CSN4 – Richieste di risorse di calcolo per il 2026

Michele Pepe e Nazario Tantalo

CSN4: 36 progetti (Iniziative Specifiche) di cui 19 fanno uso di risorse di calcolo HPC

Lattice QCD

- LQCD123 *(F. Sanfilippo)*
- NPQCD *(M. D'Elia)*
- QCDLAT *(M. Pepe)*
- SFT *(M. Panero)*
- SIM *(M.P. Lombardo)*
- GAGRA *(M. Papinutto)*

Cosmology and Astroparticle Physics

- INDARK *(M. Lattanzi)*
- NEUMATT *(R. De Pietri)*
- TEONGRAV *(B. Giacomazzo)*

Nuclear Physics

- MONSTRE *(A. Roggero)*
- NUCSYS *(M. Viviani)*

Standard Model Phenomenology

- QFTATCOL *(C. Carloni Calame)*
- PML4HEP *(R. Torre)*

Physics of the Complex Systems

- BIOPHYS *(G. La Penna)*
- ENESMA *(F. Viola)*
- FIELDTURB *(G. Gonnella)*

Quantum Information

- QUANTUM *(S. Montangero)*
- LINCOLN *(S. Pilati)*

Condensed matter

- TIME2QUEST *(A. Sindona)*

Circa 300 ricercatori

Lattice QCD

Attività prevista per il 2026: LQCD123

Computing time requests for year 2026

A) Inclusive hadronic decay of B_s meson

Motivation: Calculation of the correlation functions needed to compute the inclusive decay of the B_s meson, following the methodology presented in arXiv:2504.06063 via Hansen-Lupo-Tantalo approach, extrapolating to the physical B_s meson, adopting a specific framework to avoid signal/to/noise degradation in the computation of the needed four-point functions.

Estimated cost: 350k node-hours on Leonardo (GPU cluster)

B) isospin breaking/QED corrections to the inclusive decay of τ into hadrons

Motivation: Removing the leading systematic error on the determination of the Cabibbo angle by phenomenological comparison of the inclusive decay of the τ into hadrons. This will be achieved by including the previously neglected isospin breaking/QED contributions, extending the methodology of Phys.Rev.Lett. 132 (2024) 26, 261901

Estimated cost: 200k node-hours on Leonardo (GPU cluster)

C) Electro-unquenching effects on the hadronic vacuum contribution to the anomalous magnetic moment of muon

Motivation: finalize the calculation of the HVP of the hadron, by including the specific contributions related to the QED and isospin breaking effects in the sea (electrounquenching).

Estimated cost: 150k node-hours on Leonardo (GPU cluster)

D) Semileptonic $D \to K\ell\bar{\nu}$ and $D \to \pi\ell\bar{\nu}$ decay

Motivation: improve the calculation of the form factors related to the semileptonic decay of *D* meson, by computing the correlation function within a methodology specifically suitable for the kinematic close to maximum q^2, to cast light on the present tension between the results of ETM and FNAL collaboration.

Estimated cost: 50k node-hours on Leonardo (CPU cluster)

E) Decay rate for $h_c \to e^+e^-\eta_c$

Motivation: compute the decay rate of the charmonium $h_c \to e^+e^-\eta_c$ involving a virtual photon converting into an electron-positron pair. This extend our very recent study (arXiv:2504.16807) of the $h_c \to \gamma\eta_c$ decay (i.e. the decay to an onshell photon)

Estimated cost: 150k node-hours on Leonardo (GPU cluster)

Lattice QCD

Attività prevista per il 2026: NPQCD

Our research program concerns frontier open problems in the non-perturbative aspects of strong interactions and other QCD-like theories. We have a long-standing tradition in the use of HPC resources, also through competitive calls such as PRACE or ISCRA. Our numerical simulations are mostly based on codes developed by researchers of our team or collaborators, running on GPUs [1, 2] or standard [3] clusters, but also on other publicly available codes [4].

The main research topics to be pursued in 2026 are the following:

A) HIGH TEMPERATURE QCD, TOPOLOGY AND AXION PHENOMENOLOGY

One of the main lines of our research will be the determination of quantities relevant to axion phenomenology, in particular the so-called sphaleron rate, for which we have provided a first reliable determination for $N_f = 2 + 1$ QCD with physical quark masses [5].

Our present main task remains an extension to higher temperatures and at non-zero momentum, since this could be of particular interest for phenomenological computations concerning the thermal production of axions during the cosmological evolution. We have already presented a preliminary investigation of the two-point function of the topological charge density at non-zero momentum [6]. The extension to higher temperature will require a determination of the line of constant physics for QCD with 2+1+1 staggered flavours (i.e., including dynamical charm contributions), going down to lattice spacings small enough to reach temperature of the order of 1 Gev with good control over discretization effects. Such determination is currently under way using step scaling strategies. Simulations at high T will benefit from the use of the full QCD algorithm which implements parallel tempering on boundary conditions [7]. All the production stages will be run on GPUs (hence on Leonardo-booster).

An extension of the determination of the sphaleron rate in the presence of an external magnetic field will be of great interest in order to better interpret results that we have recently obtained in Ref. [8] for the electric conductivity in a magnetic background, in particular regarding their possible connection to the chiral magnetic effect.

Gauge configurations produced in this context will be used to determine other quantities relevant for axion phenomenology, like the finite T topological susceptibility [9], which enters the determination of axion coupling constant, hence the axion mass.

The investigation of topological properties at finite T will be pursued from several aspects. In particular, we have indications coming from global observables (cumulants of the total topological charge) that in the high temperature phase θ dependence is well described by the semiclassical dilute instanton gas approximation. We will investigate the local topological properties of high temperature configurations, in order to extract instanton (more properly caloron) properties, and investigate the interactions between topological excitations.

B) LOW ENERGY AND CONFINING PROPERTIES OF QCD AND QCD-LIKE THEORIES

We plan to finalize the determination of the so-called $l7$ low-energy constant, by applying to staggered fermions the strategies developed for twisted mass fermions [10]. The production of gauge configurations is based on GPU, while the analysis of physical observables, which takes a considerable amount of time, makes use of general purpose CPU resources.

We also plan to finalize the extension of our determination of the strong coupling in $SU(3)$ [11] to a larger number of colours. This part runs mostly on CPUs.

Building on our previous studies [12, 13, 14, 15, 16], we plan to investigate the chromoelectromagnetic tensor field generated by mesons and baryons in Quantum Chromodynamics (QCD) with (2+1) flavors. This investigation will be carried out both at zero temperature and at finite temperature. Our objective is to obtain a detailed profile of the flux tube structure and the spatial distribution of color fields and currents around static sources. At zero temperature, we also aim to gain direct insight into the phenomenon of string breaking. At finite temperature, we will study the evolution of the flux tube structure across the crossover region, with the goal of providing indications relevant to the phenomenology of the quark-gluon plasma. This part of the project will primarily utilize GPUs for the generation of gauge configurations, while the evaluation of operators on the tensor fields produced by mesons and baryons will be mostly performed on CPUs.

In Refs. [17] we determined the theta dependence of the lightest glueball mass and of the string tension, we will continue to investigate this topic by considering also the finite temperature case (screening masses), excited states and, possibly, string corrections to the static potentia. This part of the project will run mostly on CPUs.

C) PHASE DIAGRAM OF QCD AND QCD-LIKE THEORIES

We will extend our investigation of the QCD phase diagram in the presence of a constant chromomagnetic background field, building on our previous study [18]. Our goal is to clarify the connection between a possible critical chromomagnetic field and signals of partial restoration of chiral symmetry. Additionally, we aim to further investigate indications of hysteresis effects in the renormalized light and strange chiral condensates. This project is currently running on CPUs, but a GPU port is in progress.

The study of the so-called Roberge-Weiss (RW) transition of QCD will be pursued in various different ways. First, we plan to extend the study of this transition to QCD with 2+1+1 flavours, i.e. including dynamical charm contributions, investigating also the change of θ-dependence along the RW-line. Then, we plan to study the RW transition in the presence of a large number of flavours, and approaching the chiral limit, as a tool to investigate the emergence of a conformal window in many flavour QCD. This part of the project will run extensively on GPUs.

Finally, part of the computational efforts will be dedicated to the study of lower dimensional strongly coupled gauge models, to investigate the confining properties of these theories and the possible existence of continuous phase transitions which can be relevant for finite temperature transitions of 4d gauge theories. We will also investigate the phase diagram of dual models representing a possible solution to the sign problem. This part of the project will run mostly on CPUs.

D) DEVELOPMENTS IN HPC AND QUANTUM COMPUTATION

Part of our allocation will be used with the purpose of developing exploratory computational strategies in HPC and Quantum Computing (QC). In particular, on one side we plan to run benchamrk simulations of LQCD and Lattice Boltzmann on the GPUs (booster) partition and study the scalability across several nodes, using several framworks, from CUDA to OpenACC and OpenMP.

On the QC side, we plan to work on the following topics: emulation of Variational Quantum Eigensolver protocol for ground state estimation via subspace extension; emulation and optimization of mixed protocols in analog quantum pulsed control, involving functional optimization of controls acting on stochastic partial differential equations.

We also plan to investigate equilibrium and dynamical properties of lattice gauge theories, also in the framework of open quantum systems, by means of sign-problem-free quantum-inspired (tensor network) algorithms and hybrid architecture in synergy with quantum computers. These computationally intensive tensor network simulations will leverage high-performance computing resources, utilizing both CPU clusters for large-scale matrix operations and GPU acceleration for the parallelizable tensor contractions and linear algebra decompositions that are central to our approach. These quantum-inspired algorithms will allow us to explore non-equilibrium phenomena, thermalization processes, topological effects and real-time evolution in gauge field theories. We plan also to analyse quantum algorithms that could be relevant for high-energy physics problems, by means of advanced emulation tools deployed on HPC platforms, where CPU resources will handle the classical preprocessing and orchestration of quantum circuit simulations, while GPU computing will accelerate the tensor network calculations and gate operations required for realistic system sizes.

STORAGE REQUIREMENTS

Our computational program involves the production of many gauge configurations which should be stored for further analysis. This is at the basis of our requests for storage, both on disk and on tape.

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Lattice QCD

Attività prevista per il 2026: QCDLAT

Title: Non-perturbative QCD on the lattice: advancing the frontiers of extreme conditions and of precision physics

National Coordinator: Michele Pepe (Michele.Pepe@mib.infn.it)

INFN sections of people involved: Milano Bicocca, Parma, Roma Sapienza, Roma Tor Vergata

Number of Participants: 16

Description of the research activity

The purpose of this proposal is to expand the frontiers of QCD research: we push its boundaries into unexplored regimes characterized by extreme conditions and its theoretical predictions to high accuracy for searching potential signals of physics beyond the Standard Model (SM).

The lattice regularization will allow us to perform non-perturbative investigation from first principles by Monte Carlo simulations. The development of new theoretical methodologies and of innovative algorithmic techniques will be essential in pursuing our project and for attaining final numerical precisions at the percent level or less.

The research activity of this proposal involves many important and interesting phenomena, covering a broad range of energy scales. Indeed, the behavior of QCD in extreme conditions – namely at high temperature and/or at finite chemical potential – plays a central role for nuclear physics as well as for cosmology and astrophysics, and sheds light on early stages of the Universe. Precise comparisons between theory and experiments for a selected number of ElectroWeak and Strong processes may detect hints of new particles or interactions beyond our current understanding of particle physics.

The research activity of the people involved in this project crucially depends on the allocation of computer resources that INFN provides and which are also essential for being competitive when participating to national and European calls for computer time.

The project is organized in four groups of objectives and the tasks that are planned to be pursued during the year 2026 using the INFN computational resources are the following:

- **Flavour physics in the SM and beyond**: precise calculation of the hadronic contribution to the muon anomalous magnetic moment; precise determination of fundamental SM parameters; kaon-mixing matrix elements to constraint extensions of the SM; computation of isospin breaking corrections.
- **QCD in extreme conditions**: non-perturbative study of QCD up to temperatures of the order of the Electroweak scale; computation of the matching between QCD and its description by an effective action in the high temperature regime; computation of transport coefficients; search for the QCD critical point via singularity structures in the T-μ phase diagram; Lefschetz thimble approach to study systems with a sign problem.
- **Theoretical developments:** non-perturbative renormalization of the QCD energy-momentum tensor and of other composite operators; Renormalization Group evolution of fundamental SM parameters; computation of improvement coefficients of lattice operators; computation of scattering amplitudes and of time-like observables.
- **Algorithmic advances:** factorization of the fermionic determinant and multi-level algorithms; computation of spectral densities; simulations with light quarks and large volumes (master field simulations); numerical stochastic perturbation theory.

The people participating to the QCDLAT project are internationally renowned experts in the Monte Carlo simulations of QCD on the lattice exploiting HPC systems; international collaborators are involved in the research activity discussed above.

Request of computational resources at Cineca:

- **CPU**-based partition: **50 Mch**
- **GPU**-based partition: **600 Knh**

Request of computer-time allocation on HPC systems for R&D

The people participating to the project QCDLAT have performed since very long time a very intense research activity on the non-perturbative dynamics of QCD. This sort of studies can be accomplished from first principles only by numerical simulations on the lattice: they are extremely demanding from the computational viewpoint and they can be pursued only on HPC systems available at supercomputing centres.

The steady increase of the computational power of HPC systems allows on the one side to increase the accuracy of the calculations and on the other side to extend the target of the numerical investigations, however the most relevant improvements in the efficiency of the numerical computations often come from the development of new algorithms and new computational strategies.

For this reason, a very important part of the activity of QCDLAT has always been dedicated to the search of innovative numerical techniques to boost the Monte Carlo simulations of QCD on the lattice and, indeed, many methods proposed and studied by our group are now well-established computational strategies.

The study and the development of innovative numerical methods can be efficiently carried out only on small size HPC systems, with resources that can be easily accessible and with a fast stop-restart working approach that is essential when studying and testing new algorithms.

In order to continue this very important research of QCDLAT, we would like to ask to have access to 8 nodes with 192 cores each connected by a 200 Gbit/s switch InfiniBand. We are also interested in the possibility of using 8 nodes with GPUs.

Request of computational resources on Tier1/Tier2 clusters:

- **CPU**-based partition: **13.5 Mch**
- **GPU**-based partition: **70 Knh**

Request of storage space on disk

People participating to the project QCDLAT have been awarded relevant computer resources (European Calls PRACE) at supercomputing centres. In pursuing those projects, many gauge field configurations have been generated: those data are very important since the measurement of physical quantities is, in general, performed in a successive step with respect to the production of the configurations. Those data are saved on our local machines, and we would like to ask for **100 Tb of disk space** for backup.

Lattice QCD

Attività prevista per il 2026: SFT

L'iniziativa scientifica SFT dell'Istituto Nazionale di Fisica Nucleare (INFN) è dedita alla ricerca fondamentale con metodi analitici e numerici di teoria statistica dei campi; i principali temi affrontati sono all'interfaccia tra la fisica dei costituenti elementari della materia e la fisica di sistemi di materia condensata.

Le principali attività scientifiche dell'iniziativa specifica SFT che richiedono l'utilizzo di risorse di calcolo ad alte prestazioni consistono in simulazioni di teorie di campo su reticolo. Specificamente, le attività di calcolo condotte dall'iniziativa specifica SFT si contraddistinguono da quelle delle altre iniziative specifiche che hanno attività nell'ambito della teoria dei campi su reticolo per un approccio che privilegia aspetti fondamentali rispetto ad aspetti fenomenologici, e per lo studio su reticolo anche di modelli diversi rispetto alla teoria delle interazioni forti del Modello Standard (ovvero la cromodinamica quantistica).

Le attività scientifiche in programma per l'iniziativa specifica SFT durante l'anno 2026 saranno ancora in questo filone, con la prosecuzione, in particolare, di progetti di ricerca nei seguenti ambiti:

- lo studio di alta precisione di effetti previsti dai modelli di stringa bosonica nelle teorie di gauge confinanti;
- lo studio di modelli di apprendimento automatizzato applicati alla generazione di configurazioni di teorie di campo su reticolo;
- lo studio numerico di quantità associate ai fenomeni caratterizzanti i sistemi quantistici in bassa dimensione (quali le catene di spin), con una particolare attenzione allo studio delle correlazioni quantistiche e della mutua informazione quantistica;
- la simulazione numerica di sistemi quantistici in bassa dimensione.

Come avvenuto durante gli anni recenti, i risultati di questi studi numerici verranno direttamente confrontati con le previsioni analitiche derivate da modelli effettivi, da teorie conformi, o da approcci di *bootstrap*: questo approccio consentirà di dare la massima visibilità possibile (e, conseguentemente, di garantire un adeguato impatto bibliometrico) ai risultati di questi studi. In tal senso, vale la pena notare che alcuni membri di questa iniziativa specifica sono coinvolti nella collaborazione scientifica internazionale "Simons Collaboration on Confinement and QCD Strings" (https://simonsconfinementcollaboration.org), che comprende gruppi dediti ad attività numeriche accanto a gruppi dediti a studi con tecniche analitiche. La naturale predisposizione alla collaborazione scientifica con altri gruppi (in particolare a livello internazionale) dei membri dell'iniziativa scientifica SFT è testimoniata anche dalle pubblicazioni scientifiche basate su progetti di calcolo ad alte prestazioni prodotte negli ultimi anni dall'iniziativa.

Si prevede che il numero di membri dell'iniziativa specifica SFT che avranno bisogno di accesso alle risorse di calcolo Cineca durante il 2026 avrà un leggero aumento rispetto agli anni precedenti (con il reclutamento, in particolare, di alcuni nuovi dottorandi destinati a questo progetto). Per questo motivo si richiede l'assegnazione di risorse leggermente superiori rispetto all'anno in corso, e almeno in linea con le assegnazioni degli anni fino al 2024.

Lattice QCD

Attività prevista per il 2026: SIM

STRONGLY INTERACTING MATTER – SIM: PURPOSE OF THE 2025 PROJECT

We aim at performing massive studies of several aspects of Quantum Chromodynamics relevant for the study of relativistic heavy ion collisions, that include the analysis of equilibrium properties as well as the out-of-equilibrium properties of the early stages of high-energy proton-proton (pp), proton-nucleus (pA) and nucleus-nucleus (AA) collisions, and a Bayesian analysis devoted to the computation of some properties of the quark-gluon plasma (QGP).

LATTICE QCD–INFINIBAND

The equilibrium studies of the phase diagram, carried out by the INFN-Florence, will concentrate on the strongly coupled region between above pseudocritical temperature, and non-zero θ-angle. According to current observations, this region ends abruptly at T about 300 MeV, and the physics behind this sharp crossover is still under investigation. In our most recent paper A. Y. Kotov, M. P. Lombardo and A. Trunin, [arXiv:2502.15407 [hep-lat]], to appear in JHEP, we present a preliminary evidence of the disappearance of the first order transition line at $\theta = \pi$ at about 300 MeV. We would like to follow up on this by analyzing the Lee-Yang zeros using the existent configurations, and possibly generating new configurations in small volumes to follow the volume scaling. A full-fledged ISCRA project may follow (we cannot apply to EuroHPC due to conflicting interests of MpL)

EARLY STAGES OF PP, PA AND AA COLLISIONS – FARM

For the early stages of pp, pA and AA collisions, involving the INFN-Catania unit, we intend to employ the HPC-Cineca computing resources in Farm configuration. This will be the first time that the INFN-Catania unit of SIM uses HPC-Cineca resources.

Our existing code prepares an initial condition, known as the glasma, that includes initial state fluctuations, as well as quantum fluctuations obtained evolving the Wilson lines with the JIMWLK equation. Then, the evolution of the fields is studied via real-time lattice formulation of the Yang-Mills equations, which are solved in a 3+1D framework. The Farm setup will allow us to generate thousands of parallel events in a broad range of rapidity, providing statistically significant ensembles of evolved gluon fields for reliable averages. These configurations will be used to compute initial-state observables such as single-particle spectra, two-particle correlations, momentum-space correlators, and collective flow coefficients of the bulk gluonic matter. We will also investigate the dynamics of charm and beauty quarks in the early Glasma stage of pA and AA collisions, to quantify how bulk anisotropies are transferred to heavy quark degrees of freedom. Our previous works have shown that this dynamics is highly non-trivial, see for example L. Oliva et al., "Melting of $c\bar{c}$ and $b\bar{b}$ pairs in the pre-equilibrium stage of proton-nucleus collisions at the Large Hadron Collider" [arXiv:2412.07967 [hep-ph]], to appear in Phys. Rev. D, and D. Avramescu et al., "Simulating jets and heavy quarks in the glasma using the colored particle-in-cell method", Phys. Rev. D 107 (2023) 11, 114021. These studies were limited to midrapidity and neglected the quantum evolution of the initial condition, which generates a rapidity-dependent distribution. This is essential for performing theoretical calculations under conditions more comparable to experiments. Full-fledged ISCRA and EuroHPC projects may follow.

For a lattice with size $N_x = N_y = 64$ and $N_\eta = 64$ we estimated a cost of $\sim 3.6 \times 10^4$ CPU-hours per each physics scenario, derived from benchmark runs on local hardware (Lenovo workstation) for a lattice with size $N_x = N_y = 64$ and $N_\eta = 1$ and extrapolated linearly to $N_\eta = 64$. A safety margin of $\sim 20\%$ has been included to account for I/O and runtime variability. Each physics scenario corresponds to a set of parameters that characterize the geometry of the collision, and to 2×10^3 independent events. Each event runs on a CPU threads. We plan to consider at least 10 physics cases, which totally would cost $\sim 3.6 \times 10^5$ CPU-hours. Moreover, we plan to run a few simulations with a larger lattice with $N_x = N_y = 128$ and $N_\eta = 64$. With the larger lattice we plan to analyze 4 different physics cases, 2×10^3 events for each case. For each physics case we have estimated a cost of $\sim 1.44 \times 10^5$ CPU-hours, that for four physics cases would require $\sim 5.76 \times 10^5$ CPU-hours. Summing up the two contributions, our total request is of $\sim 1 \times 10^6$ CPU-hours. For the smaller lattice we have estimated ~ 350 Mb of RAM for each event, while the larger lattice size would require ~ 1.3 Gb of RAM for each event.

BAYESIAN PARAMETER ESTIMATION OF QUARK–GLUON PLASMA PROPERTIES–FARM

This project aims at the comprehensive simulation of nuclear collisions, including initial conditions, hydrodynamic evolution, and post-hadronization interactions, with the objective of constraining the parameters of the Quark-Gluon Plasma (QGP), specifically, the parameters characterizing the initial conditions and the shear and bulk viscosities — through Bayesian inference techniques, which is a widespread methodology in this field. Compared with other studies, we will make use of full 3+1 D hydrodynamic simulation, without initial state fluctuations in order to make the full project affordable in terms of CPU time. Our main goal is to demonstrate the discriminating power of spin polarization (which has not ever been employed as a data in these studies) to pin down bulk viscosity and longitudinal initial conditions. Based on an ongoing similar project of ours, our estimate of the minimum required CPU time is 1 MegaHour. Regarding RAM usage, a single average hydrodynamic event typically requires approximately 8 GB. The code itself is not parallelized, as the workflow consists in generating on the order of 5000 events for different parameters of the QGP. The post-processing stage (computation of observables, etc.) does not require major computational resources.

Lattice QCD

Attività prevista per il 2026: GAGRA

Lattice regularization of gauge theories offers a unique opportunity to compute the functional integral numerically without approximation, using Monte Carlo techniques. This allows for first-principles investigations of the low-energy, non-perturbative regime of Yang-Mills theories and QCD for any number of colours N.

The central focus of our research project is the numerical computation of the low-energy spectrum of gauge theories. Specifically, we aim to calculate the masses of the lowest-lying glueball and meson states in the large-N limit, in order to compare them with predictions from analytical models developed to solve these theories (see, e.g., Refs. [1, 2]).

Over the past two years, we have developed a code to simulate SU(N) pure gauge theories and compute two-point correlation functions of Wilson loops of various lengths. These loops are classified according to their transformation properties under the cubic group and discrete symmetries such as parity and charge conjugation. From the two-point correlators, we extract the low-lying glueball spectrum by solving the Generalized Eigenvalue Problem.

A major challenge in this computation is the long-standing issue of the exponential degradation of the signal-to-noise ratio in two-point correlation functions at large Euclidean time separations. This problem has been partially addressed in the glueball case [3], leading to state-of-the-art computations in [4]. A more recent study [5] has extended simulations up to $N = 12$ – the largest value of N simulated to date – and performed an extrapolation to $N \to \infty$. However, this study does not implement the algorithmic improvements developed in [3], and its reported uncertainties appear to be unusually small, raising tensions with previously published results (e.g., [4]) regarding the mass values of some states.

Over the past year, we have implemented and tested the two-level sampling method introduced in [3] and further investigated in [6, 7], alongside APE and stout smearing of gauge links used in the construction of Wilson loops to create or annihilate glueball states. We performed a large-scale simulation for $N = 3$, confirming that our algorithm's performance is fully consistent with those reported in [6, 7]. We extracted the low-lying glueball spectrum and compared our results with existing literature. This study will be presented at the Lattice 2025 conference.

We have recently initiated extensive new simulations to compute the glueball spectrum at larger values of N and finer lattice spacings. This will allow us to systematically take the continuum limit at each value of N and then safely extrapolate to the $N \to \infty$ limit. To carry out this project, we also plan to apply for additional computational resources through ISCRA proposals.

In the past year, we have also made significant progress in studying the meson spectrum in the large-N limit. In this case, the issue of signal degradation is less severe: the pseudoscalar channel is largely unaffected, and the problem is milder in other channels compared to glueballs. Nonetheless, even in the most recent state-of-the-art studies of meson masses at large N [8], no continuum extrapolation has been performed. To address this, we have developed a code to invert the Dirac operator and compute two-point meson correlation functions for arbitrary N. This code has been tested for $N = 3$ and $N = 4$, and we are currently using it to compute meson correlators on the same gauge ensembles generated for the glueball spectrum calculations at large N. As in the glueball case, we plan to perform continuum extrapolations at each N, and we aim to expand the set of N values used in the large-N extrapolation.

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Cosmology and Astroparticle Physics

Attività prevista per il 2026: INDARK

In 2026, computational resources will continue to be used to support the InDark activities on the development of robust tools for the analysis and scientific exploitation of observations from next-generation cosmological experiments. This includes CMB observations from the ground (Simons Observatory, CMB-S4) and from space (LiteBIRD), galaxy surveys (Euclid), gravitational wave interferometers, as well as the cross-correlation of these probes. We detail the activities in more detail in the following, with a focus on those who rely more directly on the usage of HPC resources, also giving specific examples of recent publications.

CMB B-mode polarization has been recognized as a unique probe of cosmic inflation and it will be the target of a large number of international experiments planned for the coming years. Their success, however, deeply relies on the exquisite control of systematic effects and astrophysical foreground contamination in the data. The same holds for other scientific targets, like neutrino masses and the effective number of relativistic degrees of freedom. As experiments from the ground and from space will feature a wide frequency coverage and an unprecedented number of detectors (up to 10^5), we will expand and optimise available tools for the simulation of systematic effects and foregrounds, and we will analyse their impact on the estimate of the cosmological parameters. Innovative algorithms and efficient HPC software solutions will be explored, including those based on GPUs. As an example, recently we have been developing a fast map-level emulator for maps of CMB systematics, based on the scattering transform formalism [1].

We will continue to develop and run different estimators for the Cosmic Birefringence (CB) effect. The estimators can be based on CMB maps or CMB spectra. The estimators produce estimates of the isotropic rotation angle or of the CB spectra/maps.

We develop summary statistics and field-based analyses to extract information from non-linear scales in cosmological large-scale structure - with emphasis on extracting primordial non-Gaussian parameters from different inflationary models. Our methodologies use large sets of N-body simulations and combine traditional statistical estimation with machine learning-based approaches. We also plan on developing numerical pipelines to simulate and study general relativistic effects in future galaxy surveys. [2]

We have developed a code to test parameterised Modified Gravity theories. The code, called PANDA, is a compile-time module of the parallel simulation code Gadget4 and in principle allows to simulate structure formation for any model within the Horndeski landscape. So far, the code has been tested and validated on a few target models for which exact simulations are available, namely f(R) gravity and nDGP models, showing percent-level agreement with standard codes based on a full solver of the specific field equations, at a much lower computational cost. A presentation paper describing the algorithm of PANDA is currently in preparation. Over the past year, the PANDA framework has been extended to include also other Dark Energy models such as Dark Scattering cosmologies and general interacting Dark Energy scenarios. Also, the PANDA module has been integrated with the native lightcone output capabilities of Gadget4, thereby allowing to generate self-consistent clustering+weak lensing mock observations.

We also developed a new suite of cosmological simulations for testing Dark Matter particle candidates (the AIDA-TNG simulations) that were completed in 2024 and led to the publication of the first AIDA-TNG paper, now accepted. [3]

We will investigate models beyond LCDM with available CMB and LSS data and assess the sensitivity of future experiments. Some examples of the models of interest: early Universe physics (inflation, non-adiabatic initial conditions, primordial magnetic fields); modified gravity; reionization; CB and generalized Faraday rotation through power spectrum analyses; decaying dark matter; neutrinos and other light relics (axions, sterile neutrinos, majorons). See e.g. [4] for an analysis of low-reheating temperature scenarios, or Sec. 6.1.2 of the ACT paper on extended cosmological models [5] on neutrino nonstandard interactions. This activity is based on Einstein-Boltzmann codes and associated Markov Chains MonteCarlo samplers, all massively parallelized and CPU-based.

We plan to carry out a systematic analysis of non-standard initial conditions of the Universe, as well as a non-parametric reconstruction of the primordial power spectrum, with a particular focus on large-scale structure data in combination with CMB observations, as in [6, 7]. The requested computing time is essential to carry out cosmological parameter inference using Monte Carlo techniques on current and upcoming datasets. The activities will primarily be CPU-based, with a subset relying on GPU-accelerated emulators. Depending on the specific analysis and dataset, the main codes we plan to use include CAMB, Cobaya, CosmoMC, CosmoSIS and CosmoPower.

Part of the activities are currently still using mainly CPU-based machines, as opposed to GPUs. However, we are exploiting computational time on GPU-based machines to explore the possibility of migrating a fraction of our codes to GPUs.

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Cosmology and Astroparticle Physics

Attività prevista per il 2026: NEUMATT

The request is for a total of **6 Mcore hours** on CPU data general CINECA clusters and a small amount of (~3,000 node hours) 100 kcore hours on LEONARDO-booster to perform code porting and run general GPU-optimized simulation code. The requested disk space is 10 TBytes, as the checkpoint size is of the order of 0.25TByte and full 3D output for a high-resolution simulation is of the order of 1TByte.

NEUMATT (composed of the Ferrara, LNGS, Catania, and Pisa Units) is focused on the study of the structure of neutron stars (NSs), ranging from the investigation of the relevant microphysics and its interplay with the structure and composition of compact stars and the observational implication of the neutron stars' complex and rich phenomenology to the observed signal in the universe (electromagnetic and gravitational) coming from astrophysical system that includes neutron stars. The primary focus of the computational request is to study the effect of the EOS for nuclear matter on the gravitational signal generated by Neutron Star Mergers and on the dynamics of the ejected matter.

The last years have been mainly focused on developing a new code (MIR) [6] that is now ready to perform the first set of physical simulations of the effect of real EOS and resistive effects in the dynamics of binary neutron star mergers in the presence of magnetic fields.to investigate how different models for the EoS and different astrophysical scenarios (one or two families of compact stars) affect this kind of signal. In particular, the amount of mass ejected, its entropy, and its chemical composition are key for determining the properties of the kilonovae. In particular:

- Simulations using different astrophysical scenarios for the EoS describing neutron stars, including one or two families of compact stars. They aim to determine the amount of mass ejected, its entropy, and its chemical composition, as these are key factors in determining the properties of the kilonovae.
- Study of the effect of magneto-resistive on the post-merger dynamics.

The typical cost of a 3D merger simulation (with magnetic fields) at a resolution of the order of 200 m (the minimum resolution required) for an evolution lasting 50 ms requires 237 GByte of allocated memory and is performed using 512/1024 cores and **200k core hours,** while the activation of magneto resistive double the CPU time needed. Higher resolution simulations require 2048 cores. We estimated that at least 20 configurations need to be simulated at different resolutions. This would result in an estimated 4 Mcore hours for the simulation at the highest resolution. The additional request cost of the lower-resolution simulation, as well as the development and optimization of the code, should be added, for a total of **6 Mcore hours.**

Most relevant publication for the proposal:

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Cosmology and Astroparticle Physics

Attività prevista per il 2026: TEONGRAV

The TEONGRAV collaboration is composed of 125 members in 11 research units. The current number of HPC users is 50. We need HPC resources for the following projects:

1. Numerical Relativity Simulations of Compact Binary Mergers: we shall use the publicly available Einstein Toolkit code to run simulations of compact binary mergers, neutron stars (NSs) and black holes (BHs), in order to study their gravitational wave (GW) and electromagnetic (EM) emission. The Einstein Toolkit uses a hybrid parallelization approach (OpenMP and MPI). The toolkit has been already used on CINECA CPU clusters (including LEONARDO DCGP). We recently developed a new general relativistic magnetohydrodynamic (GRMHD) code able to run on GPUs (AsterX). We plan to use this code on the GPU nodes of LEONARDO. We will also carry simulations with CPU codes such as Spritz and IllinoisGRMHD (both based on the Einstein Toolkit).

2. Numerical Relativity Simulations of Black Hole Mergers Beyond General Relativity: We will simulate the gravitational collapse of fundamental fields and BH mergers in motivated extensions of General Relativity both within an effective field theory approach and at the fully nonperturbative level. In both cases we shall use codes developed in the Einstein Toolkit, GRChombo and Simflowny, as well as domestic codes. The codes make use of CPU clusters.

3. Bayesian parameter estimation: We shall perform Bayesian inference of single GW events and population studies, both to study parameter estimation and waveform systematics, and also to assess whether current and future GW detectors can infer the properties of multiple formation channels for BH binaries. We will use the BILBY and GWpopulation infrastructures. The latter runs on GPUs. We are prototyping an innovative simulation-based inference algorithm based on neural networks for both black-hole ringdown studies and LISA data analysis. These algorithms are optimized for GPUs.

4. *N*-body simulation of stellar clusters to investigate the formation channels of compact binary mergers: We will simulate the evolution of massive stellar clusters to study the formation of compact binary mergers in dense environments. We will use the code PETAR, a high-performance code that exploits hybrid parallelization methods (MPI, OpenMP, GPU), coupled with the single and binary population synthesis codes MOBSE and SEVN. In parallel, we will use the MPI hydrodynamic code RAMSES to simulate star-forming regions and generate more realistic conditions for the *N*-body simulations.

5. Special relativistic MHD simulations of short GRB jets: We will use the PLUTO code to investigate the propagation of jets across realistic NS-NS post-merger environments, with particular attention to electromagnetic dissipation properties, using both ideal and resistive relativistic MHD. The goal is to connect our models with short GRB observations. We already performed preliminary simulations on the CINECA clusters Marconi and Galileo100. PLUTO simulations can run only on CPU (a GPU version of PLUTO is being developed).

6. Hydrodynamical simulations of Massive Black Hole formation and evolution: We will employ the public code GIZMO to study the formation and evolution of massive BHs in the cosmological context, to study in detail potential GW sources for LISA and ET. We will investigate the conditions under which these objects form and how they evolve and pair in binaries. GIZMO has been used on the Galileo100 and Marconi CINECA clusters, and is fully parallelised with MPI and OpenMP, but no GPU parallelisation is present at the moment.

7. Magnetohydrodynamical simulations of accretion discs and circumbinary discs around massive black holes: Exploiting a novel post-Newtonian and GRMHD implementation in the code GIZMO, based on the work by Lupi (2023), we will explore the transition from the Newtonian to the relativistic regime of accretion flows around single and binary massive black holes to study the electromagnetic counterparts of GW sources for LISA and ET.

Nuclear Physics

Attività prevista per il 2026: MONSTRE

Our project aims to establish a comprehensive and integrated framework for the study of atomic nuclei, nuclear reactions, and strongly interacting matter. The synergistic efforts of the various units, based on their complementary expertise in advanced many- body and computational methods, will be devoted to the study of complex nuclear phenomena occurring at different scales of energy and size. Modern ab initio techniques will be refined and applied making use of microscopic interactions, derived from nuclear effective field theories. Density functionals will be developed using ab initio and/or phenomenogical constraints and applied to the calculation of bulk, spectroscopic, and decay properties of finite nuclei throughout the whole nuclear chart, Collective modes will be studied making use of many body techniques including beyond mean-field correlations. The consistent merging of structure and reaction theories will offer the opportunity to directly compare theoretical calculations with empirical data for nuclear systems under extreme conditions, also deriving microscopic optical potentials. These investigations will also be performed by developing mathematical methods, quantum computing-based algorithms and machine learning techniques specifically tailored for the study of the nuclear many-body problem. Special attention will be devoted to the current experimental projects related to the production of rare isotopes, dark-matter detection, and the physics of electroweak interactions, including neutrino physics and double-beta decay. Combined astrophysical and terrestrial constraints, together with predictions based on state-of- the-art models, will be employed to achieve an improved, multi-faceted understanding of the nuclear equation of state.

Examples of HPC applications

SHELL model calculations

The KSHELL code, massively employed in shell-model calculations, can easily run on a Linux PC with a many-core CPU and OpenMP library, as well as on a state-of-the-art massive parallel computer with hybrid MPI+OpenMP parallel programming. It exhibits a strong scaling of the parallel computation tested on different HPC systems, included the CINECA Marconi and Galileo100 clusters. In order to store the calculated wavefunctions for all the systems we plan to calculate we need about 1Tb of storage. All the libraries needed are already installed on the CINECA machines.

RPA−based calculations

The nuclear response of atomic nuclei is calculated by using the QRPA approach for deformed systems and the Second RPA for spherical ones. From a computational point of view, the most demanding operations required these calculations are the evaluation of the matrix elements to be diagonalized and the diagonalization of the corresponding eigenvalue problem. The dimensions of the matrices are of the order of $10^7 - 10^9$. PETSC/SLEPC libraries are employed to handle the matrices and for their diagonalization, using the MPI parallel protocol. These libraries are already available on the CINECA infrastracture. The typical storage needed is of the order of 500 Gb.

Quantum Monte Carlo calculations

Nuclear structure calculations are performed using two distinct methods: the Configuration Interaction Monte Carlo code is allows for efficient parallel execution, through MPI, with up to a few hundred cores but we are planning to add also a layer parallelized using OpenMP to allow the code to scale to larger allocations; the Variational Monte Carlo calculations using Network Quantum States are instead based on the NetKet code which is designed to use GPU systems through JAX. At the moment typical simulations involve a single GPU node at a time. For both simulations the typical storage is in the hundreds of Gb.

Nuclear Physics

Attività prevista per il 2026: NUCSYS

The calculations performed thanks to the CINECA HPC resources regard the study of the structure and dynamics of nuclear systems. Recently, we have studied the following problems:

- Study of the α-particle first excited state. This is a 0^+ resonance, which structure is still largely unknown. This resonance can be studied from the "monopole" transition from the ground state, a 0+ state as well, which experimentally can be investigated via either electron scattering or $\alpha - \alpha$ scattering. In practice, we compute the transition matrix element of the electromagnetic charge operator between the ^{4}He ground-state and the $p+^3$H and $n+^3$He scattering states. The nuclear wave functions are calculated using the hyperspherical harmonic method, by starting from Hamiltonians including 2N and 3N interactions derived in Chiral Effective Field Theory. The results for the monopole form factor are in agreement with the recent electron-scattering MAMI data.

- Study of the processes $d(d,p)^3$H and $d(d,n)^3$He at energies of interest for energy production and for big-bang nucleosinthesis. We accurately solve the four body scattering problem starting from nuclear Hamiltonians which include modern two- and three-nucleon interactions, derived in chiral effective field theory (χEFT). We can obtain results for the astrophysical factor, the unpolarized differential cross section, and various single and double polarized observables. An estimate of the "theoretical uncertainty" for all these quantities is the goal of this study, obtained from calculations of the various observables at different χEFT orders.

- Effect of meson exchange currents in the beta decay of heavy nuclei. The aim of this study is to compute accurate nuclear matrix elements for the beta decay and double beta decay of ^{48}Ca, ^{76}Ge,and ^{82}Se isotopes, which are candidates for the observation of neutrinoless double beta decay, in the framework of the shell model method. The first goal has been to assess the role of both electroweak currents and many-body correlations as the origins of the well-known problem of the quenching of the axial coupling constant g_A. Calculations of matrix elements for the neutrinoless double beta decay are ongoing.

Standard Model Phenomenology

Attività prevista per il 2026: QFTATCOLL

The Project (Iniziativa Specifica) QFT@Colliders deals with the application of Quantum Field Theory techniques to the phenomenology of present and future colliders. Important searches and experimental measurements, at modern particle accelerators at energy and intensity frontiers, require the calculation of higher-order corrections to a variety of scattering processes in gauge theories of fundamental interactions. Moreover, such calculations must be available in the form of Monte Carlo event generators, in order to allow for a systematic and meaningful comparison between data and theory. An increasing level of theoretical precision is required to fully exploit the high quality of future data collected at the LHC and high-intensity e^+e^- machines. Many new physics signals are obscured by large Standard Model (SM) backgrounds: improving the accuracy of the modelling of such backgrounds is of crucial importance to explore possible regions of model parameter space, where only an excess over SM expectations and not a clearly standing resonance is expected. In addition, the study of the properties of newly discovered particles requires the availability of precise simulation tools. Precision measurements, in combination with accurate theoretical predictions, may open the way to the detection of fundamental physics phenomena not yet discovered, even if the present lack of clear direct new physics signals will persist in data of present and near-future experiments. Furthermore, the synergy between the research at the energy and intensity frontiers may allow to deeply probe the SM and eventually unravel the existence of new physics beyond it.

This ambitious theoretical program needs computational resources, which are usually CPU intensive, for code development, validation and physics studies. This is even more true because of the increasing accuracy of the Monte Carlo tools, which now aims at reaching QCD/EW NNLO accuracy matched with Parton Showers for a growing number of scattering processes.

The Monte Carlo codes which will exploit the resources are well know tools in the communitiy of high energy phenomenology, such as `GenEva` [1], `POWHEG BOX` [2], `MadGraph5_aMC@NLO` [3], `Mesmer` [4], `BabaYaga@NLO` [5] and likely more.

References

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Standard Model Phenomenology

Attività prevista per il 2026: PML4HEP

For a few years now, the High Energy Physics (HEP) community has started to substantially explore Machine Learning techniques for a diverse variety of tasks and, as such, a large number of ideas, applications, and tools are being published. This is not only the case within experimental collaborations, but also among the phenomenology and formal theory communities. Even more, as we head towards the High Luminosity era of the Large Hadron Collider (HL-LHC), in which unprecedented amount of highly complex data need to be simulated, collected, and finally analyzed, the importance of building reliable and more efficient methods, techniques, and workflows for HEP is becoming compulsory. As the community has already realized, ML plays a crucial role in this development. In particular, ML, together with new frontiers in hardware acceleration, provide a potential solution to meet the expected computing resources for simulating and reconstructing the products of the collisions and will also be essential for developing novel strategies for triggering and reconstructing data, as well as for the statistical analysis, interpretation, and preservation of such data. This represents a brand new field of research, which effectively complements the HL-LHC physics program. Furthermore, supported by the largely enhanced precision expected at the HL-LHC, dedicated ML methods will provide great opportunities to pursue data-driven searches, i.e. for anomaly detection, data quality monitoring and efficient background estimation. However, to ensure a systematic implementation of ML methods in the HEP workflows, one needs to carefully study their properties and capabilities against complex, high-dimensional data and to assess their ability to match the required precision, typically much higher than that of industrial and "real-life" applications. This program, which can go under the name of "Precision ML", cannot be separated from the development of novel techniques for hardware acceleration, the design of reliable quality metrics, and the proper assessment of the relevant uncertainties. We believe that the joint effort of experts from the INFN theory and experimental communities can help shape this Precision ML program and contribute to it.

Physics of the Complex Systems

Attività prevista per il 2026: BIOPHYS

The INF25_biophys HPC project (coordinator Giovanni La Penna) collects the activity of 7 groups involved in high-performance computing in the field of biophysics. Users of HPC resources are 41, with a significant increase with respect to 2024. Below the list of groups and the actual PIs:

- University of Roma Tor Vergata (UNITOV), Velia Minicozzi;
- Politecnico of Torino (POLITO), Andrea Gamba;
- University of Torino (UNITO), Michele Caselle;
- University of Trento (UNITN), Luca Tubiana;
- University of Napoli (UNINA), Mario Nicodemi;
- Scuola Normale Superiore of Pisa (SNS), Giuseppe Brancato;
- University of Milano (UNIMI), Guido Tiana;

Each group applies original, advanced and continuously developing computational methods, all requiring HPC resources, to different scales relevant to biology: active sites with explicit electrons; macromolecules described as atoms; coarse grained models; crowded environments; networks. Methods range from quantum mechanics, atomic interactions, polymer physics, network science, machine learning, and extended cutting-edge statistical methods.

Below is a short summary of some of the activities that will be continued in years 2025-2026.

UNITOV - Development and application of computational methods (mainly generalized statistical ensembles) to determine the structure and the dynamics of biologically relevant molecules. We use molecular dynamics at different space and time scales, based on classical and first principles models, all requiring massive HPC resources. We analyse experimental results obtained exploiting large scale facilities such as synchrotrons, free electron lasers (FEL), NMR infrastructures.

POLITO - Use of computational methods to model region/activity localization in eukaryotic cells, based on the idea that protein sorting naturally emerges from the combination of spontaneous molecular aggregation with vesicle nucleation. Effects of molecular crowding, to understand how the efficiency of sorting may depend on the number of molecular species involved, are explicitely taken into account. This task is performed by extensive numerical simulations of the model for varying numbers of molecular species and values of control parameters using parallelized computer code.

UNITO - Application of topic modelling techniques for the identification of cancer subtypes, extending a specific class of topic models to allow a multi-omics approach. The methods allow to clearly distinguish healthy from tumour samples as well as the different cancer subtypes. The integration of different layers of information is crucial for the observed classification accuracy. Our approach naturally provides the genes and the microRNAs associated to the specific topics that are used for sample organization. Recent interpretations of methods based on machine learning (large language models) in the frame of statistical physics are developed.

UNINA - Continuous development of polymer models to study the three-dimensional (3D) organization of DNA and its temporal dynamics. Investigation of the physical mechanisms (e.g. phase separation or polymer adsorption) that shape chromosome structure and control genome activity. The research will use massive parallel molecular dynamics simulations, machine learning methods and analyses of public genomic databases.

SNS - Development and application of numerical simulation methods for modeling complex macromolecular systems of biological interest through the use of various HPC resources and facilities. Investigation of the structural and dynamic properties of voltage-gated ion channels and the effects of some pathogenic mutations causing their dysfunction. Applications of deep neural networks to describe atomic interactions.

UNIMI - Combination of deep neural networks and extended replica-exchange molecular dynamics to study the conformational landscape of structurally disordered proteins and folding mechanisms.

Physics of the Complex Systems

Attività prevista per il 2026: ENESMA

1 Turbulent hemodynamics

Introduction and methods

The hemodynamics within the whole human heart will be solved using a multi–physics computational approach capable of tackling the electrophysiology, the elasto–mechanics and the fluid dynamics of the heart, along with their multi–way coupled interactions. The developed tool embodies accuracy, versatility and computational efficiency, thus allowing cardiovascular simulations in realistic conditions and it has been developed and validated by our group through comparisons with the literature, ad–hoc experiments and clinical data in a sequence of papers, see [1,2,3].

The pulsatile and transitional character of the hemodynamics is obtained by solving directly the incompressible Navier–Stokes equations using a staggered finite differences method. All spatial derivatives are discretized by central second–order accurate finite-difference schemes including the nonlinear terms and the time advancement of the solution is obtained by a low storage 3rd–order Runge-Kutta scheme. The nonlinear terms are treated explicitly, while the viscous terms are computed implicitly (or explicitly with a small time step so that the stability constraints of the viscous terms and the CFL condition for the non-linear terms are both satisfied). The elliptic equation for pressure is solved using a combination of FFTs, implemented using serial FFTW and the serial tridiagonal solver from LAPACK. Finally, all I/O larger than writing short plain text log-files is done using parallel HDF5. The parallelization of the Navier–Stokes solver is based on a domain decomposition where the Cartesian domain is split into slabs. According to this 'one-dimensional slab' parallelisation, each processor needs to store information from the neighbouring processors that is required for computing the derivatives in what is called a 'halo/ghost' layer and since the flow solver employs a second-order finite difference spatial discretisation at most one halo layer is required on each side of a slab. All the simulations will be carried out using our in–house multi–physics solver, which has been GPU accelerated using CUDA Fortran with an extensive use of CUF kernel directories that automatically run single and nested loops on the GPU device without modifying the original CPU code.

The code is complemented with various immersed boundary (IB) techniques to handle complex moving and deforming geometries. The structural mechanics is based on the Fedosov's interaction potential method [1] to account for the mechanical properties of the biological tissues, which are anisotropic and nonlinear. The electrophysiology, responsible for the active potential propagation in the cardiac tissue triggering the active muscular tension, is incorporated by means of a bidomain model [3] that can account for the different cellular models of the various portions of the heart. All these models are three–way coupled with each other, thus capturing the fully synergistic physics of the heart.

Objectives

The state-of-the-art numerical model is used not only to investigate in-silico cardiac pathologies or to test innovative medical devices, but also for fundamental studies in hemodynamics. As an example, we are carrying out a systematic Lagrangian analysis of turbulence in the left heart using high-fidelity simulations based on a patient-specific anatomical model [4]. The FSEI solver is used to simulate the whole cardiac cycle, and we track hundreds of thousands of passive tracers to explore turbulence across a wide range of time scales, from one heartbeat to fractions of the viscous time-scale. Furthermore, our analysis focuses on the impact of two key physiological parameters: heart rate (HR) and aortic valve stiffness. By comparing simulations at HR = 40, 60, and 80 bpm, we quantify the effect of cardiac frequency on velocity fluctuations. Additionally, we investigate a pathological condition involving a stiffened aortic valve, mimicking aortic stenosis, by increasing the leaflet stiffness. To characterize turbulence, we employ a set of Lagrangian statistical tools, including time correlation functions, structure functions, local scaling exponents, and flatness factors. Correlation functions reveal temporal coherence and flow memory, while structure functions and their local slopes provide insight into the scale-by-scale behavior of velocity fluctuations. Flatness, in turn, quantifies intermittency and the prevalence of rare, intense flow events. Together, these metrics allow for a comprehensive evaluation of turbulent dynamics under physiologically realistic conditions. Both the ventricle and aorta display strong intermittency with non-Gaussian velocity statistics. The aorta is characterized by more organized, advective dynamics, with intermittent features primarily driven by the sharp transitions associated with systolic ejection and subsequent deceleration. In general, the aortic (and in particular its ascending part) hemodynamics manifests stronger turbulence than the ventricle. Using a combination of 2-point correlation functions, Lagrangian structure functions, flatness factors, and local scaling exponents, we quantify how turbulent energy transport varies across scales [4]. Our findings demonstrate that Lagrangian statistics offer a powerful and sensitive framework for probing the complex dynamics of cardiovascular flow.

Essential bibliography

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[3] Viola, F., Del Corso, G., & Verzicco, R. (2023). High-fidelity model of the human heart: An immersed boundary implementation. Physical Review Fluids, 100502.

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Physics of the Complex Systems

Attività prevista per il 2026: FIELDTURB

The FIELDTURB initiative will tackle three main topics, each addressing cutting-edge research topics that require high-performance computing.

1. Complex Fluids and Complex Flows

This activity will focus on the effects of turbulent flows in multicomponent fluids. Specifically, we aim to investigate turbulent emulsions under various conditions using state-of-the-art numerical simulations. Our objectives include studying the statistics of droplet distribution, the conditions under which the expected power-law distribution is observed, and the role of intermittency. We will investigate how flow statistics are modified in the presence of an emulsion and examine the effect of surface tension in the non-stationary flow produced by a Rayleigh-Taylor configuration.

Additionally, we are committed to developing and deploying a unique tool for the community interested in data-driven fluid mechanics: an open-access database offering high-quality and high-quantity data for a series of key benchmarks for the turbulence community, including Eulerian and Lagrangian datasets. We will perform state-of-the-art LES (LARGE EDDY) simulations and use reinforcement learning (RL) to identify optimal strategies for exploiting turbulent flows.

Building on our initial observations of the transition from three-dimensional to two-dimensional turbulence in planar jets of power-law fluids at low Reynolds numbers, our research activity aims to comprehensively explore how spatial constraints impact turbulence characteristics and scaling behaviors. We plan to conduct an extensive series of direct numerical simulations, manipulating the width of the computational domain to vary the turbulent scale systematically. The research will utilize high-performance computing facilities and GPUs resources, to handle the computational demands.

We aim to perform a set of LES simulations with a new class of spectral subgrid models based on a self-similar and reversible power-law closure to minimize the impact of subgrid scales on the inertial range of fully developed turbulence. We will span a resolution from 1024^3 to 4096^3 collocation points. The latter will be a preliminary test to be extended in a dedicated project.

2. Turbulence in Quantum Fluids and Complex Plasma Flows

In this area, we aim to numerically investigate, using the Gross-Pitaevskii (GP) equation, the statistical behavior of turbulent 2D inverse and forward cascade regimes, both transient and steady, to highlight universal properties and compare our results with experimental investigations. We aim to numerically characterize, by parallel finite-difference solvers, relativistic flows exhibiting complex hydrodynamical responses in the presence of collisional dynamics at the mesoscale, involving non-trivial thermal effects.

We will also use hydro-kinetic mesoscale schemes to address the following novel topics: development of hydro-kinetic schemes capable of solving warm fluid closures for the Vlasov equations, modeling ion motion in the plasma acceleration process, and detailed characterization of thermal effects in plasma waves with quantitative assessments for the improvement/deterioration of wakefield acceleration.

3. Active and Non-Equilibrium Systems

We aim to numerically study, using cutting-edge parallel solvers, non-equilibrium phase transitions, and the role of topological defects in active systems at both the microscopic and continuum levels. Through large-scale Molecular Dynamics simulations (using the open-source software LAMMPS) of Active Brownian Particles (ABP), we will examine the collective behavior of active particles. Our focus includes investigating the role of defects in the universal character of topological transitions in ABP.

At the continuum level, we aim to model self-propelled droplets and liquid crystals in the presence of external fields and chirality. The interplay between topological defects and flow becomes particularly relevant when complex and active fluids are geometrically confined. We will apply multiphase mesoscopic 3D Lattice Boltzmann approaches, parallelized through the MPI standard, to study 3D chiral liquid crystal shells where the director field stabilizes helicoidal patterns and high-energy excitations, such as skyrmions. By adding active stress in models for multicomponent fluids in the 3D Lattice Boltzmann approach, we will also study the emergence of self-propelled directed motion in active emulsions, due to the coupling between induced flow and topological defects. These simulations requires huge system sizes (L=512,1014, 2048 in lattice units) and long numerical experimetns in order to reach the relevant space and time scales. To tackle it, we will exploit our parallel domain decompostion with MPI implemented in our LB solver, and the resources avaible at CINECA, using multi nodes runs (up to 20 nodes for each run on LEONARDO Gneral Purpose).

Quantum Information

Attività prevista per il 2026: QUANTUM

Our research group develops **Quantum TEA**, a suite of tensor network methods and algorithms designed to address a wide range of problems in quantum many-body physics, optimization, and quantum information science. A central focus is the simulation of ground state properties and time evolution in condensed matter and high-energy physics. Quantum many-body physics poses complex computational challenges that require advanced numerical tools. Among the most successful frameworks are tensor network methods, such as matrix product states (MPS) and the density matrix renormalization group (DMRG), which we extend and optimize for modern applications.

We develop algorithms that go beyond traditional one-dimensional systems to include higher-dimensional models, long-range and all-to-all interactions, and disordered systems such as spin glasses. These models are not only physically rich but also computationally relevant, as spin-glass Hamiltonians naturally map to hard combinatorial optimization problems.

A key research direction involves the simulation of lattice gauge theories (LGTs), which are central to non-perturbative studies in high-energy physics. Tensor network methods have achieved notable results in simulating LGTs in (1+1) dimensions, for both Abelian and non-Abelian gauge groups. More recently, these methods have been extended to Abelian theories in (3+1) dimensions and non-Abelian SU(2) models in (2+1) dimensions. We are particularly interested in advancing real-time simulations of scattering processes and other dynamical phenomena in gauge theories.

Complementing our many-body work, we apply tensor networks to a variety of combinatorial optimization problems, including the knapsack problem, graph coloring, and classical Potts models. Our methods also extend to quantum-inspired approaches for lattice-based and post-quantum cryptography, where understanding structure and entanglement aids in evaluating cryptographic hardness and designing efficient algorithms. Currently, we are investigating the problem of quantum compilation framed as an optimization problem and study the emergent many-body physics from the quantum circuits phase space. This bridges algorithmic design and physical intuition, aiming to support the development of efficient and noise-resilient circuits for near-term quantum devices.

A branch of our software suite is **Quantum Matcha Tea**, a quantum circuit emulator based on tensor network techniques—specifically the MPS and TTN ansatz. This tool enables efficient simulation of quantum circuits, including the modeling of noise via the quantum trajectories method. It provides a platform for benchmarking quantum algorithms with a particular focus on entanglement generation, offering insights into quantum advantage, error resilience, and circuit complexity.

Quantum Information

Attività prevista per il 2026: LINCOLN

Research Unit: LINCOLN (group IV, CSN4), Perugia Section.

Associated researchers: 5 people, 5FTE
Brodoloni Luca (PhD student, Unicam, 100%), Cantori Simone (PhD student, Unicam, 100%), Midei Giovanni (PhD student, Unicam, 100%), Pilati Sebastiano (PA, Unicam, 100%, loc. resp.), Gabriele Spada (Postdoc, Unicam, 100%).

Project title: *Simulating complex quantum systems via hybrid stochastic-neural algorithms*

Project description: The focus of our research plan is on performing accurate computer simulations of complex quantum systems via a combined use of stochastic algorithms, chiefly quantum Monte Carlo (QMC) methods, deep learning methods, as well as sparse linear algebra libraries (e.g., cupy) executed on high performance computers. First, we will address random spin models relevant to quantum simulation platforms such as Rydberg atoms trapped in optical tweezers and ion traps. One of our goals is to guide experimentalists to the observation of intriguing phases of matter due to frustrated interactions and disorder, chiefly spin-glass phases [1]. Another goal is to investigate the possible synergies between quantum computers and classical deep learning techniques [2], mostly focusing of the computational task of simulating quantum systems via an emergent paradigm, nowadays referred to as sample-based quantum diagonalization. To reach these goals, we will employ quantum Monte Carlo codes boosted by neural-network-based variational wave functions, as well as sparse eigenvalue solvers (cupy) combined with autoregressive neural networks.
Our QMC codes exploit shared memory parallelism, implemented via automatic loop parallelization in NUMBA. Furthermore, ensemble averaging of over disorder realizations can be distributed over different cores and/or nodes, with virtually no data communication. We implemented this job-farming protocol via MPI4PY. Overall, our QMC simulations exploit hybrid OPENMP-MPI parallelism and efficiently scale on multicore-multinode CPU clusters. Furthermore, we plan to train autoregressive deep neural networks, implemented in PYTORCH, while also solving large sparse linear algebra problems via cupy. Therefore, we are also requesting a smaller amount of compute time on the GPU cluster.

Requests of HPC resources for 2026:

- CPU cluster [LEONARDO-DCGP (CPU cluster)]: 448000 core hours (112cores x 10 nodes x 5h x 80 runs= 470400 core hours).
- GPU cluster [LEONARDO (GPU cluster)]: 8000 core hours (32cores x 1node x 5hours x 50 runs).

References:

[1] L. Brodoloni, S. Pilati, "*Zero-temperature Monte Carlo simulations of two-dimensional quantum spin glasses guided by neural network states*", Physical Review E 110, 065305 (2024), Editors' Suggestion

[2] S. Cantori, A. Mari, D. Vitali, S. Pilati, "Synergy between noisy quantum computers and scalable classical deep learning", EPJ Quantum Technology 11, 45 (2024)

Condensed matter

Attività prevista per il 2026: TIME2QUEST

A. Sindona[1], M. Pisarra[1], N. Logullo[1], G. Stefanucci[2], O. Pulci[2], M. Palummo[2], E. Perfetto[2], S. Achilli[3], G. Onida[3]
[1]Gruppo Collegato INFN di Cosenza (CS), [2]Sezione INFN di Roma Tor Vergata (RM2), [3]Sezione INFN di Milano (MI)

As outlined in its project summary for 2024–2026, the NemeSYS/Time2Quest Specific Initiative (SI), funded by INFN since 2017, focuses on developing and applying high-performance computational strategies to investigate excited-state properties, transport phenomena, and many-body effects in low-dimensional systems. These efforts are closely aligned with the advancement of emerging quantum information technologies.
The requested CPU hours, detailed at the end of this proposal, are essential for advancing the understanding of many-body and correlated-electron phenomena in selected heterostructures and functionalized configurations of two-dimensional materials, particularly those based on graphene and transition metal dichalcogenides. Due to reduced dielectric screening, these systems exhibit enhanced many-body interactions and support unconventional, often topologically nontrivial, quasiparticles and excitons [1–3]. These properties make them promising candidates for next-generation electronic and optoelectronic technologies, with potential applications in quantum information processing and sustainable energy.
The simulations will target three main research directions:
• **Ground-state and electronic structure.** Density-functional theory (DFT) calculations will be carried out using ABINIT [4] and QUANTUM ESPRESSO [5].
• **Excited-state properties.** Many-body perturbation theory simulations based on the GW approximation and the Bethe–Salpeter Equation (BSE) will be performed with the YAMBO code [6], optimized for GPU architectures at CINECA. M. Palummo, from the RM2 unit of this SI, is part of the YAMBO developer and superuser team.
• **Ultrafast dynamics.** Time-dependent DFT (TDDFT) simulations will employ in-house codes developed within the CS unit by A. Sindona and M. Pisarra [7, 8], as well as the CHEERS code [9], which implements nonequilibrium Green's function (NEGF) methods and is partly developed by G. Stefanucci and E. Perfetto from the RM2 unit.
The DFT step is relatively inexpensive, whereas GW, BSE, and TDDFT simulations are computationally intensive and require massive parallelization, making them well suited for the LEONARDO-Booster system.
The following topics and related simulations will support the core applications of the SI's 2026 research program:
• **Plasmon excitations and dielectric, electromagnetic, and fundamental properties** of graphene-derived, transition metal dichalcogenide–based, and magnetic systems: DFT + TDDFT + GW/BSE codes.
• **Electronic and structural properties** of low-dimensional layered materials, including twisted multilayer graphene and multilayer domains in nonporous graphene: DFT + TDDFT codes.
• **Quantum thermodynamics within a density-functional framework**, including interacting electrons in flat-band systems, electron delocalization in 2D Mott insulators, and vibronic transitions in molecules: DFT + TDDFT + GW/BSE + NEGF codes.
• **Quantum information processes**, including information transfer in spin systems, quantum kernels for data analysis, and Majorana bound states in 2D electron gases: DFT + TDDFT + NEGF codes.
In summary, the requested computational resources will enable comprehensive, state-of-the-art simulations to fully exploit quantum phenomena in low-dimensional materials, thereby driving fundamental advances in correlated electron systems confined to low dimensions and fostering innovations in quantum information processing.

CPU Time Request
LEONARDO Booster: 2000000
LEONARDO Data-Centric: 200000

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[1] K. S. Novoselov *et al.*, *Science* **353**, aac9439 (2016).
[2] M. Palummo, K. Yamashita, G. Giorgi, in *Sustainable Strategies in Organic Electronics*, pp. 391–422 (2022).
[3] L. Bastonero, G. Cicero, M. Palummo, M. Re Fiorentin, *ACS Appl. Mater. Interfaces* **13**, 36221 (2021).
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[6] D. Sangalli *et al.*, *J. Phys.: Condens. Matter* **31**, 325902 (2019).
[7] C. Vacacela Gomez, M. Pisarra, M. Gravina, J. M. Pitarke, A. Sindona, *Phys. Rev. Lett.* **117**, 116801 (2016).
[8] A. Sindona, M. Pisarra, S. Bellucci, T. Tene, M. Guevara, C. Vacacela Gomez, *Phys. Rev. B* **100**, 235422 (2019).
[9] Y. Pavlyukh, R. Tuovinen, E. Perfetto, G. Stefanucci, *Phys. Status Solidi B* **261**, 2300502 (2024).

Richieste di risorse di calcolo

- Richieste su Leonardo (Cineca)
- Rimodulazione per rientrare nella disponibilità di risorse: **100 Mch (DCGP)** e **12 Mgpuh (Booster)**
- Criteri: onerosità computazionale, storico, capacità di utilizzo completo e regolare
- Uso 2024: 160 Mch (DCGP) e 10 Mgpuh (Booster)

Richieste 2026	LEONARDO DCGP		LEONARDO booster		
Iniziativa Specifica	richiesta (corehours)	proposta (corehours)	richiesta (gpuhours)	proposta (gpuhours)	proposta (corehours)
biophys	1,000,000	650,000	250,000	250,000	2,000,000
enesma	50,000	50,000	500,000	300,000	2,400,000
fldturb	7,000,000	4,500,000	125,000	112,500	900,000
gagra	500,000	400,000	37,500	25,000	200,000
indark	1,000,000	900,000	375,000	375,000	3,000,000
lincoln	448,000	400,000	1,000	1,250	10,000
lqcd123	5,600,000	3,500,000	3,400,000	3,400,000	27,200,000
monstre	2,200,000	1,550,000	4,375	4,375	35,000
time2quest	3,210,200	1,000,000	400,000	375,000	3,000,000
neumatt	6,000,000	4,000,000	12,500	12,500	100,000
npqcd	32,000,000	22,250,000	3,400,000	3,125,000	25,000,000
nucsys	1,600,000	800,000	250,000	125,000	1,000,000
pml4hep	100,000	100,000	31,250	25,000	200,000
qcdlat	50,000,000	33,500,000	2,500,000	2,375,000	19,000,000
qftatcol	10,000,000	6,000,000	62,500	31,250	250,000
quantum	500,000	500,000	125,000	125,000	1,000,000
sft	976,460	900,000	137,500	125,000	1,000,000
sim	2,000,000	1,500,000	37,500	31,250	250,000
teongrav	14,000,000	12,500,000	500,000	500,000	4,000,000
TEST		5,000,000		681,875	5,455,000
TOTALE	**138,184,660**	**100,000,000**	**12,149,125**	**12,000,000**	**96,000,000**

- Richieste su HPC Bubbles: **2 Mch** (8 Keuro)
- Motivazione: accesso per test di ambiente software, performance e connessione tra nodi su questi nuovi sistemi HPC

Spazio di storage

- Occupazione spazio disco su Leonardo al CINECA

OCCUPAZIONE AREA WORK DI LEONARDO PER PROGETTO											
	LEONARDO-booster ()			LEONARDO-DCGP (_0)				Complessivo			
progetto	spazio occupato (TB)	spazio assegnato (TB)	percentuale occupazione spazio		spazio occupato (TB)	spazio assegnato (TB)	percentuale occupazione spazio		spazio occupato (TB)	spazio assegnato (TB)	percentuale occupazione spazio
biophys	0.80	1.00	80.2	biophys_0	0.64	1.00	64.3	biophys	1.44	2.00	72.2
enesma	0.58	1.00	57.5	enesma_0	0.00	1.00	0.0	enesma	0.58	2.00	28.8
fldturb	0.43	1.00	42.9	fldturb_0	0.00	1.00	0.0	fldturb	0.43	2.00	21.4
gagra	0.20	10.00	2.0	gagra_0	0.00	1.00	0.0	gagra	0.20	11.00	1.8
indark	0.89	1.00	88.8	indark_0	0.01	1.00	1.0	indark	0.90	2.00	44.9
lincoln	0.00	1.00	0.0	lincoln_0	0.00	1.00	0.2	lincoln	0.00	2.00	0.1
lqcd123	52.00	70.00	74.3	lqcd123_0	0.00	1.00	0.0	lqcd123	52.00	71.00	73.2
monstre	0.00	1.00	0.0	monstre_0	0.00	1.00	0.0	monstre	0.00	2.00	0.0
nemesys	0.00	1.00	0.0	nemesys_0	0.00	1.00	0.0	nemesys	0.00	2.00	0.0
neumatt	0.00	1.00	0.0	neumatt_0	0.00	1.00	0.0	neumatt	0.00	2.00	0.0
npqcd	86.00	200.00	43.0	npqcd_0	0.00	1.00	0.0	npqcd	86.00	201.00	42.8
nucsys	1.80	4.00	45.0	nucsys_0	0.19	1.00	19.0	nucsys	1.99	5.00	39.8
pml4hep	0.09	1.00	8.7	pml4hep_0	0.00	1.00	0.0	pml4hep	0.09	2.00	4.3
qcdlat	19.00	20.00	95.0	qcdlat_0	55.00	200.00	27.5	qcdlat	74.00	220.00	33.6
qftatcol	0.01	1.00	1.0	qftatcol_0	0.00	1.00	0.0	qftatcol	0.01	2.00	0.5
quantum	0.06	1.00	6.4	quantum_0	0.00	1.00	0.0	quantum	0.06	2.00	3.2
sft	0.55	1.00	54.6	sft_0	0.00	1.00	0.0	sft	0.55	2.00	27.3
sim	0.00	1.00	0.0	sim	0.00	1.00	0.0	sim	0.00	2.00	0.0
teongrav	26.00	50.00	52.0	teongrav_0	1.40	50.00	2.8	teongrav	27.40	100.00	27.4
TOTALE	***188.40***	***367.00***	***51.3***		***57.24***	***267.00***	***114.8***		***245.64***	***634.00***	***38.7***

- Non ci sono criticità; margine per accogliere eventuali necessità in corso d'anno
- Nessuna richiesta di spazio di storage su disco
- In contatto con il CNAF per l'accesso a **1.5 Pb** di tape finanziato l'anno scorso
- Nessuna richiesta incrementale di spazio di storage su tape