From Fuzzy Spacetime to Classical Reality

Laria Figurato: Ph.D. in Physics, cycle XXXVIII

Summary

This thesis investigates the interplay between quantum mechanics and gravity at the non-relativistic level, focusing on how gravitational effects may influence quantum state reduction and decoherence. The work proceeds along two directions: gravitational decoherence (Károlyházy model) and gravity-induced collapse (Diósi–Penrose model), representing two distinct pathways through which classicality might emerge from quantum theory.

On the decoherence side, we developed a generalized stochastic model of spacetime fluctuations that refines Károlyházy's original idea of metric-induced decoherence. The model overcomes inconsistencies in earlier formulations, aligns with current experimental bounds, and quantifies how stochastic gravitational potentials degrade quantum coherence without invoking wave-function collapse. By introducing generalized correlation functions, it restores consistency with known experimental bounds, narrows the viable parameter space, and identifies the conditions under which gravitational decoherence may become experimentally accessible.

On the collapse side, we analyzed the Diósi–Penrose (DP) model, which links spontaneous wave-function localization to gravitational self-energy. Using analytic and numerical methods, we derived theoretical upper bounds on the model's parameters by requiring that the collapse effectively suppress macroscopic superpositions. We 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.

More broadly, the thesis addresses one of modern physics' central challenges: reconciling quantum theory, which governs the microscopic world, with general relativity, which describes spacetime and gravitation. Collapse and decoherence models provide promising frameworks to study this interface. The DP model introduces genuinely non-unitary dynamics, offering an experimentally testable link between quantum mechanics and gravity, while the Károlyházy approach preserves unitarity but attributes decoherence to stochastic spacetime fluctuations.

Together, our results provide tighter theoretical constraints on gravitationally induced quantum effects and delineate experimentally relevant regimes. The combined results clarify under which conditions gravity could account for the quantum-to-classical transition and guide the design of future precision experiments probing the quantum–gravitational boundary.

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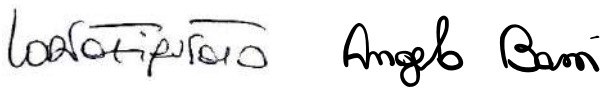

UNIVERSITÀ DEGLI STUDI DI TRIESTE
XXXVIII CICLO DEL DOTTORATO DI RICERCA IN FISICA

THESIS TITLE:

On the Classical and Quantum Aspects of Memory Effects in Open Dynamical Systems

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Thesis abstract

The richness of quantum mechanics often emerges in the attempt to extend well-established and useful notions from classical physics to the non-commutative context, where one finds not a single, but rather a multiplicity of non-equivalent possibilities. In the effort to characterize the physics of memory effects, this becomes particularly evident: indeed, to the well-defined notion of Markovianity in classical stochastic processes, there corresponds a whole hierarchy of concepts in the quantum regime (see [1–4] for comprehensive and up-to-date reviews). Over the years, indeed, many different approaches to quantum Markovian behaviour have been proposed in the context of open quantum systems, namely systems that cannot be isolated from their surrounding environments.

If the coupling with the environment is weak, a standard procedure is to rigorously perform systematic approximations in order to obtain the reduced dynamics of the system, described by a semigroup of completely positive and trace-preserving maps [5]. This kind of evolution is fully characterized from a mathematical point of view through the celebrated result of Gorini, Kossakowski, Sudarshan [6] and Lindblad [7]. Notably, the weak-coupling regime constrains not only the reduced dynamics of the system, but also the multi-time statistics of the full quantum stochastic process [8–10].

On the other hand, the dynamics of open systems that are strongly coupled to their environments is generally affected by memory effects. Different notions along the hierarchy may then be useful to characterize them, and the most appropriate one could well be context-dependent. It is though essential to clarify and deepen the understanding of the different aspects of non-Markovian behaviour, as well as the sources of discrepancy with respect to the classical regime.

This thesis revolves around three main projects, a central theme in all of them being the interplay between the classical and quantum aspects of information flows between a system and its environment. When one focuses on the reduced evolution of an open system—whether classical or quantum—non-Markovian behavior can be recognized through revivals of distances or divergences, which are typically interpreted as a backflow of information previously stored in the environment during earlier stages of the evolution [11]. It should be also noted that this interpretation is still actively debated and, therefore, should be considered with some care.

The first Chapter of the thesis is devoted to review the necessary mathematical tools for the subsequent developments and to introduce a common-ground notation in order to treat quantum and stochastic processes on the same footing. This can be achieved by exploiting the algebraic approach to quantum mechanics [12].

In Chapter 2, the quantum-classical interplay will be investigated by reducing a Markovian quantum evolution to a fixed Abelian subalgebra. The output of this procedure, which has a clear operational

interpretation, is generally a non-Markovian classical dynamics. As we shall see, backflows of information in these reduced evolutions are assisted by quantum coherences, that effectively act as an environment for the reference classical subalgebra.

Conversely, one can observe memory effects with no classical counterpart, even though they may be assisted by a classical environment. This is the case of the so-called superactivation of backflow of information (SBFI), which occurs in bipartite systems whose subsystems individually exhibit no information revivals. In Chapter 3, we shall discuss this intriguing phenomenon both from the abstract perspective of the quantum dynamical map and from the physical perspective of a concrete model. Interestingly, this purely quantum effect can be assisted by a classical memory, such as a classical Markov chain collisional environment, whereby it is triggered by sufficiently strong correlations between first-neighboring spins. The collisional approach to open quantum systems is reformulated through the algebraic approach typical of many-body physics. This treatment, on the one hand, facilitates the investigation of the SBFI phenomenon through the evaluation of system–environment correlations. Moreover, it provides the appropriate language to broaden the perspective of the reduced dynamics to include the study of the multi-time statistics of the process.

In fact, generally speaking, it is not possible to fully appreciate the physical mechanisms governing memory effects directly from the reduced dynamics, as the latter yields only the one-time marginal of the underlying full quantum stochastic process. A possible way out of this problem is finally presented in Chapter 4, by discussing a substantially refined notion of Markovianity when multi-time correlations are taken into account. This is achieved through the extraction of a quantum symbolic dynamics out of the open dynamical system as proposed by Alicki and Fannes [13, 14], basing on some earlier pioneering work by Lindblad [15]. This approach naturally drives towards a quantum version of the so-called dynamical entropy, that generalizes the entropy of Kolmogorov and Sinai to the non-commutative setting. This quantity describes the asymptotic rate of information extracted by repeated measurement on the dynamical systems. In such a context, it offers a way to study non-Markovianity and backflow of information by including the information contained in the multi-time correlation functions. Some exact results, mainly obtained through simple collisional models, are further discussed within the state-purification scheme provided by the so-called GNS construction: in this context, an interesting connection to the SBFI effect appears.

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List of publications

1. F. Benatti and G. Nichele. "Open Quantum Dynamics: Memory Effects and Superactivation of Backflow of Information". *Mathematics* 12.1 (2024). DOI: 10.3390/math12010037

2. F. Benatti, D. Chruściński, and G. Nichele. "Quantum versus classical P-divisibility". *Physical Review A* 110.5 (2024), p. 052212. DOI: 10.1103/PhysRevA.110.052212

3. F. Benatti and G. Nichele. "Superactivation of memory effects in a classical Markov environment". *Physica Scripta* 100.6 (2025), p. 065115. DOI: 10.1088/1402-4896/add57e

4. G. Nichele and F. Benatti. "Entropic Superactivation of Backflow of Information". *Quantum Economics and Finance* 2.2 (2025). DOI: 10.1177/29767032251361881

5. G. Nichele and F. Benatti. "Quantum Dynamical Entropy and non-Markovianity: a collisional model perspective". *In preparation.* (2025)

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[20] G. Nichele and F. Benatti. "Quantum Dynamical Entropy and non-Markovianity: a collisional model perspective". *In preparation.* (2025).

Title: Geophysical applications of quantum gravimeters

Summary:

Quantum gravimeters represent a new generation of instruments for measuring the local gravitational acceleration with high precision and long-term stability. Building upon the principles of atom interferometry, these devices exploit the quantum nature of matter waves to achieve in absolute gravity measurement sensitivities better than classical gravimeters based on mechanical or optical techniques.

This Thesis provides a concise overview of gravimetry and its relevance to geophysical studies, followed by an analysis of the sensitivity estimates of current quantum gravimeters. The discussion includes the effect of noise and investigation of strategies for optimizing gravimeter performance. Finally, several geophysical applications are presented. The results show the potential of quantum gravimetry to complement traditional geophysical surveys and to open new perspectives for high-resolution gravity mapping and monitoring.

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Structure and reactivity of biomimetic iron-centered 2D materials from ultra-high vacuum to near-ambient pressure.

The aim of this work was to investigate novel 2D materials based on metalorganic architectures, inspired by strategies already adopted by nature for processes such as light harvesting, chemical conversion and synthesis.[1] These systems provide a versatile platform for stabilizing single metal atoms at surfaces, with properties that can be tuned through by exploiting surface trans-effect, interaction with axial ligands, lateral coordination and peripheral residues.[2]

Specifically, we focused on iron-centered 2D materials, namely FeTPyP and hemin, deposited on weakly interacting supporting substrates such as Gr/Ir(111) and Au(111), respectively. The structural and electronic properties of the monolayers were characterized under Ultra High Vacuum (UHV) and near-ambient pressure (NAP) conditions. Subsequently, single Co adatoms were added to both systems to probe the structural and electronic response to coordination, specifically investigating their role in the reactivity toward CO and O_2.

Starting from the FeTPyP system, Scanning Tunneling Microscopy (STM) measurements revealed that the molecules self-assemble on Gr/Ir(111) into a close-packed structure, driven by intermolecular interactions between the electronegative N atoms of the pyridyl end groups and the peripheral H atoms from the neighbouring pyrrole moieties. X-ray Photoelectron Spectroscopy (XPS) shows that the Fe centers are in the +2 oxidation state.

Upon Co deposition, the latter single atoms coordinate to the pyridinic terminations, altering the lateral coupling and yielding a network with specific, density-dependent geometrical and electronic properties. While Co at the pyridinic sites is found in the +1 oxidation state, as already observed in analagous systems,[3,4] this work represents the first instance in which the metal embedded within the macrocycle is reduced upon Co coordination, forming Fe(I), a species highly reactive towards O_2.

Under NAP conditions, the monometallic layer remains inert toward O_2 and CO, whereas the bimetallic network is reactive, with both metal sites participating in the reactions. Upon O_2 exposure, Infrared-Visible Sum Frequency Generation (IR-Vis SFG) and NAP-XPS measurements reveal clear evidence of O_2 ligation and activation, highlighting potential applicative approaches. For CO exposure, IR-Vis SFG spectroscopy was employed to investigate the cooperativity and adsorption energy, at the nanometer scale for both Co- and Fe-sites as a function of Co loading. Increasing Co loading induces a stronger anti-cooperative trend among Co sites. In contrast, Fe sites exhibit a non-cooperative behavior for the low and high Co loadings, and an anti-cooperative trend at intermediate coverage. Regarding the adsorption energy, CO preferentially binds to Fe sites up to a Co loading threshold, beyond which this tendency reverses.

NAP-XPS measurements combined with Density Functional Theory (DFT) calculations enabled the determination 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 O_2, Fe is predominantly observed experimentally in the +2 oxidation state. Exposure to O_2 further oxidizes Co to +2 and Fe to +3, in excellent agreement with theoretical predictions. In contrast, under CO exposure, the residual background stabilizes Co and Fe centers in the +2 and +3 oxidation states, respectively, making a comparison with the ab initio calculations not straightforward.

To further explore the influence of molecular environment and peripheral groups on metal reactivity, a larger molecule, specifically hemin, the core component of hemoglobin, was deposited on Au(111). The resulting layer consists of a mixture of Fe-free and Fe-filled molecules due to the limited purity of the biological precursor. STM measurements and Near Edge X-ray Absorption Fine Structure (NEXAFS) analysis, reveal the presence of intact, flat-lying molecules on the surface, with the carboxylic terminations appearing as bright protrusions in the STM images when they bend out of the molecular plane.

Several molecular configurations are observed, with some carboxylic groups positioned close to the macrocycle of adjacent molecules.
Depending on the molecular arrangement, hydrogen-bond interactions can form either between the carboxylic groups of neighboring molecules or between a carboxylic termination and the iminic nitrogen atom. XPS analysis shows that the Fe centers are predominantly in the +2 oxidation state.
The reactivity of the layer was then tested toward CO and O_2 exposure, revealing distinct behavior. In the case of CO, no clear evidence of direct interaction with the hemin layer is observed at room temperature up to 0.3 *mbar* of CO, indicating that the system is close-to inert toward this gas. In contrast, O_2 stabilization occurs at 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 O_2 and stabilizing the Fe-O_2 interaction, thereby effectively reproducing the second coordination sphere observed in biological systems.[5–7]
To create a bimetallic system and fill the vacant centers, Co atoms were deposited after the formation of the hemin layer. However, Co atoms preferentially interact with the metalated hemin molecules, undergoing trans-metalation, resulting in a mixed system composed of Fe-free, Fe-filled and Co-filled species, along with an intermediate configuration in which both Co and Fe are simultaneously present within the molecular macrocycle. Upon O_2 exposure, oxygen activation occurs, due to the coexistence of Fe and Co clusters on the substrate, leading to the formation of atomic oxygen species that diffuse across the surface, where several processes, including further trans-metalation, take place.

Additional Information:

All the XPS and NEXAFS measurements were performed at the MAX IV Laboratory during several experimental campaigns at the HIPPIE and FlexPES beamlines.
STM images of the FeTPyP and FeTPyP-Co systems were acquired in collaboration with the staff of the STM laboratory of MAX IV (Dr. Nikolay Vinogradov and Dr. Eleanor Frampton), whereas STM images of the hemin and hemin+Co systems were obtained at the STM Laboratory of the Graz University (Austria) in collaboration with Dr. Maximilian Laßhofer, Prof. Martin Sterrer and Prof. Giovanni Zamborlini.

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Summary of the Thesis

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November 13, 2025

Massive black holes (MBHs, $M_{\rm BH} > 10^6\ M_\odot$), residing at the centers of massive galaxies, play a fundamental role in shaping the evolution of cosmic structures. Through a complex interplay of accretion and feedback processes, they contribute to the regulation of thermal and dynamical state of their gaseous surroundings. A small fraction of these MBHs shines as luminous active galactic nuclei (AGN), with bolometric luminosities in the range $L \sim 10^{44} - 10^{46}$ erg s^{-1}. Their signatures can eventually span the entire electromagnetic spectrum and their impact extends from sub-parsec scales—where accretion takes place—to hundreds of kiloparsecs, with the injection of collimated radio jets and inflating X-ray cavities. The well-established scaling relations linking MBH masses to the global properties of their host galaxies suggest that every MBH has likely experienced an active phase in its past, intimately coupling its growth to that of its host. Understanding the evolution of MBHs is therefore essential to unveil the physical mechanisms driving galaxy evolution. Galaxy groups and clusters, located at the nodes of the cosmic web, offer an ideal laboratory to investigate the influence of MBHs on large scales. In these extreme environments, AGN feedback profoundly affects the thermodynamics of the intracluster medium, suppressing excessive cooling and regulating star formation within massive galaxies.
In this context, the dynamical evolution of MBHs is of paramount importance. The location of a MBH within its host galaxy directly influences its accretion rate, thereby regulating the ensuing feedback processes. Moreover, the increasing resolution of multi-wavelength observations has revealed compelling evidence of close, interacting MBH systems, while the advent of gravitational-wave astronomy and multi-messenger astrophysics has opened a new observational window on MBH mergers, calling for deeper theoretical and numerical insight.

Cosmological hydrodynamical simulations tackle this challenge by following the highly nonlinear processes that govern the formation and evolution of cosmic structures. However, the need to model large and diverse environments to gain reliable statistical insights often comes at the cost of limited spatial and mass resolution. In particular, the dynamics of MBHs is typically unresolved, requiring the adoption of sub-resolution models to describe their evolution. This Thesis explores the dynamics of MBHs across a range of simulated environments — from large cosmological volumes to galaxy clusters from the DIANOGA suite - and idealized setups designed for controlled comparisons between analytical expectations and numerical modeling. All simulations presented in this Thesis are carried out with the OpenGADGET3 code, which combines a Tree–Particle-Mesh algorithm for gravitational forces with a Smoothed Particle Hydrodynamics scheme for the gas component. The code features several sub-resolution prescriptions describing star formation, stellar evolution, metal enrichment, radiative cooling, MBH accretion, and AGN feedback. A key contribution of this work is the introduction of a novel model to account for unresolved dynamical friction (DF) in OpenGADGET3, derived from the first-order Fokker–Planck approximation. This model enables a more accurate treatment of the orbital decay of MBHs and their interactions with the surrounding medium within complex environments.

In the first part of the Thesis, a novel prescription for unresolved DF has been developed and implemented in the OpenGADGET3 code. This model has been tested against two widely used ad-hoc numerical prescriptions: the repositioning method, which relocates the BH particle to the position of the most bound nearby particle, and the boosted dynamical mass approach, which artificially increases the BH mass to enhance the resolved DF. A series of simulations — including a cosmological box, a group-sized halo, and a cluster-sized halo — have been performed with the OpenGADGET3 code, maintaining identical settings for all other sub-resolution prescriptions while varying only the BH dynamical tracking method. The DF correction shows encouraging performances, matching the efficiency of the repositioning and boosted-mass methods to center the BHs within their hosts. However, the

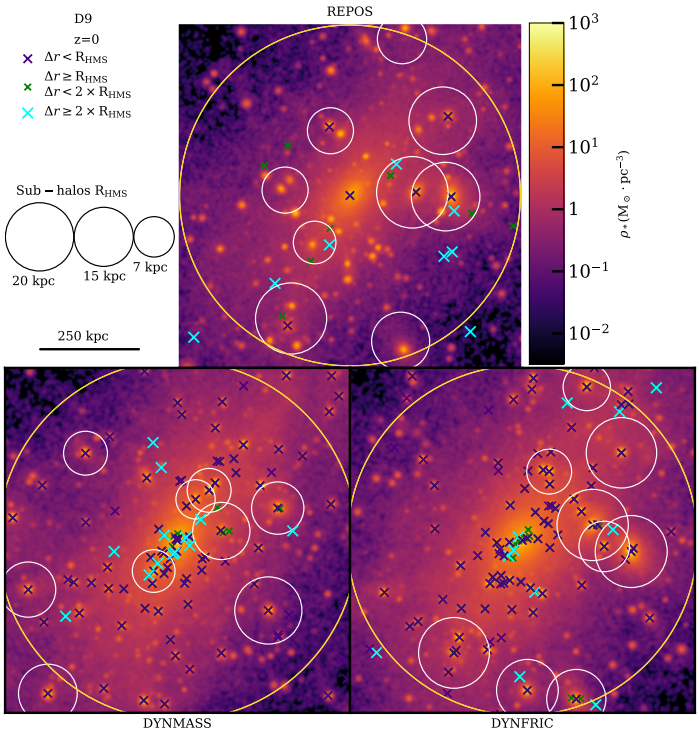

Figure 1: Demography of MBHs within the virial radius of the simulated cluster using repositioning (upper panel), dynamical mass (bottom left panel), and dynamical friction (bottom right panel). BHs are identified as crosses, with different colours according to the distance to their closest sub-halo, as indicated in the colormap.

limitations of the latter approaches become evident: the repositioning method tends to produce an excess of spurious off-centered BHs and merger events, while the boosted-mass approach often fails to reproduce timing of BH mergers. Figure 1 shows the population of MBHs located within the virial radius of the simulated cluster. In the simulation adopting the repositioning technique (upper panel), a lower occupancy of BHs within subhalos is observed, accompanied by a comparatively larger population of wandering BHs that have been displaced from their host galaxies. This analysis is part of the work published in [2].

Building on these results, the second part of the Thesis focuses on further tests within a controlled environment, where the DF performances can be reliably compared with analytical solutions. Different realizations of a dark matter only Navarro–Frenk–White halo sampled at different resolutions are evolved with a BH initially placed in the halo outskirts (at 20 kpc from the center) on a circular orbit. The BH sinking timescales and trajectories are analyzed in simulations with and without the DF correction, and compared to analytical solutions obtained with the newly developed OTIS library — a public tool designed to integrate the equations of motion of a BH embedded in a DM halo (optionally including a stellar bulge). The inclusion of the DF correction yields sinking timescales that converge well with increasing resolution and show good agreement with analytical predictions, in contrast to simulations without the correction. Figure 2 shows the orbital evolution for different halo resolutions (increasing from left to right) with (bottom row) and without (top row) the DF correction. For the two lowest resolution simulations, the DF correction is able to deliver the BH toward the halo center. A dedicated study of the challenging regime where the BH mass is smaller than that of surrounding particles further demonstrates that refining the DF formulation can increase control on BH dynamics even in this limit. The addition of a stellar bulge introduces further complexity, as two-body interactions from this component tend to heat and delay the BH orbit. Although the DF correction mitigates this effect, it still produces slightly higher initial eccentricities compared to the analytical model. A detailed discussion of this study is presented in [1] and accepted for the publication by Astronomy & Computing.

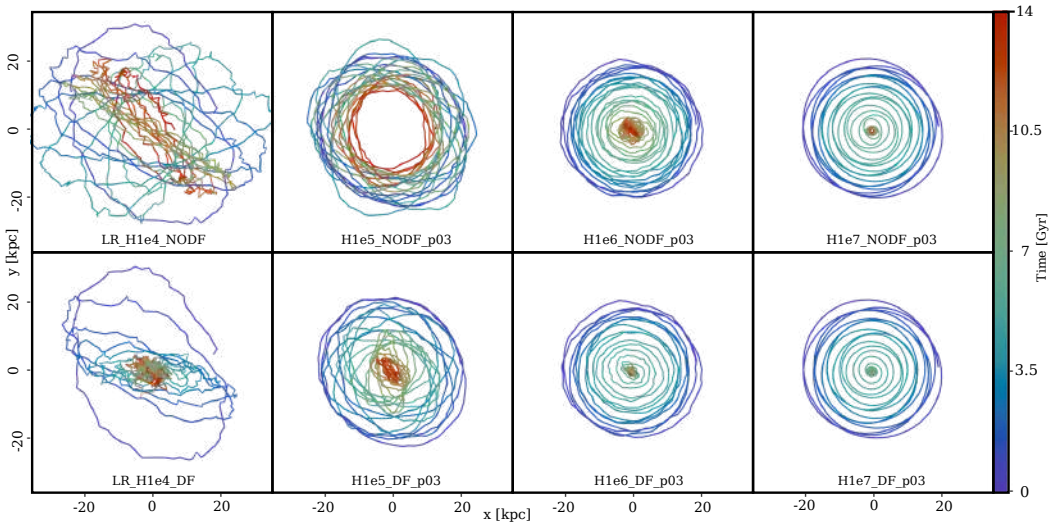

Figure 2: Orbits of a BH initially placed at 20 kiloparsecs with circular velocity in a dark matter Navarro-Frank-White halo. The halo is sampled with an increasing number of particles from left to right, from 10^4 to 10^7 particles. Bottom and top rows are showing simulation with and withouh the DF correction. Orbits are color coded with time as shown in the side colormap legend.

The third part of the Thesis explores some numerical methodologies and sub-resolution prescriptions regulating MBH feeding and feedback in OpenGADGET3. Particular attention is paid to the interplay among subtle, often overlooked, numerical techniques and to quantifying their mutual impact. Four key aspects are investigated: the role of stochastic, discrete swallowing of gas particles during BH accretion; the implementation of a cold-cloud evaporation mechanism; alternative kernel-weighting schemes for feedback energy in the low-accretion (radio) mode and the coupling between AGN-driven feedback and supernova-induced galactic winds. Starting from a fiducial configuration, a group-sized halo is re-simulated multiple times, varying one sub-resolution prescriptions at a time. The results demonstrate the high sensitivity of the intragroup medium thermodynamics to the adopted prescriptions. Even small changes in the numerical implementation can lead to significant differences in AGN activity and gas cooling histories. Within the OpenGADGET3 framework, accretion and feedback from cold gas are shown to play a dominant role, enabling episodes of significant cold accretion even at low redshift. The insights gained from these analyses have led to the development of a refined simulation setup that serves as the reference for the new-generation DIANOGA high-resolution campaign, aimed at exploring the most extreme cluster environments. In these systems, the differences between numerical implementations become even more pronounced, emphasizing the need for accurate and physically motivated models. This third study has been recently submitted to Astronomy & Computing.

In conclusion, this Thesis introduces advancements both in the physical modeling of DF and the numerical handling of accretion and feedback in cosmological simulations. The newly developed DF correction improves the physical realism of BH orbital evolution, while the systematic exploration of sub-resolution numerical techniques provides a foundation for future developments — including the coupling with new accretion models, the implementation of kinetic AGN feedback, the exploration of high-redshift environments, and the incorporation of BH spin evolution. Together, these efforts pave the way toward a more predictive framework for tracing the co-evolution of MBHs and their host galaxies across cosmic times.

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Advancing Cosmological Simulations with GPU-Enabled PINOCCHIO: From Dark Matter Halos to Cosmic Voids

Marius Daniel Lepinzan: Ph.D. in Physics, cycle XXXVIII

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1 PINOCCHIO

PINOCCHIO (PINpointing Orbit Crossing-Collapsed HIerarchical Objects) is a Lagrangian Perturbation Theory (LPT) code designed to rapidly simulate the formation and evolution of dark matter halos, starting from an initial density contrast field. The code bridges two key paradigms in structure formation theory: the Extended Press-Schechter approach, and its generalization to a more realistic ellipsoidal collapse model. These models describe the hierarchical buildup of dark matter halos as overdensities of the primordial density field evolving and collapsing under gravity. By leveraging this approximate yet accurate formulation, together with a highly parallelized structure for most of its components, PINOCCHIO offers a computationally efficient alternative to full N-body simulations. With a good degree of accuracy in reproducing overdensity summary statistics, such as the halo mass function (HMF), halo bias, and 2-point statistics, and a computational cost more than 1.000 timess lower, PINOCCHIO offers a highly efficient alternative for generating many realizations of the Universe, making it especially suitable for robust statistical analyses such as covariance matrices estimation and calibration.

In this PhD thesis, we focus on PINOCCHIO from two complementary perspectives: (i) a technical one, aimed at transitioning the code towards a fully GPU-accelerated workflow where possible, and (ii) a scientific one, exploring a novel application of PINOCCHIO to the study of cosmic voids.

1.1 Code structure

The calculation begins by generating a linear density contrast field as a realization of a Gaussian random process, which is then smoothed over a hierarchy of decreasing radii R.

The collapse times for each grid point is computed using ellipsoidal evolution, approximated through third-order LPT (3LPT). Since LPT accurately describes the dynamics up to orbit crossing (OC) events, it provides a reliable estimate for the moment when an ellipsoid collapses along its shortest axis. At this stage, the particle (or equivalently the grid point, is considered to have entered a multi-stream regime, becoming part of a dark matter halo or the filamentary network connecting halos.

Collapsed particles are grouped into halos and filaments using a algorithm named FRAGMENTATION, which mimics the hierarchical processes of accretion and merging to construct halo merger trees. The accretion of particles onto a halo, as well as the merging of two halos, is determined by comparing their predicted Eulerian positions, computed via LPT displacements, and applying a distance criterion: accretion or merging occurs when their separation falls below a threshold, which depends on the Lagrangian radius of the larger object.

Collapse times and LPT displacements are obtained efficiently in Fourier space using Fast Fourier Transforms (FFTs), since spatial derivatives become simple multiplications by the wavenumber components.

2 Rationale for GPU porting

The growing scale of simulations in computational cosmology demands increasingly efficient execution to align with the pace of advancements in scientific discovery. As High Performance Computing (HPC) platforms continue to evolve, leveraging their full potential, especially through the acceleration capabilities of Graphics Processing Units (GPUs), has become mandatory. Large simulations require hundreds of thousands core/node hours, forcing HPC facilities to operate at full capacity for extended periods. Sustaining such workloads for such amount of times leads to unsustainable energy costs, especially in an age of environmental awareness. For this reason in the last decades "green awareness" has become increasingly important, and nowadays pure performance is not enough to establish the efficiency of a scientific code. In particular, hardware and software development must advance at the same pace, and co-design is required to guarantee that scientific codes runs efficiently on modern HPC facilities.

2.1 Methodology: Porting strategy and energy measurements

The GPU porting effort began from the legacy version of the code[1], which is designed exclusively for multi-core CPU architectures, using a hybrid MPI/OpenMP approach.

Although the collapse-times calculation represents only a modest fraction of the total runtimes, it was chosen as the first target for GPU acceleration. Thanks to the modular structure of PINOCCHIO, computational kernels can be ported incrementally, and the collapse times computation, based on local operations on the Hessian of the gravitational potential described in Section 1, is an ideal first candidate, being an embarrassingly parallel problem.

To enhance both performance and portability, we offload this specific segment of the code to GPUs using OpenMP target directives. Since the original CPU-based implementation relies on the GNU Scientific Library (GSL) for interpolation routines, which does not support GPU offloading, we developed custom GPU-native interpolation (cubic spline and bilinear) routines to enable full device execution. This approach enables GPU acceleration ensuring portability across architectures, including NVIDIA and AMD platforms, and long-term maintainability.

Building on the porting effort, we evaluated also the energy impact of this GPU porting by measuring and comparing the energy consumption of CPUs and GPUs. For this purpose, we integrate the Power Measurement Toolkit (PMT), a high-level library to monitor power consumption between CPUs and GPUs, allowing us to assess the energy efficiency of the optimized code.

In parallel with the collapse times porting effort, the FFT operations required for computing the both the displacement source term and the Hessian were also ported to GPUs using the heFFTe[2] library.

2.2 Results: Porting and energy measurements

2.2.1 Collapse times calculation

Through comparative benchmarking on three major supercomputing platforms, LEONARDO (NVIDIA-based), KAROLINA (NVIDIA-based) and SETONIX (AMD-based), we demonstrate both the portability and significant performance gains of our approach. We achieve speedup factors of at least 4× on NVIDIA-LEONARDO (2× on NVIDIA-KAROLINA) and up to 8× on the AMD-based platform.

In addition, GPU offloading results in up to a 2× reduction in energy consumption, leading to an overall efficiency improvement of up to 4× on the NVIDIA-KAROLINA platform, and about an 8× reduction in energy consumption on the AMD system, corresponding to an overall efficiency improvement of 64×. On NVIDIA-LEONARDO, we did not have access to hardware-level counters required to measure energy consumption on both the CPU and GPU, hence the use of KAROLINA for these measurements. For both speedup and energy reduction, the AMD system benefits from superior architectural features.

In a simulation setup of full production, representative of typical large-scale simulation campaigns, the GPU-accelerated version of the collapse times led to a net reduction of approximately 100 seconds per run. When extrapolated to thousands of simulations (as required for robust covariance estimates), this would result in a saving of over 160000 Standard-h, representing a substantial gain in computational efficiency and resource optimization. To further validate the scientific consistency of our GPU-accelerated implementation, we compare the halo mass function (HMFs) obtained from both the CPU and GPU versions of PINOCCHIO in a full production run scenario. The agreement between the two implementations is remarkably good, with relative differences well below the 1% level across the entire mass range.

2.2.2 FFT

Benchmarking on NVIDIA-LEONARDO yields speedup factors of at least 28×. In a full production simulation setup, the GPU-accelerated version of the FFT calculation led to a net reduction of approximately 370 seconds per run. When extrapolated to thousands of simulations, this would correspond to a saving of over 590000 Standard-h.

3 Rationale for Cosmic Voids

Cosmic voids, vast underdense regions in the large-scale structure of the Universe, occupy the majority of its volume. They are promising cosmological probes that offer complementary and improved constraints on cosmological models, and their capacity to inform cosmological constraints will continue to grow in this era of large-scale surveys . Their underdense nature not only makes them less affected by non-linear gravitational dynamics, providing a unique window into the growth of structures and the properties of the Universe's expansion, but also provides unique sensitivity to the underlying cosmological model.

[1] https://github.com/pigimonaco/Pinocchio.git
[2] https://github.com/icl-utk-edu/heffte?tab=readme-ov-file

Unlike overdense structures, voids evolve in a quasi-linear regime, making them particularly well-suited for semi-analytic approaches such as PINOCCHIO. Previous studies have demonstrated the accuracy of PINOCCHIO in reproducing halo statistics, including the HMF, halo bias, and two-point clustering. However, its effectiveness in modeling other components of the cosmic web, such as voids, remains an open question.

3.1 Methodology: Cosmic Voids

To test the reliability of PINOCCHIO in predicting void statistics, we use the full N-body code OpenGADGET3 as a benchmark. Voids are identified using the VIDE toolkit, which is applied to the halo field (rather than the full matter density field) constructed from the halo catalogs of both simulations. By comparing results across different redshifts and resolutions, we assess how well PINOCCHIO reproduces the statistical and structural properties of voids over cosmic times. We investigate four key summary statistics that characterize cosmic voids: the void size function (VSF), void ellipticity function (VEF), core density function (CDF), and radial density profiles (RDP).

3.2 Results: Cosmic Voids

Across all metrics, PINOCCHIO demonstrated excellent agreement with OpenGADGET3 within statistical uncertainties, with no evidence of systematic biases. In particular:

- VSF: PINOCCHIO reproduces the void abundance as a function of size across redshift and resolution, with a level o agreement comparable to that achieved for HMF in overdense regions. Differences at large void sizes are attributed to resolution-dependent halo clustering effects.
- VEF: the ellipticity distributions show excellent consistency across multiple redshifts, suggesting that PINOCCHIO captures the large-scale tidal influence on void shapes.
- CDF: PINOCCHIO performs particularly well at low core densities, where its LPT-based approach is expected to be most accurate. Deviations at higher core densities are mild and resolution-dependent, likely related to FRAGMENTATION and small-halo statistics.
- RDP: the stacked radial density profiles agree well across all redshifts, reinforcing PINOCCHIO's reliability in reproducing the structure, environment, and evolution of voids.

Across all these statistics, the differences between PINOCCHIO and OpenGADGET3 results remain mostly within $\pm 10\%$ variation range and below the 2σ deviation level. Overall these results demonstrate that PINOCCHIO reproduces void summary statistics with good accuracy, particularly in the underdense regime where linear and quasi-linear dynamics dominate. This makes it a promising tool for cosmological applications involving voids, especially in the context of upcoming large-volume surveys such as Euclid and LSST, where computational efficiency and statistical robustness are crucial.

4 General Conclusion

In this thesis, we advanced PINOCCHIO both technically and scientifically. On the technical side, we demonstrated that key components of the code can be efficiently ported to GPUs, achieving substantial performance gains and significant reductions in energy consumption across multiple HPC architectures. On the scientific side, we showed that PINOCCHIO reliably reproduces void statistics when benchmarked against full N-body simulations, extending its validated applicability beyond halo-based analyses. Together, these results establish PINOCCHIO as both an efficient and accurate framework for large-scale cosmological simulations, well-suited for the demands of current and upcoming survey programs.

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Title: Quantum Algorithms for Cosmological Simulations

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Modern cosmology relies heavily on large-scale numerical simulations to describe the complexity of cosmic structure formation from the initial conditions established by the physics of the primeval Universe. These simulations are used to bridge the gap between theoretical models and observations. Specifically, what is considered to be the standard cosmological model has been validated by extensive observational campaigns and describes a Universe dominated by Dark Matter (DM) and Dark Energy (DE), whose fundamental nature remains unknown. This cosmological framework is fully characterized by a set of *cosmological parameters*. The aim of modern cosmology is to constrain these parameters by comparing observational data from large-scale surveys with accurate model predictions. This requires generating extensive ensembles of simulations with identical initial conditions but varying parameter values. However, achieving both the required computational speed and spatial resolution pushes classical computers to their limits, imposing severe computational demands.

In this context, quantum computing (QC) emerges as a promising paradigm for efficient realization of large-scale cosmological simulations. While quantum algorithms have demonstrated potential exponential speedups in fields such as quantum chemistry, their application to cosmology remains largely unexplored. This thesis investigates how quantum computers can accelerate cosmological simulations, serving as a pathfinder study in this emerging field.

Cosmological simulations describe the evolution of perturbations in the DM distribution, which under gravitational influence determine where large-scale structures form and evolve.
Cosmological simulations describe the evolution of perturbations in the DM distribution, which under gravitational influence determine where large-scale structures form and evolve. The first part of this work focuses on developing algorithms for direct simulation of such perturbations, building upon the correspondence shown by Mocz et al. (2018) between the Vlasov-Poisson (VP) equation, describing evolution of perturbations in a self-gravitating collisionless fluid, and the Schrödinger-Poisson (SP) equation. This correspondence suggests that SP, being inherently quantum-mechanical, may serve as an optimal candidate for quantum algorithmic implementation.

The first chapter of the Thesis provides an overview of the standard cosmological model and the role of DM in large-scale structure formation, including different DM types. I introduce the VP equation governing perturbation evolution and review the main classical numerical methods for its integration: N-body methods, direct integration methods, and Schrödinger methods, with particular emphasis on the latter.

This is followed by a concise introduction to quantum computing, establishing the essential concepts such as qubits, quantum gates, unitary evolution, and quantum algorithms, alongside the current state of quantum hardware and its limitations.

In the third chapter, I conduct a detailed comparison of N-body, direct integration, and Schrödinger methods for the VP equation to identify the regime where SP best approximates VP solutions for cold DM scenarios. I developed four classical numerical solvers: two direct integration methods, one N-body method, and one quantum-inspired Schrödinger-based method. During development of the direct VP solvers, I discovered that the widely-used flux-conservation method exhibits artificial adhesion behavior at shell crossing. I traced this erroneous behavior to the initial conditions used for cold DM distributions and addressed the issue by implementing a spectral solver with slight regularization, which proved most suitable for this scenario. These results are presented in Cappelli et al. (2025), published by IEEE.
With properly implemented direct solvers, I performed comparative 1D and 2D simulations across all three methods using different initial conditions. The results demonstrate precise agreement between the VP and coarse-grained SP solutions in the classical limit $\hbar/m \to 0$. These findings will be presented in Cappelli et al. (in preparation).

Building on these findings, Chapter 4 investigates whether quantum algorithms can accurately reproduce DM evolution using the SP equation. I propose a variational quantum algorithm for real-time 1D SP evolution using 5 qubits. The algorithm operates in two stages: first solving the Poisson equation, then performing time evolution through inversion of an evolution matrix $\mathcal{M}$. I demonstrate that the required number of qubits scales logarithmically with the problem scale $\hbar/m$, while circuit depth scales logarithmically with spatial resolution. These results appear in Cappelli et al. (2024), published by APS.

Chapter 5 documents attempts to extend the algorithm to higher-dimensional simulations. While achieving improved time-step efficiency and implementing superior variational ansätze, I encountered fundamental chal-

lenges with regularization of the evolution matrix $\mathcal{M}$. Additionally, the variational circuit architecture requires a number of measurements scaling as $1/\epsilon^2$, where ϵ denotes the target precision. These challenges demonstrated the intrinsic limit in the implementation of a variational algorithm for SP and prompted a shift in focus toward direct approaches. Specifically, I investigated Carleman embedding [Carleman, Torsten (1932)] of the SP equation, but found that the nonlinearity strength precludes accurate approximation even at third order.

The final chapter shifts focus from full DM simulations to accelerating specific, computationally expensive components of classical codes by offloading calculations to quantum computers. Specifically, I address the fixed-radius neighbor search (FRANS) problem, which is central to calculating gravitational forces in N-body methods and hydrodynamical smoothed-particle hydrodynamics (SPH) simulations.
The proposed solution is named QFRANS, a quantum algorithm based on amplitude amplification for the FRANS problem. The algorithm identifies all pairs in a database that are closer than a given distance. The total complexity in the worst-case scenario is $\mathcal{O}(M^{1/2}N^2)$, where M is the number of neighboring pairs and N is the number of particles, and it uses $\mathcal{O}(\log N)$ qubits. By employing extra ancilla qubits, the circuit depth can be reduced to $\mathcal{O}(N \log N)$ at the cost of $\mathcal{O}(N)$ qubits for unstructured datasets, or $\mathcal{O}(\text{poly}(\log N))$ qubits for structured datasets. The primary limitation regarding ancilla qubits is currently imposed by state preparation algorithms. With future developments, this could prove to be a promising approach to the FRANS problem.

This work represents a first step toward quantum algorithms for DM simulations. While the results presented in this Thesis are definitely promising, we encountered numerous challenges in identifying an algorithm that could provide a breakthrough by fully exploiting quantum advantage. Direct integration of the SP equation is a complex problem better suited for the fault-tolerant regime of quantum computers. The study would benefit from a deeper and more comprehensive analysis, employing different techniques such as continuous variables, nonlinear Schrödingerization [Jin et al. (2024)], or alternative linearization approaches. The FRANS problem appears most promising currently, though state preparation remains the principal challenge. With quantum random access memory (QRAM), the algorithm could provide advantages over classical methods, while other search algorithms merit further investigation.

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Abstract

Simulations of two-dimensional crystalline and amorphous oxides

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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.