

# 2022 December 16<sup>th</sup> - Building A - Room 128/129

8h50 - 9h00 : OPENING (Pasquale CALABRESE)

9h00 - 9h45	APC	Group Intro (Alessandro BRESSAN) Giulia CAPURRI - Astrophysics & Cosmology with Gravitational Waves Lumen BOCO - High redshift quasar problem and its solution
9h45 - 10h30	АРР	Group Intro (Enrico BARAUSSE) Marco CRISOSTOMI - Testing gravity with gravitational waves Pranjal RALEGANKAR - Probing hidden sectors with early universe cosmology
10h30 - 11h00		Coffee Break
llh00- llh45	СМ	Group Intro (Giuseppe SANTORO) Andrea TIRELLI - Hydrogen at high pressures by Machine Learning and Quantum Monte Carlo Paolo PEGOLO - Topology, oxidation states, and charge transport in ionic conductors
11h45 - 12h30	TSDS	Group Intro (Roberto TROTTA) Eszter SZEKELY - What neural networks learn and other methods don't - the case of higher-order statistics Riccardo MARGIOTTA - Optimal control attacks: online label poisoning
12h30 - 14h15		Lunch

14h15 - 15h00	MSBP	Group Intro (Cristian MICHELETTI) Valerio PIOMPONI - Molecular Dynamics Simulations of Modified RNA Matching Denaturation Experiments Zahra Ahmadian DEHAGHANI - Topologically interlocked ring polymers
15h00 - 15h30		Coffee Break
15h30 - 16h15	SP	Group Intro (Andrea GAMBASSI) Stefano SCOPA – Generalized Hydrodynamics and its quantum fluctuations Francesco CODAGNONE - The call of Quantum Integrability for Cold Atoms
16h15 - 17h00	TPP	Group Intro (Marco SERONE) Saman SOLTANI – Black holes under the microscope: a holographic perspective Francesco GAROSI - From the Earth to the sky through fundamental physics

Coordinator Intro: 5/15min – Contributions: 15/20min (with questions)

# **Local Organisation Committee**

Mario COLLURA Angelo ROSA Pasquale CALABRESE Stefano LIBERATI

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# Contributions

# Astrophysics and Cosmology (APC)

**Speaker:** Giulia CAPURRI **Title:** Astrophysics & Cosmology with Gravitational Waves **Abstract:** TBA

## Speaker: Lumen BOCO

Title: High redshift quasar problem and its solution

Abstract: Understanding the growth of supermassive black holes is one of the main quests for modern extragalactic astrophysics. Indeed recent observations of quasars powered by extremely massive black holes at very high redshift have revealed some weaknesses of the standard Eddington accretion scenario. During my talk I will review the high redshift quasar problem and I will discuss a novel mechanism for supermassive black hole growth we have devised to solve it. This envisages the migration of stellar black holes, via gaseous dynamical friction, toward the central regions of galaxies and their subsequent mergers to grow an intermediate mass black hole (heavy seed). Subsequent gas accretion onto such heavy seed will lead the central black hole to become supermassive in a very short timescale, providing a viable solution to the high redshift quasar tension.

I will conclude discussing the perspectives to test this mechanism via the detection of gravitational waves produced by merger events between the migrating compact objects and the growing central BH with future ground and space-based detectors such as the Einstein Telescope (ET) and the Laser Interferometer Space Antenna (LISA).

# Astroparticle Physics (APP)

## Speaker: Marco CRISTOSOMI

## Title: Testing gravity with gravitational waves

**Abstract:** Gravitational waves from compact binary coalescences provide access to the strong field and highly dynamic regime of gravity. I will present some of the ongoing efforts to test General Relativity in this regime, the current state and future prospects.

## Speaker: Pranjal RALEGANKAR

Title: Probing hidden sectors with early universe cosmology

**Abstract**: No fundamental requirement exists for all particles to interact with the Standard Model gauge forces. Consequently, there could naturally be a hidden sector of particles that have gone undetected and dark matter could reside in it. A hidden sector of particles could have a different temperature than the plasma formed by the Standard Model particles in the early universe. Such a hidden sector can alter early universe cosmology from the assumed behavior in a variety of ways and lead to interesting observational consequences. In this talk, I discuss three such consequences: an enhancement in sub-Earth mass dark matter microhalos, an inhomogeneous distribution of helium to hydrogen ratio in different galaxies, and a significant abundance of dark radiation.

## Theory and Numerical Simulation of Condensed Matter (CM)

Speaker: Andrea TIRELLI Title: Hydrogen at high pressures by Machine Learning and Quantum Monte Carlo **Abstract:** In this talk I will overview some recent developments on the study of hydrogen at planetary conditions leveraging a new technique combining the accuracy of quantum Monte Carlo ab-initio simulations with the efficiency of a Machine Learning. Such a technique is based on kernel regression in combination with state-of-the-art methods to describe atoms in a systems. I will show some examples benchmarking the quality of the method and try to motivate the importance and need of having highly accurate ML models. This is a joint work with G. Tenti, K. Nakano and S. Sorella.

#### Speaker: Paolo PEGOLO

#### Title: TOPOLOGY, OXIDATION STATES, AND CHARGE TRANSPORT IN IONIC CONDUCTORS

Abstract: Recent theoretical advances, based on a combination of concepts from Thouless' topological theory of adiabatic charge transport and a newly introduced gauge-invariance principle for transport coefficients, have permitted to connect (and reconcile) Faraday's picture of ionic transport---whereby each atom carries a well-defined integer charge---with a rigorous quantum description of the electronic charge-density distribution, which hardly suggests its partition into well-defined atomic contributions. Interestingly, by relaxing some general topological conditions, charge may be transported in ionic conductors without any net ionic displacements. This phenomenology can be connected with the well-known Marcus-Hush theory of electron transfer, which reflects the topology of adiabatic paths drawn by atomic trajectories. As a significant byproduct, this permits to classify different regimes of ionic transport according to the topological properties of the electronic structure of the conducting material.

## Theoretical and Scientific Data Science (TSDS)

### Speaker: Eszter SZEKELY

**Title:** WHAT NEURAL NETWORKS LEARN AND OTHER METHODS DON'T - THE CASE OF HIGHER-ORDER STATISTICS **Abstract:** A common explanation for the recent success of neural networks in machine learning is that they are great *feature extractors*: their structure, a composition of simple functions with parameters that can be tuned to the data, allows them to hone into those characteristics of a data set that are pertinent for a given task. From a theoretical point of view, however, it remains an active area to verify this statement. For example, what problems can be learnt by neural networks, rather than by other methods that have a *fixed* feature map, like kernel machines? We study this problem in a controlled setting by training neural networks and kernel machines on a data set with synthetic images. We find a regime with low signal-to-noise ratio, where neural networks consistently beat kernel machines, especially when the task depends on the higher-order correlations in the data beyond the covariance matrix. We relate the performance of both methods to a phase transition in the higher-order correlation moments, which is of independent interest.

### Speaker: Riccardo MARGIOTTA

### Title: Optimal control attacks: online label poisoning

Abstract: Artificial neural networks are powerful mathematical models that are changing our technologies. However, they are vulnerable to adversarial attacks: small ad-hoc perturbations of input data that can strongly alter the models' output. Understanding such attacks is key to designing effective defense strategies and building reliable models. Previous studies have mainly explored static attacks, where the training dataset is constant and available to the attacker upfront. Instead, little attention was devoted to the online setting, where attacks and training co-occur on a stream of incoming data. In this work, we consider attacks on online learners training on labeled (input-output) data, where the attacker may perturb the current label to manipulate the learning dynamics. Crafting the best possible attacks can be formalized as an optimal control problem, which

we tackle using greedy strategies and deep reinforcement learning agents. We first address the simplest case of attacking a single neuron in the teacher-student setup. This controlled setting allows us to gain theoretical insights. We then extend our analysis to neural networks and consider applications to real datasets. Our results show that greedy attacks are nearly optimal and that the model robustness increases with the batch size of incoming data.

## Molecular and Statistical Biophysics (MSBP)

## Speaker: Valerio PIOMPONI

Title: MOLECULAR DYNAMICS SIMULATIONS OF MODIFIED RNA MATCHING DENATURATION EXPERIMENTS Abstract: Post-transcriptional modifications of RNA are the object of growing interest in the community, since they have been shown to be functional in a variety of biological processes, and consist of biochemical alterations of nucleotides that can directly impact RNA structure and/or dynamics. The N6-methyladenosine (m6A) is the most prevalent chemical modification in messenger RNAs and has been observed both in coding and non-coding RNAs, showing the capability of regulating interaction of RNA with proteins. Although m6A is widely studied by the RNA community, the number of applications of molecular dynamics (MD) simulations to N6-methylated RNAs reported to date is still limited. MD is a powerful tool to access structural dynamics of RNA at the atomistic level, but the quality of the simulations strongly rely on the quality of the force fields parameters used. For these reasons, we made an effort to improve the quality of the m6A force field by fitting parameters to denaturation experiments performed on m6A-containing duplexes and NMR measurements that estimate the populations of m6A \emph{syn/anti} isomers. Our fitting strategy makes use of achemical free-energy calculations, which allows us to estimate the destabilization induced by the methylation on duplexes, by integrating along an alchemical path describing the transformation of a standard adenine into its N6-methylated version. In my talk, I will show the results of our fitting, illustrating how the refinement of 6 charges of the nucleobase plus the addition of a torsional potential allows us to significatively improve the agreement between computations and experiments. Furthermore, I will show how the alchemical computations methods we set up for m6A, plus the improved force field parameters that we derived, can be used in further studies to quantitatively estimate the impact of modifications on RNA structural dynamics and in binding affinities between RNA and proteins.

## Speaker: Zahra Ahmadian DEHAGHANI

### Title: TOPOLOGICALLY INTERLOCKED RING POLYMERS

Abstract The topology of polymers plays a significant role in their in- and out-of-equilibrium behavior in melts and solutions. An emerging and still underexplored class of topological polymers are polycatenanes, a linear chainmail of mechanically interlocked ring polymers. Despite recent advances in synthesizing these structures, not much is known about their statics, dynamics and rheological properties. Using molecular dynamic simulation, we explore the effect of topology in polycatenane behavior in good and bad solvent. By using equivalent conventional polymers as a term of reference, we discuss how the linear chainmail topology alters the global properties of the polycatenane in bad solvent, including its entanglement.

## Statistical Physics (SP)

**Speaker:** Stefano SCOPA **Title:** Generalized Hydrodynamics and its quantum fluctuations Abstract: The study of the out-of-equilibrium properties of quantum many-body systems is a notoriously hard problem, due to the exponential increase of the Hilbert space with the number of the system's components. In the case of quantum integrable models, a large-scale description of the dynamics is attained by means of an Euler hydrodynamic theory with infinitely many conservation laws, dubbed Generalized Hydrodynamics (GHD). Employing GHD, one can give accurate predictions of the experimental measures on the transport properties of the quantum model. But despite its great predictive power, GHD (like any hydrodynamic theory) does not capture important quantum effects, such as equal-time correlations among different points and zero-temperature entanglement. A way to account for these missing quantum effects is established by Quantum GHD, where an effective field theory description of the leading quantum fluctuations is incorporated over the evolving GHD background. In this short talk, I wish to provide a non-technical overview of GHD and its re-quantization, focusing on the results that this research path enabled us to collect so far.

### Speaker: Francesco CODAGNONE

#### Title: The call of Quantum Integrability for Cold Atoms

Abstract: Recent developments in cooling and optical trapping of cold atoms open exciting opportunities for experimental studies of interacting systems under well controlled conditions, with a remarkable achievement being the quasi-one-dimensional quantum gases. Low-dimensional systems play an important role in physics because there exist exact solutions for a number of such models: this happens when the systems in question are integrable. Here we discuss how, taking advantage of the richness of integrable theories, we are able to investigate the properties one-dimensional systems of cold atoms. with particular attention devoted to the case of the integrable, supersymmetric bose-fermi mixture.

## **Theoretical Particle Physics (TPP)**

Speaker: Soltan SAMANI Title: BLACK HOLES UNDER THE MICROSCOPE: A HOLOGRAPHIC PERSPECTIVE Abstract: TBA

**Speaker:** Francesco/Giulio BARNI **Title:** From the Earth to the sky through fundamental physics **Abstract:** TBA