CSN4 - Risorse di calcolo per il 2025

Bologna, 5 Settembre 2024

Leonardo Cosmai, Michele Pepe



Projects in Computational Theoretical Physics

Lattice QCD

LQCD123 NPQCD **QCDLAT** SFT SIM GAGRA

Cosmology and Astroparticle Physics

TEONGRAV INDARK NEUMATT

Physics of Complex Systems

BIOPHYS FIELDTURB ENESMA

~ 300 researchers

Nuclear Physics

MONSTRE **NUCSYS**

Condensed Matter



Particle Physics Phenomenology

QFTATCOL PML4HEP

> Quantum Information

QUANTUM LINCOLN



Activities planned by the **Computational Theoretical Physics projects in 2025**

L. Cosmai, M. Pepe - CSN4 2024









Lattice QCD

Study of QCD in extreme conditions



- Lattice QCD is an essential tool for obtaining precise first-principle theoretical predictions of the hadronic processes underlying many key experimental searches.
- As experimental measurements become more precise, lattice QCD will play an increasingly important role in providing the necessary matching theoretical precision.

Precision studies of flavor physics, within and beyond the Standard Model



LATTICE 2024

The latest lattice QCD results related to the **muon g-2 problem** have significantly reduced the discrepancy between theoretical predictions and experimental measurements. The new calculations now differ from the experimental measurements by only 0.9 standard deviations. This finding is critical as it challenges the previously observed tension between experiment and theory, which had fueled speculation about new physics beyond the Standard Model.



LQCD123 (F. Sanfilippo)

1 - Computation time requests for year 2025

A) Continuation of the generation of a fifth lattice spacing of 2+1+1 QCD configurations, with physical pion mass: O(200) trajectories with very fine lattice spacing (ensemble "cE112" L = T/2 =5.46 fm, a=0.049 fm), using the framework discussed in *PoS* LATTICE2022 (2023) 340, arXiv:2212.06635.

Motivation: increase the statistics and improve a key ensemble needed to properly extrapolate to the continuum limit the observables involving heavy quarks and/or large transferred momentum, such as the semileptonic decays of *B* mesons.

Estimated cost: 250k node-hours on Leonardo (GPU cluster)



B) determination of the rate of the $B_s \rightarrow \phi \gamma$ decay.

Motivation: studying a rare FCNC decay, suppressed in the Standard Model (SM), but experimentally measured, allows to test the accuracy of SM and constrain New Physics. Only a very old quenched calculation is available to date.

Estimated cost: 250k node-hours on Leonardo (GPU cluster)



C) determination of the two-pion states interaction, describing the ρ resonance on a lattice.

Motivation: predict from the first principles, the $e^+e^- \rightarrow \pi^+\pi^-$ cross section, to cast light on the discrepancy recently emerged between CMD3 and KLEO/BABAR experiments, strictly related to the muon g-2 puzzle

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



D) Weak annihilation contribution to the inclusive semileptonic decays of heavy mesons

Motivation: include the neglected contribution in our approach for the calculation of the inclusive semileptonic decays of heavy mesons, presently the largest systematic error in our recent study, published in JHEP 07 (2022) 083. The calculation will use HLT method, applied to gluonicdisconnected contraction computed using the one-end-trick.

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



E) Charming-penguin contributions to $b \rightarrow s$ transition

Motivation: explore the feasibility of the calculation of the charming-penguin contribution to the correlation function of $b \rightarrow s$ transition, needed to properly treat the long-distance contribution arising from charm loop, presently estimated by means of models. The method we aim to apply, if successful, will allow to study precisely a whole new class of processes, where such a contribution is expected to be sizable.

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

2 - Storage requests for year 2025 (and following)

1) 1 Pb of disk space on Leonardo for the storage of the gauge configurations on Leonardo

The gauge configurations customarily used in our project needs to be stored on Leonardo machine, which will be used for most of the projects. The requirements is of 1 Pb of disk space, to accommodate the subset of gauge configurations more frequently used. They will be migrated from the 2024 project, and partially downloaded from Julich computing center (Germany) where a full repository is available.

2) 5 Pb of disk +10 Pb tape space to store the low-lying eigenvectors of the Dirac operator

We recently developed a variation of the Low-Mode-Averaging approach, which will allow to greatly improve the statistical accuracy of our future calculations, at a little additional **computational cost**. Indeed the approach is based on the improvement of the infrared part of the correlation functions alone, therefore it requires only the evaluation of suitable matrix elements between the used stochastic sources and the low-lying eigenvectors of the Dirac operator. This usage of the eigenvectors has a numerical cost <u>much reduced</u> with respect to the main calculation, nonetheless induces a great numerical gain in the computation.

The eigenvectors have been computed on Leonardo machine, for ensembles B64 and C80, along the EuroHPC project EHPC-EXT-2023E01-007, with an approximate cost of 15Mcorehours, and a disk occupation of approximately 5 Pb. The eigenvectors for ensembles D96 and E112 are presently under production and will require approximately twice this amount of resources, owing to the larger volumes involved.

To leverage the cost of future applications of the LMA method, the computed eigenvectors needs to be <u>permanently stored (>3 years)</u>, and recalled when needed, to be processed to build the IR part of the correlation function of interest. For the set of mentioned gauge ensembles, this **requires** approximately 15 Pb of disk. Achieving persistency of such amount of data is outside the scope of the project where they are getting generated, therefore we request to grant us the needed space. The storage allocation <u>might be split between disk and tape</u>, with a suggested 5 Pb Disk + 10 Pb tape. The tape disk might be not directly connected to Leonardo, provided high-speed connection is available to the Leonardo machine, where the calculations will be most typically run.

(M. D'Elia)

HPC Research Program for year 2025, I.S. 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 2025 are the following:



A) HIGH TEMPERATURE QCD, TOPOLOGY AND AXION PHENOMENOL-OGY

In the last year, we have put the basis for a considerable progress to be achieved in the next future. In particular, we have recently finalized [5] the extension to full QCD of the algorithm to defeat topological freezing originally developed for Yang-Mills theories in Ref. [6], which implements parallel tempering on boundary conditions.

The new algorithm will be used to approach extremely fine lattices (with lattice spacings going down to 10^{-2} fm), in order to study the topological properties of QCD (in particular, the topological susceptibility [7]) with physical quark masses for temperatures of the order of 1 GeV, which are those relevant to axion phenomenology.

A preliminary task for this project will be represented by the determination of a line of constant physics, going down to such small lattice spacings, for the discretized theory (adopting improved staggered fermions) with 2+1+1 flavours, since at such high temperatures the contributions from dynamical charm quarks cannot be neglected any more.

All the production stages will be run on GPUs (hence on Leonardo-booster), with two different levels of parallelization, the first represented by the parallel tempering algorithm itself, which runs multiple RHMC simulations for different copies of the gauge system, the second represented by the distribution of each single copy over multiple GPUs. That will allow us to scale very efficiently to $O(10^2)$ GPUs used in parallel for a single run.

Gauge configurations produced in this context will be used to determine other quantities relevant for 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 [8].

We plan to extend the determination of the sphaleron rate to higher temperatures and, at the same time, we aim at computing the same quantity at non-zero momentum, since this could be of particular interest for phenomenological computations concerning the thermal production of axions during the cosmological evolution.

Furthermore, a 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. [9] for the electric conductivity in a magnetic background, in particular regarding their possible connection to the chiral magnetic effect.



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

In Ref. [10] we have provided a continuum extrapolated determination of the chiral condensate and of other low energy constants of QCD by numerical simulations with staggered fermions at the physical point. We plan to extend this program with the determination of other low

energy constants entering at the second order of chiral perturbation theory, in particular the so-called *l*7 constant, by applying to staggered fermions the strategies developed for twisted mass fermions [11]. In this case, the production of gauge configurations will be based on GPU, however the analysis of physical observables, which takes a considerable amount of time, will make use of general purpose CPU resources.

As a further line of research, we plan to extend our recent determination of the strong coupling in SU(3) [12] to a larger number of colours. This part will run mostly on CPUs.

Based on our previous studies [13, 14, 15, 16, 17], we plan to investigate the structure of flux tubes in Quantum Chromodynamics (QCD) with (2+1) flavours at finite temperature using physical quark masses. We aim to understand how the shape of the flux tube and the distribution of color fields and currents around static sources evolve across the deconfinement transition. Additionally, we will explore the impact of a constant chromomagnetic background field on the flux tubes. This part of the project will run mostly on GPUs for generating gauge configurations. The operators measurements will be handled mainly on CPUs

A precision determination of the flux tube properties and a comparison with effective string theory predictions for the static quark-antiquark potential will be performed in pure gauge theories, extending results of Refs. [18, 19, 20] with and without the insertion of a θ -term, with and without the addition of a trace deformation in the case of compactified theories. This part of the project will run mostly on CPUs.

C) PHASE DIAGRAM OF QCD AND QCD-LIKE THEORIES

We will pursue our efforts in the study of the phase diagram of QCD in the presence of external background fields [21], by completing a study regarding the dependence of the Roberge-Weiss transition on magnetic background fields. At the same time, we plan to start an investigation of the dependence of the chiral transition of QCD, both with and without background fields, on the number of flavours. This part of the project will run extensively on GPUs.

We will also investigate the QCD phase diagram under the influence of a constant chromomagnetic background field. Our goal is to determine how this field affects the deconfinement temperature. This project component currently runs on CPUs, but a port to GPUs is underway.

Finally, part of the computational efforts will be dedicated to the study of lowwer dimensional strongly coupled gauge models coupled to fermionic fields, in order 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.

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.

NPQCD (cont'd) (M. D'Elia)

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QCDLAT (M. Pepe)

QCDLAT INFN Research Project of the Theory Group (CSN4)

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:** 20

Description of the research activity

The aim of this proposal is to advance the frontiers of QCD research by exploring poorly known regimes characterized by extreme conditions and achieving high-accuracy theoretical predictions to search for potential signals of physics beyond the Standard Model (SM). Working in the framework of the lattice regularization, we will conduct non-perturbative investigations from first principles through Monte Carlo simulations. The development of new theoretical methodologies and innovative algorithmic techniques will be crucial to our project, enabling us to achieve numerical precisions at the percent level or better.

This proposal encompasses a wide range of significant and interesting phenomena across various energy scales. The behavior of QCD under extreme conditions – such as high temperatures and finite chemical potential – is crucial for nuclear physics, cosmology, and astrophysics, providing insights into the early stages of the Universe. Precise comparisons between theoretical predictions and experimental results for selected Electroweak and Strong processes may reveal new particles or interactions, expanding 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 2025 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 searching for BSM physics; precise determination of fundamental SM parameters; kaon-mixing matrix elements to constraint extensions of the SM; computation of isospin breaking corrections; precise determination of the matrix elements of ΔF=2 four-quark operators.
- QCD in extreme conditions: computation of transport coefficients in the Yang-Mills theory; calculation of non-static mesonic screening masses in QCD up to T≈100 GeV; 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 energy-momentum tensor; 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; shifted boundary conditions for QCD at finite T; simulations with light quarks and large volumes (master field simulations); numerical stochastic perturbation theory applied to chemical potential.

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: 60 Mch
- GPU-based partition: 400 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 tape

People participating to the project QCDLAT have been awarded relevant computer resources (European Calls PRACE, EuroHPC) 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.

Thus, it is important to store those configurations in a long-term way so that one can access at any time that Database to measure new quantities that have turned out interesting to compute. Considering that also many other configurations will be produced, we would like to confirm the request of 500 Tb of storage on tape.

Iniziativa scientifica SFT (Statistical Field Theory)

SFT (M. Panero)

Attività di ricerca previste per il 2025

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.

Le principali attività scientifiche che coinvolgono il calcolo ad alte prestazioni rientrano nell'ambito delle simulazioni di teorie di campo su reticolo. 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 una attenzione principalmente rivolta ad aspetti fondamentali, che vengono talvolta affrontati in modelli-giocattolo semplificati rispetto alle teorie che descrivono i sistemi fisici realizzati in natura, per un carattere di trasversalità per ciò che concerne le teorie fisiche che vengono studiate (che vanno da quelle orientate alla fisica delle particelle elementari alle alte energie a quelle mirate alla fisica della materia condensata e ai sistemi quantistici), per una buona produttività ed un buon impatto scientifico in relazione alle risorse investite, e per l'apertura a numerose collaborazioni internazionali.

Si prevede che il numero di ricercatori/ricercatrici coinvolti in queste ricerche durante il 2025 rimanga stabile (o abbia un leggero aumento) rispetto agli anni precedenti, in cui le risorse allocate sono state utilizzate con profitto. Quindi si auspica una conferma della frazione di budget riservato a questa iniziativa specifica (rispetto al quadro generale delle attività teoriche dell'INFN) in linea con le assegnazioni degli anni precedenti.

Le principali linee di ricerca previste per il 2025 comprendono:

- . Uno studio sistematico della ricostruzione di funzioni spettrali da reticolo, con una particolare attenzione all'analisi di decadimenti semileptonici dei mesoni pesanti, generalizzando il lavoro già pubblicato in JHEP 07 (2022) 083, in collaborazione con l'iniziativa specifica LQCD123.
- Lo studio dei dettagli della struttura del tubo di flusso in teorie di Yang–Mills basate su invarianza locale rispetto ai gruppi SU(N).
- . Lo studio dell'entropia di entanglement in teorie quantistiche in bassa dimensione, con particolare attenzione alla teoria scalare in 1 + 1 dimensioni.
- Lo studio del modello di Potts quantistico a tre stati con un campo esterno in 1 + 1 dimensioni, analizzando numericamente l'evoluzione del modello dopo che questo viene sottoposto ad un "quench" ovvero ad una variazione improvvisa del campo esterno.



SIM (M.P. Lombardo)

SIM: Strongly Interacting Matter

Utenti: MpL, Andrey Kotov, Anton Trunin, e collaboratori, Aldo Cotrone e studenti/collaboratori

Twisted Mass Fermions - Lattice QCD a temperatura finita

Da alcuni anni usiamo la formulazione twisted mass per studiare la fisica della QCD ad alta temperatura, ovvero a temperature comprese tra la temperatura critica Tc e 3-4 Tc.

La motivazione di questi studi è triplice: in primo luogo, si tratta di caratterizzare la regione studiata dagli esperimenti di collisioni di ioni pesanti ultrarelativistici; secondariamente, c'e' un interesse teorico generale nelle questioni associate al comportamento critico della QCD, anche in relazione alla possibile esistenza di crossover ad alta temperatura di natura incerta. In terzo luogo, vorremmo usare i risultati delle misure di topologia con metodi gluonici e fermionici per migliorare i limiti sulla massa dell'assioma in QCD, e tentare una misura diretta del potenziale dell'assione nell'intorno di Tc.

Piu' in dettaglio, vorremmo generare configurazioni tra Tc e 2Tc, nella regione del crossover, con masse fisiche dei quark, e per diversi coupling. Useremo i parametri individuati da ETMC, e temperature e volumi saranno scelti per estendere e completare gli ensemble esistenti (maggiori dettagli sul piano dei run sono ovviamente disponibili su richiesta). Queste configurazioni verranno usate per i seguenti studi:

- Analisi di un crossover molto rapido osservato intorno a T 300 MeV la cui natura è tuttora poco chiara. I risultati che stiamo analizzando adesso confermano questo crossover veloce, segnalato anche da grandi fluttuazioni. Le osservabili includono condensato e suscettività chiare
- Nuove misure del condensato chirale, utilizzando una proposta da ETMC a temperatura zero, in collaborazione con membri della collaborazione.
- Osservazione del ripristino della simmetria nello spettro mesonico, in particolare nel settore scalare vogliamo investigare il comportamento del pione che si ipotizza possa sopravvivere la transizione chirale. Di nuovo in collaborazione con ETMC vorremmo misurare lo spettro eta- eta' per precisare i risultati che gia' abbiamo sul solo eta'
- Utilizzo delle osservabili topologiche per la massa e potenziale dell'assioma in QCD

2) Transizioni di fase in teorie olografiche

Si tratta di risolvere problemi di ottimizzazione e ODE/PDE, utilizzando soprattutto un nodo alla volta, ma anche sperimentando parallelismo. Si tratta di allocazioni esplorative, che usano una quantita' molto limitata di risorse

L. Cosmai, M. Pepe - CSN4 2024

GAGRA (M. Papinutto)



1. GAGRA RESEARCH PROJECT

The lattice regularisation of gauge theories offers the unique possibility of computing the functional integral numerically without any approximation through Monte Carlo techniques. One can thus obtain theoretical informations about the low-energy, non-perturbative regime of Yang-Mills theories and OCD with any number of colours N.

The main interest of our research project is the numerical computation of the low-energy spectrum of gauge theories. We are thus planning to compute the lowest glueballs and mesons masses in the large-N limit in order to compare them against the predictions of the models developed to solve analytically such theories (see e.g. Ref. [1,2]).

In the last two years we have written a code for the simulation of SU(N) pure gauge theories and the computation of the two-point correlation functions of Wilson loops of several lengths, classified according to the transformation properties under the cubic group and discrete symmetries (parity and charge conjugation). From the two-point correlators we have implemented the extraction of the low-lying glueball spectrum through the solution of the Generalized Eigenvalue Problem.

This computation faces the long standing problem of the exponential deterioration of the signal-to-noise ratio of the two-point correlation functions at large Euclidean time. This problem has been partially solved in the glueball case [3] allowing for the state of the art computations in [4]. After this study a new one [7] has been recently presented which goes up to N = 12 (the largest value of N ever simulated so far) and perform an extrapolation to $N = \infty$. The latter does not implements the algorithmic improvement developed in [3] and presents errors which seems exceedingly small, giving rise to tensions in the values of the mass of some states with respect to previous published results (e.g. in [4]).

In the last year we have implemented and tested the two-level sampling proposed in [3] and investigated in [5,6], together with the smearing of gauge links used to build the Wilson loops which creates or annihilates the glueball states. We are presently running a large scale simulation for N = 3 in order to test the performances of the algorithm, extract the low-lying glueball spectrum and test it against the results present in the existing literature. This study will be presented at the Lattice 2024 conference.

In the coming year we thus plan to start new extensive simulations to compute the lowlying glueball spectrum at large values of N and small lattice spacings, in order to be able to perform systematically the continuum limit at each N and then a safe extrapolation to the $N = \infty$ limit.

In the case of the meson spectrum, the problem of the exponential deterioration of the signal-to-noise ratio does not affects the pseudoscalar channel while in the other channels is less dramatic than in the glueball case. Despite this, even in the most recent/state of the art study of meson masses at large-N [8], no continuum limit has been taken. We are presently writing the code to compute two-point meson functions at arbitrary values of N, planning to perform a study in which the continuum limit is taken for each N, possibly increasing the number of N on which the large-N limit is taken.

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COSMOLOGY AND ASTROPARTICLE PHYSICS

L. Cosmai, M. Pepe - CSN4 2024



TEONGRAV (B. Giacomazzo)

TEONGRAV collaboration is composed of 108 members in 10 research units. The current number of HPC users is 33. We need HPC resources for the following projects:

(1) 5. Special relativistic MHD simulations of short GRB jets: We will use the PLUTO code to **1. Numerical Relativity Simulations of Compact Binary Mergers**: we shall use the publicly investigate the propagation of jets across realistic NS-NS post-merger environments, with particular available Einstein Toolkit code to run simulations of compact binary mergers, neutron stars (NSs) and attention to electromagnetic dissipation properties, using both ideal and resistive relativistic MHD. The black holes (BHs), in order to study their gravitational wave (GW) and electromagnetic (EM) emission. goal is to connect our models with short GRB observations. We already performed preliminary The Einstein Toolkit uses a hybrid parallelization approach (OpenMP and MPI). The toolkit has been simulations on the CINECA clusters Marconi and Galileo100. PLUTO simulations can run only on already used on CINECA CPU clusters (including LEONARDO DCGP). A new version of the toolkit CPU (a GPU version of PLUTO is being developed). able to run on GPUs is currently being developed, and is going to be tested on the GPU nodes of LEONARDO.

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 **0** 2. Numerical Relativity Simulations of Black Hole Mergers Beyond General Relativity: We will context, to study in detail potential GW sources for LISA and ET. We will investigate the conditions simulate the gravitational collapse of fundamental fields and BH mergers in motivated extensions of under which these objects form and how they evolve and pair in binaries. GIZMO has been used on General Relativity both within an effective field theory approach and at the fully nonperturbative level. the Galileo100 and Marconi CINECA clusters, and is fully parallelised with MPI and OpenMP, but no In both cases we shall use codes developed in the Einstein Toolkit and in GRChombo, as well as GPU parallelisation is present at the moment. domestic codes. The codes make use of CPU clusters.

1 7. Magnetohydrodynamical simulations of accretion discs and circumbinary discs around **0** 3. Bayesian parameter estimation: We shall perform Bayesian inference of single GW events and massive black holes: Exploiting a novel post-Newtonian and GRMHD implementation in the code population studies, both to study parameter estimation and waveform systematics, and also to assess GIZMO, based on the work by Lupi (2023), we will explore the transition from the Newtonian to the whether current and future GW detectors can infer the properties of multiple formation channels for relativistic regime of accretion flows around single and binary massive black holes to study the BH binaries. We will use the BILBY and GWpopulation infrastructures. The latter runs on GPUs. We electromagnetic counterparts of GW sources for LISA and ET. 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.

INDARK (M. Lattanzi)

InDark - Description of the research program for 2025 M. Lattanzi for the InDark affiliates

In 2025, 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), as well as galaxy surveys (Euclid), as well as their cross-correlation. We detail the activities in more detail in the following.

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.



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.

We have now completed the implementation of the new code for parameterised Modified Gravity theories that was started in 2022. The code, called PANDA, is a compile-time module of the parallel simulations 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. We will develop and test statistical methods for next generation CMB and LSS experiments, such as Simons Observatory, CMB-S4, LiteBIRD, Euclid, including validation phase on synthetic datasets through Monte Carlo analysis.

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). This activity is based on Einstein-Boltzmann codes and associated Markov Chains MonteCarlo samplers, all massively parallelized and CPU-based.

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.

NEUMATT (R. De Pietri)

Scientific project for the year 2025 (**NEUMATT**)

NEUMATT (composed of the Ferrara, LNGS, Catania, and Pisa Units) is focused on the study of the The typical cost of a 3D merger simulation (with magnetic fields) at a resolution of the order of 200 m (the structure of neutron stars (NSs), ranging from the investigation of the relevant microphysics and its minimum resolution required) for an evolution lasting 50 ms requires 237 GByte of allocated memory and interplay with the structure and composition of compact stars and the observational implication of the is performed using 512/1024 cores and **200k core hours**, while the activation of magneto resistive double neutron stars' complex and rich phenomenology to the observed signal in the universe (electromagnetic the CPU time needed. Higher resolution simulations require 2048 cores. We estimated the need to and gravitational) coming from astrophysical system that includes neutron stars. The main focus of the simulate at least 20 configurations at different resolutions. That would lead to an estimate of **4 Mcore** computational request is to study the effect of the EOS for nuclear matter on the gravitational signal **hours** for the simulation at the best resolution. The additional request cost of the lower resolution generated by Neutron Star Mergers and on the dynamics of the ejected matter. The study of this effect is simulation and the development and optimization of the code should be added, for a total of 76 Mcore particular timing with the start on May 24, 2023 of Observing Run 4 (O4) that will last to June 2025 and in hours- The request allocation amounts to 6 Mcore hours on CPU clusters (Like Leonardo CPU cluster). A anticipation of observing period O5 expected for the middle of 2027 by the LVK interferometers. In that small amount of ~3000 node hours (100000 corehours) is requested on GPU machines to start code period is expected, at least one event like GW170817 with a multi messenger observation of a binary porting. The requested disk space is 10TByte since checkpoint size is of order 0.25 TByte and full 3D neutron star merger that will need to be interpreted to infer the properties of the EOS. output for a high resolution simulation is order 1TByte.

The request aims to fulfill the need for the final development of the required codes with enough resources to validate the developing codes needed to describe the dynamics of matter effectively described by genuine EOS (developed and studied by the group) and the magnetoresistive preparatory to performing PRACE allocation for large-scale simulations. The last years were mainly focused on developing a new code (MIR) in the testing and validation phase [2]. The system is now ready to perform the final validation and the first set of physical simulations of the effect of real EOS and resistive effect in the dynamics of binary neutron star mergers in the presence of magnetic fields.

The amounts of requested computational resources are motivated to simulate the mergers of compact stars in numerical relativity and the subsequent kilonovae light curves: we aim to investigate how different models for the EoS and different astrophysical scenarios (one or two families of compact stars) affect those kinds of signals. In particular, the amount of mass ejected, its entropy, and its chemical composition are vital for determining the properties of the kilonovae. one of the missing ingredients is the effect of the dissipative process (like resistive effects) on the dynamics of magnetic fields (resistive magneto-hydro-dynamics).

Most relevant publication for the proposal:

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study the effect of resistivity in Neutron Star dynamics", in preparation.





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PHYSICS OF COMPLEX SYSTEMS

L. Cosmai, M. Pepe - CSN4 2024





BIOPHYS (G. La Penna)

The INF24_biophys project (coordinator Giovanni La Penna) collects the activity of 7 groups involved in high-performance computing in the field of biophysics. Useres of HPC resources are 29. 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 and advanced computational methods, all requiring HPC resources, to different scales relevant to biology: 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 2024-2025. 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 and free electron lasers (FEL).

POLITO - We use a computational model that we have recently introduced 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. We take into account the effects of molecular crowding to understand how the efficiency of sorting may depend on the number of molecular species involved. 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 - We apply topic modelling techniques for the identification of cancer subtypes, extending a specific class of topic models to allow a multi-omics approach. We are able 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.
 UNINA - We develop polymer models to study the three-dimensional (3D) organization of DNA and its temporal dynamics. We investigate 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 - Research activities are focused on the development and application of numerical simulation methods for modeling complex macromolecular systems of biological interest through the use of various HPC resources and facilities. We investigate the structural and dynamic properties of voltagegated ion channels and the effects of some pathogenic mutations causing their dysfunction. We are also applying deep neural networks to describe atomic interactions.

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

FIELDTURB (G. Gonnella)

INFN Computational Resource Requests for 2025

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 nonstationary 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. Besides this community service, we intend to further tackle problems related to modeling the evolution of turbulent quantities from a subset of partial observations, and to develop data reconstruction and data assimilation tools using both data-driven and physics-informed machine learning architectures for idealized high Reynolds number flows of theoretical and applied interest. 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 also plan to simulate the 2D Navier Stokes to check the presence of hidden symmetries in the inertial range of a passive scalar advected by the flow, for which we need high-resolution simulations up to 16384² grid points.

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. Within the GP model, we plan to systematically investigate the generation and characteristic features of waves depending on the shape and velocity of the moving obstacle. 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 and studying the effect of the diffusion properties of clusters of active particles at the collective level.

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. A classification of topologically charged defect lines in 3D will also help in deepening the connection between these non equilibrium topological configurations, occuring in active turbulence states, and Majorana quasis particles. 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 decomposition 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).

ENESMA (F. Viola)

Project description

Turbulent hemodynamics

The main objective of the project is to carry out a direct numerical simulation of the whole cardiac hemodynamics, The code is complemented with various immersed boundary (IB) techniques to handle complex moving and solving up to the smallest fluid dynamics spatial scale (~ 40μ m) and investigate the transitional nature of the deforming geometries. The structural mechanics is based on the Fedosov's interaction potential method [1] impulsive jets originated by the chambers contraction, namely aortic, mitral, tricuspid and pulmonary jets. We to account for the mechanical properties of the biological tissues, which are anisotropic and nonlinear. The will consider the case of a healthy heart with an ejection fraction of about 65% beating at 70 bpm, the experience electrophysiology, responsible for the active potential propagation in the cardiac tissue triggering the active of the group in the cardiac modelling will ensure a fast start of the project. This is also a preliminary step before muscular tension, is incorporated by means of a bidomain model [3] that can account for the different cellular investigating pathologic cases. models of the various portions of the heart. All these models are three-way coupled with each other, thus The hemodynamics within the whole human heart will be solved using a multi-physics computational approach capturing the fully synergistic physics of the heart.

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.

Essential bibliography

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NUCLEAR PHYSICS

L. Cosmai, M. Pepe - CSN4 2024





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MONSTRE (A. Roggero)

MONSTRE:

MOdeling Nuclear STructure and REactions

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 nuclear response of atomic nuclei is calculated by using the QRPA approach for deformed systems and The KSHELL code, massively employed in shell-model calculations, can easily run on a Linux PC with a manythe Second RPA for spherical ones. From a computational point of view, the most demanding operations required core CPU and OpenMP library, as well as on a state-of-the-art massive parallel computer with hybrid MPI+OpenMP these calculations are the evaluation of the matrix elements to be diagonalized and the diagonalization of the parallel programming. It exhibits a strong scaling of the parallel computation tested on different HPC systems, corresponding eigenvalue problem. The dimensions of the matrices are of the order of $10^7 - 10^9$. PETSC/SLEPC included the CINECA Marconi and Galileo100 clusters. In order to store the calculated wavefunctions for all the libraries are employed to handle the matrices and for their diagonalization, using the MPI parallel protocol. These systems we plan to calculate we need about 1Tb of storage. All the libraries needed are already installed on the libraries are already available on the CINECA infrastructure. The typical storage needed is of the order of 500 Gb. CINECA machines.

RPA-based calculations (Random Phase Approximation)

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.





NUCSYS (M. Viviani)

Note: in 2024 some researchers (L. Coraggio, N. Itaco, G. Di Gregorio), associated before to the I.S. MONSTRE, moved to I.S. NUCSYS. However, the corehours assigned to NUCSYS have not increased with respect to the previous years, making difficult to complete a series of calculations performed in collaboration (matrix elements of the weak current operators needed for the study of weak interaction of nuclei, see project 1 below). For that reason, for 2025 we kindly ask for a substantial increase of core-hours.

The scientific projects which will be developed using the CINECA resources are:

1) Weak interaction in nuclei. Weak interaction processes provide unique probes of the physics of nuclei and fundamental symmetries and play a central role in astrophysics. Surprisingly, key aspects of this well-known decays remain a puzzle. In particular, when calculations of Gamow-Teller transitions of the spin-isospin-lowering operator are confronted with experiment, some renormalization, or "quenching" q, of the axial current is needed, with a typical q = 0.75 in shell-model. We study these processes within the framework of the realistic shell model (RSM). It provides a consistent approach to derive effective Hamiltonians and decay operators. In fact, the bare matrix elements of the NN potential, and of any transition operator, are renormalized with respect to the truncation of the full Hilbert space into the reduced shell-model model space, to account for the neglected degrees of freedom. We have successfully employed RSM to study, for different nuclei, allowed and forbidden single β -decay, the 2v $\beta\beta$ -decay, and to predict the nuclear matrix elements of their 0vββ-decay. To further validate our theoretical framework, we plan to extend our study to ordinary muon capture (OMC) decay process. This is a semileptonic weak interaction process quite like electron capture (EC), with the momentum exchange involved in, Q \approx 50 – 100 MeV, as for 0v $\beta\beta$ -decay. The computation of the wave functions is computationally challenging due to the high dimensionality of the problem, therefore it requires an HPC cluster and an efficient parallel code. We will employ KSHELL, a recently developed shellmodel code that utilizes hybrid OpenMP-MPI for massive parallel computation. KSHELL's performance has been validated on various HPC systems, including CINECA clusters.



2) **Study of the D-T fusion with polarized nuclei.** The fusion reaction d(3H,n)4He and d(3He,p)4He are critical processes for the designs of fusion reactors. Up to now, only a few ab-initio theoretical studies of these reactions exist, performed with rather approximate versions of nucleon-nucleon (NN) interaction [Nat.Comm. **10**, 351 (2019)]. We plan to perform the study of these reactions using state-of-the-art NN and three-nucleon interactions derived within the framework of the chiral effective field theory. The solution of the five-body scattering problem will be tackled using accurate numerical method (the hyperspherical harmonic technique). Moreover, we plan to calculate the cross section also for polarized initial particles. In such a case, using crude models, it was speculated that the rate would increase by a 50%. We plan to verify this hypothesis using our more accurate approach, by estimating also the "theoretical uncertainty" deriving from our incomplete knowledge of the nuclear interaction. We plan to use codes based on both CPUs and GPUs parallel computation. This work is the extension of our study of the d(d,n)3He and d(d,p)3H reactions performed using CINECA resources in past years [Phys. Rev. Lett. **130**, 122501 (2023)].

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L. Cosmai, M. Pepe - CSN4 2024





TIME2QUEST (NEMESYS) (A. Sindona)

Time2Quest [CINECA HPC resources - Research Program]

A. Sindona¹, M. Pisarra¹, G. Stefanucci², O. Pulci², M. Palummo², S. Achilli³, G. Onida³ ¹Gruppo Collegato INFN di Cosenza, ²Sezione INFN di Roma Tor Vergata, ³Sezione INFN di Milano

As expressed in its project proposal, the specific initiative (SI) Time2Quest aims at exploring highly demanding computational strategies to unravel excited state properties, collective excitations, transport phenomena and other many-body effects in low dimensional systems of uttermost importance for quantum information processing.

The requested cpu hours are needed to progress towards the microscopic understanding of the electronic and optical properties of suitably combined and functionalized classes of two-dimensional materials, along with related layered heterostructures. This is important not only from fundamental but also applicative point of view. Indeed, due to the 'naked' nature to the environment of their electronic states and low dielectric screening, emergent quantum phenomena are theoretically predicted and experimentally observed. Moreover, they are promising candidates for novel electronic and opto-electronic devices from quantum technologies to energy saving and production. Specifically the main focus will be on graphene-like and chalcogen-based 2D/layered materials. Both classes of materials, in these last years, have shown enhanced many-body effects due to low-dielectric screening and peculiar, often topological, quasi-particles and excitons [1-3].

For the ground-state and electronic structure simulations we plan to use the density functional theory (DFT) codes Abinit [4] and Quantum-ESPRESSO [5] and the many body perturbation theory (MBPT) code Yambo [6]. All these packages are well configured and GPU-parallelized on the galileo 100 and leonardo clusters of the CINECA consortium. MP from the unirm2 unit of the present SI is a member of the developer/superuser team of YAMBO. We also plan to use specific time-dependent density functional theory (TDDFT) codes developed with the unics unit of the present SI [7].

DFT will provide geometries and Kohn-Sham (KS) electronic structures using local/semi-local forms for the exchange-correlation functional. Quantitatively correct electronic structures will be computed by performing many body GW calculations and the use of less expensive, hybrid xc-functionals will be tested. Excitonic optical properties will be calculated within linear response theory, by solving the many body Bethe-Salpeter Equation (BSE). This method provides a deep analysis of (intra- and inter-) excitons (energies, spatial localization, weights in terms of singleparticle states). Momentum forbidden and spin forbidden excitons which are crucial to understand exciton dynamics after light-excitation, will be also characterized. Exciton radiative lifetimes will be estimated by applying by using a fully ab-initio method developed by MP and collaborators [8]. Non-radiative lifetimes (electron-electron/phonon interactions) can be estimated from the spectral width of the self-energy in the particle and hole sector, by employing recent advances in electron-phonon scattering computations [9]. Due to the modulation of the opto-electronic properties from the number of layers, we will address not only monolayer but also multilayer forms with a particular focus on homo and hetero-bilayers, where twisting angle has been demonstrated recently to be a further degree of freedom to play with.



The DFT step requires moderate computational resources, being essentially a self-consistent one-particle approach. On the other hand, the TDDFT, GW, BSE and, in general, MBPT steps are highly demanding, and can be efficiently run only on HPC resources, such as the above-mentioned clusters of the CINECA consortium. The requested CPU time can be used to set up one of the applications proposed in the research program of the present SI for 2025.

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PARTICLE PHYSICS PHENOMENOLOGY

L. Cosmai, M. Pepe - CSN4 2024





QFTATCOL (C. Carloni Calame)

QFT@Colliders

July 3, 2024

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 at the LHC. 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 community of high energy phenomenology, such as GenEva [1], POWHEG BOX [2], MadGraph5_aMC@NLO [3], Mesmer [4], BabaYaga@NLO [5] and possibly more.

References

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- [5] wwww.pv.infn.it/~hepcomplex/babayaga.html



PML4HEP (R. Torre)

Precision Machine Learning for High Energy Physics (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.



QUANTUM INFORMATION

L. Cosmai, M. Pepe - CSN4 2024





FIG. 3. Ground state phase diagram of Rydberg atom Hamiltonian. To detect the phase transition lines of a Ry-





QUANTUM (S. Montangero)

INFN Quantum Padova: Breve descrizione del progetto scientifico

The Quantum Information and Matter group of the University of Padova is involved in research at the interface of quantum science, many-body physics, high-energy physics, and condensed matter.



We tackle fundamental problems in complex many-body quantum systems, where we are interested in emergent phenomena in basic spin systems and more sophisticated models of condensed matter and lattice gauge theories. We investigate the properties of various macroscopic quantum phenomena: superfludity, supercondictivity, Bose-Einstein condensation, and laser coherence. In particular, the main topics of our research activity are: BCS-BEC crossover with ultracold atoms, topological stuctures in neutral and charged superfluids, macroscopic quantum tunneling with Josephson junctions, and quantum physics in curved geometries.

These problems are closely related to the field of quantum technologies, a second large interest of our group. Part of our group is actively developing and improving quantum information protocols and algorithms. We use quantum optimal control and advanced tensor network techniques for developing and benchmarking new protocols or quantum simulation schemes, i.e., quantum circuits and quantum simulators. We employ various quantum-inspired methods, e.g., to solve optimization problems.

On the other hand, quantum simulations allow us to use relatively simple quantum mechanical systems to infer properties of other, more complex ones. We are in contact with leading experimental groups who use Rydberg atoms arrays trapped in optical tweezers. In collaboration with them, we preform quantum simulations of lattice gauge theories and related models.

Many activities in the group are tied together by the use of a common tool – tensor network methods. These are an advanced numerical technique which provides efficient and accurate methods for the simulation of strongly correlated quantum many-body systems. The development of new techniques and algorithms and their efficient implementation is a very lively activity in our group.

Moreover, the research group is leading the development of the open-source software Quantum TEA, is maintaining the open-source optimal control software QuOCS together with its international partners. Furthermore, the projects align with the INFN Quantum initiative and the ALINFN initiative.

Due to the variety of applications and research directions, we encounter all types of simulations from data parallel CPU-simulations to GPU-accelerated jobs.







Prof. Sebastiano Pilati Università di Camerino Scuola di Scienze e Tecnologie Sezione di Fisica Via Madonna delle Carceri

I-62032 Camerino (MC) - ITALY.

Request of HPC Resources for 2025: INFN LINCOLN, Perugia-Camerino

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

Associated researchers: 6 people, 6FTE

Brodoloni Luca (PhD student, Unicam, 100%), Cantori Simone (PhD student, Unicam, 100%), Di Patti Francesca (RTDB, UniPG, 100%), Midei Giovanni (PhD student, Unicam, 100%), Pilati Sebastiano (PA, Unicam, 100%, loc. resp.), Gabriele Spada (Postdoc, Unicam, 100%).

Project title: Neural Monte Carlo simulations of quantum spin glasses



Project description: The experiments performed with quantum simulation platforms, such as Rydberg atoms in optical tweezers or ion traps, offer new venues to study the physics of disordered quantum systems and the possible emergence of quantum spin-glass phases. Notably, these experiments allow one to engineer the Hamiltonian parameters essentially at will, thus allowing a one-to-one comparison against theoretical models. This opportunity calls for accurate theoretical predictions based on state-of-the-art computational techniques. In recent years, the Camerino Unit has developed self-learning projective quantum Monte Carlo (QMC) algorithms to simulate quantum Ising models with random couplings [1]. These algorithms are suitable for providing unbiased predictions to guide the explorations of spin-glass physics in Rydberg-atom or trapped-ion experiments. Notably, these QMC methods exploit neural networks as guiding variational phase functions. In a first study, we have shown that the spin-glass quantum phase transition in the paradigmatic Edwards-Anderson model can be precisely located [2]. Notably, the studies of spin-glass phenomena require averaging over large ensembles of different (random) realizations of the disorder. This significantly increases computational demands.

Our QMC codes exploit shared memory parallelism, implemented via automatic loop parallelization in NUMBA, to propagate the population of random walkers needed in projective QMC algorithms. Furthermore, ensemble averaging can be distributed over different cores and/or nodes, with virtually no data communication. We implemented this job-farming protocol via MPI4PY. Overall, our simulations exploit hybrid OPENMP-MPI parallelism, and efficiently scale on multicore-multinode CPU clusters. Furthermore, we plan to train deep neural networks, implemented in PYTORCH, to perform supervised learning of quantum many-body systems, following a growing research line on which our Unit is continually active [3]. Therefore, we are also requesting a smaller amount of compute time on a GPU cluster.

Requests of HPC resources for 2025:

- CPU cluster [LEONARDO-DCGP (CPU cluster) or GALILEO 100]: 470400 core hours (112cores x 10 nodes x 6h x 70 runs= 470400 core hours).
- GPU cluster [LEONARDO (GPU cluster)]: 9600 core hours (32cores x 1node x 6hours x 50 runs).

References:

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Camerino (MC) July 3th, 2024 Sebastiano Pilati (University of Camerino, Res. Loc. of LINCOLN, Perugia Section)

Cineca-INFN agreement 2024

L. Cosmai, M. Pepe - CSN4 2024





CSN4+CSN2+CSN5

LEONARDO-booster

da	1-Feb-2024	а	3-Sep-2024	#giorni	215		
							consumo
							atteso da
							linearizzazi
	budget	consumo	consumo/b	residuo			one mensile
account	(corehours)	(corehours)	udget (%)	(corehours)	residuo%	#giorni	(corehours)
INF24_biophys_1	2,500,000	306,137	12.25	2,193,863	87.75	215	1,472,603
INF24_euclid_1	1,000	0	0.00	1,000	100.00	215	589
INF24_fldturb_1	3,000,000	250,072	8.34	2,749,928	91.66	215	1,767,123
INF24_indark_1	5,000,000	974,393	19.49	4,025,607	80.51	215	2,945,205
INF24_litebird_1	1,000	0	0.00	1,000	100.00	215	589
INF24_lqcd123_1	20,400,000	10,516,128	51.55	9,883,872	48.45	215	12,016,438
INF24_neumatt_1	30,000	18,559	61.86	11,441	38.14	215	17,671
INF24_npqcd_1	18,000,000	9,286,517	51.59	8,713,483	48.41	215	10,602,740
INF24_qcdlat_1	11,600,000	3,866,473	33.33	7,733,527	66.67	215	6,832,877
INF24_teongrav_1	3,000,000	2,704,996	90.17	295,004	9.83	215	1,767,123
INF24_enesma_1	4,000,000	3,335	0.08	3,996,665	99.92	215	2,356,164
INF24_gagra_1	350,000	207	0.06	349,793	99.94	215	206,164
INF24_Ihc_1	1,000,000	44,378	4.44	955,622	95.56	215	589,041
INF24_lincoln_1	200,000	0	0.00	200,000	100.00	215	117,808
INF24_Ispe_1	1,000	0	0.00	1,000	100.00	215	589
INF24_monstre_1	80,000	2,797	3.50	77,203	96.50	215	47,123
INF24_nemesys_1	2,000,000	465,453	23.27	1,534,547	76.73	215	1,178,082
INF24_nucsys_1	1,000,000	287,314	28.73	712,686	71.27	215	589,041
INF24_pmlhep_1	2,375,000	182,286	7.68	2,192,714	92.32	215	1,398,973
INF24_qftatcol_1	5,000,000	0	0.00	5,000,000	100.00	215	2,945,205
INF24_quantum_1	300,000	155,397	51.80	144,603	48.20	215	176,712
INF24_sft_1	800,000	528,550	66.07	271,450	33.93	215	471,233
INF24_sim_1	3,000,000	2,787,051	92.90	212,949	7.10	215	1,767,123
INF24_test_1	11,990,000	1,453	0.01	11,988,547	99.99	215	7,062,603
INF24_virgo_1	1,000	0	0.00	1,000	100.00	215	589
INF24_cubic_1	1,000	0	0.00	1,000	100.00	215	589
INF24_et_1	1,000	0	0.00	1,000	100.00	215	589
INF24_anna_1	36,000	0	0.00	36,000	100.00	215	21,205
INF24_brainsta_1	192,000	90,358	47.06	101,642	52.94	215	113,096
INF24_miro_1	131,000	19,229	14.68	111,771	85.32	215	77,164
TOTALE	95,990,000	32,491,083	33.85	63,498,917	66.15	215	56,542,055

L. Cosmai, M. Pepe - CSN4 2024

	corehours	%
LATTICE	26,986,379	83.06
ASTRO	3,697,948	11.38
COMPLEX	559,544	1.72
NUCLEAR	290,111	0.89
CONDMAT	465,453	1.43
PHENOMEN	182,286	0.56
QUANTUM	155,397	0.48
EXPERIMENTS	153,965	0.47
TOTAL	32,491,083	100.00



(consumo effettivo)/(c

onsumo

atteso da

linearizzazi

one mensile

del budget)

20.79

0.00

14.15

33.08

0.00

87.51

105.02

[%]









			LEONAF	RDO-boos	ster								LEONAF	RDO-boos	ster			
	da 1-Feb-2024	l a	3-Sep-2024	giorni	215	5				da 1-1	Feb-2024	ć	a 3-Sep-2024	#giorni	215	;		
account	budget (corehours)	consumo (corehours)	consumo/b udget (%)	residuo (corehours)	residuo%	#giorni	consumo atteso da linearizzazi one mensile (corehours)	(consumo effettivo)/(c onsumo atteso da linearizzazi one mensile del budget) [%]	account	bud (cor	lget rehours)	consumo (corehours)	consumo/b udget (%)	residuo (corehours)	residuo%	#giorni	consumo atteso da linearizzazi one mensil (corehours	i c
INF24_blophys_1	3 000 000	250 072	8.34	2,193,803	91.66	215	1 767 123	3 14 15	INF24_euclid_1		1,000	(0.00	1,000	100.00	21	5 58	39
INF24 indark 1	5.000.000	974.393	19.49	4.025.607	80.51	215	2.945.205	5 33.08	INF24_litebird_1		1,000	(0.00	1,000	100.00	21	5 <u>5</u> 58	39
INF24 lgcd123 1	20,400,000	10,516,128	51.55	9,883,872	48.45	215	12,016,438	87.51	INF24_Ispe_1		1,000	(0.00	1,000	100.00	21	5 58	39
INF24_neumatt_1	30,000	18,559	61.86	11,441	38.14	. 215	17,671	1 105.02	INF24_virgo_1		1,000	(0.00	1,000	100.00	21	<u>5 58</u>	39
INF24_npqcd_1	18,000,000	9,286,517	51.59	8,713,483	48.41	215	10,602,740	87.59	INF24_cubic_1		1,000	(0.00	1,000	100.00	21	5 58	39
INF24_qcdlat_1	11,600,000	3,866,473	33.33	7,733,527	66.67	215	6,832,877	7 56.59	INF24_et_1		1,000	(0.00	1,000	100.00	21	5 58	39
INF24_teongrav_1	3,000,000	2,704,996	90.17	295,004	9.83	215	1,767,123	3 153.07	TOTALE		6,000		0.00	6,000	100.00	21	5 3,53	34
INF24_enesma_1	4,000,000	3,335	0.08	3,996,665	99.92	215	2,356,164	4 0.14										
INF24_gagra_1	350,000	207	0.06	349,793	99.94	. 215	206,164	4 0.10										
INF24_Ihc_1	1,000,000	44,378	4.44	955,622	95.56	215	589,041	1 7.53										
INF24_lincoln_1	200,000	0 0	0.00	200,000	100.00	215	117,808	3 0.00										
INF24_monstre_1	80,000	2,797	3.50	77,203	96.50	215	47,123	3 5.94										
INF24_nemesys_1	2,000,000	465,453	23.27	1,534,547	76.73	215	1,178,082	2 39.51										
INF24_nucsys_1	1,000,000	287,314	28.73	712,686	71.27	215	589,041	1 48.78							stor			
INF24_pmlhep_1	2,375,000	182,286	7.68	2,192,714	92.32	215	1,398,973	3 13.03										
INF24_qftatcol_1	5,000,000	0	0.00	5,000,000	100.00	215	2,945,205	5 0.00		da 1-	-Feb-2024		a 3-Sep-2024	l #giorni	215	5		
INF24_quantum_1	300,000	155,397	51.80	144,603	48.20	215	176,712	2 87.94										(
INF24_sft_1	800,000	528,550	66.07	271,450	33.93	215	471,233	3 112.16										e
INF24_sim_1	3,000,000	2,787,051	92.90	212,949	7.10	215	1,767,123	3 157.72										(
INF24_test_1	11,990,000	1,453	0.01	11,988,547	99.99	215	7,062,603	3 0.02										E
TOTALE	95,625,000	32,381,496	33.86	63,243,504	66.14	215	56,327,055	5 57.49									consumo	



			LEONAF	<mark>RDO-boos</mark>	ster			
da	1-Feb-2024	а	3-Sep-2024	#giorni	215			
account	budget (corehours)	consumo (corehours)	consumo/b udget (%)	residuo (corehours)	residuo%	#giorni	consumo atteso da linearizzazi one mensile (corehours)	(r e c a li c d [
INF24_anna_1	36,000	0	0.00	36,000	100.00	215	21,205	
INF24_brainsta_1	192,000	90,358	47.06	191,953	99.98	215	113,096	
INF24_miro_1	131,000	19,229	14.68	130,985	99.99	215	77,164	
TOTALE	359,000	109,587	30.53	358,969	99.99	215	211,466	





CSN4+CSN2+CSN5

LEONARDO-GP

da	1-Mar-2024	а	3-Sep-2024	#aiorni	186		
				J			
							consumo
							atteso da
	budgot	consumo	consumo/b	rosiduo			linearizzazi
account	(corehours)	(corehours)	udget (%)	(corehours)	residuo%	#giorni	(corehours)
INF24 biophys 2	990.000	684.376	69.13	305.624	30.87	186	548.03
INF24 cubic 2	127.000	0	0.00	127.000	100.00	186	70.30
INF24 enesma 2	11,000	192	1.75	10,808	98.25	186	6,08
INF24_et_2	440,000	0	0.00	440,000	100.00	186	243,57
INF24_euclid_2	4,231,270	0	0.00	4,231,270	100.00	186	2,342,31
INF24_fldturb_2	6,133,840	6,110,270	99.62	23,570	0.38	186	3,395,51
INF24_gagra_2	443,920	160,497	36.15	283,423	63.85	186	245,74
INF24_indark_2	600,000	5,347	0.89	594,653	99.11	186	332,14
INF24_Ihc_2	601,000	125,658	20.91	475,342	79.09	186	332,69
INF24_lincoln_2	418,000	355,305	85.00	62,695	15.00	186	231,39
INF24_litebird_2	1,620,710	0	0.00	1,620,710	100.00	186	897,17
INF24_Iqcd123_2	13,060,000	9,019,935	69.07	4,040,065	30.93	186	7,229,64
INF24_Ispe_2	297,160	0	0.00	297,160	100.00	186	164,49
INF24_monstre_2	1,106,430	0	0.00	1,106,430	100.00	186	612,48
INF24_nemesys_2	254,390	33,623	13.22	220,767	86.78	186	140,82
INF24_neumatt_2	1,210,740	919,388	75.94	291,352	24.06	186	670,23
INF24_npqcd_2	33,005,290	18,233,362	55.24	14,771,928	44.76	186	18,270,78
INF24_nucsys_2	1,110,000	637,625	57.44	472,375	42.56	186	614,46
INF24_pmlhep_2	202,000	250,838	124.18	-48,838	-24.18	186	111,82
INF24_qcdlat_2	62,909,310	62,228,210	98.92	681,100	1.08	186	34,824,79
INF24_qftatcol_2	2,803,500	2,109,295	75.24	694,205	24.76	186	1,551,93
INF24_quantum_2	2,026,540	875,574	43.21	1,150,966	56.79	186	1,121,83
INF24_sft_2	776,460	20,193	2.60	756,267	97.40	186	429,82
INF24_sim_2	1,110,000	1,113,639	100.33	-3,639	-0.33	186	614,46
INF24_teongrav_2	8,810,040	9,192,622	104.34	-382,582	-4.34	186	4,876,98
INF24_test_2	22,341,000	2,486,441	11.13	19,854,559	88.87	186	12,367,33
INF24_virgo_2	2,000	0	0.00	2,000	100.00	186	1,10
INF24_anna_2	300,000	0	0.00	300,000	100.00	186	166,07
INF24_brainsta_2	2,000	0	0.00	2,000	100.00	186	1,10
INF24_miro_2	601,000	0	0.00	601,000	100.00	186	332,69
TOTALE	167,544,600	114,562,390	68.38	52,982,210	31.62	186	92,747,90

			corehours
		LATTICE	93,262,277
neu		ASTRO	10,117,357
130		COMPLEX	6,794,838
ne		NUCLEAR	637,625
		CONDMAT	33,623
		PHENOMEN	2,360,133
24.88		QUANTUM	1,230,879
3.15		EXPERIMENTS	125,658
0.00		TOTAL	114,562,390
0.00			
9.95 5.21			
1 61			
37.77			
53.55	QUANTUM		
0.00	1.1%		
24.76	PHENOMEN		
0.00	2.1%		



%

81.41

8.83

5.93

0.56

0.03

2.06

1.07

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100.00









	LEONARDO-GP									
da	1-Mar-2024	а	3-Sep-2024	#giorni	186					
account	budget (corehours)	consumo (corehours)	consumo/b udget (%)	residuo (corehours)	residuo%	#giorni	consumo atteso da linearizzazi one mensile (corehours)	(consumo effettivo)/(c onsumo atteso da linearizzazi one mensile del budget) [%]		
INF24_biophys_2	990,000	684,376	69.13	305,624	30.87	186	548,036	124.88		
INF24_enesma_2	11,000	192	1.75	10,808	98.25	186	6,089	3.15		
INF24_fldturb_2	6,133,840	6,110,270	99.62	23,570	0.38	186	3,395,519	179.95		
INF24_gagra_2	443,920	160,497	36.15	283,423	63.85	186	245,741	65.31		
INF24_indark_2	600,000	5,347	0.89	594,653	99.11	186	332,143	1.61		
INF24_Ihc_2	601,000	125,658	20.91	475,342	79.09	186	332,696	37.77		
INF24_lincoln_2	418,000	355,305	85.00	62,695	15.00	186	231,393	153.55		
INF24_lqcd123_2	13,060,000	9,019,935	69.07	4,040,065	30.93	186	7,229,643	124.76		
INF24_monstre_2	1,106,430	0	0.00	1,106,430	100.00	186	612,488	0.00		
INF24_nemesys_2	254,390	33,623	13.22	220,767	86.78	186	140,823	23.88		
INF24_neumatt_2	1,210,740	919,388	75.94	291,352	24.06	186	670,231	137.17		
INF24_npqcd_2	33,005,290	18,233,362	55.24	14,771,928	44.76	186	18,270,786	99.80		
INF24_nucsys_2	1,110,000	637,625	57.44	472,375	42.56	186	614,464	103.77		
INF24_pmlhep_2	202,000	250,838	124.18	-48,838	-24.18	186	111,821	224.32		
INF24_qcdlat_2	62,909,310	62,228,210	98.92	681,100	1.08	186	34,824,797	178.69		
INF24_qftatcol_2	2,803,500	2,109,295	75.24	694,205	24.76	186	1,551,938	135.91		
INF24_quantum_2	2,026,540	875,574	43.21	1,150,966	56.79	186	1,121,835	78.05		
INF24_sft_2	776,460	20,193	2.60	756,267	97.40	186	429,826	4.70		
INF24_sim_2	1,110,000	1,113,639	100.33	-3,639	-0.33	186	614,464	181.24		
INF24_teongrav_2	8,810,040	9,192,622	104.34	-382,582	-4.34	186	4,876,986	188.49		
INF24_test_2	22,341,000	2,486,441	11.13	19,854,559	88.87	186	12,367,339	20.10		
TOTALE	159,923,460	114,562,390	71.64	45,361,070	28.36	186	88,529,058	129.41		



			LEON	<mark>ARDO-GI</mark>	2			
da	1-Mar-2024	а	3-Sep-2024	#giorni	186			
account	budget (corehours)	consumo (corehours)	consumo/b udget (%)	residuo (corehours)	residuo%	#giorni	consumo atteso da linearizzazi one mensile (corehours)	(co eff on att lin on de [%
INF24_cubic_2	127,000	0	0.00	127,000	100.00	186	70,304	
INF24_et_2	440,000	0	0.00	440,000	100.00	186	243,571	
INF24_euclid_2	4,231,270	0	0.00	4,231,270	100.00	186	2,342,310	
INF24_litebird_2	1,620,710	0	0.00	1,620,710	100.00	186	897,179	
INF24_Ispe_2	297,160	0	0.00	297,160	100.00	186	164,499	
INF24_virgo_2	2,000	0	0.00	2,000	100.00	186	1,107	
TOTALE	6,718,140	0	0.00	6,718,140	100.00	186	3,718,970	

CSN5

	LEONARDO-GP								
da	1-Mar-2024	а	3-Sep-2024	#giorni	186				
	budget	consumo	consumo/b	residuo			consumo atteso da linearizzazi one mensile	(co eff on att lin on de [%	
account	(corehours)	(corehours)	udget (%)	(corehours)	residuo%	#giorni	(corehours)		
INF24_anna_2	300,000	0	0.00	300,000	100.00	186	166,071		
INF24_brainsta_2	2,000	0	0.00	2,000	100.00	186	1,107		
INF24_miro_2	601,000	0	0.00	601,000	100.00	186	332,696		
TOTALE	903,000	0	0.00	903,000	100.00	186	499,875		





CSN4+CSN2+CSN5

	MARCONI-A3									
da	1-Feb-2024	а	27-Jul-2024	#giorni	177					
account	budget (corehours)	consumo (corehours)	consumo/b udget (%)	residuo (corehours)	residuo%	#giorni	consumo atteso da linearizzazi one mensile (corehours)	(consumo effettivo)/(c onsumo atteso da linearizzazi one mensile del budget) [%]		
INF24_biophys	300,000	315,201	105.07	-15,201	-5.07	177	145,479	216.66		
INF24_euclid	500,000	28,656	5.73	471,344	94.27	177	242,466	11.82		
INF24_fldturb	700,000	205,262	29.32	494,738	70.68	177	339,452	60.47		
INF24_INDark	100,000	102,011	102.01	-2,011	-2.01	177	48,493	210.36		
INF24_IIteDira	249,000	216,831	87.08	32,169	12.92	177	120,748	179.57		
INF24_IQC0123	1,500,000	380.264	0.00	1,500,000	100.00	177	103 073	200.68		
INF24_neumati	3 300 000	1 311 031	97.32 30.73	1 088 060	60.27	177	1 600 274	200.08		
INF24_npqcu	5,000,000	2 680 235	53.60	2 310 765	46.40	177	2 424 658	110 54		
INF24_qcdiat	800,000	779 960	97.50	2,319,703	2 51	177	387 945	201.05		
INF24_enesma	1 000	0	0.00	1 000	100.00	177	485	0.00		
INF24 gagra	25.000	21.078	84.31	3.922	15.69	177	12.123	173.86		
INF24 Ihc	1.000	0	0.00	1.000	100.00	177	485	0.00		
 INF24 lincoln	30,000	0	0.00	30,000	100.00	177	14,548	0.00		
 INF24_Ispe	41,000	13,835	33.74	27,165	66.26	177	19,882	69.58		
INF24_monstre	160,000	13,549	8.47	146,451	91.53	177	77,589	17.46		
INF24_nemesys	40,000	25,609	64.02	14,391	35.98	177	19,397	132.02		
INF24_nucsys	150,000	0	0.00	150,000	100.00	177	72,740	0.00		
INF24_pmlhep	1,000	0	0.00	1,000	100.00	177	485	0.00		
INF24_qftatcol	150,000	6,494	4.33	143,506	95.67	177	72,740	8.93		
INF24_quantum	40,000	3,458	8.65	36,542	91.36	177	19,397	17.83		
INF24_sft	120,000	63,537	52.95	56,463	47.05	177	58,192	109.19		
INF24_sim	150,000	0	0.00	150,000	100.00	177	72,740	0.00		
INF24_test	1,042,000	0	0.00	1,042,000	100.00	177	505,299	0.00		
INF24_virgo	1,000	0	0.00	1,000	100.00	177	485	0.00		
INF24_cubic	17,000	0	0.00	17,000	100.00	177	8,244	0.00		
INF24_et	60,000	0	0.00	60,000	100.00	177	29,096	0.00		
INF24_anna	40,000	0	0.00	40,000	100.00	177	19,397	0.00		
INF24_brainsta	1,000	0	0.00	1,000	100.00	177	485	0.00		
INF24_miro	81,000	0	0.00	81,000	100.00	177	39,279	0.00		
TOTALE	15,000,000	6,176,011	41.17	8,823,989	58.83	177	7,273,973	84.91		

L. Cosmai, IVI. Pepe - CSIN4 2024

	corehours	%
LATTICE	4,075,881	66.00
ASTRO	1,271,235	20.58
COMPLEX	520,463	8.43
NUCLEAR	13,549	0.22
CONDMAT	25,609	0.41
PHENOMEN	6,494	0.11
QUANTUM	3,458	0.06
EXPERIMENTS	259,322	4.20
TOTAL	6,176,011	100

EXPERIMENTS









MARCONI-A3										MAR	CONI-A3					
d	a 1-Feb-2024	а	27-Jul-2024	#giorni	177					da 1-Feb-2024	а	27-Jul-2024	#giorni	177		
account	budget (corehours)	consumo (corehours)	consumo/b udget (%)	residuo (corehours)	residuo%	#giorni	consumo atteso da linearizzazi one mensile (corehours)	(consumo effettivo)/(c onsumo atteso da linearizzazi one mensile del budget) [%]	account	budget (corehours)	consumo (corehours)	consumo/b udget (%)	residuo (corehours)	residuo%	#giorni	consumo atteso da linearizzazi one mensile (corehours)
INF24_biophys	300,000	315,201	105.07	-15,201	-5.07	17	7 145,479	9 216.66	INF24_euclid	500,000	28,656	5.73	471,344	94.27		177 242,466
INF24_fldturb	700,000	205,262	29.32	494,738	70.68	17	7 339,452	2 60.47	INF24_litebird	249,000	216,831	87.08	32,169	12.92		177 120,748
INF24_indark	100,000	102,011	102.01	-2,011	-2.01	17	48,49	3 210.36	INF24_Ispe	41,000	13,835	33.74	27,165	66.26		177 19,882
INF24_IQC0123	1,500,000	0	0.00	1,500,000	100.00	1,	7 7 727,39	7 0.00	INF24_virgo	1,000	0	0.00	1,000	100.00		485
INF24_neumatt	400,000	389,204	97.32	1 088 060	2.08	17	7 193,97	3 200.08		17,000	0	0.00	17,000	100.00		177 8,244
INF24_npqca	5,000,000	2 680 235	53.60	2 310 765	46.40	17	7 1,000,274	+ 01.93 8 110 54	INF24_et	60,000	0	0.00	60,000	100.00		177 29,096 177 420.024
INF24_qculat	800,000	779 960	97.50	2,319,703	40.40	17	7 2,424,030	5 201.05	TOTALE	808,000	259,322	29.88	008,078	70.12		420,921
INF24_teolograv	1 000	119,900	97.50	1 000	100.00	17	7 307,94	5 0.00								
INF24 gagra	25,000	21.078	84.31	3,922	15.69	17	7 12.12	3 173.86								
INF24 Ihc	1,000	0	0.00	1,000	100.00	17	7 48	5 0.00								
INF24 lincoln	30.000	0	0.00	30.000	100.00	17	7 14.548	8 0.00								
INF24 monstre	160,000	13,549	8.47	146,451	91.53	17	7 77,589	9 17.46								
 INF24_nemesys	40,000	25,609	64.02	14,391	35.98	17	7 19,39	7 132.02								
INF24_nucsys	150,000	0	0.00	150,000	100.00	17	77 72,740	0.00								
INF24_pmlhep	1,000	0	0.00	1,000	100.00	17	7 48	5 0.00					CONI-A3			
INF24_qftatcol	150,000	6,494	4.33	143,506	95.67	17	77 72,740	0 8.93		da 1-Feb-2024	а	27-Jul-2024	#giorni	177		
INF24_quantum	40,000	3,458	8.65	36,542	91.36	17	7 19,39	7 17.83								
INF24_sft	120,000	63,537	52.95	56,463	47.05	17	7 58,192	2 109.19								
INF24_sim	150,000	0	0.00	150,000	100.00	17	77 72,740	0.00								
INF24_test	1,042,000	0	0.00	1,042,000	100.00	17	7 505,299	9 0.00								consumo
TOTALE	14,010,000	5,916,689	42.23	8,093,311	57.77	17	6,793,89	0 87.09								atteso da
									account INF24_anna INF24_brainsta INF24_miro <i>TOTALE</i>	budget (corehours) 40,000 1,000 81,000 122.000	consumo (corehours) 0 0 0	consumo/b udget (%) 0.00 0.00 0.00	residuo (corehours) 40,000 1,000 81,000 122.000	residuo% 100.00 100.00 100.00 100.00	#giorni	Iinearizzazi one mensile (corehours) 177 177 177 39,279 177 59.162

CSN2





CSN4+CSN2+CSN5

GAL	ILE	01	00

da	1-Feb-2024	а	3-Sep-2024	#giorni	215			
account	budget (corehours)	consumo (corehours)	consumo/b udget (%)	residuo (corehours)	residuo%	#giorni	consumo atteso da linearizzazi one mensile (corehours)	(consumo effettivo)/(c onsumo atteso da linearizzazi one mensile del budget) [%]
INF24_biophys_0	19,998	17,035	85.18	2,963	14.82	215	11,780	144.61
INF24_euclid_0	229,998	5,019	2.18	224,979	97.82	215	135,478	3.70
INF24_fldturb_0	300,003	77,490	25.83	222,513	74.17	215	176,714	43.85
INF24_indark_0	39,999	15,874	39.69	24,125	60.31	215	23,561	67.37
INF24_litebird_0	99,000	24,498	24.75	74,502	75.25	215	58,315	42.01
INF24_lqcd123_0	499,998	0	0.00	499,998	100.00	215	294,519	0.00
INF24_neumatt_0	79,998	102,135	127.67	-22,137	-27.67	215	47,122	216.75
INF24_npqcd_0	1,350,000	0	0.00	1,350,000	100.00	215	795,205	0.00
INF24_qcdlat_0	2,149,998	98,526	4.58	2,051,472	95.42	215	1,266,437	7.78
INF24_teongrav_0	300,000	263,600	87.87	36,400	12.13	215	176,712	149.17
INF24_enesma_0	999	0	0.00	999	100.00	215	588	0.00
INF24_gagra_0	9,999	0	0.00	9,999	100.00	215	5,890	0.00
INF24_Ihc_0	999	1	0.10	998	99.90	215	588	0.17
INF24_lincoln_0	10,998	8,305	75.51	2,693	24.49	215	6,478	128.20
INF24_Ispe_0	16,998	12,117	71.28	4,881	28.72	215	10,013	121.02
INF24_monstre_0	60,000	34,082	56.80	25,918	43.20	215	35,342	96.43
INF24_nemesys_0	15,000	12,956	86.37	2,044	13.63	215	8,836	146.63
INF24_nucsys_0	60,000	61,137	101.90	-1,137	-1.90	215	35,342	172.98
INF24_pmlhep_0	100,998	56,057	55.50	44,941	44.50	215	59,492	94.23
INF24_qftatcol_0	60,000	0	0.00	60,000	100.00	215	35,342	0.00
INF24_quantum_0	15,000	0	0.00	15,000	100.00	215	8,836	0.00
INF24_sft_0	49,998	38,862	77.73	11,136	22.27	215	29,451	131.96
INF24_sim_0	60,000	0	0.00	60,000	100.00	215	35,342	0.00
INF24_test_0	387,999	0	0.00	387,999	100.00	215	228,547	0.00
INF24_virgo_0	999	0	0.00	999	100.00	215	588	0.00
INF24_cubic_0	6,999	0	0.00	6,999	100.00	215	4,123	0.00
INF24_et_0	24,000	0	0.00	24,000	100.00	215	14,137	0.00
INF24_anna_0	15,999	0	0.00	15,999	100.00	215	9,424	0.00
INF24_brainsta_0	999	0	0.00	999	100.00	215	588	0.00
INF24_miro_0	33,000	0	0.00	33,000	100.00	215	19,438	0.00
TOTALE	5,999,976	827,694	13.79	5,172,282	86.21	215	3,534,232	23.42

corehours	%
137,388	16.60
381,609	46.11
94,525	11.42
95,219	11.50
12,956	1.57
56,057	6.77
8,305	1.00
41,635	5.03
827,694	100.00
	corehours 137,388 381,609 94,525 95,219 12,956 56,057 8,305 41,635 827,694









GALILEO100										
da	1-Feb-2024	а	3-Sep-2024	#giorni	215					
account	budget (corehours)	consumo (corehours)	consumo/b udget (%)	residuo (corehours)	residuo%	#giorni	consumo atteso da linearizzazi one mensile (corehours)	(consumo effettivo)/(c onsumo atteso da linearizzazi one mensil del budget) [%]		
INF24_biophys_0	19,998	17,035	85.18	2,963	14.82	215	11,780	144.6		
INF24_fldturb_0	300,003	77,490	25.83	222,513	74.17	215	176,714	43.8		
INF24_indark_0	39,999	15,874	39.69	24,125	60.31	215	23,561	67.3		
	499,998	0	0.00	499,998	100.00	215	294,519	0.0		
INF24_neumatt_0	79,998	102,135	127.67	-22,137	-27.67	215	47,122	216.7		
INF24_npqcd_0	1,350,000	0	0.00	1,350,000	100.00	215	795,205	0.0		
INF24_qcdlat_0	2,149,998	98,526	4.58	2,051,472	95.42	215	1,266,437	1.1		
INF24_teongrav_0	300,000	263,600	87.87	36,400	12.13	215	1/6,/12	149.1		
INF24_enesma_0	999	0	0.00	999	100.00	215	588	0.0		
INF24_gagra_0	9,999	0	0.00	9,999	100.00	215	5,890	0.0		
INF24_Ihc_0	999	1	0.10	998	99.90	215	588	0.1		
INF24_lincoln_0	10,998	8,305	75.51	2,693	24.49	215	6,478	128.2		
INF24_monstre_0	60,000	34,082	56.80	25,918	43.20	215	35,342	96.4		
INF24_nemesys_0	15,000	12,956	86.37	2,044	13.63	215	8,836	146.6		
INF24_nucsys_0	60,000	61,137	101.90	-1,137	-1.90	215	35,342	172.9		
INF24_pmlhep_0	100,998	56,057	55.50	44,941	44.50	215	59,492	94.2		
INF24_qftatcol_0	60,000	0	0.00	60,000	100.00	215	35,342	0.0		
INF24_quantum_0	15,000	0	0.00	15,000	100.00	215	8,836	0.0		
INF24_sft_0	49,998	38,862	77.73	11,136	22.27	215	29,451	131.9		
INF24_sim_0	60,000	0	0.00	60,000	100.00	215	35,342	0.0		
INF24_test_0	387,999	0	0.00	387,999	100.00	215	228,547	0.0		
TOTALE	5,571,984	786,060	14.11	4,785,924	85.89	215	3,282,128	23.9		



GALILEO100										
da	1-Feb-2024	а	3-Sep-2024	#giorni	215					
account	budget (corehours)	consumo (corehours)	consumo/b udget (%)	residuo (corehours)	residuo%	#giorni	consumo atteso da linearizzazi one mensile (corehours)	(con effet onsu attes linea one del k [%]		
INF24_euclid_0	229,998	5,019	2.18	224,979	97.82	215	135,478			
INF24_litebird_0	99,000	24,498	24.75	74,502	75.25	215	58,315			
INF24_Ispe_0	16,998	12,117	71.28	4,881	28.72	215	10,013			
INF24_virgo_0	999	0	0.00	999	100.00	215	588			
INF24_cubic_0	6,999	0	0.00	6,999	100.00	215	4,123			
INF24_et_0	24,000	0	0.00	24,000	100.00	215	14,137			
TOTALE	377,994	41,634	11.01	336,360	88.99	215	222,654			

CSN5

GALILEO100										
da	1-Feb-2024	а	3-Sep-2024	#giorni	215					
account	budget (corehours)	consumo (corehours)	consumo/b udget (%)	residuo (corehours)	residuo%	#giorni	consumo atteso da linearizzazi one mensile (corehours)	(co effe ons atte line one del [%]		
INF24_anna_0	15,999	0	0.00	15,999	100.00	215	9,424			
INF24_brainsta_0	999	0	0.00	999	100.00	215	588			
INF24_miro_0	33,000	0	0.00	33,000	100.00	215	19,438			
TOTALE	49,998	0	0.00	49,998	100.00	215	29,451			







Cineca-INFN agreement 2025

L. Cosmai, M. Pepe - CSN4 2024



<u>Cineca-INFN agreement 2025: computing resources</u>

LEONARDO-booster: 96 Mcorehours LEONARDO-GP: 100 Mcorehours GALILEO100: 6 Mcorehours

L. Cosmai, M. Pepe - CSN4 2024



CSN4 2025										
PROGETTO	RICHIESTE CPU (corehours)	PROPOSTE CPU (corehours)	RICHIESTE GPU (corehours)	PROPOSTE GPU (corehours)	P G ((
BIOPHYS	1,500,000	900,000	3,000,000	2,500,000						
ENESMA	1,000	1,000	3,000,000	2,000,000						
FIELDTURB	7,500,000	5,500,000	3,000,000	2,000,000						
GAGRA	700,000	299,000	550,000	300,000						
INDARK	1,000,000	500,000	2,000,000	2,000,000						
LINCOLN	470,400	300,000	9,600	9,600						
LQCD123	10,000,000	3,000,000	27,000,000	26,500,000						
MONSTRE	250,000	160,000	20,000	20,000						
NEMESYS (TIME2QUEST)	3,000,000	300,000	65,000	65,000						
NEUMATT	6,000,000	1,750,000	100,000	100,000						
NPQCD	32,000,000	22,000,000	27,000,000	26,500,000						
NUCSYS	3,000,000	800,000	2,000,000	2,000,000						
PML4HEP	200,000	200,000	1,000,000	1,000,000						
QCDLAT	60,000,000	48,000,000	20,000,000	18,000,000						
QFTATCOL	12,500,000	2,000,000	500,000	500,000						
QUANTUM	1,500,000	800,000	750	750						
SFT	2,000,000	400,000	960,000	750,000						
SIM	1,000,000	340,000	500,000	500,000						
TEONGRAV	12,000,000	7,500,000	6,000,000	6,000,000						
TEST		5,250,000		5,254,650						
TOTALE	154,621,400	100,000,000	96,705,350	96,000,000						

1.5 PB tape (richieste su CALC4_TIER1)



Other computing resources

L. Cosmai, M. Pepe - CSN4 2024



Main computing resources in Europe



LUMI supercomputer **375 PFlop/s** - **FINLAND**

- LUMI-G (accelerated partition) 2978 nodes with 4 AMD MI250x GPUs and a single 64 cores AMD **EPYC** "Trento" CPU. **379.70 PFlop/s HPL**
- <u>LUMI-C (CPU partition)</u> 2048 CPU-based compute nodes (128 cores/node AMD EPYC)

LEONARDO supercomputer 250 PFlop/s - ITALY

- LEONARDO-booster
- 512 (8 x 64) GB RAM DDR4 3200 MHz 2 x NVidia HDR 2×100 Gb/s cards
- LEONARDO-GP 1536 nodes

2x Intel Sapphire Rapids, 56 cores, 4.8 GHz 512 (16 x 32) GB RAM DDR5 4800 MHz **3xNvidia HDR cards 1x100Gb/s cards** 8 TB NVM

LISA-GPU (> 100 PFlops HPL) LISA-CPU (>6 PFlops HPL)

https://eurohpc-ju.europa.eu/supercomputers/our-supercomputers_en







3456 nodes 1 x CPU Intel Xeon 8358 32 cores, 2,6 GHz 4 X Nvidia custom Ampere GPU 64GB HBM2



MARENOSTRUM 5 275 PFlop/s - SPAIN

- MareNostrum 5 ACC (Accelerated Partition) 1120 nodes based in Intel Sapphire rapids (64 cores/node) and Nvidia Hopper GPUs (4 GPUs/node). 230 PFlops HPL
- MareNostrum 5 GPP (General) **Purpose Partition**) 6408 nodes based in Intel Sapphire rapids (112 cores/ node). 45 PFlops HPL





Main computing resources in Europe



MELUXINA supercomputer 12.81 PFlop/s - LUXEMBOURG



KAROLINA supercomputer 9.59 PFlop/s - CZECH Republic



(*) 10¹⁸ Flop/s

will be the first EuroHPC exascale(*) supercomputer (@Julich-Germany)

DISCOVERER supercomputer 4.51 PFlop/s - BULGARIA



DEUCALION supercomputer 7.22 PFlop/s - PORTUGAL





6.92 PFlop/s - SLOVENIA







Database Theoretical **Computational Physics** Projects

L. Cosmai, M. Pepe - CSN4 2024



Information starting from 2019





• Grants for computing resources ~ 1 Gcorehours

- (\sim 100 applications to competitive calls)
- **Articles produced with resources from the** agreement Cineca-INFN ~ 450
- Talks produced with resources from the agreement **Cineca-INFN** ~ 350
- Master or PhD thesis with resources from the agreement Cineca-INFN ~ 150



