DOTTORANDO / *PHD STUDENT*	
COGNOME / *SURNAME*	**NOME / *NAME***
FIGURATO	LARIA
CORSO DI DOTTORATO / *PHD COURSE*	**CICLO / *CYCLE***
PHYSICS	XXXVIII
SUPERVISORE (COGNOME, NOME) / *SUPERVISOR (SURNAME, NAME)*	
BASSI, ANGELO	
CO-SUPERVISORE (EVENTUALE) (COGNOME, NOME) / CO-*SUPERVISOR IF APPLICABLE (SURNAME, NAME)*	
DONADI, SANDRO CARLESSO, MATTEO	

BREVE RELAZIONE SULL'ATTIVITÀ DI RICERCA / *CONCISE PROGRESS REPORT (RESEARCH ACTIVITIES)*

(max 2500 caratteri, spazi esclusi/ *max 2500 characters excluding blanks*)

The research addresses the interplay between quantum mechanics and gravity, focusing on how gravitational effects may influence quantum state reduction and decoherence. The work proceeds along two complementary lines: Gravitational Decoherence (Károlyházy model) and Gravity-Induced Collapse (Diósi–Penrose model).

Regarding the first line, we developed a generalized stochastic model of spacetime fluctuations that overcomes inconsistencies in earlier formulations and aligns with current experimental bounds. This approach refines Károlyházy's original idea of metric-induced decoherence, quantifying how stochastic gravitational potentials degrade quantum coherence without invoking wave-function collapse. Our analysis narrows the viable parameter space and identifies conditions under which gravitational decoherence may become experimentally accessible.

Regarding the second one, we analyzed the Diósi–Penrose (DP) model, which links spontaneous wave-function collapse to gravitational self-energy. Using analytic and numerical methods, we derived upper bounds on the model's parameters by requiring suppression of observable macroscopic superpositions. We further explored scaling laws for the collapse time as a function of mass, geometry, and dimensionality, and extended the framework to include non-Markovian (memory) effects.

Together, these studies delineate distinct gravitational pathways—stochastic decoherence versus objective collapse—by which classicality may emerge from quantum theory. The results provide tighter theoretical constraints and guide the design of future precision experiments at the quantum–classical boundary.

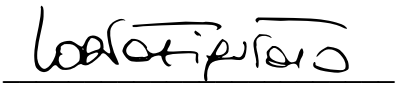
ATTIVITÀ FORMATIVE / *TRAINING ATTENDED BY THE PHD STUDENT*			
TIPO / *TYPE* Corso/Seminario/Workshop/ Convegno/Stage/Altro (specificare) – *Course/Seminar/Workshop/Conference/Stage/ Other (specify*)	**TITOLO / *TITLE***	**SEDE / *LOCATION***	***PERIODO (DAL AL)* / TIME PERIOD (FROM TO)**
WORKSHOP	"A LOOK AT THE INTERFACE BETWEEN GRAVITY AND QUANTUM THEORY - 2025 EDITION"	SAN VITO DI CADORE, (IT)	22-26/07/2025
DOCTORAL SCHOOL	"FUNDAMENTAL PROBLEMS IN QUANTUM PHYSICS 2025"	TRIESTE, (IT)	17-19/06/2025
WORKSHOP	"CONTROL OF QUANTUM SYSTEMS @ERLANGEN [CONQUER24]"	ERLANGEN, (GER)	11-13/12/2024
WORKSHOP	"DICE2024"	CASTIGLIONCELLO (IT)	16-20/09/2024
DOCTORAL SCHOOL	"FUNDAMENTAL PROBLEMS IN QUANTUM PHYSICS 2024"	TRIESTE, (IT)	10-12/09/2024
DOCTORAL SCHOOL	"EMERGENCE OF CLASSICALITY: NEW PERSPECTIVES ON MEASUREMENTS IN QUANTUM THEORY"	DUBLIN, (IRE)	15-19/06/2024
WORKSHOP	"A LOOK AT THE INTERFACE BETWEEN GRAVITY AND QUANTUM THEORY - 2024 EDITION"	SAN VITO DI CADORE, (IT)	2-4/06/2024
WORKSHOP	"MODERN ODYSSEY: QUANTUM GRAVITY MEETS QUANTUM COLLAPSE AT ATOMIC AND NUCLEAR PHYSICS ENERGY SCALES IN THE COSMIC SILENCE"	TRENTO, (IT)	3-7/06/2024
WORKSHOP	"AS FOR THE CAT. . . MODELS AND INTERPRETATIONS OF QUANTUM MECHANICS"	TRIESTE, (IT)	10/05/2024
DOCTORAL SCHOOL	"FUNDAMENTAL PROBLEMS IN QUANTUM PHYSICS 2023"	TRIESTE, (IT)	15 /09/2023
WORKSHOP	"A LOOK AT THE INTERFACE BETWEEN GRAVITY AND QUANTUM THEORY"	CALALZO DI CADORE, (IT)	11-13/07/2023

ATTIVITÀ DI DIDATTICA E DI RICERCA / *TEACHING AND RESEARCH ACTIVITIES HELD BY THE PHD STUDENT*	
TIPO / *TYPE*	**TITOLO / *TITLE***
ATTIVITÀ TUTORIALI E DIDATTICO INTEGRATIVE SVOLTE / *TUTORING ACTIVITIES*	LECTURES: • "ITALIAN QUANTUM WEEKS" , "GIOVANI QUANTISTICI @TRIESTE" , (GORIZIA, 2023) INVITED LECTURER
SEMINARI TENUTI DAL DOTTORANDO / *SEMINARS HELD BY THE PHD STUDENT*	• "ON THE TESTABILITY OF THE KA'ROLYHA'ZY MODEL" SEMINAR GIVEN TO THE GROUP OF PROF. A. BASSI, UNIVERSITY OF TRIESTE • "ON THE EFFECTIVENESS OF THE COLLAPSE IN THE DIO'SI-PENROSE MODEL" SEMINAR GIVEN TO THE GROUP OF PROF. A. BASSI, UNIVERSITY OF TRIESTE
PUBBLICAZIONI SCIENTIFICHE / *SCIENTIFIC PUBLICATIONS* riferimenti bibliografici completi delle pubblicazioni presenti nel catalogo ArTS / *full bibliographic references of the publications submitted to the ArTS catalog*	PUBLICATIONS: • ON THE TESTABILITY OF THE KA'ROLYHA'ZY MODEL, MODEL, L. FIGURATO, A. BASSI, AND S. DONADI, NEW JOURNAL OF PHYSICS 26, 013001 (2024) • ON THE EFFECTIVENESS OF THE COLLAPSE IN THE DIO'SI-PENROSE MODEL, L. FIGURATO, M. DIRINDIN, J. L. GAONA-REYES, M. CARLESSO, A. BASSI, AND S. DONADI, NEW JOURNAL OF PHYSICS 26, 113004 (2024)
PRESENTAZIONI A CONGRESSI, POSTER, ABSTRACT ETC / *PRESENTATIONS AT CONFERENCES, POSTERS,* ABSTRACTS, se pubblicato, riportare i riferimenti bibliografici / *if published provide full bibliographic references*	TALKS: • ON THE EFFECTIVENESS OF THE COLLAPSE IN THE DIO'SI-PENROSE MODEL "DICE2024" (2024) • ON THE EFFECTIVENESS OF THE COLLAPSE IN THE DIO'SI-PENROSE MODEL "FUNDAMENTAL PROBLEMS IN QUANTUM PHYSICS 2024" (2024) • ON THE EFFECTIVENESS OF THE COLLAPSE IN THE DIO'SI-PENROSE MODEL "A LOOK AT THE INTERFACE BETWEEN GRAVITY AND QUANTUM THEORY - 2024 EDITION" (2024) • ON THE EFFECTIVENESS OF THE COLLAPSE IN THE DIO'SI-PENROSE MODEL "MODERN ODYSSEY: QUANTUM GRAVITY MEETS QUANTUM COLLAPSE AT ATOMIC AND NUCLEAR PHYSICS ENERGY SCALES IN THE COSMIC SILENCE" • ON THE TESTABILITY OF THE KA'ROLYHA'ZY MODEL "FUNDAMENTAL PROBLEMS IN QUANTUM PHYSICS 2023" (2023) • ON THE TESTABILITY OF THE KA'ROLYHA'ZY MODEL "A LOOK AT THE INTERFACE BETWEEN GRAVITY AND QUANTUM THEORY" (2023) POSTERS: • "EMERGENCE OF CLASSICALITY: NEW PERSPECTIVES ON MEASUREMENTS IN QUANTUM THEORY" (2024) POSTER PRIZE

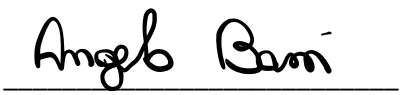
Data compilazione /*Date,*

8 November 2025

Firma dottorando/*PhD student's signature*



Firma supervisore/*Supervisor's signature*



DOTTORANDO / *PHD STUDENT*	
COGNOME / *SURNAME* NICHELE	**NOME / *NAME*** GIOVANNI
CORSO DI DOTTORATO / *PHD COURSE*	**CICLO / *CYCLE***
PHYSICS	XXXVIII
SUPERVISORE (COGNOME, NOME) / *SUPERVISOR (SURNAME, NAME)*	
BENATTI FABIO	
CO-SUPERVISORE (EVENTUALE) (COGNOME, NOME) / *CO-SUPERVISOR IF APPLICABLE (SURNAME, NAME)*	

BREVE RELAZIONE SULL'ATTIVITÀ DI RICERCA / *CONCISE PROGRESS REPORT (RESEARCH ACTIVITIES)*

(max 2500 caratteri, spazi esclusi/ *max 2500 characters excluding blanks*)

My PhD research has developed along three main lines, with the overall purpose of comparing and contrasting classical and quantum non-Markovian stochastic processes. A central concept throughout the thesis is that of backflow of information (BFI), whose interpretation and physical characterization are still object of debate.

i. Classical Reduction of Quantum Dynamics ([2]). Both for classical and quantum systems, one often identifies BFI as revivals of distinguishability between states, occurring whenever the dynamics is not P-divisible, i.e. not contractive. Restricting a quantum process to any fixed maximally Abelian (i.e. commutative) subalgebra yields a classical stochastic process. However, if the original process is P-divisible, the classically reduced process need not be such, the typical example being that of a unitary evolution. Conversely, for some paradigmatic examples of purely dissipative processes, P-divisibility is preserved by the classical reduction. The main finding of this project is the construction of a purely dissipative quantum evolution whose classical restriction loses P-divisibility. The corresponding classical revivals of distinguishability have been then interpreted as quantum coherence-assisted BFI, in full analogy with the open-system scenario.

ii. Superactivation of Memory Effects ([1,3,4]). In the quantum regime there are also memory effects with no classical counterpart. This is the case of two independently evolving parties that do not show revivals when considered independently, but do so when statistically coupled. This effect, called superactivation of backflow of information (SBFI), can also occur via a classical stationary environment, as in the case of two qubits each coupled to a classical Markov chain [3]. Moreover, no entanglement is required. The study of SBFI led to (a) its phenomenological characterization through quantum correlations (beyond entanglement); (b) a constructive way to witness SBFI in terms of entropic quantities [4]; (c) its physical characterization in terms of the growth and collapse of system–environment correlations [3].

iii. Dynamical Entropy and non-Markovianity. The physical mechanisms underlying memory effects are very difficult to infer from the dynamical map only, since the latter is just the one-time marginal of an underlying stochastic process. We then studied the Alicki–Lindblad–Fannes dynamical entropy for open systems, that can be computed by having access to the multi-time statistics. We exactly computed the ALF entropy for the collisional model described in ii) and further provided an example of zero dynamical entropy, mimicking the behavior of a reversible evolution. The ALF entropy has also been operationally interpreted through the state-purification scheme provided by the GNS construction. A link to the SBFI effect naturally emerged in the latter context.

ATTIVITÀ FORMATIVE / *TRAINING ATTENDED BY THE PHD STUDENT*

TIPO / *TYPE*	**TITOLO / *TITLE***	**SEDE / *LOCATION***	***PERIODO (DAL AL)* / TIME PERIOD (FROM TO)**
Corso/Seminario/Workshop/			

Convegno/Stage/Altro (specificare) – *Course/Seminar/Workshop/Conference/Stage/ Other (specify)*			
SCHOOL	MATHEMATICAL ASPECTS OF QUANTUM MECHANICS - WINTER SCHOOL https://indico.math.cnrs.fr/event/9899/	INSTITUT DE MATHÉMATIQUES DE TOULOUSE, PAUL SABATIER UNIVERSITY, TOULOUSE, FRANCE	15 – 19 JANUARY 2024
SCHOOL	SUMMER SCHOOL ON QUANTUM CHAOS, DISSIPATION AND INFORMATION https://indico.fysik.su.se/event/8493/	NORDITA, STOCKHOLM, SWEDEN	16–20 SEPTEMBER 2024
CONFERENCE	54 SYMPOSIUM ON MATHEMATICAL PHYSICS https://fizyka.umk.pl/smp/smp54/	INSTITUTE OF PHYSICS, NICOLAUS COPERNICUS UNIVERSITY, TORUŃ, POLAND	8-11 JUNE 2023
CONFERENCE	IQIS2023 – ITALIAN QUANTUM INFORMATION SCIENCE CONFERENCE https://iqis2023.it/	UNIVERSITY OF TRIESTE	18-22 SEPTEMBER 2023
CONFERENCE	55 SYMPOSIUM ON MATHEMATICAL PHYSICS https://fizyka.umk.pl/smp/smp55/	INSTITUTE OF PHYSICS, NICOLAUS COPERNICUS UNIVERSITY, TORUŃ, POLAND	21-22 JUNE 2024
CONFERENCE	56 SYMPOSIUM ON MATHEMATICAL PHYSICS https://fizyka.umk.pl/smp/smp56/	INSTITUTE OF PHYSICS, NICOLAUS COPERNICUS UNIVERSITY, TORUŃ, POLAND	13-15 JUNE 2025
CONFERENCE	IQIS2025 – ITALIAN QUANTUM INFORMATION SCIENCE CONFERENCE https://events.unibo.it/iqis-2025	ALMA MATER STUDIORIUM - UNIVERSITY OF BOLOGNA	8-11 SEPTEMBER 2025
CONFERENCE	111° CONGRESSO NAZIONALE SIF - SOCIETÀ ITALIANA DI FISICA https://www.sif.it/attivita/congresso/111	UNIVERSITY OF PALERMO	23-26 SEPTEMBER 2025
SHORT-TIME VISIT	SCIENTIFIC VISIT - DEPARTMENT OF MATHEMATICAL PHYSICS	INSTITUTE OF PHYSICS, NICOLAUS COPERNICUS UNIVERSITY, TORUŃ, POLAND	22-26 APRIL 2024
WORKSHOP	WORKSHOP ON THE PEER REVIEW PROCESS	UNIVERSITY OF TRIESTE	13-14 MAY 2024

ATTIVITÀ DI DIDATTICA E DI RICERCA / *TEACHING AND RESEARCH ACTIVITIES HELD BY THE PHD STUDENT*

TIPO / *TYPE*	**TITOLO / *TITLE***
ATTIVITÀ TUTORIALI E DIDATTICO INTEGRATIVE SVOLTE / *TUTORING ACTIVITIES*	
SEMINARI TENUTI DAL DOTTORANDO / *SEMINARS HELD BY THE PHD STUDENT*	i. SEMINAR "*TENSOR PRODUCTS OF DYNAMICAL MAPS AND SUPERACTIVATION OF BACKFLOW OF INFORMATION*", DEPARTMENT OF MATHEMATICAL PHYSICS, INSTITUTE OF PHYSICS, TORUŃ (POLAND), 23 APRIL 2024

PUBBLICAZIONI SCIENTIFICHE / *SCIENTIFIC PUBLICATIONS* riferimenti bibliografici completi delle pubblicazioni presenti nel catalogo ArTS / *full bibliographic references of the publications submitted to the ArTS catalog*	[1]. F. BENATTI, G. **NICHELE,** OPEN QUANTUM DYNAMICS: MEMORY EFFECTS AND SUPERACTIVATION OF BACKFLOW OF INFORMATION, *MATHEMATICS 12*, 37.(2024) https://doi.org/10.3390/math12010037 [2]. F. BENATTI, D. CHRUŚCIŃSKI, **G. NICHELE** (2024). QUANTUM VERSUS CLASSICAL P-DIVISIBILITY. *PHYSICAL REVIEW A*, *110*(5), 052212. (2024) https://doi.org/10.1103/physreva.110.052212 [3]. F. BENATTI, **G. NICHELE,** SUPERACTIVATION OF MEMORY EFFECTS IN A CLASSICAL MARKOV ENVIRONMENT. *PHYSICA SCRIPTA*, *100*(6), 065115. (2025) https://doi.org/10.1088/1402-4896/add57e [4]. **G. NICHELE,** F. BENATTI, ENTROPIC SUPERACTIVATION OF BACKFLOW OF INFORMATION. *QUANTUM ECONOMICS AND FINANCE*, *FIRST ONLINE,* (2025). https://doi.org/10.1177/29767032251361881
PRESENTAZIONI A CONGRESSI, POSTER, ABSTRACT ETC / *PRESENTATIONS AT CONFERENCES, POSTERS,* ABSTRACTS, se pubblicato, riportare i riferimenti bibliografici / *if published provide full bibliographic references*	i. **POSTER** - "QUANTUM VERSUS CLASSICAL *P*-DIVISIBILITY" – 55 SYMPOSIUM ON MATHEMATICAL PHYSICS, INSTITUTE OF PHYSICS, TORUŃ (POLAND), JUNE 2024 ii. **POSTER** - "QUANTUM VERSUS CLASSICAL *P*-DIVISIBILITY" – SUMMER SCHOOL ON QUANTUM CHAOS, DISSIPATION AND INFORMATION, NORDITA, STOCKHOLM (SWEDEN), SEPTEMBER 2024, AVAILABLE AT https://indico.fysik.su.se/event/8493/attachments/5920/7647/nichele_giovanni_posternordita.pdf iii. **INVITED TALK** - "NON-MARKOVIAN OPEN QUANTUM SYSTEMS AND DYNAMICAL ENTROPY: A COLLISIONAL MODEL PERSPECTIVE" – 56 SYMPOSIUM ON MATHEMATICAL PHYSICS, INSTITUTE OF PHYSICS, TORUŃ (POLAND), JUNE 2025, ABSTRACT AVAILABLE AT https://fizyka.umk.pl/smp/smp56/Abstr_56T.pdf iv. **CONTRIBUTED TALK** - "NON-MARKOVIAN OPEN QUANTUM SYSTEMS AND DYNAMICAL ENTROPY: A COLLISIONAL MODEL PERSPECTIVE" – IQIS2025, BOLOGNA, SEPTEMBER 2025, ABSTRACT AVAILABLE AT https://events.unibo.it/iqis-2025/conference-program/booklet_finale-2.pdf/@@download/file/BOOKLET_FINALE-4.pdf v. **CONTRIBUTED TALK** – "SUPERACTIVATION OF BACKFLOW OF INFORMATION IN A CLASSICAL MARKOV ENVIRONMENT", 111° CONGRESSO SIF, PALERMO, SEPTEMBER 2025, ABSTRACT AVAILABLE AT https://static.sif.it/SIF/resources/public/files/congr25/atti-congresso-111_2025.pdf

Data compilazione /*Date,*
Trieste, 07/11/2025

_____

Firma dottorando/*PhD student's signature*

_____

Firma supervisore/*Supervisor's signature*

_____

DOTTORANDO / *PHD STUDENT*	
COGNOME / *SURNAME*	**NOME / *NAME***
RODRIGUES DE SOUZA JUNIOR	IVALDEVINGLES
CORSO DI DOTTORATO / *PHD COURSE*	**CICLO / *CYCLE***
PHYSICS	XXXVIII
SUPERVISORE (COGNOME, NOME) / *SUPERVISOR (SURNAME, NAME)*	
TROMBETTONI, ANDREA	
CO-SUPERVISORE (EVENTUALE) (COGNOME, NOME) / CO-*SUPERVISOR IF APPLICABLE (SURNAME, NAME)*	
BRAITENBERG, CARLA	

BREVE RELAZIONE SULL'ATTIVITÀ DI RICERCA / *CONCISE PROGRESS REPORT (RESEARCH ACTIVITIES)*

(max 2500 caratteri, spazi esclusi/ *max 2500 characters excluding blanks*)

This doctoral research focused on the physical-mathematical modeling, simulation, and geophysical applications of quantum gravimeters. Initially, detailed descriptions of two- and three-level atomic systems were developed, with emphasis on atom–light interaction and on the fundamental principles of atomic interferometry. The study addressed the role of $\pi/2$ and π Raman pulses in Mach–Zehnder interferometers, relating the accumulated phase difference to the local gravitational acceleration.

Moreover, the influence of the temporal shape of the pulses was investigated, and an in-depth analysis of the sensitivity function was developed, which is used to characterize the noise sources that affect the interferometer. The analyses were based on the fact that the relationship between the Rabi frequency and the duration of the laser pulses directly determines the transitions between the atomic states and, consequently, the interferometric response of the system.

The main activities carried out during the doctoral research involved computational numerical analyses performed using synthetic data. In this context, a numerical simulation of the temporal evolution of the probability density function was developed using the split-operator method. This approach made it possible to evaluate the effects of the laser pulse phases on the final interferometer measurement, as well as to study the phase accumulated along the atomic trajectory as a result of the applied acceleration.

Computational geophysics techniques were also employed to generate synthetic gravimetric anomalies, which made it possible to assess the capability of quantum gravimeters to detect subsurface heterogeneities. Geophysical inversion methods, such as Tikhonov regularization and the generalized inverse, were applied to estimate density distributions from the simulated anomalies. These concepts were then used to evaluate the applicability of the quantum gravimeters to four-dimensional gravimetric monitoring in the context of fluid substitution.

During the development of the research activities, a scientific collaboration was established with the Physics Group at the University of Florence. This collaboration took place through a visit to the University of Florence, where it was possible to engage in discussions on modeling strategies and noise analysis.

ATTIVITÀ FORMATIVE / *TRAINING ATTENDED BY THE PHD STUDENT*

TIPO / *TYPE* Corso/Seminario/Workshop/ Convegno/Stage/Altro (specificare) – *Course/Seminar/Workshop/Conference/Stage/Other (specify)*	**TITOLO / *TITLE***	**SEDE / *LOCATION***	***PERIODO (DAL AL)* / TIME PERIOD (FROM TO)**
COURSE	MODERN TOOLS FOR COMPUTATIONAL PHYSICS	TRIESTE (ICTP-MIRAMARE)	FROM 03/2025 TO 04/2025
COUSE	INTRODUCTION TO BAYESIAN METHODS	TRIESTE (UNIVERSITY OF TRIESTE - VIA ALFONSO	FROM 08/05/2023 TO 18/05/2023

		VALERIO)	
COURSE	ADVANCED QUANTUM MECHANICS AND SELECTED APPLICATIONS TO QUANTUM COMPUTATION	TRIESTE (ICTP-MIRAMARE)	FROM 23/05/2023 TO 25/07/2023
COURSE	STATISTICAL FIELD THEORY	TRIESTE (ICTP-MIRAMARE)	FROM 15/05/2023 TO 06/2023
COURSE	COMPLETE POSITIVITY IN QUANTUM INFORMATION	TRIESTE (ICTP-MIRAMARE)	FROM 19/10/2023 TO 29/11/2023
COURSE	LOW TEMPERATURE PHYSICS: QUANTUM FLUIDS AND SUPERCONDUCTIVITY	TRIESTE (ICTP-MIRAMARE)	FROM 01/2024 TO 02/2024
WORKSHOP	MAWI SCHOOL ON COMPUTATIONAL METHODS FOR ULTRACOLD QUANTUM MATTER	GRENOBLE (FRANCE)	FROM 25/03/2024 TO 29/03/2025

ATTIVITÀ DI DIDATTICA E DI RICERCA / *TEACHING AND RESEARCH ACTIVITIES HELD BY THE PHD STUDENT*	
TIPO / *TYPE*	**TITOLO / *TITLE***
ATTIVITÀ TUTORIALI E DIDATTICO INTEGRATIVE SVOLTE / *TUTORING ACTIVITIES*	
SEMINARI TENUTI DAL DOTTORANDO / *SEMINARS HELD BY THE PHD STUDENT*	”QUANTUM GRAVMETERS”, SEMINAR AT UNIVERSITY OF FLORENCE (22/3/2025) – “GEOPHYSICAL APPLICATIONS OF QUANTUM SENSORS”, INFORMAL STUDENT PRESENTATION DURING THE SCHOOL “COMPUTATIONAL METHODS FOR ULTRACOLD QUANTUM MATTER”, LPMMC, GRENOBLE (26/3/2024)
PUBBLICAZIONI SCIENTIFICHE / *SCIENTIFIC PUBLICATIONS* riferimenti bibliografici completi delle pubblicazioni presenti nel catalogo ArTS / *full bibliographic references of the publications submitted to the ArTS catalog*	THE FOLLOWING TWO MANUSCRITPS ARE CURRENTLY IN THE COMPLETION STAGE AND WILL BE SUBMITTED PRIOR TO THE PHD DEFENSE: I. RODRIGUES DE SOUZA JUNIOR ET AL., “THEORY AND APPLICATIONS OF ULTRACOLD QUANTUM GRAVIMETERS: AN INTROUDCTION FOR GEOPHYSICISTS” I. RODRIGUES DE SOUZA JUNIOR ET AL., “TIME-DEPENDENT PHASE ESTIMATION: THEORETICAL ASPECTS AND GEOPHYSICAL APPLICATIONS””

PRESENTAZIONI A CONGRESSI, POSTER, ABSTRACT ETC / *PRESENTATIONS AT CONFERENCES, POSTERS,* ABSTRACTS, se pubblicato, riportare i riferimenti bibliografici / *if published provide full bibliographic references*	

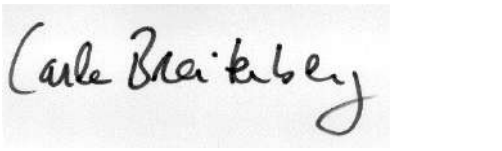
Data compilazione /*Date,*

____21/11/2025____

Firma dottorando/*PhD student's signature*

_____

Firma supervisore/*Supervisor's signature*



_____

DOTTORANDO / *PHD STUDENT*	
COGNOME / *SURNAME* NAMAR	**NOME / *NAME*** ALESSANDRO
CORSO DI DOTTORATO / *PHD COURSE*	**CICLO / *CYCLE***
PHYSICS	38
SUPERVISORE (COGNOME, NOME) / *SUPERVISOR (SURNAME, NAME)*	
VESSELLI ERIK	
CO-SUPERVISORE (EVENTUALE) (COGNOME, NOME) / CO-*SUPERVISOR IF APPLICABLE (SURNAME, NAME)*	
SCARDAMAGLIA MATTIA	

BREVE RELAZIONE SULL'ATTIVITÀ DI RICERCA / *CONCISE PROGRESS REPORT (RESEARCH ACTIVITIES)*

(max 2500 caratteri, spazi esclusi/ *max 2500 characters excluding blanks*)

My research activity focused on the growth and characterization of novel 2D materials based on metalorganic architectures. In particular, I investigated iron-based materials, starting from FeTPyP and hemin as molecular precursors. Although both molecules share the same core, a macrocycle containing a central Fe atom, they differ in the peripheral functional groups: pyridinic terminations in the former and carboxylic groups in the latter. These materials offer a nature-inspired strategy to cage single metal atoms, and when deposited on a substrate, the properties of their reactive centers can be tuned through surface trans effect and lateral interactions. The aim of my PhD work was to characterize the structural and electronic properties of these materials under Ultra High Vacuum (UHV) and Near-Ambient Pressure (NAP) conditions, highlighting how distinct properties emerge from the same macrocycle when the chemistry of the peripheral groups is varied. Subsequently, Co atoms were coordinated in both systems and the structural and electronic properties of the modified systems were investigated in UHV as well as under reactive conditions.

FeTPyP and FeTPyP-Co on Gr/Ir(111)

Scanning Tunneling Microscopy (STM) measurements reveal that FeTPyP molecules self-assemble on the Gr/Ir(111) system into a close-packed structure, stabilized by intermolecular interactions between the electronegative N atoms of the pyridyl end groups and the peripheral H atoms from the neighboring pyrrole moieties. Deposition of Co atoms induces distinct structural and electronic modifications, including the unexpected reduction of the Fe oxidation state from +2 to +1.

Under NAP conditions, significant differences were observed between the monometallic FeTPyP layer and the bimetallic FeTPyP-Co network. The monometallic layer remained inert toward O2 and CO, whereas the bimetallic network exhibits clear reactivity, with both metal centers participating in the reactions. In the presence of O2, Infrared-Visible Sum Frequency Generation (IR-Vis SFG) and NAP-X-ray Photoelectron Spectroscopy (NAP-XPS) measurements provided clear evidence of O2 ligation and activation. CO adsorption was also studied by IR-Vis SFG spectroscopy, probing the cooperative effects and adsorption energies at both metal sites as a function of Co loading.

NAP-XPS combined with Density Functional Theory (DFT) calculations allowed the assignment of the oxidation states of both metal centers. Upon Co deposition, both Fe and Co are theoretically compatible with a +1 oxidation state. However, due to the high reactivity of Fe(I) toward O2, Fe is predominantly observed experimentally in the +2 oxidation state. Exposure to O2 further oxidizes Co and Fe to +2 and +3 oxidation states, respectively, in excellent agreement with theoretical predictions. In contrast, under CO exposure, the experimental results diverged from theory due to the residual oxygen presence under the experimental conditions.

Hemin and hemin+Co on Au(111)

To explore the influence of the molecular environment and peripheral functional groups on the reactivity, hemin, the core component of hemoglobin, was deposited on Au(111). STM and Near Edge X-ray Absorption Fine Structure (NEXAFS) measurements confirmed the formation of an ordered layer containing both Fe-free and Fe-filled species, due to the limited purity of the biological precursor. Different molecular configurations were observed, involving

hydrogen-bonding interactions between carboxylic groups of neighboring molecules or between a carboxylic group, overlapping the macrocycle of an adjacent molecule, and the iminic nitrogen atom.
The reactivity of the layer was then tested toward CO and O2 exposure. For CO adsorption, no direct interaction with the hemin layer was observed at room temperature up to 0.3 mbar of CO, indicating that the system is inert toward this gas. In contrast, O2 stabilization occurs at the Fe sites when carboxylic terminations are positioned near the centers of neighboring molecules. In this configurations, carboxylic groups mimic the distal histidine in oxyhemoglobin and oxymyoglobin, forming hydrogen bonds with O2 and stabilizing the Fe-O2 interaction, thereby effectively reproducing the second coordination sphere observed in biological systems. To create a bimetallic structure, Co atoms were deposited after the formation of the hemin layer, with the aim of occupying the vacant metal centers. Surprisingly, Co preferentially interacts with the hemin molecules, resulting in a system composed of Fe-free, Fe-filled and Co-filled species, along with an intermediate configuration in which both Co and Fe were simultaneously present within the molecular macrocycle. Upon O2 exposure, O2 activation occurred, leading to the formation of atomic oxygen atom species that diffused across the surface, where several processes, including trans-metalation, took place.

Synchrotron Activities, Scientific Collaborations and Research Period Abroad

All XPS data were collected at the MAX IV Laboratory (University of Lund, Sweden), where I had the opportunity to participate to several experimental campaigns at HIPPIE and FlexPES beamlines. At the HIPPIE beamline, I contributed to the following research proposals: ID 20221030 “Self-metalation of tetrapyrroles at the gas-solid interface.”, ID 20230232 “2D bio-mimetic materials towards the second coordination sphere: an in situ spectroscopic characterization of the active site ligation environment in a synthetic cobalamin-based 2D material.”, ID 20231301 “Cooperativity effects in a FeTPyP-Co metalorganic framework on graphene: the role of electronic configurations and local coordination.”, ID 20240093 “From 2D metalorganic frameworks to the second coordination sphere: reactivity of one-armed porphyrins at surfaces”. At the FlexPES beamline, I was involved in proposal ID 20240091 “From 2D metalorganic frameworks to the second coordination sphere: electronic and geometric structure of one-armed porphyrins at surfaces”.
During my PhD I also spent a six-month research period at MAX IV Laboratory, specifically at the HIPPIE beamline. During this time, I assisted the beamline staff with the following proposals: ID 20231733 “Studying subsurface carbon segregation in a palladium catalyst during methane oxidation” and ID 20240738 “Self-sustained oscillations studied with new tr-APXPS methods”. In addition, I contributed to the installation and testing of a monochromatic X-Ray source on the solid-gas endstation of HIPPIE beamline, which is now available for users to perform sample pre-characterization before official beamtime session. I also collaborated with the STM laboratory staff to acquire STM images of both FeTPyP and FeTPyP-Co systems. Moreover, I had the opportunity to conduct an in-house research project at HIPPIE (proposal ID 20241097), in which I further investigated the properties of FeTPyP/FeTPyP-Co and hemin/hemin+Co systems from UHV up to NAP conditions.
Furthermore, during my period abroad, I also had the possibility to participate in an experimental campaign at ALBA synchrotron (Barcelona, Spain) specifically at the BL29-BOREAS beamline with the following proposal ID 2024028422 entitled “Ferromagnetism on 2D bimetallic organic framework”.

ATTIVITÀ FORMATIVE / *TRAINING ATTENDED BY THE PHD STUDENT*

TIPO / *TYPE* Corso/Seminario/Workshop/ Convegno/Stage/Altro (specificare) – *Course/Seminar/Workshop/Conference/Stage/ Other (specify)*	**TITOLO / *TITLE***	**SEDE / *LOCATION***	***PERIODO (DAL AL)* / TIME PERIOD (FROM TO)**
SUMMER SCHOOL	SPECTROSCOPY SUMMER SCHOOL	LUND (Sweden)	AUGUST 21ST-AUGUST 25TH (2023)
CONFERENCE	ECSCD-16/ICSOS-14	WIEN (AUSTRIA)	JUNE 2ND – JUNE 6TH (2025)
CONFERENCE	APXPS 2025	NEW YORK (UNITED STATES)	DECEMBER 9TH-DECEMBER 12TH (2025)
PHD COURSE	FREE ELECTRON LASER AND SYNCHROTRON-BASED SPECTROSCOPIES: GETTING TO THE NANOMETER WITH FEMTOSECOND RESOLUTION	TRIESTE (ITALY)	MAY 20TH- JUNE 1ST (2023)
PHD COURSE	X-RAY ABSORPTION SPECTROSCOPY	TRIESTE (ITALY)	JULY 10TH- JULY 14TH (2023)
PHD COURSE	NANOSTRUCTURE IN	TRIESTE (ITALY)	NOVEMBER 20TH-DECEMBER

	CATALYSIS		6TH (2023)
PHD COURSE	INFRARED SPECTROSCOPY: FROM MACRO TO NANOSCALE ON THE MOLECULES OF LIFE	TRIESTE (ITALY)	JUNE 1ST-JUNE 15TH (2023)
PHD COURSE	INTRODUCTION TO DENSITY FUNCTIONAL THEORY	TRIESTE (ITALY)	APRIL 18TH- MAY 5TH (2023)
PHD COURSE	CHARACTERIZATION OF 2D SAM PROPERTIES	TRIESTE (ITALY)	MARCH 28TH-APRIL 10TH (2024)
PHD COURSE	2D SELF-ASSEMBLED MONOLAYERS	TRIESTE (ITALY)	JULY 5TH- JULY 25TH (2024)
PHD COURSE	IMAGING WITH X-RAY FUNDAMENTALS AND APPLICATIONS	TRIESTE (ITALY)	DECEMBER 10TH-DECEMEBR 22ND (2023)

ATTIVITÀ DI DIDATTICA E DI RICERCA / *TEACHING AND RESEARCH ACTIVITIES HELD BY THE PHD STUDENT*	
TIPO / *TYPE*	**TITOLO / *TITLE***
ATTIVITÀ TUTORIALI E DIDATTICO INTEGRATIVE SVOLTE / *TUTORING ACTIVITIES*	
SEMINARI TENUTI DAL DOTTORANDO / *SEMINARS HELD BY THE PHD STUDENT*	
PUBBLICAZIONI SCIENTIFICHE / *SCIENTIFIC PUBLICATIONS* riferimenti bibliografici completi delle pubblicazioni presenti nel catalogo ArTS / *full bibliographic references of the publications submitted to the ArTS catalog*	Title: Scalable bottom-up synthesis of Co-Ni-doped graphene Authors:Valeria Chesnyak, Mirco Panighel, Alessandro Namar, Ayesha Farooq, Matus Stredansky, Giovanni Comelli, Cristiana Di Valentin & Cristina Africh Journal: Science advances Doi:https://dx.doi.org/10.1126/sciadv.ado8956 Title: Single atom coordination in a manganese–cobalt bi-metallic framework on graphene: geometric and electronic structures Authors: Stefania Baronio, Michela De Col, Davide Bidoggia, Alessandro Namar, Mattia Scardamaglia, Mirko Cinchetti, Giovanni Zamborlini, Paolo Giannozzi & Erik Vesselli Journal: Nanoscale Doi:https://dx.doi.org/10.1039/d5nr01383f Title: Carbon subsurface traffic jam as driver for methane oxidation activity and selectivity on Palladium surfaces Authors: Ulrike Küst, Rosemary Jones, Julia Prumbs, Alessandro Namar, Mattia Scardamaglia, Andrey Shavorskiy & Jan Knudsen Journal: Nature Communications Doi:https://dx.doi.org/10.1038/s41467-025-63088-9
PRESENTAZIONI A CONGRESSI, POSTER, ABSTRACT ETC / *PRESENTATIONS AT CONFERENCES, POSTERS,* ABSTRACTS, se pubblicato, riportare i riferimenti bibliografici	• Poster presentation delivered at the Spectroscopy Summer School attended at the Max IV Laboratory (Lund, Sweden) with the title:" An in situ spectroscopic and vibrational surface characterization of a protein's solvation: the case of vitamin B12/Au(111)" • Poster presentation delivered at the APXPS 2025 Workshop in New York (United States), titled: "Bio-inspired Surface Catalysis: Hemin Reactivity".

/ *if published provide full bibliographic references*	• Oral presentation delivered at the ECSCD-16/ICSOS-14 Conference in Wien (Austria) entitled: "Cooperativity in a graphene-supported FeTPyP-Co metalorganic network: the role of electronic and geometric structure."

Data compilazione /*Date,*

19/11/2025

Firma dottorando/*PhD student's signature*

Firma supervisore/*Supervisor's signature*

DOTTORANDO / *PHD STUDENT*	
COGNOME / *SURNAME* DAMIANO	**NOME / *NAME*** ALICE
CORSO DI DOTTORATO / *PHD COURSE*	**CICLO / *CYCLE***
FISICA	XXXVIII
SUPERVISORE (COGNOME, NOME) / *SUPERVISOR (SURNAME, NAME)*	
STEFANO BORGANI	
CO-SUPERVISORE (EVENTUALE) (COGNOME, NOME) / CO-*SUPERVISOR IF APPLICABLE (SURNAME, NAME)*	
MILENA VALENTINI	

BREVE RELAZIONE SULL'ATTIVITÀ DI RICERCA / *CONCISE PROGRESS REPORT (RESEARCH ACTIVITIES)*

(max 2500 caratteri, spazi esclusi/ *max 2500 characters excluding blanks*)

Massive black holes (MBHs), sitting at the centres of massive galaxies, contribute to the evolution of cosmic structures through accretion and feedback mechanisms. A minority of them shine in Active Galactic Nuclei (AGN), affecting scales from sub-parsec accretion flows to cluster-scale jets and cavities. Tight empirical correlations between MBH mass and galaxy properties suggest that every MBH has undergone active phases, linking its growth to that of its host.

The MBH interplay with the surrounding medium modulates the accretion and feedback efficiencies, therefore the location where the BHs reside and their dynamical evolution is of primary importance. Moreover, electromagnetic signatures and recent gravitational-wave detections are revealing interacting and merging MBH systems, further motivating accurate dynamical modelling.

Cosmological hydrodynamical simulations follow the nonlinear cosmic structure formation but lack the resolution to accurately capture MBH-related processes, requiring sub-resolution prescriptions governing their formation, accretion, feedback and dynamics.

Within my reasearch activity, I investigated the evolution and modelling of sub-resolution prescriptions for BH–specially focusing on MBH dynamics—in cosmological simulations. I contributed in the development of the OpenGADGET3 code (Dolag et al. , in prep.), and carried out simulations focused on:

- the development of a novel dynamical friction (DF) correction for the unresolved contribution of DF in simulations. Tested against ad-hoc approaches—repositioning and boosted dynamical mass—it reproduces efficient orbital decay while avoiding their drawbacks, such as spurious off-centred BHs or incorrect merger timing;

- the assessment and refinement of the novel DF correction in controlled experiments, as dark-matter halos eventually coupled with a stellar bulge. The model yields sinking timescales in good agreement with analytical predictions derived using the publicly released OTIS library, which I

developed at the scope;

- the analysis of numerical prescriptions governing MBH accretion and feedback, including stochastic gas swallowing, cold-cloud evaporation, kernel-weighted energy deposition, and coupling with supernova-driven winds. Those experiments led to the development of a new simulation campaign of galaxy clusters.

Overall, the work presented in my Thesis advances both the physical modelling of MBH dynamics and the numerical treatment of accretion and feedback, providing a foundation for future developments such as kinetic feedback, improved accretion physics, high-redshift studies, and spin evolution.

ATTIVITÀ FORMATIVE / *TRAINING ATTENDED BY THE PHD STUDENT*

TIPO / *TYPE* Corso/Seminario/Workshop/ Convegno/Stage/Altro (specificare) – *Course/Seminar/Workshop/Conference/Stage/ Other (specify)*	**TITOLO / *TITLE***	**SEDE / *LOCATION***	***PERIODO (DAL AL)* / TIME PERIOD (FROM TO)**
SCHOOL	MICHIGAN COSMOLOGY SUMMER SCHOOL	UNIVERSITY OF MICHIGAN- REMOTE	2-6 JUNE 2023
SEMINAR	USCVIII MEETING	UNIVERSITÀ DI CATANIA	15-18 JUNE 2023
COLLABORATION MEETING	HYDROSIM MEETING	SESTO-ITALY	10-14 JULY 2023
SEMINAR	CONFERENCE OF THE ITALIAN PHYSICAL SOCIETY	UNIVERSITÀ DI FISCIANO	10-16 SEPTEMBER 2023
WORKSHOP	THE PROBLEMATIC EXISTENCE OF MASSIVE BLACK HOLES AT Z>6	IFPU - TRIESTE	16-20 OCTOBER 2023
SEMINAR	THE ORIGIN OF SUPERMASSIVE BLACK HOLES	SESTO-ITALY	10-14 JUNE 2024
SEMINAR	SPOKE 3 GENERAL MEETING	ISOLA D'ELBA	5-9 MAY 2024
SCHOOL	INAF HPC SCHOOL FOR ASTROPHYSICS	CNR - BOLOGNA	4-12 JULY 2024
COLLABORATION MEETING	HYDROSIM MEETING	UNIVERSITY OF LUBIANA	28-31 JULY 2024
WORKSHOP	MIAPBP WORKSHOP ON AGN	MIAPBP- GARCHING (MUNICH)	24 MARCH – 4 APRIL 2024
SEMINAR	YOUNG ASTRONOMERS ON ACTIVE GALACTIC NUCLEI	UNIVERSITY OF SOUTHAMPTON	1-4 SEPTEMBER 2025
WORKSHOP	UNRAVELING LITTLE RED DOTS	IFPU-TRIESTE	27-31 OCTOBER 2025
STAGE	-	UNIVERSITY OF ZURICH	7 JANUARY – 24 MARCH 2025

ATTIVITÀ DI DIDATTICA E DI RICERCA / *TEACHING AND RESEARCH ACTIVITIES HELD BY THE PHD STUDENT*

TIPO / *TYPE*	TITOLO / *TITLE*
ATTIVITÀ TUTORIALI E DIDATTICO INTEGRATIVE SVOLTE / *TUTORING ACTIVITIES*	
SEMINARI TENUTI DAL DOTTORANDO / *SEMINARS HELD BY THE PHD STUDENT*	- 24th May 2023 - PhD and PostDoc seminars, Astronomical Observatory of Trieste (Italy). - 14th September 2023 - Conference of the Italian Physical Society, University of Salerno, Fisciano (Italy). - 16th October 2024 - The problematic existence of massive black holes at z>6.Workshop at ICTP (Trieste). - 13th November 2025 -End of PhD cycle seminar.
PUBBLICAZIONI SCIENTIFICHE / *SCIENTIFIC PUBLICATIONS* riferimenti bibliografici completi delle pubblicazioni presenti nel catalogo ArTS / *full bibliographic references of the publications submitted to the ArTS catalog*	**Damiano A.,** Valentini M., Borgani S., Tornatore L., Murante G., Ragagnin A., Ragone-Figueroa C., Dolag K., "Dynamical friction and the evolution of black holes in cosmological simulations: A new implementation in OpenGadget3", A&A, V**olume** 692, December 2024 **Damiano A.,** Borgani S., Valentini M., Murante G., Tornatore L., Strakos P., Jaros M., "Dynamical friction and massive black hole orbits: analytical predictions and numerical solutions", acctepted for publication on Astronomy&Astrophysics **Damiano A.,** Borgani S., Murante G., Valentini M., Tornatore L., Taffoni G., **"**Numerical solutions for black hole feeding and feedback in cosmological simulations with OpenGADGET3**",** submitted for the publication to Astronomy&Computing
PRESENTAZIONI A CONGRESSI, POSTER, ABSTRACT ETC / *PRESENTATIONS AT CONFERENCES, POSTERS,* ABSTRACTS, se pubblicato, riportare i riferimenti bibliografici / *if published provide full bibliographic references*	• 13th June 2023- INAF- Spoke 3 General Meeting University of Catania (Italy). Contributed talk. • 15th June 2023 - INAF-USC VIII Workshop, University of Catania (Italy). Contributed talk. • 14th July 2023 - Hydrosim meeting Sexten Center for Astrophysics, Sesto (Italy). Contributed talk. • 13th July 2024 - The origin of Supermassive Black Holes Sesto (Italy). Contributed talk. • 28th July 2024 - The OpenGadget3 code meeting. Lubijana (Slovenia) Contributed talk. • 24th April 2025 – MiaPbP workshop on Active Galactic Nuclei , Munich (Germany). Contributed talk.

	• 26th May 2025 – Spoke3 Technical Meeting, Perugia (Italy). Contributed talk. 1st September 2025 - Young Astronomers on Active Galactic Nuclei, Southampton (England). Contributed talk.

Data compilazione /*Date,*

20/11/2025

Firma dottorando/*PhD student's signature*

ALICE DAMIANO

Firma supervisore/*Supervisor's signature*

STEFANO BORGANI

DOTTORANDO / *PHD STUDENT*	
COGNOME / *SURNAME* LEPINZAN	**NOME / *NAME*** MARIUS DANIEL
CORSO DI DOTTORATO / *PHD COURSE*	**CICLO / *CYCLE***
FISICA	XXXVIII
SUPERVISORE (COGNOME, NOME) / *SUPERVISOR (SURNAME, NAME)*	
MONACO PIERLUIGI	
CO-SUPERVISORE (EVENTUALE) (COGNOME, NOME) / *CO-SUPERVISOR IF APPLICABLE (SURNAME, NAME)*	
CASTRO TIAGO, LUCA TORNATORE	

BREVE RELAZIONE SULL'ATTIVITÀ DI RICERCA / *CONCISE PROGRESS REPORT (RESEARCH ACTIVITIES)*

(max 2500 caratteri, spazi esclusi/ *max 2500 characters excluding blanks*)

My research focused on both the optimization and the scientific extension of PINOCCHIO, a Lagrangian Perturbation Theory based code for fast cosmological simulations. The first research direction addressed performance and energy efficiency. The original version of PINOCCHIO relied on CPU-based parallelization; therefore, I led the porting of its main computational kernels to GPUs. The collapse-time calculation, which is highly parallel, was the first target, requiring the development of GPU-native interpolation routines to replace CPU-bound (GSL) libraries and ensure portability across NVIDIA and AMD architectures. In parallel, the FFT components used to compute displacements and tidal tensors were accelerated using the heFFTe library. Benchmarking on the LEONARDO, KAROLINA, and SETONIX supercomputers demonstrated speedups of up to 8× for collapse-time evaluation and up to 28× for FFTs, together with substantial reductions in power consumption. These results show that GPU acceleration provides both faster runtime and improved energy efficiency, enabling large simulation campaigns needed for cosmological inference.

The second research direction evaluated and expanded the scientific applicability of PINOCCHIO. Using halo catalogs from PINOCCHIO and from full N-body simulations (OpenGADGET3), cosmic voids were identified with the VIDE toolkit and compared across redshifts and resolutions. The void size function, ellipticity, core densities, and radial density profiles all showed good agreement within statistical uncertainties, demonstrating that PINOCCHIO reproduces void properties reliably in the quasi-linear regime and can therefore be used to study void-based cosmological probes.

In parallel to this main work, I also investigated a machine-learning–based image deblending technique for the Euclid mission (I'm an active Consortium member since 2022), now in the final testing phase against the legacy pipeline. A 3D generalization, led by me, of the same algorithm was applied to replace the PINOCCHIO fragmentation (halo-finding) procedure in Lagrangian space, showing promising initial results for improved halo reconstruction.

Overall, this work strengthens both the computational performance and the scientific applicability of PINOCCHIO, enabling faster and more energy-efficient simulations for upcoming large-volume cosmological surveys.

ATTIVITÀ FORMATIVE / *TRAINING ATTENDED BY THE PHD STUDENT*

TIPO / *TYPE* Corso/Seminario/Workshop/ Convegno/Stage/Altro (specificare) – *Course/Seminar/Workshop/Conference/Stage/Other (specify)*	TITOLO / *TITLE*	SEDE / *LOCATION*	*PERIODO (DAL AL)* / TIME PERIOD (FROM TO)
CONFERENCE	SPOKE 3 GENERAL MEETING	CATANIA	12/06/2023-14/06/2023
WORKSHOP	INAF USCVIII: CALCOLO CRITICO	CATANIA	15/06/2023-16/06/2023
SUMMER SCHOOL	SUMMER SCHOOL ON PARALLEL COMPUTING	BOLOGNA (CINECA)	03/07/2023-14/07/2023
CONFERENCE	EUCLID CONSORTIUM MEETING	COPENHAGEN	19/07/2023-23/07/2023
WORKSHOP	SPOKE 3 TECHNICAL MEETING	TRIESTE	09/09/2023-11/09/2023
CONFERENCE	UNIVERSUM 2024	ROMA	21/02/2024-23/02/2024
VISITING PERIOD	COSMIC VOIDS COLLABORATION	MONACO DI BAVIERA (LMU)	27/05/2024-27/08/2024
CONFERENCE	SPOKE3 GENERAL MEETING	ISOLA D'ELBA	05/06/2024-09/06/2024
CONFERENCE	EUCLID CONSORTIUM MEETING	ROMA	17/06/2024-21/06/2024
CONFERENCE	CLUSTER4	TRIESTE	10/09/2024-13/09/2024
WORKSHOP	HACKATHON (CSCS)	LUGANO	07/10/2024-11/10/2024
WORKSHOP	SPOKE3 TECHNICAL MEETING	BOLOGNA	17/12/2024-18/12/2024
CONFERENCE	EUCLID CONSORTIUM MEETING + ESLAB	LEIDEN	24/03/2025-28/03/2025
WORKSHOP	SPOKE3 TECHNICAL MEETING	PERUGIA	26/05/2025-29/05/2025
CONFERENCE	TRACING COSMIC EVOLUTION WITH GALAXY CLUSTER - V	SESTO PUSTERIA	07/07/2025-11/07/2025
SUMMER SCHOOL	ADVANCED SCHOOL ON PRECISION COSMOLOGY AND DARK MATTER	FIRENZE	25/08/2025-31/08/2025
ANNUAL MEETING	OU-MER (EUCLID) F2F MEETING	ROMA	20/10/2025-22/10/2025

ATTIVITÀ DI DIDATTICA E DI RICERCA / *TEACHING AND RESEARCH ACTIVITIES HELD BY THE PHD STUDENT*

TIPO / *TYPE*	TITOLO / *TITLE*
ATTIVITÀ TUTORIALI E DIDATTICO INTEGRATIVE SVOLTE / *TUTORING ACTIVITIES*	
SEMINARI TENUTI DAL DOTTORANDO / *SEMINARS HELD BY THE PHD STUDENT*	• INAF OATS POSTDOC/PHD SEMINARS CYCLE 12/04/2025: "ADVANCING FAST COSMOLOGICAL SIMULATIONS: RECENT DEVELOPMENTS IN THE PINOCCHIO CODE"
PUBBLICAZIONI SCIENTIFICHE / *SCIENTIFIC PUBLICATIONS* riferimenti bibliografici completi delle pubblicazioni presenti nel catalogo ArTS / *full bibliographic references of the publications submitted to the ArTS catalog*	• LEPINZAN ET AL. (2025)." TRACING COSMIC VOIDS WITH FAST SIMULATIONS". A & A, ACCEPTED FOR PUBLICATION (arXiv:2506.19506) • LEPINZAN ET AL. (2025)."ACCELERATING COSMOLOGICAL SIMULATIONS ON GPUS: A PORTABLE APPROACH USING OPENMP". A & C, SUBMITTED TO "VSI: HPC IN COSMOLOGY AND ASTROPHYSICS" SPECIAL ISSUE (arXiv:2510.02873) • LACOPO, LEPINZAN ET AL. (2025)."ACCELERATING COSMOLOGICAL SIMULATIONS ON GPUS: A STEP TOWARDS SUSTAINABILITY AND GREEN-AWARENESS" ". A & C, SUBMITTED TO "VSI: HPC IN COSMOLOGY AND ASTROPHYSICS" SPECIAL ISSUE"

	• Euclid Collaboration: P. Monaco, G. Parimbelli, M. Y. Elkhashab, J. Salvalaggio, T. Castro , M. D. Lepinzan et al. (2025) , "Euclid preparation. Simulating thousands of Euclid spectroscopic skies", A & A, accepted for publication (arXiv:2507.12116) • Euclid Collaboration: E. Romelli,....., M. D. Lepinzan et al. (2025) , "Euclid Quick Data Release (Q1): From images to multiwavelength catalogues: the Euclid MERge Processing Function", A & A, accepted for publication (arXiv:2503.15305)
PRESENTAZIONI A CONGRESSI, POSTER, ABSTRACT ETC / *PRESENTATIONS AT CONFERENCES, POSTERS, ABSTRACTS,* se pubblicato, riportare i riferimenti bibliografici / *if published provide full bibliographic references*	• Technical Meeting Spoke 3, October 9-11, 2023, Università degli studi di Trieste Piazzale Europa 1, https://indico.ict.inaf.it/event/2532/ • Spoke3 - Monthly WP1-2 Meeting, online, https://indico.ict.inaf.it/event/2744 • UniVersum, February 21-23, 2024, Sapienza Università di Roma, Piazzale Aldo Moro, 5, https://docs.google.com • Spoke3 General Meeting, May 05-09, 2024, Hotel Hermitage, Isola d'Elba, https://indico.ict.inaf.it/event/2752 • CLUSTER4, September 10-13, 2024, Università di Trieste, Trieste, https://sites.google.com/view/cluster4ts/ • Technical Meeting Spoke 3, December 17-19, 2024, Research Area of Bologna, Bologna, https://indico.ict.inaf.it/event/3001/ • Technical Meeting Spoke 3, May 26-29, 2025, Hotel Giò Jazz & Wine, Perugia, https://indico.ict.inaf.it/event/3173/ • Tracing Cosmic Evolution with galaxy Cluster - V, July 07-11, 2025, Sesto Pusteria, Contributed Poster https://www.sextenfora.eu/event/sestocluster2025/

Data compilazione /*Date*,
19/11/2025

Firma dottorando/*PhD student's signature*

Firma supervisore/*Supervisor's signature*

DOTTORANDO / *PHD STUDENT*	
COGNOME / *SURNAME* CAPPELLI	**NOME / *NAME*** LUCA
CORSO DI DOTTORATO / *PHD COURSE*	**CICLO / *CYCLE***
FISICA	XXXVIII
SUPERVISORE (COGNOME, NOME) / *SUPERVISOR (SURNAME, NAME)*	
STEFANO ORGANI	
CO-SUPERVISORE (EVENTUALE) (COGNOME, NOME) / CO-*SUPERVISOR IF APPLICABLE (SURNAME, NAME)*	
GIUSEPPE MURANTE	

BREVE RELAZIONE SULL'ATTIVITÀ DI RICERCA / *CONCISE PROGRESS REPORT (RESEARCH ACTIVITIES)*

(max 2500 caratteri, spazi esclusi/ *max 2500 characters excluding blanks*)

During my PhD, I focused on developing quantum algorithms to accelerate cosmological simulations of the dark-matter distribution. Building on my Master's thesis, I developed a variational algorithm for solving the Schrödinger–Poisson (SP) equation, and investigated the complexity and resource scaling; the result is published in Physical Review Research (Cappelli et al. (2024)). The algorithm works by splitting the problem into two parts: the solution of the Poisson equation and the time evolution. This work was built around the possibility that the SP equation can approximate the Vlasov–Poisson (VP) equation, governing dark-matter evolution [P. Mocz et al. (2018)], but only in the limit where the dynamical dispersion scale $\hbar$/m→0. In order to investigate when this correspondence holds and how the classical limit emerges I developed four numerical solvers entirely from scratch: one for SP, two for VP, and one VP N-body integrator. I discovered that VP integration for cold dark matter suffers from artificial viscosity effects, which can be resolved by using smoothed initial conditions and a spectral solver. These results were published and presented at PDP 2025 in Torino [Cappelli et al. (2025)]. With the newly developed VP solver I compare the results from VP–N-body and SP simulation in 1D and 2D. We found that the correspondence holds when the SP results are obtained at higher resolution and then smoothed onto a lower resolution. The codes are optimized to run in parallel and there is a paper in production about this topic.

I then focused on improving the quantum SP variational algorithm, identifying the intrinsic limitations of this approach. Specifically, I found that the matrix governing the time evolution part is ill-posed and the regularization process becomes particularly difficult when trying to scale up the problem. Subsequently, I explored a quantum algorithm based on linearizing SP through Carleman embedding [Carleman (1932)], but this method also showed fundamental constraints. I therefore turned to accelerating computationally intensive subroutines in classical dark-matter simulation codes. In particular, I developed a quantum neighbor-search algorithm using amplitude amplification, obtaining promising theoretical results that are not yet practically applicable due to current hardware and software limitations. This work is now under review for publication.

ATTIVITÀ FORMATIVE / *TRAINING ATTENDED BY THE PHD STUDENT*

TIPO / *TYPE* Corso/Seminario/Workshop/ Convegno/ Stage/Altro (specificare) – *Course/Seminar/ Workshop/Conference/Stage/Other (specify)*	**TITOLO / *TITLE***	**SEDE / *LOCATION***	***PERIODO (DAL AL)* / TIME PERIOD (FROM TO)**
COURSE	*Formation of cosmic structures*	TRIESTE	SPRING 2023
COURSE	*Introduction to parallel computing*	TRIESTE	SPRING 2023
COURSE	*Advanced quantum mechanics and selected applications to quantum*	TRIESTE	SPRING-SUMMER 2023
COURSE	*Cosmologia 2*	TRIESTE	FALL 2023
WINTER SCHOOL	WINTER SCHOOL ON QUANTUM MACHINE LEARNING	TRENTO	9-13 DECEMBER 2024
SUMMER SCHOOL	EQAI 2025	LIGNANO	1-5 SEPTEMBER 2025
WORKSHOP	GITLAB	TRIESTE	03/02/25; 06/02/25

ATTIVITÀ DI DIDATTICA E DI RICERCA / *TEACHING AND RESEARCH ACTIVITIES HELD BY THE PHD STUDENT*	
TIPO / *TYPE*	**TITOLO / *TITLE***
ATTIVITÀ TUTORIALI E DIDATTICO INTEGRATIVE SVOLTE / *TUTORING ACTIVITIES*	
SEMINARI TENUTI DAL DOTTORANDO / *SEMINARS HELD BY THE PHD STUDENT*	Seminar on "Quantum algorithms for Cosmological simulations" at LRZ Garching, 6 March 2024, presentation Seminar on "Quantum Variational algorithm for Schrodinger-Poisson" at Bologna, 18 October 2024. Seminar on "Searching for quantum algorithms for Cosmological simulations" at Osservatorio di Trieste, 09/07/2025

PUBBLICAZIONI SCIENTIFICHE / *SCIENTIFIC PUBLICATIONS* riferimenti bibliografici completi delle pubblicazioni presenti nel catalogo ArTS / *full bibliographic references of the publications submitted to the ArTS catalog*	ON ARTS CATALOG: AUTHOR = {CAPPELLI, L. AND TACCHINO, F. AND MURANTE, G. AND BORGANI, S. AND TAVERNELLI, I.}, TITLE = {FROM VLASOV-POISSON TO SCHRÖDINGER-POISSON: DARK MATTER SIMULATION WITH A QUANTUM VARIATIONAL TIME EVOLUTION ALGORITHM}, YEAR = {2024}, JOURNAL = {PHYSICAL REVIEW RESEARCH}, VOLUME = {6/2024},URL = {HTTPS://JOURNALS.APS.ORG/PRRESEARCH/ABSTRACT/10.1103/PHYSREVRESEARCH.6.013282}, DOI = {10.1103/PHYSREVRESEARCH.6.013282}, PUBLISHED, BUT NOT ON ARTS CATALOG: 1.Numerical limits in the integration of Vlasov-Poisson equation for Cold Dark Matter; Luca Cappelli, Giuseppe Murante, Stefano Borgani, Farida Farsian, Nicoló Parmiggiani, Alessandro Rizzo, Gabriele Panebianco, Andrea Bulgarelli, Francesco Schilliró, Carlo Burigana, Vincenzo Cardone, Massimo Meneghetti, Giuseppe Sarracino, Roberto Scaramella, Vincenzo Testa, Tiziana Trombetti;; 2025 33rd Euromicro International Conference on Parallel, Distributed, and Network-Based Processing (PDP), Turin, Italy, 2025, pp. 431-438, doi: 10.1109/PDP66500.2025.00067. published, but only contributed: 1. Benchmarking Quantum Convolutional Neural Networks for Signal Classification in Simulated Gamma-Ray Burst Detection; Farida Farsian, Nicoló Parmiggiani, Alessandro Rizzo, Gabriele Panebianco, Andrea Bulgarelli, Francesco Schilliró, Carlo Burigana, Vincenzo Cardone, Luca Cappelli, Massimo Meneghetti, Giuseppe Murante, Giuseppe Sarracino, Roberto Scaramella, Vincenzo Testa, Tiziana Trombetti; 2025 33rd Euromicro International Conference on Parallel, Distributed, and Network-Based Processing (PDP), Turin, Italy, 2025, pp. 372-380, doi: 10.1109/PDP66500.2025.00059. 2. The Application of Quantum Fourier Transform in Cosmic Microwave Background Data Analysis ; Farsian Farida, Trombetti Tiziana, Burigana Carlo, Schilliro Francesco, Bulgarelli, Andrea, Cardone Vincenzo, Cappelli Luca, Meneghetti Massimo, Murante Giuseppe, Rizzo Alessandro, Sarracino Giuseppe, Graziotti Irene, Scaramella Roberto, Testa Vincenzo; 2025 IEEE International Conference on Quantum Software (QSW), Helsinki, Finland, 2025, pp. 250-256, doi: 10.1109/QSW67625.2025.00037.

PRESENTAZIONI A CONGRESSI, POSTER, ABSTRACT ETC / ***PRESENTATIONS AT CONFERENCES, POSTERS,*** **ABSTRACTS,** se pubblicato, riportare i riferimenti bibliografici / *if published provide full bibliographic references*	1) INAF USCVIII meeting, 15-16 June 2023, Catania, contributed talk 2) Hydrosim Meeting, 17-21 July 2023,,Sexten, contributed talk 3) Quantum Computing and Simulation Workshop, 11-13 October 2023, Venice, poster 4) INAF SPOKE 10 Meeting, 21-22 November 2023, Bologna, presentation 5) INAF SPOKE 10 Meeting, 15-18 April 2024 Napoli, presentation 6) Workshop on Quantum Simulation for fluid dynamics and cosmology, 22-29 July 2024, IFPU, presentation 7) INAF SPOKE 10 Meeting, 11-15 November 2024, Bologna, presentation 8) Winter School on Quantum Machine Learning, 9-13 December 2024, Trento, poster 9) PDP conference, 11-15 March 2025, Turin, contributed talk: Presented the paper: L. Cappelli, G. Murante and S. Borgani, "Numerical limits in the integration of Vlasov-Poisson equation for Cold Dark Matter," 2025 33rd Euromicro International Conference on Parallel, Distributed, and Network-Based Processing (PDP), Turin, Italy, 2025, pp. 431-438, doi: 10.1109/PDP66500.2025.00067. 10) Hydrosim meeting 28-31 July 2025, Trieste (07/2025), contributed talk

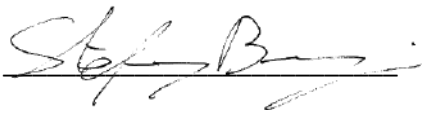
Data compilazione /*Date,*

21/11/2025

_____

Firma dottorando/*PhD student's signature*

Firma supervisore/*Supervisor's signature*



DOTTORANDO / *PHD STUDENT*	
COGNOME / *SURNAME* DIRINDIN	**NOME / *NAME*** MARCO
CORSO DI DOTTORATO / *PHD COURSE*	**CICLO / *CYCLE***
PHYSICS	XXXVIII
SUPERVISORE (COGNOME, NOME) / *SUPERVISOR (SURNAME, NAME)*	
COSLOVICH DANIELE	
CO-SUPERVISORE (EVENTUALE) (COGNOME, NOME) / CO-*SUPERVISOR IF APPLICABLE (SURNAME, NAME)*	
PERESSI MARIA	

BREVE RELAZIONE SULL'ATTIVITÀ DI RICERCA / *CONCISE PROGRESS REPORT (RESEARCH ACTIVITIES)*

(max 2500 caratteri, spazi esclusi/ *max 2500 characters excluding blanks*)

Over the last 20 years the study of low-dimensional systems has been extremely prolific, giving rise to new technological applications and new developments for fundamental research. In this context, two-dimensional network-forming oxides represent an intriguing and understudied class of materials, characterized by low-density network structures formed by covalent bonds. So far, only a couple of these systems have been synthesized, such as silica bilayers and boron-oxygen compounds. The physics of their three-dimensional equivalents is extremely rich and still debated, with an intricate interplay between polymorphism, diverse superstructural units and medium-range order. There are inherent difficulties in measuring the structure of these three-dimensional networks and this has significantly hindered our understanding of them. The synthesis of two-dimensional allotropes thus offers a unique opportunity to use standard surface techniques to examine their structure and dynamics, making these materials ideal benchmarks for testing and developing theories on network-forming glasses.

In this thesis, we use a combination of ab initio techniques, large-scale classical simulations and rigorous comparison with experiments to describe the structure of two-dimensional crystalline and amorphous oxides at different length scales. Using experimental data, we develop an effective classical potential for the silica bilayer, which is able to reproduce fine structural details of experimental samples. We use this potential to study the glassy behavior of the system at low temperatures and to assess the relationship between structure and dynamics. For a boria monolayer, we devise an algorithm to perform a systematic search for crystalline polymorphs, and we use it to predict from first principles the structure of a recently synthesized boron-oxygen crystal. Using ab initio techniques, we characterize the structure, electronic properties and substrate interactions of the synthesized system, achieving an excellent agreement with the experimental data. After characterizing the crystalline monolayer, we focus on the amorphous structure, developing an algorithm to recover the atomic positions from the experimental images. This allows us to provide a first characterization of this new glassy system.

Our results highlight the connection between atomic local environment and network topology, and suggest a strong similarity between different two-dimensional network-forming oxides. We also identify peculiar behaviors in these two-dimensional systems, such as the presence of large transient crystalline domains in the thermodynamically stable low-temperature liquid, which may point to a profound difference between glassy structure in two- and three-dimensions.

ATTIVITÀ FORMATIVE / *TRAINING ATTENDED BY THE PHD STUDENT*

TIPO / *TYPE* Corso/Seminario/Workshop/ Convegno/Stage/Altro (specificare) –	**TITOLO / *TITLE***	**SEDE / *LOCATION***	***PERIODO (DAL AL)* / TIME PERIOD (FROM TO)**

Course/Seminar/Workshop/Conference/Stage/ Other (specify)			
Course	Modern tools for computational physics	Department of Physics University of Trieste	From April 2022 to May 2022
Course	Introduction to parallel computing	Department of Physics University of Trieste	From March 2022 to April 2022
Course	Introduction to density functional theory	Department of Physics University of Trieste	From October 2023 to November 2023
Course	Neural networks	SISSA	From March 2025 to April 2025

ATTIVITÀ DI DIDATTICA E DI RICERCA / *TEACHING AND RESEARCH ACTIVITIES HELD BY THE PHD STUDENT*	
TIPO / *TYPE*	**TITOLO / *TITLE***
ATTIVITÀ TUTORIALI E DIDATTICO INTEGRATIVE SVOLTE / *TUTORING ACTIVITIES*	
SEMINARI TENUTI DAL DOTTORANDO / *SEMINARS HELD BY THE PHD STUDENT*	• *Are glasses different in Flatland? Insights from a model of 2d amorphous silica*, Miramare Campus, Department of Physics (Trieste, Italy), January 29, 2025
PUBBLICAZIONI SCIENTIFICHE / *SCIENTIFIC PUBLICATIONS* riferimenti bibliografici completi delle pubblicazioni presenti nel catalogo ArTS / *full bibliographic references of the publications submitted to the ArTS catalog*	• T. Zio, M. Dirindin, C. Di Giorgio, M. Thaler, B. Achatz, C. Cepek, I. Cojocariu, M, Jugovac, T. O. Mente¸s, A. Locatelli, L. L. Patera, A. Sala, G. Comelli, M. Peressi, C. Africh, *Two-dimensional diboron trioxide crystal composed by boroxol groups*, Science, 390(6768), 95-99 (2025) (DOI: https://doi.org/10.1126/science.adv2582) • M. Dirindin, D. Coslovich, *Glassy dynamics and local crystalline order in two-dimensional amorphous silica*, J. Phys. Chem. B, 129, 3, 1095–1108 (2025) (DOI: https://doi.org/10.1021/acs.jpcb.4c06881) • L. Figurato, M. Dirindin, J. L. Gaona-Reyes, M. Carlesso, A. Bassi, S. Donadi, *On the effectiveness of the collapse in the Diosi–Penrose model*, New Journal of Physics, 26(11), 113004 (2024) (DOI: https://doi.org/10.1088/1367-2630/ad8c77)
PRESENTAZIONI A CONGRESSI, POSTER, ABSTRACT ETC / *PRESENTATIONS AT CONFERENCES, POSTERS,* ABSTRACTS, se pubblicato, riportare i riferimenti bibliografici / *if published provide full bibliographic references*	**CONTRIBUTED TALK:** • *Glassy dynamics and local crystalline order in two-dimensional amorphous silica*, NOMATEN Centre of Excellence, (Warsaw, Poland), September 19, 2025 • *From single bond to line defects: a case study from a novel two-dimensional network-forming material*, E-MRS 2025 Fall Meeting, University of Technology in Warsaw (Poland), September 18, 2025. The talk received the award for the best PhD student presentation. • *Glassy dynamics and local crystalline order in two-dimensional amorphous silica*, 10th International Discussion Meeting on Relaxations in Complex Systems (10 IDMRCS), (Barcellona, Spain), July 24, 2025 • *From single bond to line defects: a case study from a novel two-dimensional network-forming material*, Young Reseachers' Meeting of the European Theoretical Spectroscopy Facility (ETSF YRM 2025), SISSA (Trieste, Italy), May 26, 2025

	POSTERS: • *Exploring two-dimensional crystalline phases of boron oxide on Pt(111),* 22nd International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Internation Center for Theoretical Physics (Trieste, Italy), January 08-10, 2025 • *Structure and dynamics of two-dimensional network-forming materials*, Liquid Matter Conference 2024, Mainz (Germany), September 22-27, 2024 • *Structure and dynamics of two-dimensional network-forming materials*, Course Topology and Materials at the International School of Physics "Enrico Fermi", Varenna (Italy), July 17-22, 2024 • *Exploring a stochastic cost function landscape: the case of 2d amorphous silica*, Deep Modeling for Molecular Simulation 2023 school, Princeton University (United States of America), July 11-14, 2023

Data compilazione /*Date,*

20/11/2025

Firma dottorando/*PhD student's signature*

Firma supervisore/*Supervisor's signature*