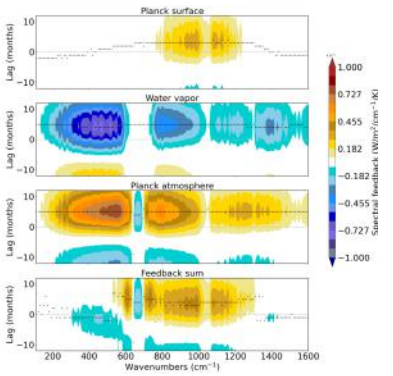
We used two datasets derived from observations of the **Infrared Atmospheric Sounding Instrument (IASI)** and the **Atmospheric Infrared Sounder (AIRS)** to calculate the **spectral ENSO signal.**



- Strong positive response within the O_3 absorption band (at 1043 cm-1), peak at lag = +3 months – channels sensitive to O_3 and T
- Positive contribution at the wings of the CO_2 absorption band, peak at lag = +3 months – channels sensitive to tropospheric T
- Negative contribution at the center of the CO_2 absorption band, peak at lag = +5 months – channels sensitive to stratospheric T
- Positive contribution within the atmospheric windows, peak at lag = +2 months – channels sensitive to H_2O and surface T

Testing climate models with spectral OLR observations

CMIP multi model mean ENSO feedbacks and feedback sum:



The **radiative change driven by surface and atmospheric temperature and water vapor** field simulated by CMIP6 models is calculated using **spectral radiative kernels and climate models outputs**. Then, the lagged regressions analysis has been performed to study the time evolution of the corresponding **Planck surface and atmosphere, and water vapor ENSO feedback**.

The **final step** of the work will involve assessing the performance of climate models by **comparing their ENSO feedback with that obtained from IASI and AIRS satellite observations**. The spectral dimension will allow us to **disclose biases that may be hidden by spectral compensation** when the corresponding broadband OLR value is considered.

Comprehensive Identification of Tick Species and Tick-Borne Pathogen Co-Infections in Wildlife and Domestic Animals from Malawi

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INTRODUCTION

Ticks are major **vectors of pathogens** affecting **human** and **animal health**. In **sub-Saharan Africa**, most tick species transmitting livestock and human **diseases** are native and often originate from wildlife. However, the role of wild animals in the epidemiology of **tick-borne pathogens** (**TBPs**) in southern Africa remains poorly understood. Climate change, urbanization, deforestation, and shifts in human–animal–environment interactions have **increased TBP risk**, while global travel and trade have heightened the likelihood of introducing **exotic tick species** into Europe. Understanding TBP circulation in tropical regions is therefore essential to anticipate **changes in tick and pathogen distributions** and to strengthen surveillance aimed at preventing disease outbreaks.

METHODS

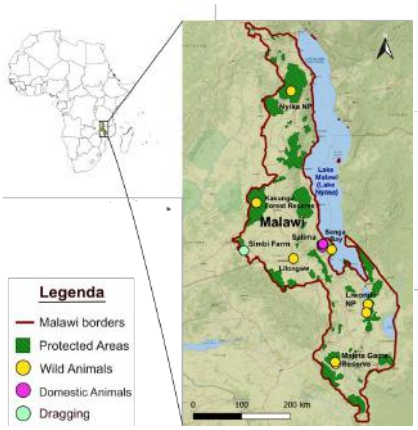

Figure 1. Map of the study sites.

Between **2015 and 2021**, ticks were collected from **wild** and **domestic animals** in four communities in Malawi. Collection sites are shown in **Figure 1**. Ticks were sorted by host, stored in labeled vials, and preserved in 95% ethanol.

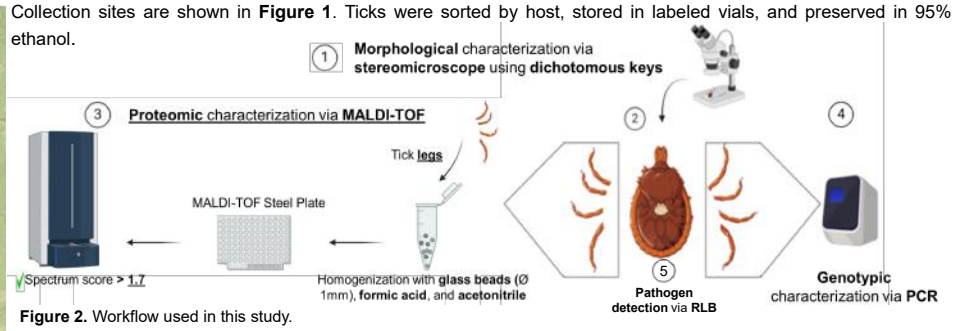

Figure 2. Workflow used in this study.

Ticks were **morphologically** identified, and each specimen was then dissected into three subsets: four legs for **MALDI-TOF MS identification** and four legs for **molecular identification** targeting the 16S rRNA and COI genes. DNA was extracted from the idiosome of representative female specimens (**n=200**) and analyzed by **Reverse Line Blot** (**RLB**) for pathogen detection, which allows the simultaneous identification of *Ehrlichia/Anaplasma spp*. and *Theileria/Babesia spp.* (**Figure 2**).

RESULTS

Overall, **995 ticks** were collected from Malawi. The identified species included ***Amblyomma exornatum, A. marmoreum, A. tholloni, A. variegatum, Haemaphysalis elliptica, Hyalomma rufipes, Ixodes schillingsi, Rhipicephalus appendiculatus, R. carnivoralis, R. decoloratus, R. microplus R. sanguineus***, and ***R. zambeziensis***. (**Figure 3**).

A. exornatum Host: Varanus | ***A. tholloni*** Host: Elephant | ***Amblyomma spp.*** Host: Unknown | ***R. appendiculatus*** Host: Impala | ***R. carnivoralis*** Host: Lion

Figure 3. Tick species collected in this study. Courtesy of IZSLER.

RLB screening revealed that 31% of the specimens tested positive for ***Anaplasma/Ehrlichia spp***. and 31% for ***Theileria/Babesia spp.*** (**Figure 4**).

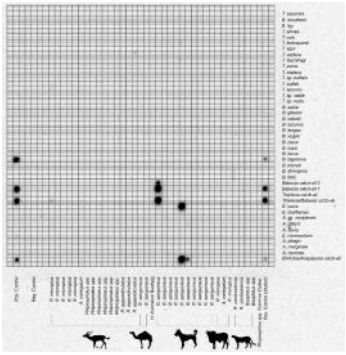

Figure 4. X-ray film showing some of the results of the RLB hybridization assay.

The most infected tick genus was ***Amblyomma spp.***, with 45% of samples positive for *Theileria/Babesia spp.*, followed by ***Rhipicephalus spp***. (22%). Positive *Anaplasma/Ehrlichia* samples were found in 37% of *Amblyomma* ticks and 27% of *Rhipicephalus* ticks. **Co-infections** with *Anaplasma/Ehrlichia spp.* and *Theileria/Babesia spp.* were detected in **18%** of the samples (**Figure 5**).

Figure 5. Heatmap illustrating pathogen occurrence in tested tick specimens.

DISCUSSION AND CONCLUSION

These preliminary findings reveal a high diversity of **TBPs in wildlife** and **domestic hosts** in **Malawi**. RLB proved effective for detecting multiple and concurrent infections, supporting its use in large-scale surveillance. In a context with limited baseline data, this approach requires refinement through targeted PCR assays and expanded screening. Establishing a **curated database** of tick species and associated pathogens will enhance **regional surveillance** and help assess spillover risks at the wildlife–livestock–human interface.

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Faculty of Veterinary Science

Improving predictability of Extreme Precipitation applying an ensemble-based approach

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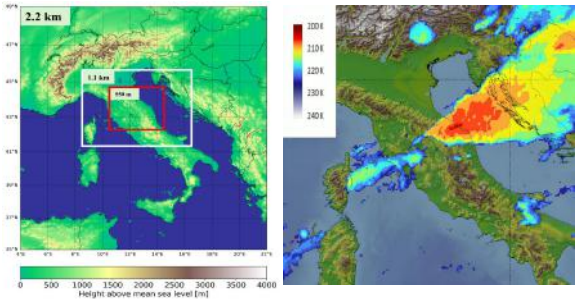
Using 500-m ICON simulations, we show that very high-resolution modelling can capture the intense rainfall behind the 2022 Marche flood much more accurately. By resolving convection and testing different initial conditions, the approach greatly improves realism and strengthens forecast confidence.

The methodology



Left: Domains used for the numerical simulations. Right: Observed structure of the Marche flooding storm from satellite

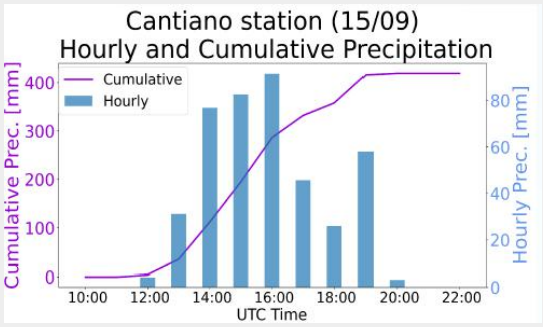
We are using the ICOsahedral Non-hydrostatic model (ICON) version 2.6.6 developed by a collaboration between DWD, MPI, DKRZ, CSCS, and KIT.

2.2 km horizontal resolution grid Limited-Area model (LAM) setup to solve convection and 65 vertical levels for 10 ensemble mebers, with varying initial conditions. The domain is centred over Italy, including Mediterranean Sea and portions of the neighbouring countries (longitude 3**°**-22**°**, latitude 34**°**-49**°**). We use IFS forecast data for initial (I.C.) and boundary conditions (B.C.) converted into ICON-based B.C. and I.C.

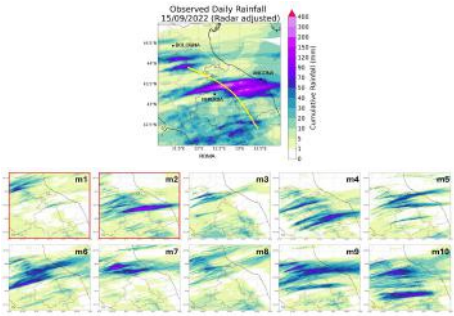
The event

A continental cut-off low over Spain led to the development of strong south-westerly winds. These winds transported high amounts of water vapour from exceptionally warm Mediterranean sea, boosting cloud formation and precipitation. The main operational models failed in forecasting the correct intensity and alocation, underestimating precipitation.

The rain gauges recorded exceptional amounts of rain: the SIAP station of Cantiano collected more than 400 mm of water in just 7 hours, between *14:00* and *21:00* (local time) of 15 September, with a peak of 92 mm at 18:00.



The simulations



High-resolution ensemble with different initial conditions

Using the operational COSMO turbtran and turbdiff turbulence scheme, this high-resolution ensemble was done with online two-way nesting between the domains. The spatial variability of the single members points out that the initial and boundary conditions played a crucial role in such event. The spatial distribution of the thunderstorm in m2 recalls almost perfectly the precipitation distribution of the primary thunderstorm that hit the mountains, with broad precipitation bands exceeding 120 mm and peaks over 150 mm.

Multimodal experimental protocols for GAG quantification in articular cartilage using low field NMR

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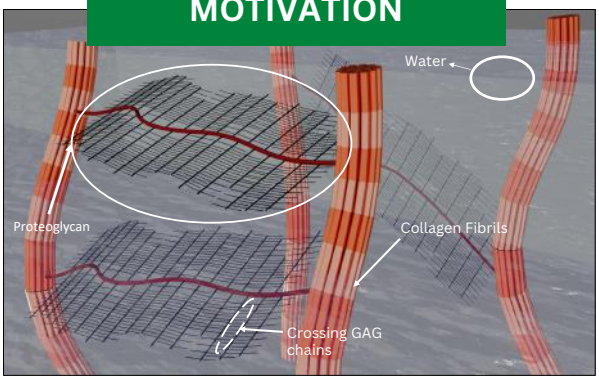
Osteoarthritis (OA) is an irreversible and degenerative disorder that affects **articular cartilage (AC)**. Currently, no screening methods have been established for the **early detection of asymptomatic patients**. To address this issue, the present study investigated the **feasibility of quantifying glycosaminoglycan (GAG)**, the first component to be degraded during OA, **concentration in AC using low-field nuclear magnetic resonance (NMR)**.

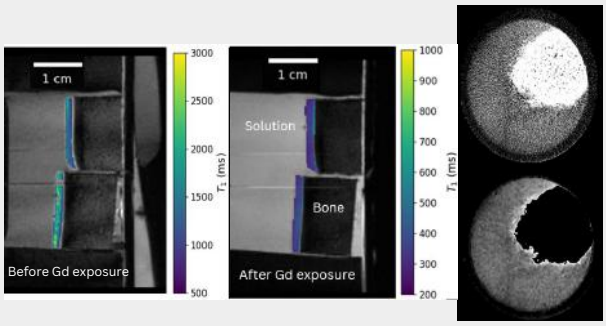
MOTIVATION



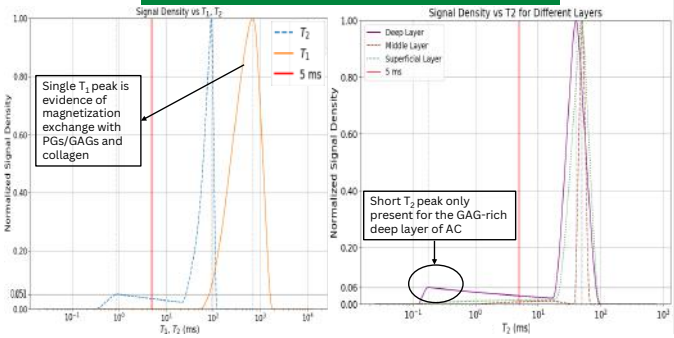
The development of OA requires **widespread and frequent screening**, discouraging high field MRI and CT based techniques. **Low field ^{1}H NMR signal inversion**, the process of computing the distribution of relaxation times of hydrogen atoms, **is potentially sensitive to changes in GAG (and proteoglycan, an ensamble of GAGs) concentration** due to them acting as a solid restricting structure to water molecules in the tissue. **Recent publications** on NMR studies of AC mainly focus on qualitatevely assessed or artificially degraded tissue, **limiting the interpretability of the results**. **This work proposes two experimental protocols that combine GAG quantification and NMR measurements while identifying parameters of interest for further study**.

MATERIALS AND METHODS

NMR measurements were performed employing a single-sided instrument (B_0 **= 0.327 T**). The data were inverted via the UPEN algorithm to obtain the **distribution of relaxation times T_1 and T_2**. Signal fraction of the fast-decaying (short) T_2 component and novel parameters such as the full width at half maximum of the distributions were then **correlated with the GAG concentration measured from two reference methods**. The **dGEMRIC** technique was implemented via **T_1 mapping** of 8 bovine samples with a **3T clinical scanner**. Contrast-enhanced X-ray computed tomography (**CE-CT**), the second reference method, was employed on 10 samples exposed to the **CA4+ cationic contrast agent**.



RESULTS



Among the observed (Spearman) **correlations**, those between **GAG concentration and short T_2 signal fraction** (ρ = 0.54) **and FWHM** (ρ = -0.54), **T_1 peak value** (ρ = 0.54), **its skewness** (ρ = 0.60) **and its average value** (ρ = 0.65) **are of particular interest**. These, along with supporting parameters and observations, allow the identification of **two water «pools»**: **one constrained by the crossing GAG chains and the other by proteoglycans more broadly**.
Future work aims to include a larger number of samples in order to establish the aforementioned features as **early OA biomarkers**, together with the extension of the two protocols to other NMR techniques such as **fast field cycling and susceptibility mapping**.

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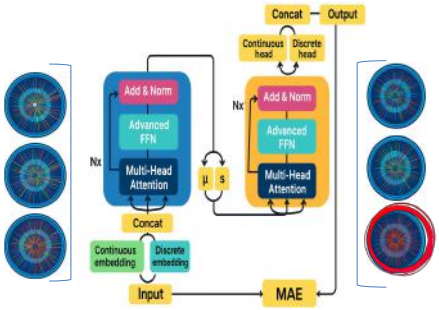
"AUGUSTO RIGHI"

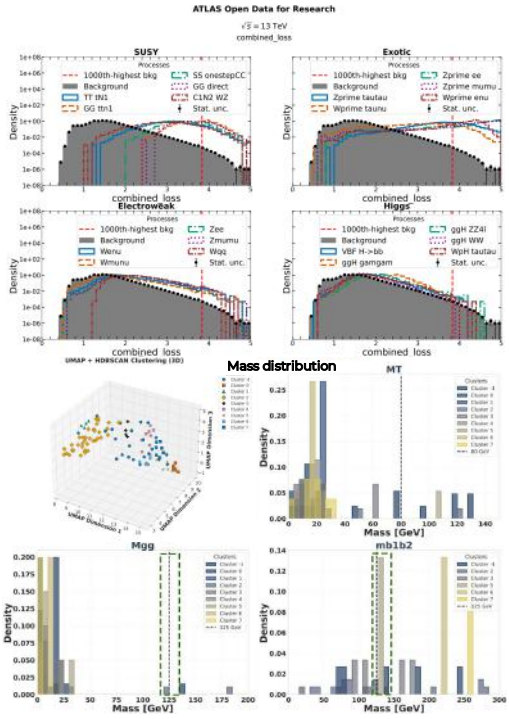
AI-Assisted Analysis to Enhance Discovery Potential in High Energy Physics

Asrith Krishna Radhakrishnan, Maximiliano Sioli, Lorenzo Rinaldi

ML Model

- Masked-attention Transformer [1] handles ~40% missing data and heterogeneous HEP features.
- SHAP pruning + embeddings create a compact, informative feature space.
- Learns correlations from raw objects (jets, leptons, MET, topology) without preselection.
- Background reconstruction gives a model-agnostic anomaly score (log(DM), z-score).
- Scalable ROOT RDataFrame + Dask + TF streaming workflow.
- UMAP [3] + HDBSCAN [4] expose anomalies in ATLAS Run-2 Open Data.





Category	Signal	AUC	Signal	AUC	Signal	AUC
SUSY	TT tN1	0.9906	GGM HinoZh	0.9772	TT higgsino RPV	0.9961
SUSY	GG ttn1	0.9968	TT RPVdirectBL	0.9986	SS onestepCC	0.9960
SUSY	GG direct	0.9977	Stau Stau	0.8724	C1N2 WZ	0.9646
SUSY	SM N2C1p	0.7927	GGM N1N2C1	0.9915	–	–
Exotic	Zprime tautau	0.9960	Wprime qq	0.9967	Wprime taunu	0.9885
Exotic	Zprime ee	0.9998	Zprime bb	0.9971	Zprime mumu	0.9980
Exotic	Wprime enu	0.9987	DM A	0.9634	Wprime munu	0.9949
Exotic	Zprime tt	0.9968	LQd	0.9979	WpL tblep	0.9964
Exotic	WpL tbhad	0.9970	DM 4-top scalar	0.9899	–	–
Higgs	VBF H→bb	0.7942	ggH gamgam	0.8870	ggH ZZ4l	0.7766
Higgs	ttH dilep	0.9358	ttH gamgam	0.9680	VBFH gamgam	0.9162

Results

- Validation: SM events reconstruct with low loss, while BSM events show higher reconstruction loss.
- Clustering: UMAP + HDBSCAN identifies structured anomaly groups; clusters 2 and 5 each reach 3.72σ significance in the p-value study, with key discriminating features highlighted via Cohen's d.
- Physics insight: These clusters contain events with mass features near Higgs-like di-b-jet and di-photon regions, indicating localized phase-space anomalies.
- The observed patterns demonstrate strong SM-BSM separation and provide interpretable handles for targeted follow-up searches

Conclusion

- Unsupervised: Masked Tab-Transformer on low-level variables, no signal assumptions.
- Sparse/mixed features: Handles ~40% missing data, creates rich embeddings.
- Anomaly scoring: Mahalanobis based reconstruction flags rare/BSM events.
- Clustering: UMAP + HDBSCAN identifies anomalous classes; key features via Cohen's d.
- Scalable & domain-independent: Applicable for HEP and other large tabular datasets.
- Future: Extend to full Run-2 and other datasets; improve BSM sensitivity.

Introduction

- Traditional HEP supervised searches are powerful but biased by predefined hypotheses.
- Modern experiments (LHC) generate large datasets, making unsupervised anomaly detection essential for uncovering rare, and unseen patterns.
- We developed a Masked Tab-Transformer autoencoder pipeline, trained on ATLAS Run-2 data [2] , that learns correlations from raw data and finds anomalies without bias.
- A scalable, distributed pipeline (ROOT RDataFrame + Dask + TMVA TensorFlow batch gen [5]) processes millions of HEP events efficiently.
- Framework is domain-independent , enabling anomaly detection in HEP and other large-scale tabular datasets.

References

[1] Arik & Pfister, TabTransformer, AAAI 2021, arXiv:2012.06678.
[2] ATLAS Open Data, doi:10.7483/OPENDATA.ATLAS.9HK7.P5SI
[3] L. McInnes et al., arXiv:1802.03426 [stat.ML]
[4] R.J.G.B. Campello et al., Adv. Knowl. Discov. Data Min. (2013), Springer, ISBN 978-3-642-37456-2
[5] ROOT TMVA, RBatchGenerator TF (2024),root.cern.ch

Computational material physics: from density functional theory to molecular dynamics with machine learning potentials

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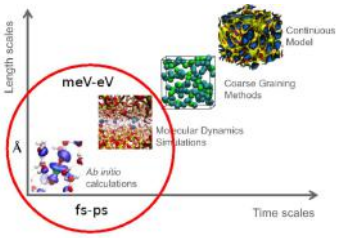
Computational Methods for Material Physics

What can we simulate?

Non-unique time and length scales → no unique theory, model or code



Ab initio: material properties from first principles solving the *quantum mechanical Shrödinger equation* numerically

+ In principle able to obtain 'exact' solutions at the electrons level
- Small system, time-consuming

The many-body problem

In condensed matter physics, to accurately describe the properties of a system, i.e. a molecule or a crystal, it is crucial to identify its equilibrium structure. This corresponds to find the solution of the time independent Shrödinger equation for the coupled nuclear and electronic Hamiltonian. In principle this might be achieved solving the many-body problem:

$$\hat{H}\Psi(\mathbf{r}_1,...,\mathbf{r}_N,\mathbf{R}_1,...,\mathbf{R}_M) = E\Psi(\mathbf{r}_1,...,\mathbf{r}_N,\mathbf{R}_1,...,\mathbf{R}_M)$$

With:

$$\hat{H} = \hat{T}_e + \hat{T}_I + \hat{V}_{e-e} + \hat{V}_{I-I} + \hat{V}_{e-I}$$

PROBLEM: the equation depends on all the 3Nx3M coordinates → Solution is unfeasable to compute! Approximations are needed.

Born-Oppenheimer approximation

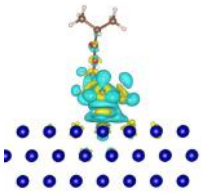
Nuclei are stationary compared to the electrons, because they are much heavier.

Many-body hamiltonian in B-O (frozen nuclei) approximation:

$$\left[\hat{T}_e + \hat{V}_{ee} + \hat{V}_{en}\right]\psi_e(\{\mathbf{r}\};\{\mathbf{R}\}) = E_e(\{\mathbf{R}\})\psi_e(\{\mathbf{r}\};\{\mathbf{R}\})$$

FIRST PRINCIPLES METHODS

- Density Functional Theory (DFT)
- Hartree-Fock Theory (HF)
- DFT+HF → Hybrid functional
- GW (quasiparticles)
- Bethe-Salpeter equation (BSE, electron-hole)
- Ab initio Molecular Dynamics (AIMD)
- Diagrammatic Monte Carlo



Basic idea behind DFT

The electronic charge density uniquely determines all the properties of the system.

Solving the many-body problem is reduced to determine a function dependent on 3 variables!

Material properties from quantum mechanics

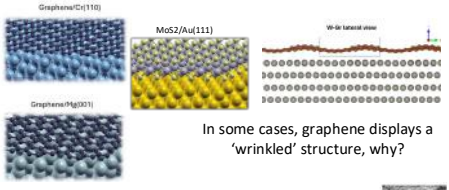
The importance of interfaces and surfaces in materials science

Applications in a wide range of fields

Optoelectronics | Catalysis | Energy storage | Tribology

2D materials on metals

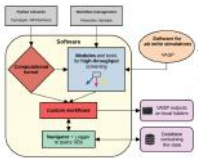
Graphene and MoS2 → strong in-plane covalent bonds and weak perpendicular van der Waals interactions



In some cases, graphene displays a 'wrinkled' structure, why?

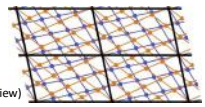
Metal-on-Metal contacts

Adhesion energy, a measure of the strength by which two surfaces bind together, ultimately dictates the mechanical behavior and failure of interfaces.



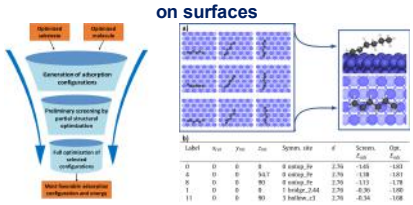
TribChem : high-throughput software to study properties of solid-solid interfaces

Combining different lattice periodicities



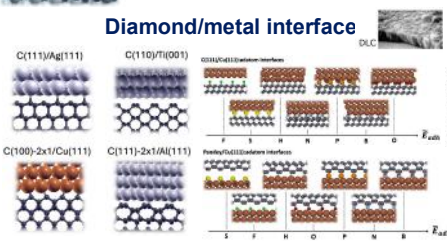
Fe/Cu (top view)

Software development for molecular adsorption on surfaces

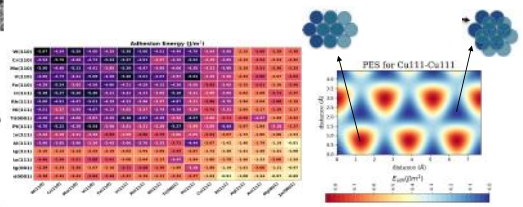


E. Pedretti et al., Computer Physics Communications **291**, 108827 (2023)

Diamond/metal interface



E. Damiani et al., Carbon **230**, 119555 (2024)



P. Restuccia et al., ACS Appl. Mater. Interfaces **15**, 19624 (2023)

Machine learning potentials for accurate large scale molecular dynamics

Principles of Molecular dynamics

1. $E(R_1, R_2, ...R_N)$ interaction energy
2. $F_i = -\nabla E(R_i)$ atomic force on atom i
3. Integrate the equation of motion:
4. $a_i = F/m \xrightarrow{\text{integration}} R_i'$

Molecular dynamics

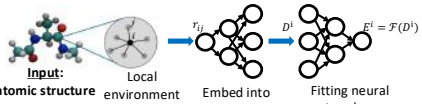
$E(R_1, R_2, ...R_N)$

***Ab initio* MD**
$H\Psi = E\Psi$
solve Schrödinger for **electrons**
☺ High accuracy
☹ High cost

Classical MD
$E = S_{ij}\, v(r_{ij})$
parametric form mimicing electrons
☺ High efficiency
☹ Questionable accuracy

Machine Learning MD
Fitted by **neural network** trained with *ab initio* data
☺ High accuracy
☺ High efficiency

Machine learning interatomic potentials (MLIPs) in a nutshell

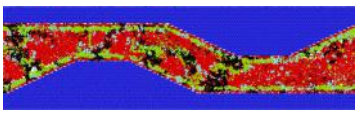


Large scale simulations: applications to tribology and catalysis

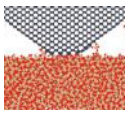
Train MLIPs on DFT data → **Near-*ab initio* accuracy**, without computing charge density: **much lower computational cost**

Efficiency gain > 1000x increase on simulated system size and time scales:

- instead of few hundred atoms, we can easily simulate **>100K/1M atoms**
- instead of tens of picoseconds of molecular dynamics, we can reach **> 10-100 ns**



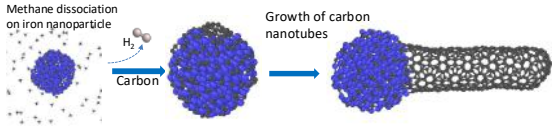
Research on lubricant additives to reduce friction in steel contacts. With MLIP simulations, we can study additive solubility, clustering, adsorption and protective film formation that prevents scuffing in engines.



Research on atomic-scale wear at diamond-silica interfaces, of great interest to semiconductor industry. MLIP simulations shows how bonds across the diamond-silica interface result in detachment of carbon atoms, slowly flattening the asperities.

Hydrogen production without CO_2 emission

MLIP simulations guide experimental research, allowing to understand atomistic processes and improving catalyst design



Descriptors represent how the network «sees» the atomic environments: similar environments will be close in feature space (descriptors).

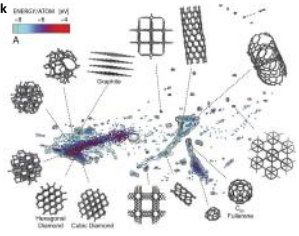
Many MLIP architectures, with many different descriptors:

- **DeePMD:** deep neural network
  Zeng, Jinzhe, et al, 159.5 (2023).

$$(\mathscr{R}^i)_j = \left\{\frac{1}{r_{ij}}\ \frac{x_{ij}}{r_{ij}}\ \frac{y_{ij}}{r_{ij}}\ \frac{z_{ij}}{r_{ij}}\right\}$$

$$\mathscr{D}^i = \frac{1}{N_c^2}(\mathscr{G}^i)^T(\mathscr{R}^i)(\mathscr{R}^i)^T\mathscr{G}^i_<$$

embedding (learnable) matrix



PCA of descriptor for different phases carbon.
P. Rowe et al, 153.3 (2020).

- **MACE:** message passing **graph** network
  I. Batatia, et al, 35 (2022): 11423-11436.

Atoms are nodes, connected by edges. Features of the local environment of each atom are passed to the neighbors through graph connections.

Phd Day -2025

ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

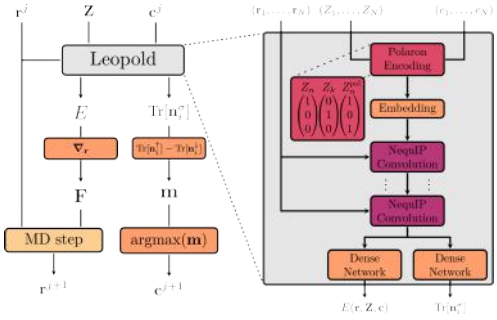
DIPARTIMENTO
DI FISICA E ASTRONOMIA
"AUGUSTO RIGHI"

MACHINE LEARNING POTENTIALS FOR LOCALIZED CHARGE DYNAMICS IN MATERIALS

LUCA LEONI, DEPARTMENT OF PHYSICS AND ASTRONOMY

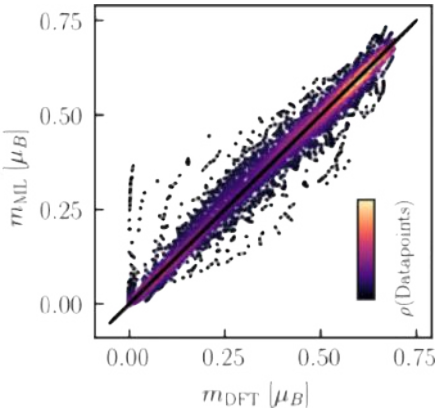
LEOPOLD

LEOPOLD is a state of the art equivariant convolutional graph neural network built on top of the NequIP architecture and implemented in JAX. The model accounts for the presence of the localized charge by assigning a *charge state* to every atom which assumes value 1 or 0 based on where the localized charge is at the moment. In this way the model can predict energy and forces accounting also for the changes due to the charge presence. Alongside them, the model predict the magnetization on every atom, so that the charge state can be updated based on its highest value.



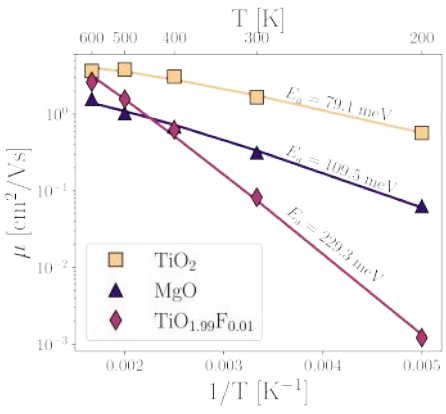
VALIDATION

To validate the results obtained by LEOPOLD we took a series of charge jumps predicted from the trained model and checked that the magnetization alligned well with the DFT predicted one. This allowed to check that the charge movement of predicted by Machine Leaning was physcial and accurate up to DFT level.



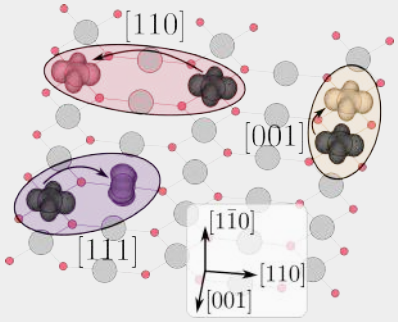
RESULTS

LEOPOLD was used to study three different charge defects: hole polaron in MgO, electron polaron in rutile-TiO2 and doped rutile TiO2. In both cases the models were trained on data obtained from a 10ps FPMD and then runned for 10ns using Machine Learning molecular dynamics. From the obtained trajectories it's we extracted the diffusion coefficients, showing for the first time a prediction of the temperature trend of polaron's mobilities.



MOTIVATION

Charge localization lies at the core of several physical phenomena that highly influences different materials properties, such as: conductivity, optical excitations,(photo) catalysis, and photovoltaic.
Unfortunately, the hopping motion of localized states, renders predicting such properties too expensive for first-principles Molecular Dynamics (FPMD) approaches. In this work we created LEOPOLD, a Machine Learning framework that allows to perform to perform such simulation at a fraction of the cost.



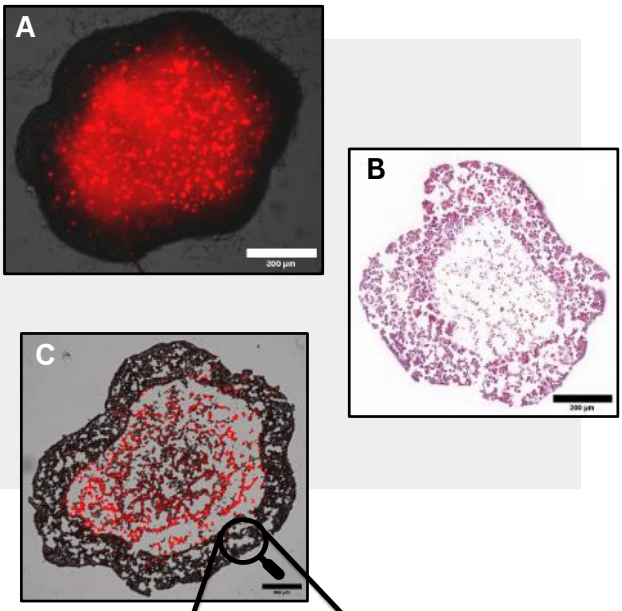
2.5D analysis of 3D spheroids for cancer stem cells isolation.

Mariachiara Stellato [1], Viktor Pal [2], Akos Diosdi [2,3], Maria Harmati [2], Daniel Remondini [1], Nicola Normanno [4], Gastone Castellani [5,6], Filippo Piccinini [4,5], Peter Horvath [2,3].

[1] Department of Physics and Astronomy "Augusto Righi" (DIFA), University of Bologna, Italy; [2] Synthetic and System Biology Unit, HUN-REN Biological Research Centre (BRC), Szeged, Hungary; [3] Single-Cell Technologies Ltd, Szeged, Hungary; [4] IRCCS Istituto Romagnolo per lo Studio dei Tumori (IRST) "Dino Amadori", Meldola (FC), Italy; [5] Department of Medical and Surgical Sciences (DIMEC), University of Bologna, Italy; [6] IRCCS Azienda Ospedaliero-Universitaria di Bologna S.Orsola, Bologna, Italy.

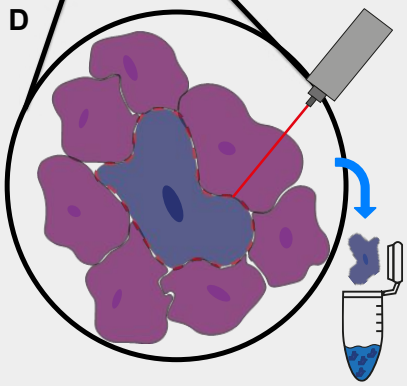
OBJECTIVES

Cancer stem cells (CSCs) are gaining significant attention in cancer research due to their unique traits, which make them more resistant to conventional anti-cancer drugs and therapies. To better understand their role and develop treatments that address their drug resistance, CSCs can be studied in controlled environments, such as 3D multicellular spheroids. In particular, interactions between CSCs and Mesenchymal Stem Cells (MSCs) have been shown to influence tumor development. Isolating single cells from CSCs-MSCs cocultures can help to better understand their behavior and resistance to drug treatments.

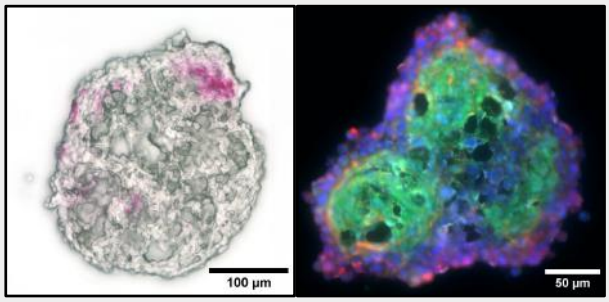


MATERIALS AND METHODS

For isolating single cells, we use a sectioning protocol that reduces the culture into a sequence of 2D sections that can be analysed to identify and collect the cells of interest through laser-based techniques into an Eppendorf tube. Although this method is really promising, the process of sectioning spheroids using a microtome or cryostat inevitably leads to damages. This limitation restricts the ability to perform reliable studies on the morpho-biological properties of selected cells [1]. Starting from this knowledge, we have developed a protocol that optimizes the extraction of the single cells from the spheroids tuning the dimension of the section not to compromise the morphology of the cells. This innovation opens opportunities for conducting radiomics studies on the single cells.



CONCLUSIONS



We performed several experiments to test the possibilities of this new technique with spheroids of different sizes and created with different cell lines, including MSCs and cancer cells. The results showed that it is possible to retrieve single cells from various spheroids' coordinates without damaging them. This method is a first step in being able to extract single selected cells without enzymatic digestion. A future step of this technique is to develop a system of micro-pipettes that allows to successfully penetrate the spheroid and retrieve selected cells without the need for sectioning.

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Cation Engineering in 2D Sn-Based Perovskites: Morphological Evolution and Degradation Behavior

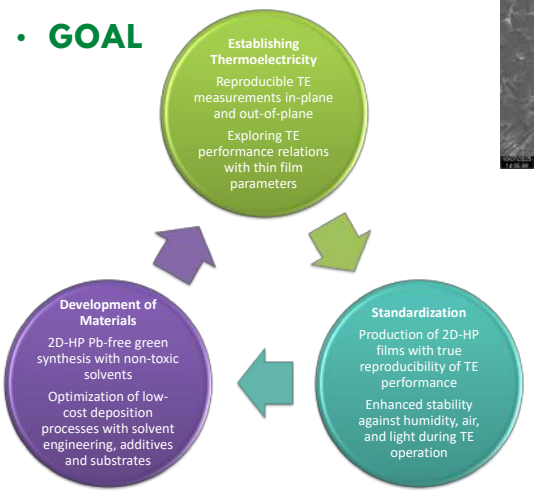
Usman Qumar, Samet Ocak, and Silvia Milita Alma Mater, University of Bologna in collabortion with CNR-ISMN

usman.qumar2@unibo.it

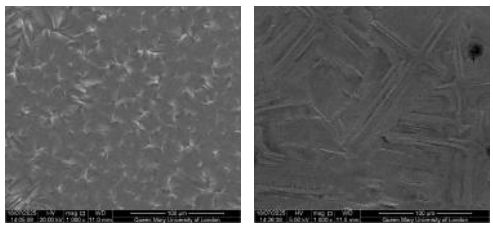
• SOLVENT EFFECT & FABRICATION

- Films of $(PEA)_2SnI_4$ and $(FPEAI)_2SnI_4$ prepared Using spin coating

• GOAL



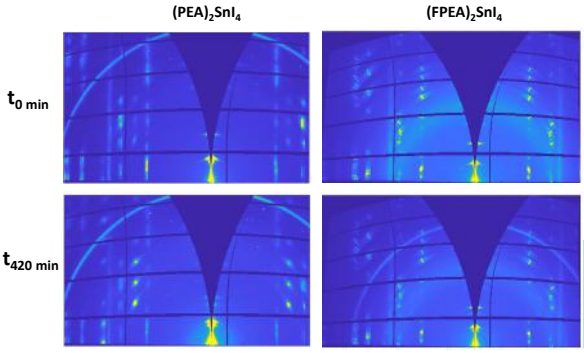
DMF | DMF 80:20 DMSO

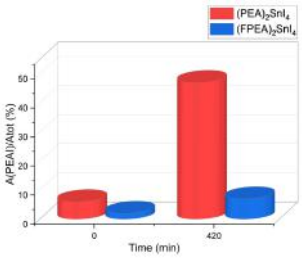


- Changing domain size and shape

• STABILITY TEST (PEAI VS FPEAI)

- degradation of PEAI increased over time
- while FPEAI remained stable.

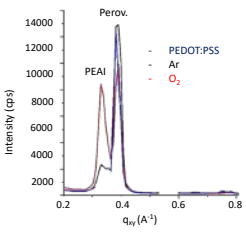


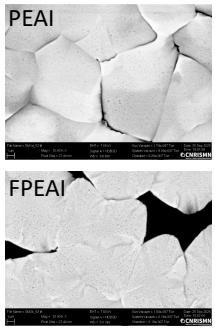


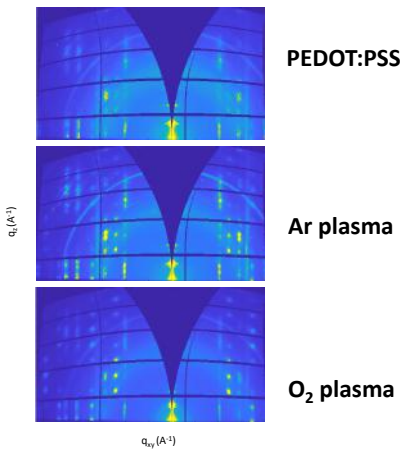
Sample	$A_{(PEAI)}/A_{(tot)}$ (t_0 min)	$A_{(PEAI)}/A_{(tot)}$ (t_{420} min)	Change (Δ)
$(PEA)_2SnI_4$	6%	47%	+41%
$(FPEA)_2SnI_4$	2%	7%	+5%

• SUBSTRATE EFFECT & STRUCTURE

- Changing cations,
- change morphology



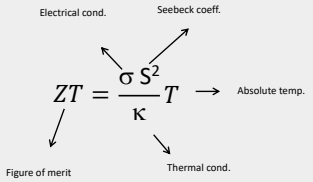


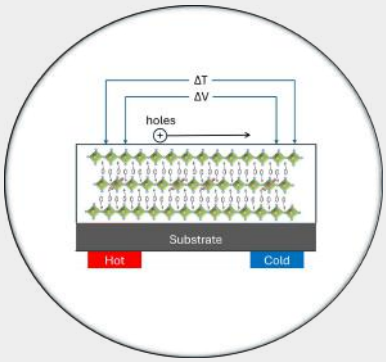


• INTRODUCTION

- High S
- Electron-crystal → moderate σ
- Phonon-glass → ultra*low* κ

👍	Lead-free
👍	Increased S without substantial decrease of σ
👍	Improved stability against moisture
👎	Instability in air
👎	If not engineered, low conductivity





• CONCLUSION

- Fluorinated cations effectively suppress structural changes
- Both systems show promising electrical conductivity, supporting their potential for device applications in future.

References:

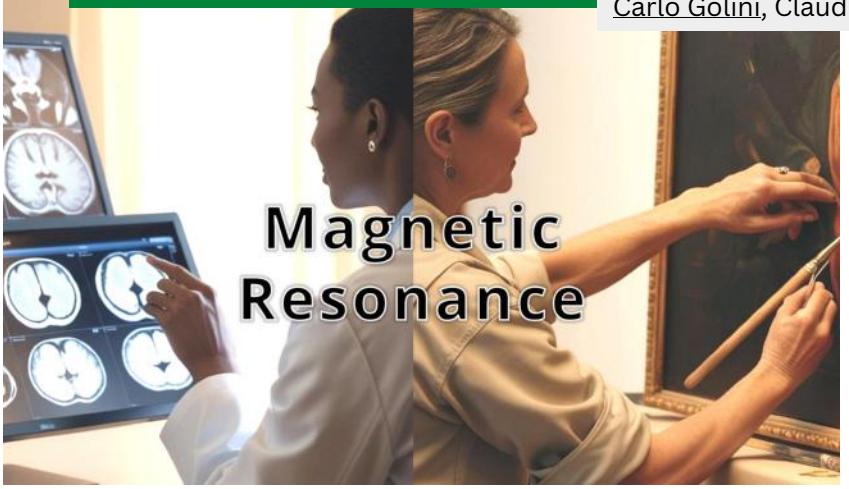
S. J. Yang, D. Kim, J. Choi, S. H. Kim, K. Park, S. Ryu, K. Cho, Enhancing Thermoelectric Power Factor of 2D Organometal Halide Perovskites by Suppressing 2D/3D Phase Separation. *Adv. Mater.* 2021, 33, 2102797.

Y. Liu, P. Chen, X. Qiu, J. Guo, J. Xia, H. Wei, H. Xie, S. Hou, M. He, X. Wang, Z. Zeng, L. Jiang, L. Liao, Y. HuLiu. Doping of Sn-based two-dimensional perovskite semiconductor for high-performance field-effect transistors and thermoelectric devices. iScience 2022,25, 4.

FROM PATIENTS TO PAINTINGS: LOOKING BEYOND THE SURFACE

ALMA MATER STUDIORUM UNIVERSITÀ DI BOLOGNA | DIPARTIMENTO DI FISICA E ASTRONOMIA AUGUSTO RIGHI

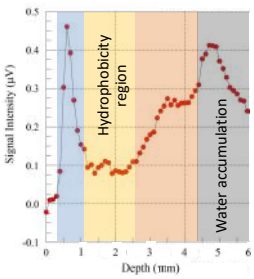
Carlo Golini, Claudia Testa, Leonardo Brizi, Juergen Frick



"Doctors and restorers both hold a masterpiece in their hands: human life and artwork": this research will make them feel less alone in their choice

Development and application of quantitative physical methodologies for non-destructive diagnostic characterization in the fields of cultural heritage and medicine

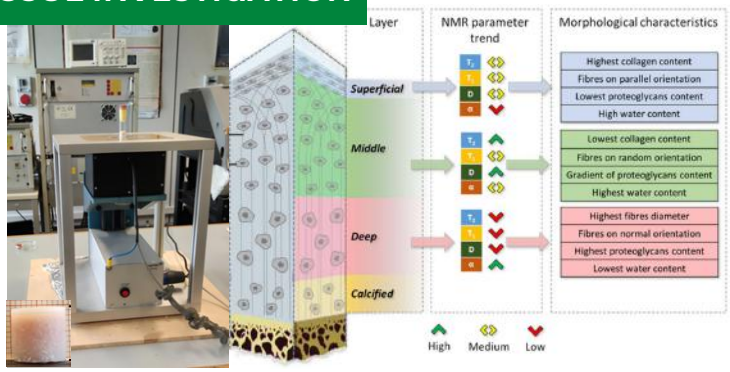
CULTURAL HERITAGE CONSERVATION



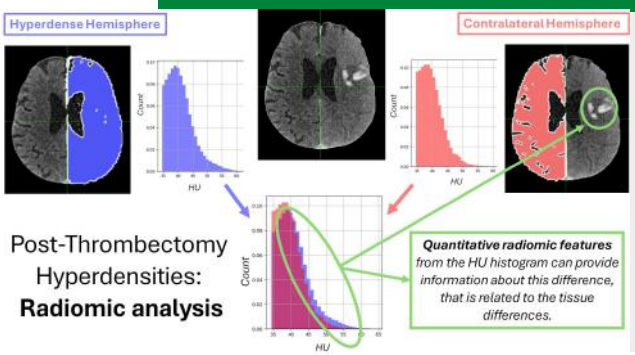
This research consists in the application of portable low-field nuclear magnetic resonance (NMR) relaxometry on materials of interest for cultural heritage.
In addition to laboratory tests, NMR measurements were performed directly in situ at the following restoration sites: the cemetery of Hoppenlau (Stuttgart, Germany), the Holy Thursday altarpiece at the Freising Cathedral (Bavaria, Germany), the late-Roman burial chamber at Reichertsberg (Trier, Germany) and the Ottonian frescoes at the Collegiate Church of Saints Peter and Orso (Aosta, Italy).

CARTILAGE TISSUE INVESTIGATION

A multi-parametric analysis of low-field NMR relaxometric measures was performed on ex vivo bovine cartilage samples. NMR parameters were demonstrated as robust markers for discriminating between cartilage zones (superficial, middle and deep).
The variations of mobility and content of water, content of proteoglycans, and collagen structure in the cartilage tissue are suitable indicators for osteoarthritis severity. Thus, characterizing this biological system through NMR parameters can help deepen the knowledge about the cartilage changes occurring in this disease.



CEREBRAL STROKE ANALYSIS



In the imaging field, two projects has been developed about stroke effects on patients. (Left) A radiomic analysis on post-thrombectomy hyperdensity CT scans to determine which clinical factor influence most. (Right) A CT Perfusion images analysis to refine the definition of the ischemic core (irreversely damaged tissue) and the penumbra (salvageable tissue).