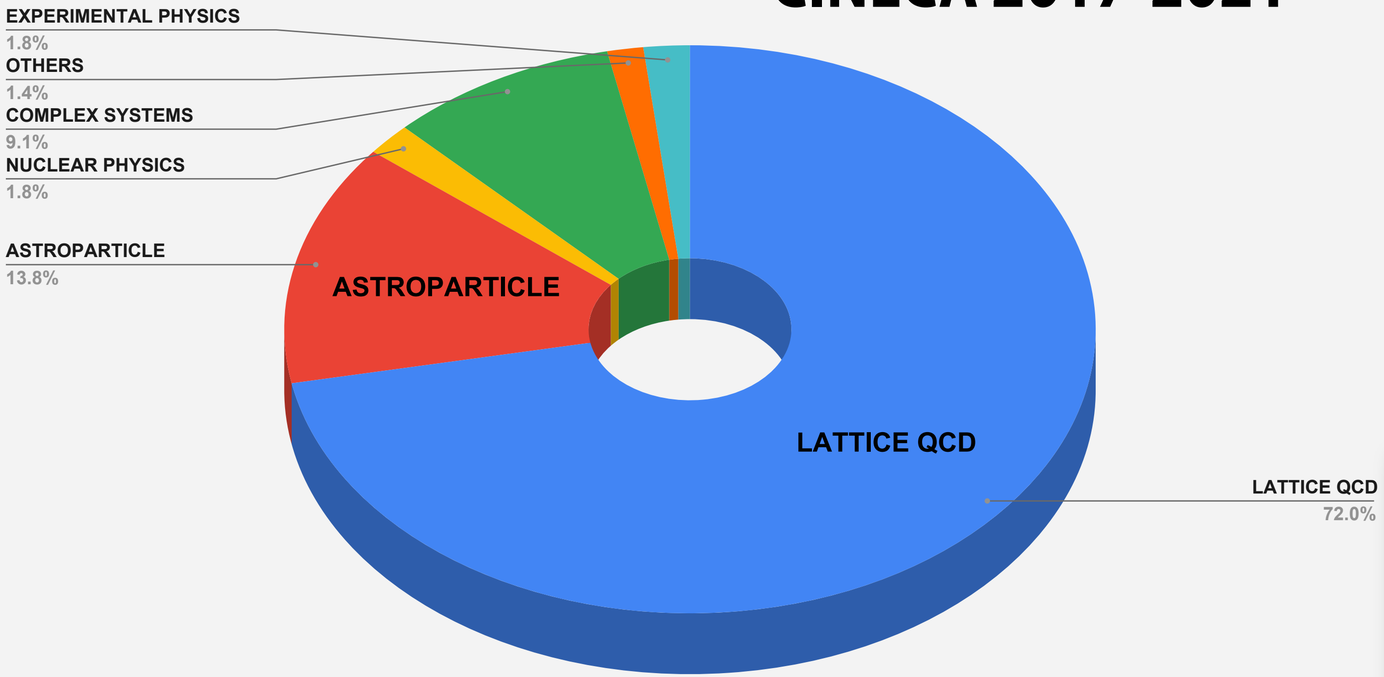
CSN4 - Risorse di calcolo per il 2023

Leonardo Cosmai, Michele Pepe

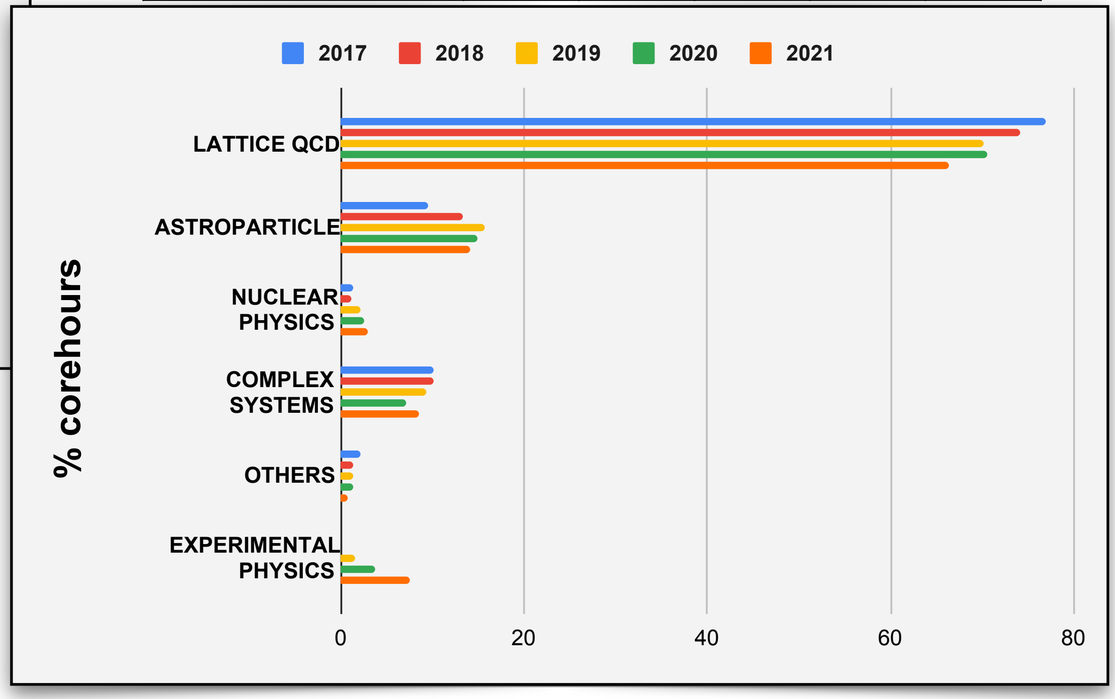
Roma, 6 Settembre 2022

HPC COMPUTING RESOURCES 2017-2021



AREA	corehours	%
LATTICE QCD	687,787,117	72.0
ASTROPARTICLE	131,826,951	13.8
NUCLEAR PHYSICS	17,546,676	1.8
COMPLEX SYSTEMS	87,396,389	9.1
OTHERS	13,724,017	1.4
EXPERIMENTAL PHYSICS	17,596,432	1.8
TOTAL	*955,877,582*	*100*

%corehours	2017	2018	2019	2020	2021
LATTICE QCD	76.97	74.09	70.06	70.62	66.31
ASTROPARTICLE	9.49	13.34	15.64	14.80	14.06
NUCLEAR PHYSICS	1.24	1.05	2.17	2.45	2.86
COMPLEX SYSTEMS	10.09	10.10	9.25	7.10	8.51
OTHERS	2.21	1.43	1.35	1.28	0.80
EXPERIMENTAL PHYSICS			1.53	3.75	7.46



Le risorse di calcolo

Andamento storico (2012-2021)

RISORSE INFN SULLE MACCHINE CINECA A PARTIRE DA SETTEMBRE 2012 (Mcorehours)						
	FERMI	GALILEO	MARCONI (A1)	MARCONI (A2)	MARCONI (A3)	MARCONI100
Set 2012 - Dic 2013	115					
2014	110					
2015	100	15				
2016	100	15				
2017		15	18	120		
2018			9	120	164	
2019				120	164	
2020					164	10
2021					110	21

2018	ASSEGNAZIONE (Mcorehours)	CONSUMO (Mcorehours)	CONSUMO/ASSEGNAZIONE (%)
MARCONI (A1)	9.00	4.90	54.44%
MARCONI (A2)	120.00	119.00	99.17%
MARCONI (A3)	164.00	141.00	85.98%

2019	ASSEGNAZIONE (Mcorehours)	CONSUMO (Mcorehours)	CONSUMO/ASSEGNAZIONE (%)
MARCONI (A2)	120.00	119.20	99.33%
MARCONI (A3)	166.10	162.80	98.01%

2020	ASSEGNAZIONE (Mcorehours)	CONSUMO (Mcorehours)	CONSUMO/ASSEGNAZIONE (%)
MARCONI (A3)	169.00	163.00	96.45%
MARCONI100	10.11	11.93	117.98%

2021	ASSEGNAZIONE (Mcorehours)	CONSUMO (Mcorehours)	CONSUMO/ASSEGNAZIONE (%)
MARCONI (A3)	102.25	73.25	71.64%
MARCONI100	20.70	14.50	70.05%

Le macchine al CINECA (2012-…)

	processor	#cores/ node	#accelerators/ node	#nodes	#cores	(peak perf)/node [GFlop/s]	(peak perf)/core [GFlop/s]	peak performance [PFlop/s]	start date	end date
FERMI	IBM PowerA2	16		10,240	163,840	204.8	12.8	2.1	01-Sep-2012	18-Jul-2016
GALILEO	Intel Haswell	16		516	8,256	1,170.0	73.1	0.6	01-Feb-0205	20-Nov-2017
MARCONI-A1 (Broadwell)	Broadwell	36		1,512	54,432	1,300.0	36.1	2.0	04-Jul-2016	26-Sep-2018
MARCONI-A2 (KNL)	Knights Landing (KNL)	68		3,600	244,800	3,000.0	44.1	10.8	04-Jan-2017	01-Jan-2020
MARCONI-A3 (SKL)	Skylake	48		3,188	153,024	3,200.0	66.7	10.2	07-Aug-2017	
MARCONI100	IBM Power AC922	32	4 nVidia V100	980	31,360	32,000.0	1,000.0	31.4	04-May-2020	
GALILEO100	Intel Xeon Platinum	48	2 V100 (su 36 nodi)	554	26,592	3,530.0	73.5	2.0	15-Oct-2021	

Le risorse di calcolo

Le risorse computazionali oltre l'Accordo CINECA-INFN *(e.g. periodo 2017-2019)*

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  agreement CINECA-INFN dal 2012 parzialmente finanziato da:
  - progetto premiale SUMA (0.5 Meuro: GALILEO)
  - progetto HPC_HTC (CIPE) (1.5 Meuro: MARCONI-SKL)

- 

Partnership for Advanced Computing in Europe (PRACE)

- **Italian SuperComputing Resource Allocation - ISCRA**

	# progetti	corehours
CINECA-INFN AGREEMENT (2017-2019)		*730,000,000*
ISCRA-C	45	20,615,000
ISCRA-B	40	205,440,950
PRACE	30	925,928,640
ALTRE RISORSE INTERNAZIONALI	11	367,000,000
TOTALE		*1,518,984,590*
GRAN TOTALE		*2,248,984,590*
Lavori pubblicati (con uso di risorse HPC)	*315*	

- **Moltiplicatore per accesso a risorse ISCRA e PRACE: 2,250,000,000/730,000,000 = 3**

Le sigle della CSN4 che fanno uso di risorse di calcolo HPC

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

Cosmology and Astroparticle Physics:
- INDARK *(M. Lattanzi)*
- NEUMATT *(R. De Pietri)*
- TEONGRAV *(B. Giacomazzo)*

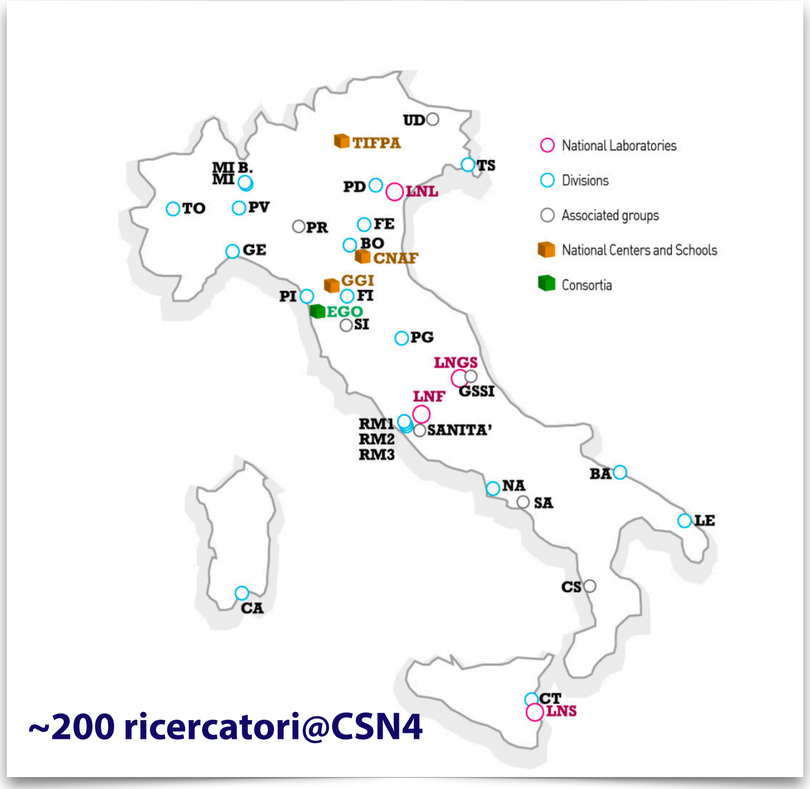
Nuclear Physics:
- MONSTRE *(N. Itaco)*
- NUCSYS *(M. Viviani)*

Standard Model Phenomenology:
- QFTATCOL *(C. Carloni Calame)*

Physics of the Complex Systems:
- BIOPHYS *(S. Morante)*
- ENESMA *(C. Presilla)*
- FIELDTURB *(G. Boffetta)*

Quantum Information:
- QUANTUM *(S. Montangero)*

Condensed matter:
- NEMESYS *(A. Sindona)*



~200 ricercatori@CSN4

Lattice QCD

Projects: LQCD123, NPQCD, QCDLAT, SFT, SIM, GAGRA

LQCD123

Physics activity: QCD + QED phenomenology

QED CORRECTIONS TO LEADING HADRONIC CONTRIB. (a_μ) OF $g_\mu - 2$

PRD99(**2019**) + update in progress

$$\frac{\delta a_\mu^{HVP}(ud)}{a_\mu^{HVP}(ud)} = 0.0115(18)_{stat+fit}(21)_{input}(20)_{chir}(19)_{FVE}(9)_{cont}$$

$$= 0.0115(40)$$

$$a_\mu^{HVP}(ud) = 619.0(17.8)\cdot 10^{-10}$$

$$\delta a_\mu^{HVP}(ud) = 7.1(2.5)\cdot 10^{-10}$$

ℓ_7 low energy constant

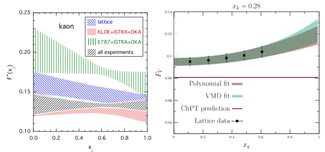
PRD 104, 074513 (**2021**)

ISCRA22B - EπC

REAL & VIRTUAL PHOTON EMISSION

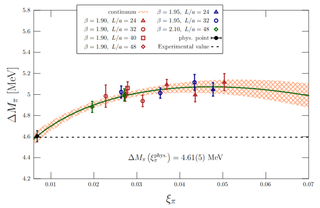
PRD103,1 (**2021**), PRD103,5 (**2021**)

and arXiv:2202.03833 (to appear on PRD)



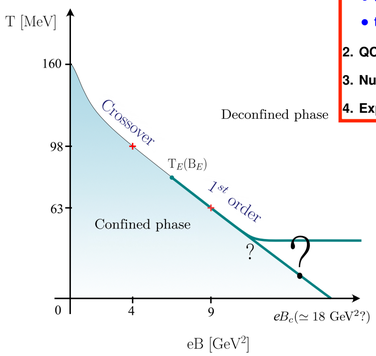
$M_{\pi^+} - M_{\pi^0}$ theoretical prediction to $\mathcal{O}(\alpha)$

arXiv:2202.11970



NPQCD

1. QCD in extreme conditions
   - finite temperature and density
   - phase diagram in strong magnetic backgrounds
   - color confinement and deconfinement
   - topological properties and axion phenomenology
2. QCD-like theories (Large-N limit, universality)
3. Numerical approaches to quantum gravity (CDT)
4. Exploratory exercises in Quantum Computing

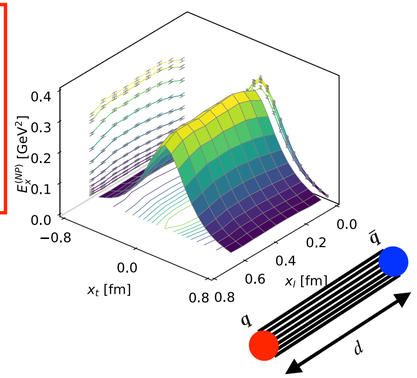


Critical endpoint found in the QCD Phase Diagram in a magnetic background

M. D'Elia, L. Maio, F. Sanfilippo and A. Stanzione, "Phase diagram of QCD in a magnetic background," Phys. Rev. D 105, 034511 (2022)

Editors' suggestion

based on NPQCD and Iscra-B QGPSMF HP10B9REXC



The non-perturbative chromoelectric field obtained by subtracting the perturbative contribution

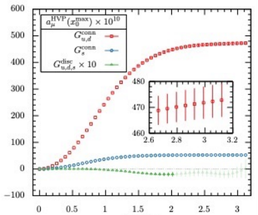
M. Baker, V. Chelnokov, L. Cosmai, F. Cuteri, and A. Papa, "The flux tube profile in full QCD", POS Lattice 2021

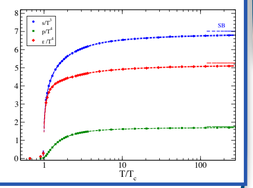
based on NPQCD and Iscra-B HP10BUL8OZ

QCDLAT

The Physics

- **Theme 1: QCD and flavour physics in the SM and beyond**
  $(g-2)_\mu$, ΔF=2 in SM and beyond, CP violation in K, D and B mixing and decays
- **Theme 2: QCD at high temperature**
  Equation of State, screening masses, transport coefficients, topology (axions)...
  Study of QCD phase diagram by simulations with an imaginary chemical potential
- **Theme 3**: **Theoretical developments**
  NP renormalization: quark masses, energy-momentum tensor, ΔF=2 operators in SM and beyond, …., . NSPT, improvement, . . .





SFT

Research focus: Strongly interacting quantum theories describing *condensed matter* and *elementary particles*:

- Statistical field theories in and out of equilibrium
- Entanglement in quantum systems
- Topological phases of matter
- Conformal field theory
- Integrable models

HPC-intensive activities:

- Conformal field theory and conformal perturbation theory *vs.* Monte Carlo simulations of lattice gauge theories
- Lattice simulation of topological objects in statistical models
- Free energies from non-equilibrium Markov-chain Monte Carlo & machine learning for lattice field theory
- Strong dynamics with matter fields in multiple representations: lattice simulation of SU(4) lattice gauge theory for new physics beyond the Standard Model

SIM

SIM

Research Topics

Critical and pseudocritical behaviour in QCD

Phenomenology of the Quark Gluon Plasma

QCD axions and topology of strong matter

Dense matter: methods and models

Machine Learning for phase transitions

LQCD123

Computation time requests for year 2023

A) State-of-the-art simulations of QCD with 2+1+1 dynamical quarks with physical pion mass

A1) Continuation of gauge ensemble cA.080.64 (L = T/2~ 6 fm, a~0.095 fm) with O(1000) trajectories and related measurements.
Motivation: needed to have a further lattice spacing (the coarsest in the present ETMC setup) for better control of continuum extrapolations in the charm and bottom flavour physics, see PRD 104 (2021) 7; 074520, PRD 104 (2021) 7, 074515; PRD 103 (2021) 1, 014502.

Estimated cost 50k node-hours on M100/LEONARDO (GPU cluster)

A2) Very large volume gauge ensemble cB.072.128 (L = T/2 = 10.5 fm, a=0.082 fm):
with O(500) trajectories.
Motivation: compute the (long distance part of) the Hadronic Vacuum Polarization contribution to g_μ -2 and, by spectral density methods, the R-ratio of $e^+e^- \rightarrow$ (hadrons) at different CoM energies, see e-Print: 2206.15084, submitted to Phys.Rev.D for publication; Phys.Rev.D 99 (2019) 9, 094508.

Estimated cost 350k node-hours on M100/LEONARDO (GPU cluster)

B) A bsm-mass-generation mechanism (PhysRevLett 123, (2019) 061802) in two different lattice regularizations: computation of quark propagators and derived observables using quenched bosonic field configuration on lattices L^3x 2L with linear size L/a < 30 .
Motivation: studying the level of universality and predictive power of a recently proposed (PRD 92 (2015) 5, 054505) mechanism of elementary fermion mass generation based on a sofar unnoticed non-perturbative fermion chiral anomaly.

Estimated cost is 7 M core-hours on MARCONI-A3/LEONARDO (CPU cluster)

C) Determination of leptonic decay constants with very high precision, by means of calculation of the needed two point function with high-statistics directly at the physical point, along the line of Phys.Rev.D 104 (2021) 7, 074520. Determination of the unitarity bounds for semileptonic B meson decay along the line of our recent PRD 104 (2021) 5, 054502.
Motivation: increase the accuracy of the Unitary Triangle tests of the CKM matrix, by decreasing the statistical and systematic uncertainties related to the involved hadronic matrix elements.

Estimated cost 200k node-hours on M100/LEONARDO (GPU cluster)

D) Determination of form factors for the real and virtual radiative leptonic decay of mesons, of the form $P \rightarrow \ell\nu\gamma$ computed on several kinematics, with the needed infrared cancellation along the line of *PRD* 103 (2021) 1, 014502 and *Phys.Rev.D* 105 (2022) 11, 114507, with simulations carried out at the physical pion mass, for several pseudoscalar mesons of phenomenological interest.
Motivation: the real radiative emission is needed to increase the accuracy of the determination of the CKM matrix elements beyond the precision of %, at which QED and radiative corrections cannot be neglected. This is especially interesting for heavy mesons for which no effective theory can be used to take into account the radiative effects. The virtual radiative emission offers additional channels to determine the CKM matrix elements from channel not affected by helicity suppression.

Estimated cost: 8 M core-hours on MARCONI-A3/LEONARDO (CPU cluster)

Risorse ottenute da call competitive (ultimi 3 anni)

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PRA17-4394:  45M core hours su MARCONI (KNL)
PRA20-5171:  76M core hours su Marconi100
PRA22-5171: 66M core hours su Marconi100
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NPQCD

HPC Research Program for year 2023, 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 GPU [1, 2] or standard [3] clusters, but also on other publicly available codes [4].

The main research topics to be pursued in 2023 are the following:

A) QCD PHASE DIAGRAM

We have recently found first evidence for a critical endpoint in the phase diagram of QCD in the presence of a magnetic background field [5]. That opens the way for a number of planned investigations:

- extensive simulations, with lattice spacings down to ~ 0.05 fm and lattices of at least 3 fm in spatial size, in order to locate the critical endpoint and determine the latent heat along the first order line [mostly running on GPU, estimated cost 200K nodehours]
- measurement of various other quantities of phenomenological interest close to the critical endpoint, in particular topological or transport quantities, such as the electric conductivity [mostly running on CPU on gauge ensembles produced in previous point, estimated cost 3Mcorehours]
- combined simulations at non zero-magnetic background field and imaginary chemical potential, in order to reveal a possible connections with the critical endpoint expected at finite baryon chemical potential [mostly running on GPU, estimated cost 100K nodehours]

B) QCD TOPOLOGY AND AXION PHENOMENOLOGY

A recent study of ours [6] has shown that a careful study of QCD topology at finite temperature, in particular reaching T $\sim$ 1 GeV and above, which is the range relevant for axion phenomenology, requires a careful consideration of various systematic effects. We find agreement with the power law behaviour predicted by semiclassical arguments, but a tension in the overall normalization. Future progress can be based on the developement of efficient numerical codes which improve the sampling of topological modes, like the one developed recently by our group [7]. We plan to continue and combine our recent efforts in these directions, in order to refine our present determinations and possibly reach higher temperatures, that will require large efforts on lattice with lattice spacings down to ~ 0.02 fm [mostly running on GPU, estimated cost 200K nodehours]

C) QCD flux tubes and deconfinement transition

We plan to study the spatial distribution of all components of the color fields created by a static quark and antiquark in (2+1)-flavor QCD with physical quark masses. We have identified the components of the measured chromoelectric field transverse to the line connecting the quark-antiquark pair with the transverse components of an effective Coulomb-like field E_C associated with the quark sources. The next step is subtracting E_C from the total simulated chromoelectric field E yields a non-perturbative, primarily longitudinal chromoelectric field E_{NP}, which to be identified as the confining field. We expect to find evidence of the "string breaking" phenomenon. We plan to study also the distribution of (chromo)magnetic currents and electric charges near the sources [8, 9]. We plan to extend the study of the spatial distribution of all components of the color fields created by a static quark and antiquark to the case of the SU(3) pure gauge theory at nonzero temperature. We will attempt also in these case to separate the longitudinal chromelectric field into nonperturbative and Coulomb- (or Yukawa-) like parts. We also plan to study the effect on the spatial distribution of color fields of external fields, such as a chromomagnetic field or the effect of a baryonic chemical potential. [Estimated cost 200 knodehours GPU, 5 Mcorehours CPU]

D) Other projects [estimated total cost 100 knodehours GPU, 7 Mcorehours CPU]
We list here a number of other projects planned for next year, which will be running on both GPU and CPU HCPC resources and complete our demand for computational resources:

- investigation of lattice QCD at non-zero temperature and density through effective Polyakov loop models in dual formulations and in the static approximation for the quark determinant, both with Wilson and staggered fermions [10].
- properties of the staggered Dirac operator and investigation of QCD chiral properties through staggered spectral projectors [GPU for production, CPU for analysis]
- study of gauge theories with a double compactification, with or without a trace deformation
- interplay between local and global symmetries in lattice gauge models, with the principal aim of characterizing the models whose critical behaviour is associated to an effective field theory with local gauge symmetry.
- confining properties of QCD in the region around the crossover temperature.

Risorse ottenute da call competitive (ultimi 3 anni)

- **PRACE:** AXTRO (call 13) and SISMAF (call 9)
- **ISCRA-B:** HP10BWSSLC, HP10BLQLBY, HP10BQMUVT, HP10B36BYO, HP10BA76RL, HP10BX8GQE, HP10BZV1G1, HP10BA5QTA, HP10BSRSMS, HP10B4P9OZ, HP10B9REXC, HP10B2J1PH, HP10CIN32X (last 4 in the last 3 years)

References

[1] C. Bonati, E. Calore, S. Coscetti, M. D'Elia, M. Mesiti, F. Negro, S. F. Schifano, G. Silvi and R. Tripiccione, Int. J. Mod. Phys. C **28**, no.05, 1750063 (2017) doi:10.1142/S0129183117500632 [arXiv:1701.00426 [hep-lat]].

[2] C. Bonati, E. Calore, M. D'Elia, M. Mesiti, F. Negro, F. Sanfilippo, S. F. Schifano, G. Silvi and R. Tripiccione, Int. J. Mod. Phys. C **29**, no.01, 1850010 (2018) doi:10.1142/S0129183118500109 [arXiv:1801.01473 [hep-lat]].

[3] https://github.com/sunpho84/nissa

[4] https://web.physics.utah.edu/ detar/milc/

[5] M. D'Elia, L. Maio, F. Sanfilippo and A. Stanzione, Phys. Rev. D **105**, no.3, 034511 (2022) doi:10.1103/PhysRevD.105.034511 [arXiv:2111.11237 [hep-lat]].

[6] A. Athenodorou, C. Bonanno, C. Bonati, G. Clemente, F. D'Angelo, M. D'Elia, L. Maio, G. Martinelli, F. Sanfilippo and A. Todaro, [arXiv:2208.08921 [hep-lat]].

[7] C. Bonanno, C. Bonati and M. D'Elia, JHEP **03**, 111 (2021) doi:10.1007/JHEP03(2021)111 [arXiv:2012.14000 [hep-lat]].

[8] M. Baker, P. Cea, V. Chelnokov, L. Cosmai, F. Cuteri and A. Papa, Eur. Phys. J. C **80**, no.6, 514 (2020) doi:10.1140/epjc/s10052-020-8077-5 [arXiv:1912.04739 [hep-lat]].

[9] M. Baker, V. Chelnokov, L. Cosmai, F. Cuteri and A. Papa, [arXiv:2207.08797 [hep-lat]].

[10] O. Borisenko, V. Chelnokov, E. Mendicelli and A. Papa, Nucl. Phys. B **965**, 115332 (2021) doi:10.1016/j.nuclphysb.2021.115332 [arXiv:2011.08285 [hep-lat]].

QCDLAT

QCDLAT
INFN Research Project of the Theory Group (CSN4)

Title: Next generation lattice field theory for searching new phenomena in particle physics
National Coordinator: Leonardo Giusti (Leonardo.Giusti@mib.infn.it)
INFN sections of people involved: Milano Bicocca, Parma, Roma1, Roma2
Number of Participants: 17

Description of the research activity

The main objective of this project is to search for new fundamental phenomena in Nature by advancing the theoretical knowledge on strongly interacting theories in the Standard Model and beyond. We will strive for developing new theoretical and computational tools to cast into a coherent fundamental theory existing and forthcoming experimental results from the LHC as well as from many other high-energy experiments. We will carry out precise studies of the dynamics of the strong interactions from first principles within the lattice field theory setup. We aim at computations with a precision of percent or less. This is the accuracy required for the interpretation and the analysis of the wealth of experimental results expected both for sub-nuclear matter and for the quark-gluon plasma.

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 2023 using the INFN computational resources are the following:

QCD and flavour physics in the Standard Model and beyond: working on the determination of the hadronic contribution to $(g-2)_\mu$ using a multi-level Monte Carlo and with a target accuracy of a few permille, precise determination of fundamental Standard Model parameters, weak matrix elements for leptonic, semi-leptonic and $\Delta S = 2$ transitions;

QCD at high temperature and finite density: study of the phase diagram in the temperature - chemical potential plane, with a precise calculation of the QCD Equation of State and of the screening masses at μ=0 up to temperatures of O(100) GeV. We will also keep on investigating the QCD phase diagram via multi-point Padé approximants, computed via imaginary baryonic chemical potential simulations. In particular, lower temperatures will be probed, focusing on the chiral transition regime.

Theoretical developments: study of non-perturbative renormalization of fundamental parameters and composite operators, Lefschetz thimbles and chiral symmetry breaking. Perturbative calculations around non-trivial vacua (instantons) will be performed by numerical methods, moving from current Quantum Mechanics computations to (simple) applications in Field Theories.

Computational strategies: fermion determinant factorization, multi-level Monte Carlo, Lefschetz thimbles, master field simulations, numerical stochastic perturbation theory;

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

Request of computational resources at Cineca:

- **CPU**-based partition: **30 Mch**
- **GPU**-based partition: **250 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 128 cores each (e.g., 2x AMD Epyc Rome 64 cores or similar) connected by a 200 Gbit/s switch InfiniBand. In the first stage of algorithmic development, we would use the 8 nodes in 2 sets of 4 nodes each; once the general setup of the new algorithm is defined, the final, fine tuning, stage is accomplished on the whole system of 8 nodes.**

Request of storage space on tape

People participating to the project QCDLAT have been awarded relevant computer resources (European Calls PRACE) at supercomputing centres. In pursuing those projects, many gauge field configurations have been generated: those data are very important since the measurement of physical quantities is, in general, performed in a successive step with respect to the production of the configurations.

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 ask 500 Tb of storage on tape.**

Risorse ottenute da call competitive (ultimi 3 anni)

Approximatively 180 MChours granted by PRACE and ISCRA

SFT

SFT Scientific Initiative – Planned Research Activities for 2023

1. **Spectral reconstruction in gauge theories with fermions in multiple representations** With collaborators from Edinburgh and from Rome, we are extending our previous study of composite-Higgs models reported in Eur. Phys. J C 79 (2019) 638 with the novel spectral-reconstruction technique proposed by two of us in Phys. Rev. D 99 (2019) 094508. The calculations are done with a customized version of the GRID lattice QCD code developed in Edinburgh, which will be ported to graphics processing units (GPUs).

2. **Non-perturbative analysis of inclusive semileptonic decays of heavy mesons** Following our work recently published in JHEP 07 (2022) 083 with collaborators from Rome, Zurich and Tsukuba, we will carry out a systematic study of inclusive semileptonic decays of heavy mesons through the analysis of four-point correlation functions in lattice QCD configurations shared with us by the Extended Twisted-Mass Collaboration. In particular, the extrapolations to the large-volume and to the continuum limits will be undertaken, and comparisons with analytical predictions from heavy-quark effective theory and the operator-product expansion will be performed.

3. **Thermal behavior of composite dark matter in the early universe** In collaboration with researchers from Milan and from Swansea, the equation of state of a composite-dark-matter model, based on a strongly coupled symplectic gauge theory, will be derived through lattice simulations. The nature of the deconfining transition of this model, and its potential implications for primordial gravitational waves, will also be studied.

4. **Stochastic normalizing flows and Monte Carlo calculations out of equilibrium** The formalism recently developed in JHEP 07 (2022) 015, which connects deep generative models used in the field of machine learning with numerical simulation methods based on annealed importance sampling and on non-equilibrium statistical mechanics, will be applied to study non-perturbatively different quantum field theories in various dimensions, at a computational cost dramatically reduced with respect to conventional Monte Carlo methods. For this project we are already using GPUs.

5. **Entanglement entropy from non-equilibrium Monte Carlo calculations** The study of entanglement entropy (a measure of entanglement, one of the fundamental properties of quantum systems) in statistical models with the techniques proposed by an SFT member in Phys. Rev. E 95 (2017) 062132 will be extended to consider the entropic c-function. Having already obtained very encouraging results in the analytically solvable Ising model in two dimensions, we will analyze the three-dimensional Ising model, which is dual to a very simple, yet non-trivial, gauge theory. This project will be carried out adapting an existing code that runs on GPUs.

6. **Hagedorn states and low-energy description of** $\mathrm{U}(1)$ **gauge theory in three dimensions** In collaboration with researchers from Bern, we will carry out a high-precision study of compact U(1) gauge theory in three dimensions at finite temperature through Monte Carlo calculations using multi-cluster algorithms. The study is expected to reveal the existence of non-trivial high-energy states in the spectrum of this theory, which could not be easily accessed through conventional simulations, and which, as was recently discussed in JHEP 03 (2022) 115, in JHEP 05 (2019) 068, in Phys. Rev. D 98 (2018) 054513 and in JHEP 07 (2015) 143, have the potential to reveal important details about the low-energy behavior of confining gauge theories.

7. **Non-commutative regularization of** $\mathrm{SU}(N)$ **group manifolds for quantum simulation** Following the work done by one of us in JHEP 05 (2007) 082, a non-commutative regularization of $\mathrm{SU}(N)$ group manifolds will be worked out, and its application for quantum simulation will be studied through classical simulations, with the goal of providing a systematically improvable, resource-efficient, and symmetry-preserving discretization scheme for quantum simulation of the gauge theories underlying the Standard Model of elementary-particle physics.

SIM

SIM - Strongly Interacting Matter

We plan to continue and extend to new directions our study of Strongly Interacting Matter at extreme conditions of temperature by lattice simulations of Quantum Chromodynamics with twisted mass Wilson fermions. Twisted mass Wilson fermions have been developed by the Roma colleagues and are particularly well suited to deal with chiral symmetry. By "extreme temperatures" we mean temperatures explored by current LHC experiments, from about 150 to 400 MeV. In this range there is a phase transition to a plasma phase (Quark Gluon Plasma), which is the most recent cosmological transition. The highest temperatures afford the possibility of studying properties of the QCD axion.

Within previous runs we have generated a set of ensembles for several pion masses, ranging from physical $m_\pi = 139$ MeV up to heavy regime $m_\pi \simeq 400$ MeV. The charm and strange masses are set to their physical values. The latter is a significant characteristic of our simulations, since a dynamical charm is normally not included in high temperature studies, even if it is known to have an impact on thermodynamics. For a recent publication see e.g. A. Y. Kotov, M. P. Lombardo and A.Trunin, Phys. Lett. B **823** (2021), 136749, for an brief overview EPJ Web Conf. **258** (2022), 05012. A full set of references is available on spires.

Our goals for the simulations in the year 2023 include the following:

1. Current statistics does not allow to measure all observables with good statistical accuracy. In particular we would like to enhance the study of axion properties including the potential. We plan to increase statistics for existing ensembles. Estimated CPU-time: 1500000 core hours.
2. The results for the physical pion mass were generated only for one lattice spacing. Due to recent tuning of the parameters of ETMC (Extended Twisted Mass Collaboration), simulations now can be performed with other lattice spacings. We plan to generate new configurations for physical pion mass and smaller lattice spacing. Estimated CPU-time: 2500000 core hours.
3. Using older and new configurations we plan to attack a recent observed, unexpected property of the QCD plasma, namely the existence of an anomalous threshold at temperatures of about 300 MeV. To this end the following observables are going to be measured: meson screening masses, chiral observables. A joint analysis of heavy quark potential and monopoles with the group of V. Bornyakov is planned. Required GPU-time: 1500 node-hours, for at least an initial study for the new, more demanding observables. A full re-analysis of the chiral condensate may be more expensive.
4. We plan to study the application of machine learning techniques and methods for identifying phase transitions in QCD and QCD-like theories, a project initiated with Lucio Anderlini and Andrea Palermo, preliminary results presented at Lattice2021. As the first step, we would consider the pure Yang-Mills theory, which does not require huge computational resources, and afterwards continue the study on the ensembles generated with dynamical fermions. Estimated GPU-time: 1500 node-hours, for an initial study. The need would increase for a full, detailed study including continuum limit and finite volume scaling in Yang Mills.

Possible usage of GPU resources

Our request comprises already GPU projects [tasks 3,4]. The request, as indicated, may benefit from a larger allocation. Generation of the new configurations with ETMC code [tasks 1,2] at the moment can be performed only on the CPU machine.

If a request arises to use only GPU, we see two possibilities: if the GPU porting of ETMC code is ready, then tasks 1 and 2 will be ported on GPU. If not, we are prepared to shift the configuration generation on other machines, and extend the GPU simulations for machine learning and observables as described in the text.

In short, it seems possible to convert our entire request for CPU's to GPU's. In concreteness, that would require some more careful timing, and some reorganization of our planning.

Further computational resources

We plan to apply to ISCRA resources. The request maybe more GPU or CPU oriented depending on the outcome of this INFN request. We cannot apply to EuroHPC resources as M.P. Lombardo chairs the EuroHPC panel for particle physics.

Risorse ottenute da call competitive (ultimi 3 anni)

```
2022–2025 Dirac
vedi attachment per dettagli(le allocazioni vengono aggiustate ogni quattro mesi)
146.000 Mcore–h su AMD–Rome @ Data Intesive Leicester nel 2022


2019–2021 ISCRA
1250000 standard hours MARCON2 +
103642 M100


2016–2019 PRACE
23 000 000 core hours on FERMI +
10 000 000 core hours on MARCONI (KNL) +
8 500 000 core hours on MARCONI (KNL)
```

Cosmology and Astroparticle Physics

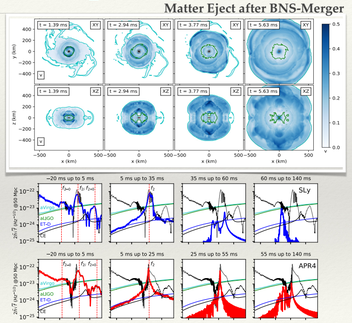
Projects: TEONGRAV, NEUMATT, INDARK

NEUMATT

NEUtron star MATTer - Computing Activity

- National Coordinator : **Alessandro Drago** (Univ. Ferrara)
  INFN-CT: Fiorella Burgio, Antonino Del Popolo, Hans-Josef Schulze, Isaac Vidaña **INFN-FE**: Michal Bejger, Roberto De Pietri, Alessandro Drago, Alessandra Feo, Andrea Lavagno, Giuseppe. **INFN-LNGS**: Massimo Mannarelli, Francesco Vissani, Giulia Pagliaroli. **INFN-MI**: Pierre Pizzochero. **INFN-PI**: Ignazio Bombaci, Domenico Logoteta
- **Main topic: GRAVITATIONAL WAVE SIGNAL FROM THE MERGE OF BINARY NEUTRON STARS**
- **New research in progress on the R-mode excitation of Neutron Stars as Gravitational Waves-source.**
- **Full 3D-simulation of Einstein Equation coupled to matter of the merger. Post-merger signal + study of the the ejected matter. Equation of State effect on the signal.**
- Recent works: ApJ 881 122 (2019), Phys. Rev. D 101, 064052 (2020) + PhD. + MS.Th + work in preparation.

Matter Eject after BNS-Merger



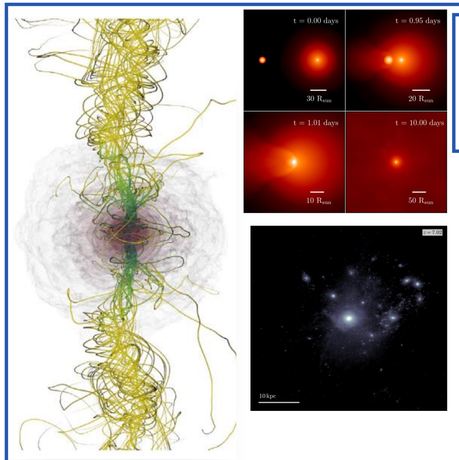
post-merger GWfrequency is changing with time….

INDARK

Dark energy and matter, axions, neutrinos, modified gravity

Markov Chain Monte Carlo codes interfaced with Boltzmann codes

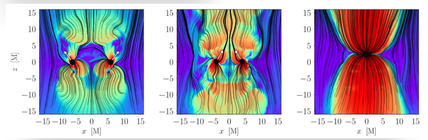
TEONGRAV

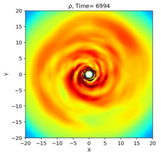


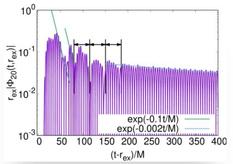
Hydrodynamics and magnetohydrodynamics simulations using state of the art codes in both the Newtonian and the General Relativistic regime

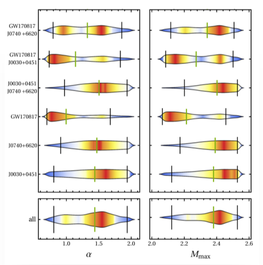
In the field of numerical simulations of compact objects, TEONGRAV performs hydrodynamics and magnetohydrodynamics simulations using state of the art codes in both the Newtonian and the General Relativistic regimes. Main recent projects include:

- Model the gravitational wave emission from horizonless, multicenter geometries within the "fuzzball" paradigm of string theory (Roma 1)
- Model gravitational and electromagnetic emission from neutron stars (Firenze, Milano-Bicocca, Padova, TIFPA, Trieste)
- Accretion disks around Kerr black holes (Firenze)
- Simulations of binaries neutron stars beyond General relativity (Trieste)
- Exploring the dynamics of massive black hole binaries embedded in circumbinary discs (Milano-Bicocca)
- Model electromagnetic counterparts of supermassive black hole mergers (Milano-Bicocca)
- Model dynamical evolution and formation of stellar-mass and supermassive black holes via N-body simulations (Milano-Bicocca, Padova)



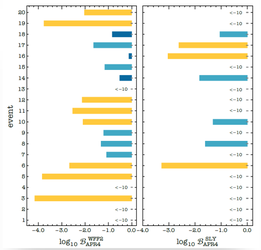


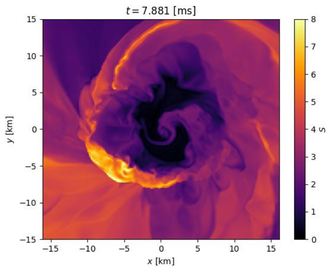




Analysis of observational data and numerical simulations of compact objects

- Develop efficient data analysis strategies which use gravitational-wave observations of binary neutron stars to test the nuclear equations of state of neutron star matter (Roma 1, GSSI).
- Exploit multimessenger observations to constrain fundamental properties of hadron interactions within the neutron star cores (Roma 1, GSSI).
- Inference of nuclear equation of state properties and nucleosynthesis yields from compact binary mergers (TIFPA)
- Machine learning techniques to analyze gravitational waves from black hole binaries (Milano-Bicocca)
- Model selection for detector characterization in Pulsar Timing Arrays (Milano-Bicocca)
- Inferring population distribution parameters using non-parametric methods (Milano-Bicocca)





INDARK

InDark - Description of the research program for 2023

M. Lattanzi for the InDark affiliates

In 2023, computational resources will 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 will develop and run different estimators for the Cosmic Birefringence (CB) effect, the in-vacuo rotation of the linear polarization plane of photons during propagation caused by parity violating EM (e.g. photon-axion coupling). The estimators can be based on CMB maps or CMB spectra. The estimators produce estimates of the isotropic rotation angle (if we consider an isotropic effect) or of the CB spectra/maps (if we consider an anisotropic effect).

We plan to continue our simulation-based study of galaxy clustering on non-linear scales, aimed at measuring both cosmological and primordial non-Gaussian parameters in different inflationary scenarios. Our current pipeline includes a joint power spectrum and bispectrum analysis and has been so far tested in real space. In the coming year, we intend to: extend the analysis to redshift space; add extra-summary statistics, which can be sensitive to higher order correlation functions (e.g. wavelets); apply the procedure to the actual analysis of BOSS data.

We are currently developing a new N-body simulation code for extended cosmologies based on the Gadget-4 code which was publicly released in 2021. This code will allow to run cosmological simulations for any model defined through the Effective Field Theory of Dark Energy formalism, also including large-scale relativistic effects by exploiting the synergy with the relativistic code Gevolution. We expect to have the first production version of this new code by the end of the year. Therefore, in 2023 we expect to be able to proceed with the first cosmological simulations of EFToDE models with this new code.

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 are: 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.

We foresee that these activities will continue to use mainly CPU-based machines, as opposed to GPUs. However, we plan to exploit computational time on GPU-based machines to explore the possibility of migrating a fraction of our codes to GPUs.

In general, as we come closer to the actual data taking stage (SO will be deployed in 2024, Euclid is scheduled for launch in 2023) an increase in computing needs is expected for the coming year. Thus, our activity will likely intensify, which might lead to higher computational needs, both in terms of machine-hours and storage space (to store simulations etc). Moreover, the personnel affiliated to InDark is continuously increasing. Some of the members who have joined recently were heavily relying, in 2022, on HPC resources other than CINECA. These resources will not be available to them anymore in 2023. For all these reason, it would be good to increase the currently allocated time by 25-50%.

Risorse ottenute da call competitive (ultimi 3 anni)

- **EuKEy: 33333 Standard Hours**
- **EuNuComp: 32000 Standard Hours**
- **DZSH: 750000 Standard Hours**
- **DZS: 50000 Standard Hours**

NEUMATT

RICHIESTE CALCOLO (NEUMAT 2023)

To simulate Binary Neutron Star (BNS) systems with both Hadronic Stars and Quark Stars, we need a new resistive magneto-hydrodynamics code (within the Einstein toolkit) that will allow describing the phase-transition between neutron matter and quark matter. This new code will require extensive testing and the execution of HPC scaling performance tests to apply for European union HPC grants.

The collaboration research project also aims to assess the effect of the EOS on the gravitational signal from the merger of Compact (Neutron Star, Hybrid Star, Quark Stars) Binary Systems. The simulation results will be used to create initial data for code describing the formation of a kilonova signal (developed by the new members of the collaboration and collaborator).

Inside the convection INFN-CINECA, we requested computing hours

- Total HPC computing resources (expressed in core-hours) on machines with **CINECA CPU**: **9 Mcorehours** (9,000,000), to be subdivided as
  - 4 MCore hours (MARCONI-A3)
  - 5 MCore hours (LEONARDO (CPU cluster)).
- • Total HPC computing resources (expressed in node-hours) on the machines with **CINECA GPU**: **50k node-hours** (50.000).

The request is targeted at the non-GPU systems, while for GPU systems we require a small initial budget to start porting the code to GPU systems and run ML Equation of State codes.

The CPU-based system resource will be used to simulate Binary Neutron Stars mergers with realistic Equation of State developed by the IS to match and compare the effect of the EOS to the real signal that would be detected by the LIGO/Virgo/Cagra collaboration that is resuming observation on March 2023 and that it is expected to observer O(5) BNS merger with likely O(1) matching EM kilonova/GRB signal. That would require at least 20 simulations of adapted BNS simulation, each costing order of 0.5 Mcorehous.

We do also request 10 TByte of tape storage resources at CNAF to save and preserve the output of the simulations.

TEONGRAV

2023 TEONGRAV HPC Activities

In 2023 we will use HPC resources to continue our numerical investigation on compact object dynamics and their formation. Since most of our codes have not been ported yet to GPU, most of our request is for time on CPU clusters.
Our research will focus in particular on the following topics:

1. Numerical Relativity Simulations of Compact Binary Mergers
2. Formation Channels of Compact Object Binaries
3. Numerical Relativity Simulations of Black Hole Mergers Beyond General Relativity
4. Bayesian parameter estimation with Markov chain Monte Carlo

1. Numerical Relativity Simulations of Compact Binary Mergers: We will simulate systems composed of two neutron stars or of a neutron star and a black hole. We will use fully general relativistic hydrodynamics and magnetohydrodynamics codes, including our new Spritz code and the WhiskyTHC code, both state-of-the-art codes in Numerical Relativity. In some of the simulations we will also include the effect of neutrino emission and absorptions. We will study the merger and post-merger dynamics of these systems in order to investigate the gravitational wave (GW) emission and the possibility to detect them with current and future ground based detectors, such as Virgo and Einstein Telescope. We will also investigate those scenarios in which relativistic jets may be emitted and further evolve the jet propagation in order to better assess the production of short gamma-ray bursts and of their afterglow emission. We will also consider ejected matter and the production of heavy elements via r-process nucleosynthesis and the connected kilonova emission. In a dedicated project, we will study the possible effect of a phase transition to quark matter at supranuclear densities and finite temperatures. In particular we will study systematics effects due to the different implementations of the phase transition.
We will also consider the dynamics of accretion disks around supermassive black hole mergers. These are candidates for the future space-based LISA mission. Our simulations will focus on the electromagnetic counterparts that could be associated with these events by using fully general relativistic magnetohydrodynamics codes, such as the IllinoisGRMHD code within the Einstein Toolkit. We will consider the effect of the plasma configuration and of the black hole binary properties on the electromagnetic emission.

2. Formation Channels of Compact Object Binaries: We will investigate the formation channels of binary compact objects with isolated and dynamical evolution. For the isolated evolution, we have developed and optimized the new population synthesis code SEVN (C++), which can run in parallel over multiple nodes. For the dynamical evolution of binary black holes, we recently developed the semi-analytic code FASTCLUSTER (python), which can generate >1e6 binary black hole mergers per day per single core with a fast numerical algorithm. For more complex simulation, we are co-developing the code PeTar (CUDA, C++ and MPI) with the group of Prof Long Wang (Sun-Yat-Sen University). We will extract estimates of the merger rate density evolution of binary compact objects with the semi-analytic code CosmoRate (python). Our final goal is to do model selection of our models versus the data of the LIGO-Virgo collaboration by means of hierarchical Bayesian analysis.

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

4. Bayesian parameter estimation with Markov chain Monte Carlo: We shall perform Bayesian inference of single GW events and population studies, both to study parameter estimation and waveform systematics, and also to assess whether current and future GW detectors can infer the properties of multiple formation channels for black-hole binaries. We will use the BILBY and pyCBC infrastructures.

Risorse ottenute da call competitive (ultimi 3 anni)

2019: 2 ISCRA B ed 1 ISCRA C (totale 4.2 M core hours)
2020: 2 ISCRA B, 2 ISCRA C, 1 PRACE (totale 16.8 M core hours)
2021: 2 ISCRA C e 2 DECI (totale 4.4 M core hours)
2022: 4 ISCRA C (totale 0.4 M core hours)

QCD Phenomenology

QFTATCOLLIDER

QFT@Colliders [BO, CS, FI, MIB, PV]

- ⇝ Application of Quantum Fiedl Theory to phenomenology of present and future hadron and lepton colliders
- ⇝ Development of Monte Carlo event generators, for meaningful comparison of Theory predictions vs Experimental measurements
- ⇝ Simulation of Standard Model and BSM processes, both for backgrounds and signal
- ⇝ Steadily increasing complexity in theory predictions: higher-order radiative corrections (NLO, NNLO, ...), both in QCD and EW theory, to processes with more and more external particles
- ⇝ CPU intensive computer codes due to multi-loop matrix elements evaluation, Monte Carlo integration and event generation, highly parallelizable
- ✓ QFT@Colliders gets typically 0.4 Mcorehours per year on Marconi under INFN-Cineca HPC agreement
- ✓ MIB won 10 ISCRA C grants (2018-20), for a total of 0.25 Mch on Marconi, 0.22 Mch on Galileo and 23 Kch on Marconi100
- ✓ Furthermore, under a UNIMIB-CINECA agreement, $\simeq$ 2 Mch (effective) on Marconi A3 (2019-22).

QFTATCOLLIDER

QFT@Colliders

July 25, 2022

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 will be 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.

In this context, members of the Project plan to continue the development of the `POWHEG BOX` and `GENEVA` event generators: the use of CPU time both at the validation level and also to perform very simple simulations is quite intense. This is particularly true also in view of the increasing accuracy of these generators that aim to reach the NNLO accuracy in QCD and the NLO accuracy in the electroweak interaction, for a growing number of processes.

In particular they will focus on continuing the implementation of the NNLL′ resummation of the zero-jettiness spectrum for $t\bar{t}$ production in `GENEVA`.

They will also extend the diboson production in `GENEVA` to the production of four leptons in all possible channels (same flavor ZZ, WW and WZ) with the inclusion of the gluon-induced four-lepton production at NLO+NLL′.

In parallel with the study of the previous processes, they plan to work, for the first time, on the combined QCD and QED NLO corrections to inclusive Drell-Yan production and in association with a hard jet/photon, matched to parton shower in `POWHEG`.

Finally, they will perform numerical studies of heavy quark mass contributions to the double parton distributions (DPDs) coming from a perturbative splitting of the standard parton distribution functions.

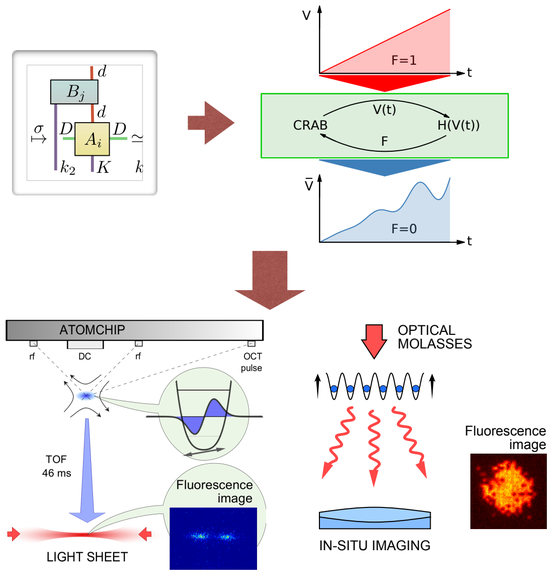
Another research in which members of the Project are actively involved is related to the CERN MUonE experiment. MUonE aims at a new and independent determination of the leading order contribution to the muon anomalous magnetic moment, through a high-precision measurement of the hadronic contribution to the running of the QED coupling constant in elastic $\mu e \to \mu e$ events. The extremely high precision required by the experiment (at the level of 10^{-5}) requires the development of high precision event generators for data analysis, which include exact NNLO QED corrections and resummation of higher orders at least in leading logarithmic approximation. Such geneators are under active development and the evaluation of exact matrix elements at NNLO in QED is a CPU intensive task (up to 1/1.5 s per phase space point on a sigle core).

Simulations and phenomenological studies for SM processes at future e^+e^- (FCC-ee, CEPC) and $\mu^+\mu^-$ colliders are also foreseen.

Quantum Information

QUANTUM

S. MONTANGERO'S GROUP RESEARCH LINES



- Development of efficient (classical and quantum) simulation and control techniques
- Simulation of interesting physics
- Define and probe fundamental limits given by energy, time and information constrains
- Experimental verification of theoretical optimal protocols

QUANTUM

Quantum Theory Group (S. Montangero)

This theoretical physics project aims to open new perspectives in the study of extended quantum many-body systems, with particular focus on the strongly correlated ones, and quantum circuits. The properties of the quantum phases of matter depend on the spatial dimensions of the system. It is well known that in two and three dimensions there is a great variety of possible states of matter and phase transitions with a phenomenology which results much richer than one dimensional case. However, in order to analyze higher-dimensional systems, it is necessary to develop new sophisticated numerical techniques. In this project, we are going to develop efficient software modules for simulating these systems via Tensor Network algorithms. In particular, we are going to explore the possibilities offered by High Performance Computing (HPC) platforms equipped with graphics processing units (GPUs). These components could drastically reduce the computational time required by the basic tensor operations, such as tensor multiplications, contractions and singular value decompositions. With the opportunity to work on HPC clusters with multiple GPUs, we aim to push the limits of tensor networks implementations and thereby set a new benchmark for simulating quantum circuits and solving the Schrodinger equation for quantum many-body systems. Our activity will focus on:

- non-abelian lattice gauge theories;
- quantum circuits and quantum algorithms;
- digital twins of quantum processing units;
- condensed-matter models for closed and open quantum systems;
- tensor network and quantum machine learning models;

For all these models, the simulation time can last from some hours to one month for a single data point. In order to reconstruct the physical phenomena, we need to collect at least ten to one hundreds data points in the different regimes of the model parameters. For example, we have recently performed computations of the ground-states of lattice gauge theories in three-spatial dimensions and we have noticed that our code needs a total time of about one month. In order to reduce the time-to-solution, our efforts are currently devoted to explore the different strategies to exploit tensor network operations, such as tensor contractions on GPUs, and MPI parallelism within our algorithms for ground-state searching or real-time dynamics. A proof-of-concept has been developed during the CINECA GPU Hackathon 2022. Furthermore, we are actively collaborating with the Quantum Lab of CINECA and we have given introductions to tensor network methods during their workshops.

In detail, we will focus on:

- perform simulations of non-abelian SU(2) lattice gauge theory in two-spatial dimensions;
- extend tensor network methods for lattice gauge theories to real-time dynamics;
- perform ground-state simulations of Hubbard-like Hamiltonians in two-dimensions;
- perform finite-temperature simulations for Rydberg systems;
- analysis of quantum processing unit hardware with digital twin systems;
- analysis of quantum error correcting codes with quantum circuits;
- analysis of tensor network machine learning algorithms;

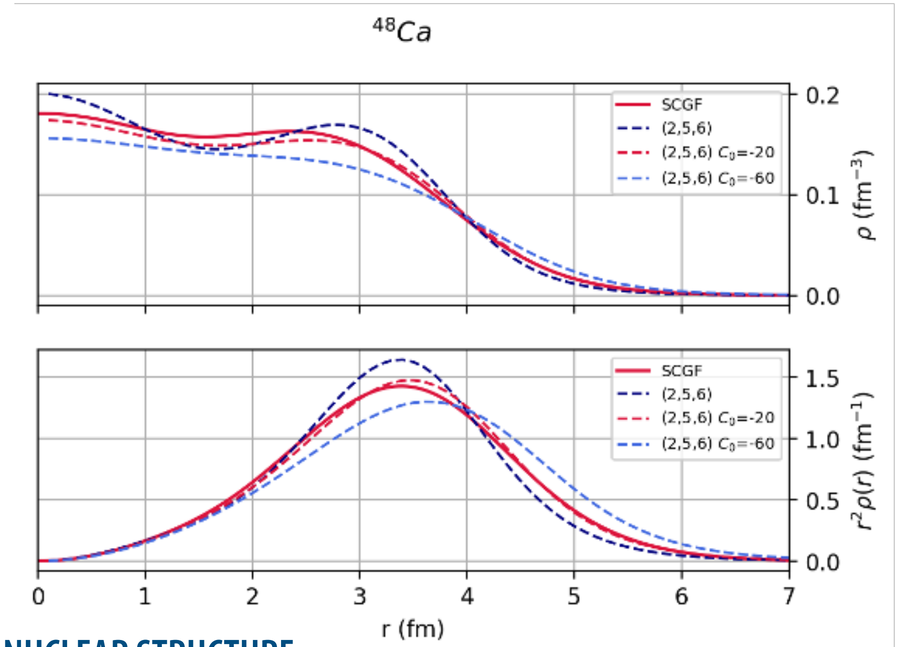
The allocation of resources will allow us to pursue those research goals which require a Tier-0 cluster like MARCONI or GALILEO and continue the successful support for our publications via computational hours at CINECA.

Nuclear Physics

Projects: MONSTRE, NUCSYS

MONSTRE

MOdeling Nuclear STructure and REactions



NUCLEAR STRUCTURE

NUCLEAR REACTIONS

DENSITY FUNCTIONALS

MANY-BODY METHODS

NUCSYS

Astrophysical factor for d(d,p) H & d(d,n) He reactions

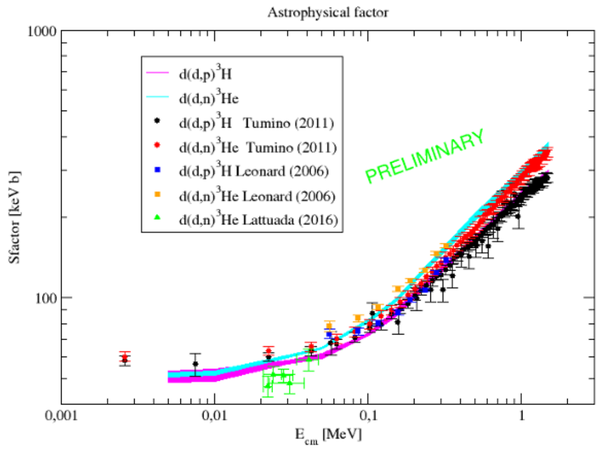
Problem:
- No ab initio calculations
- Large uncertainties from experiments [Yeh, Olive, & Fields, 2021]
- This uncertainty affects the output of BBN codes

Rates of the reactions d(d,p) H & d(d,n) He with polarized fuel

Interest:
- For d+ He reactors, the possibility to suppress the production of neutron from d(d,n) He **(Quintic suppression factor)**
- The possibility to control the direction of emission of neutrons (products emitted preferably in a direction)

→"Lean neutron reactors" reduction of the cost of the walls, more safety, less induced radioactivity, etc.

Quintic suppression factor = σ /σ ratio between the fusion cross section with polarized deuterons and the unpolarized cross section



Iniziativa Specifica MONSTRE
MOdeling Nuclear Structure and REactions

MONSTRE

Attività di ricerca in HPC per il 2023

Lo scopo principale del progetto MONSTRE è quello di costruire un quadro unificato per lo studio dei nuclei atomici, delle reazioni nucleari e della materia fortemente interagente. In tale contesto, le attività di ricerca che fanno ricorso a risorse HPC svolgono un ruolo estremamente rilevante.

In particolare, durante l'anno 2023 saranno sviluppate le seguenti linee di ricerca.

- Utilizzo di metodi Quantum Monte Carlo (AFDMC) per lo studio dei nuclei e della materia nucleare infinita, con l'obiettivo di determinarne non solo l'equazione di stato, ma anche la funzione di risposta nel limite statico.
- Sviluppo di tecniche di funzioni di Green (SCGF) per la materia nucleare e per i nuclei. Per i nuclei finiti esiste un codice altamente efficiente per CPU, utilizzato con interazioni chirali. Al momento si tratta di un ibrido MPI/OpenMP; la struttura del codice, molto dispendioso dal punto di vista dell'algebra lineare, si presta però ad un suo adattamento su GPU. A questo proposito, sarà valutata l'integrazione di librerie matematiche quali Magma o NVIDIA cuSOLVER o cuTENSOR.
- Realizzazione di uno studio basato sulla tecnica dei Neural-Network Quantum States per la descrizione dei sistemi quantistici a molti corpi introdotta da Carleo e Troyer.
- Esecuzione di calcoli in 3D della struttura di vortici in stelle di neutroni, basati sulla teoria di Hartree-Fock-Bogoliubov.
- Calcolo degli elementi di matrice nucleari di interesse per esperimenti con sonde elettrodeboli (p.e. doppio decadimento beta senza emissione di neutrini) mediante la realizzazione di Large Scale Shell-Model Calculations.

Risorse ottenute da call competitive (ultimi 3 anni)

```
1) IscraC:
A three-body chiral interaction for nuclear structure calculations of
heavy nuclei
Acronym: Ch3B
Code: HP10C8TBT0
Validity:6/08/2019-6/12/2020
Budget: 245.000 local hours su Marconi A2 + 8100 local h su Marconi100

2)IscraB:
Calculation of the Nuclear matrix element of Neutrinoless double beta
decay using realistic shell model approach
Acroym: NLDBD
Code: HP10B51E4M
Validity  9/10/ 2019 to  9/03/2021
Budget: 750.000 su Galileo + 45000 su M100+875.000 su Marconi A2

3)Prace_icei
Neutrinoless double beta decay of 100Mo
08-10-2020: creazione progetto al 22/10 /2021
Budget: 1.6M local hours su Marconi100

4)IscraC:
Quenching effect of two-body currents on the axial vector constant g_a
Acronym: QTBGA
Thursday, 10 March, 2022 to Saturday, 10 December, 2022
Budget 100.000 local hours su G100
```

NUCSYS

I.S. NUCSYS

CPU core-hours (Marconi or G100) 1,000,000
GPU core-hours (M100 or G100) 200,000

Descrizione dell'attivita' prevista nel 2023

Nel 2023 abbiamo previsto concludere lo studio delle reazioni che coinvolgono 4 nucleoni, in particolare le reazioni di fusione d(d,p)3H, d(d,n)3He e d(d,gamma)4He. L'interesse di queste reazioni e' legato 1) al problema dell'abbondanza del deuterio nella Big-Bang Nucleosynthesis (BBN) [1] e 2) alla conoscenza dei rate di fusione nel caso di deuterio polarizzato, con l'obiettivo di fornire utili informazioni alla progettazione di reattori a fusione funzionanti con combustibile polarizzato. Per i rate di reazione polarizzate attualmente non sono disponibili dati sperimentali. E' stato comunque ipotizzato che l'uso di combustibile polarizzato dovrebbe portare vari vantaggi: la soppressione dell'emissione di neutroni ed il possibile migliore controllo della direzione dei prodotti emessi [2]. Questo permetterebbe la progettazione di reattori di piu' basso costo e di piu' facile gestione. Lo studio teorico di queste reazioni e' quindi fortemente richiesto ed abbiamo gia' realizzato un primo lavoro [3]. Ma affinche' i rate calcolati teoricamente siano di effettiva utilita', bisogna riuscire anche ad avere una stima precisa dell'incertezza teorica, legata principalmente all'incompleta conoscenza della dinamica nucleare. Si propone di stimare quest'incertezza teorica eseguendo vari calcoli impiegando interazioni nucleari derivate ad ordini crescenti della "chiral perturbation theory"; questo permetterebbe sia la possibilita' di poter estrapolare il valore dei rate di fusione ad "ordine infinito", ma anche di poter avere una stima dell'errore legato al troncamento della teoria perturbativa, che allo stato attuale raggiunge il N4LO. Il codice per studiare le reazioni a 4 nucleoni e' molto be rodato e si tratterebbe di runnare vari casi con diverse interazioni ed energie. Le core-hours di CPU richieste dovrebbero coprire parzialmente il completamento di questo progetto, per cui e' stata anche sottomessa una richiesta di core-hours tramite un bando ISCRA.

Inoltre stiamo sviluppando un nuovo codice per estendere questo studio teorico alle reazioni con A>4, come le reazioni 3H(d,n)4He, 3He(d,p)4He, e 4He(d,gamma)6Li. L'interesse delle prima due reazioni e' di nuovo legato alla produzione di energia nei reattori, sempre per il caso di combustibili polarizzati [2] (in questo caso e' stato ipotizzato che i rati aumentino di un fattore 1.5). La terza reazione e' di interesse per l'astrofisica, in particolare per la formazione del 6Li, e per la soluzione del "Li puzzle" della BBN [4]. Questo nuovo codice e' scritto per sfruttare la potenza di calcolo delle GPU, e per questo e' stata avanzata la richiesta di utilizzo di 200,000 ore di M100 o G100. Il codice e' in fase di test, e si prevede completarlo entro la fine del 2022.

[1] O. Pisanti, G. Mangano, G. Miele, and P. Mazzella, JCAP **04**, 020 (2021)
[2] G. Ciullo, Springer Proc. in Phys. **187**, 1 (2016)
[3] M. Viviani, L. Girlanda, A. Kievsky, D. Logoteta, and L.E. Marcucci, arXiv:2207.01433
[4] See, for example, A. Gnech, PhD Thesis, arXiv:2012.08431

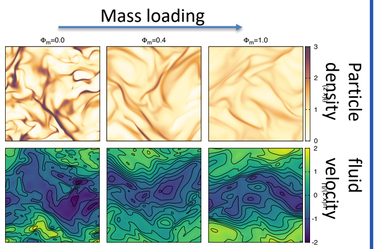
Physics of Complex Systems

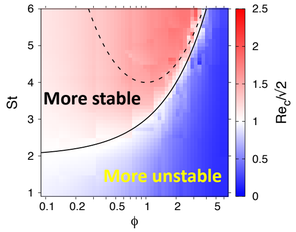
Projects: BIOPHYS, FIELDTURB, ENESMA

FIELDTURB

Dusty Kolmogorov flow

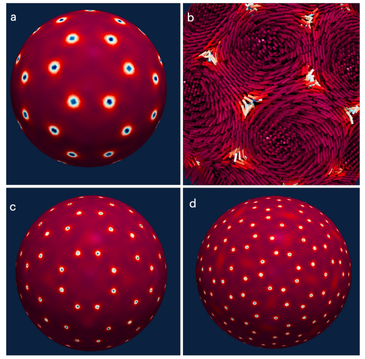
Particles suspended in a fluid exert feedback forces that can significantly impact the flow, altering the turbulent drag and velocity fluctuations. We studied flow modulation induced by particles heavier than the carrier fluid in a Eulerian two-way coupled model. The problem was studied with direct numerical simulations of the turbulent Kolmogorov flow, allowing for studying the momentum balance and the turbulent drag in the absence of boundaries.
A. Sozza, M. Cencini, S. Musacchio, G. Boffetta. *Phys. Rev. Fluids* **5**, 094302 (2020)





Particles suspended do not only alter the drag in turbulent flows, but can also alter the stability properties of the flow when close to the transition from laminar to turbulent flow. We studied by DNS how stability is modified by particles at both changing their mass loading and Stokes time, and compared the result to analytical predictions obtained with multiple scale expansion.
A. Sozza, M. Cencini, S. Musacchio, G. Boffetta. *J. Fluid Mech.* **931**, A26 (2022)

Cholesteric shells: Amorphous phases (blue fog) and finite quasicrystals



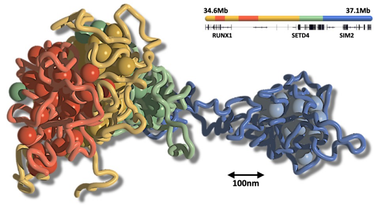
We use lattice Boltzmann parallel simulations to study what phases form when a cholesteric liquid crystal is confined to a thin shell surrounding a curved closed surface. For spherical shells, the curved geometry introduces a geometric frustration making the regular hexagonal lattice of half-skyrmions (b) observed on flat geometries disappear. At small shell radii we observe the formation of finite quasicrystals which consist of regular polygonal mixtures (a-c). As the radius of confinement is increased, these regular structures give space to amorphous arrangements with multifarious variety of double twist polygons scattered with no rule (d).

White spots pin point topological defects surrounding half-skyrmions (see zoom of (a) in panel (b))

Cholesteric shells: two dimensional blue fog and finite quasicrystals, L.N. Carenza, G. Gonnella, D. Marenduzzo, G. Negro, E. Orlandini
Physical Review Letters 128 (2), 027801,(2022).

BIOPHYS

Investigation of the three-dimensional structure of the mammalian genome and its links with gene regulation at the single-molecule level by use of extensive Molecular Dynamics computer simulations.

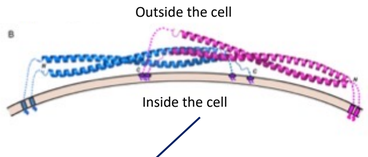


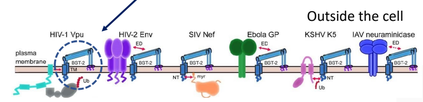
DNA Folding

Structural properties of proteins and protein assemblies (Fig.2 Covid2-orf7 and orf8, in interaction with BST2)

Viral proteins may forbid BST2 antiviral action through Zn-mediated disulfide bond disruption

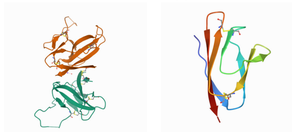
Roma2





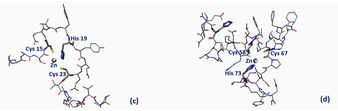
Viral proteins known to interfere with BST2 antiviral activity

CoVid accessory proteins



orf8 (PDB:7JTL)

orf7a (PDB:6W37)



Possible Zn binding sites

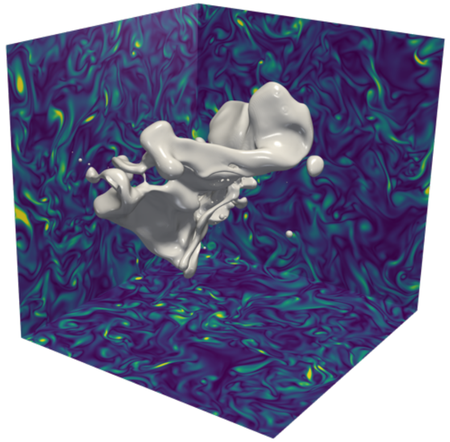
FIELDTURB

FieldTurb

The 2023 numerical research activity.

The numerical activity of the units spans several topics, from classic single-phase and multiphase turbulence to active matter and biological systems.

We will study two cases of non-ideal transport in classic fluid turbulence.
We will study the ability of microswimmers (e.g. oceanic phytoplankton and bacteria) to migrate or orient within a turbulent flow on the basis of local velocity gradients (units of Torino and Roma 2).
We will also use the HPC infrastructure for the study of coupled fluid-structure systems. In particular, we will investigate the dynamics of elastic fibres in turbulent flows (unit of Genova)



Oil droplet breaking in a turbulent flow (numerical simulation)

Regarding multiphase flows, we will study the physics of turbulent emulsions in anisotropic flow conditions. We will investigate how the droplets affect the momentum and energy balance of the flow while simultaneously studying the alterations of droplet size distributions induced by the flow anisotropies (unit of Torino).

A few activities will regard active matter and biological systems.
By using particle-based and coarse-grained field models, we will simulate large systems of non-interacting self-propelled colloids in 2D and 3D, both with and without hydrodynamic interactions, to study in detail the phase behaviour and aggregation kinetics.
We also use Polymer-based models and Molecular dynamics simulations to disentangle the intricate interaction between chromatin structure, dynamics, and gene expression.
At a higher coarse-grained level, we make use of large-scale Lattice Boltzmann simulations to study morphology and the flow patterns of active emulsions both in 2D and 3D to investigate self-motility modes and ordering mechanisms (unit of Bari).

Risorse ottenute da call competitive (ultimi 3 anni)

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Alessandra Lanotte, Unita' Lecce
2019 Project EU-PRACE 19th Call
SPECTRA Universality of Kolmogorov spectrum in non ideal turbulent flows
56 M core-hours Marconi KNL (Cineca)

Luca Biferale, Unita' di Roma 2
2019 PRA17_4374
TURB-ROT - Inverse and direct cascades in rotating turbulent flows
60 M core-hours Marconi 2 (Cineca)

Guido Boffetta, Unita' di Torino
2019 Iscra B
Pourun - Turbulent convection in porous media
4 M core-hours su Marconi KNL

Guido Boffetta, Unita' di Torino
2020 Iscra Covid
TurboPuf - Transport of droplets by turbulent multiphase puff
2 M core-hours su Galileo

Stefano Musacchio, Unita' di Torino
2022 EuroHPC proposal
Anisotropy in turbulent emulsions
richieste 3.58 M core-hours su MeluXina (under revision)
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BIOPHYS

The INF22_biophys project (coordinator Silvia Morante) collects the activity of 7 groups involved in high-performance computing in the field of biophysics. Below the list 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), Pietro Faccioli;
- University of Napoli (UNINA), Mario Nicodemi;
- Scuola Normale Superiore of Pisa (SNS), Giuseppe Brancato;
- University of Milano (UNIMI), Guido Tiana;

Each group applies orignal, advanced and novel computational methods, all requiring HPC resources, to different scales, ranging from macromolecules described as atoms, to 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 performed in year 2023.

UNITOV -
Development and application of computational methods (mainly generalized statistical ensembles) to determine the structure and the dynamics of biologically relevant molecules. Combining different scales by molecular dynamics, classical and ab initio calculations, all requiring massive HPC resources. Analysis of experimental results obtained exploiting large scale facilities such as synchrotrons and free electron lasers (FEL).

The principal lines of research in 2023 are:

1. the optimization of the hydrogenase enzyme in selected microalgae strains for the sustainable production of hydrogen;
2. the role of Zn ions in the SARS-CoV-2 virus strategy to escape the immune response mediated by the BST2 (tetherin) host protein;
3. the behaviour of trimeric proteins, like TRAF2 and spike protein;
4. understanding molecular events in ageing processes (ion trafficking), cancer (frataxin) and cell degeneration (amyloid peptides).

References:
DOI: 10.1002/open.202100217
DOI: 10.3390/molecules27061955

POLITO -
To localize different activities to distinct region, eukaryotic cells developed an elaborate system to sort and distill specific proteins into submicrometric lipid vesicles, destined to be transported towards appropriate intracellular destinations by active mechanisms. Disruption of this system leads to disease states, such as cancer. While the biochemical basis of protein sorting has been extensively investigated, a systemic view of the process is still lacking.

Recently, a computational model have been introduced, based on the idea that protein sorting naturally emerges from the combination of spontaneous molecular aggregation with vesicle nucleation. The model predicts that the sorting process is optimal in a specific range of aggregation rates, in good agreement with observations performed on primary endothelial cells.

We investigate the case when several molecular species are sorted in parallel, to account for the possible effects of molecule crowding and to understand how the efficiency of sorting may depend in principle 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.

References:
DOI: 10.1103/PhysRevLett.126.088101

UNITO -
Topic models are algorithms introduced for discovering hidden topics or latent variables in large, unstructured text corpora. Leveraging on analogies between texts and gene expression profiles, these algorithms can be used to find structures in expression data. Our work presents an application of topic modeling techniques for the identification of cancer subtypes. In particular, we extended a specific class of topic models to allow a multiomics approach. We were able to clearly distinguish healthy from tumor 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.

References:
DOI: 10.3390/cancers12123799
DOI: 10.3390/cancers14051150

UNINA -
The research activity will focus on the development of polymer models to study the three-dimensional (3D) organization of DNA and its temporal dynamics. In particular, we will 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.

References:
DOI: 10.1038/s41467-022-31856-6
DOI: 10.1016/j.celrep.2022.110601

Risorse ottenute da call competitive (ultimi 3 anni)

ISCRA approved Projects within the IS:

- 4 IscraC projects on Marconi 100 for a total of 128 k core-hours;
- 2 IscraC projects on Marconi 100 for a total of 95 k core-hours
- Iscra B on Marconi 100 of 1.6 M core-hours
- ISCRA-HP10CCZ4KN
- ISCRA-HP10CCZ4KN
- ISCRA C 20’ of quantum computing time on the D-WAVE quantum annealer
- ISCRA C project 30,000 hours on CiNECA

NEMESYS

Time2Quest [HPC resources - research program]

S. Bellucci[1], A. Sindona[2], M. Pisarra[2], G. Stefanucci[3], O. Pulci[3], M. Palummo[3], S. Achilli[4], G. Onida[4]
[1]LNF, [2]UNICS, [3]UNIRM2, [4]UNIMI

As expressed in its project proposal, the specific initiative 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/layered materials. 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 configure and parallelized in the marconi, marconi 100, and galileo 100 clusters of the CINECA consortium. MP from the unirm2 unit of the present IS 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 IS [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 single-particle 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 marconi, marconi 100, and galileo 100 clusters of the CINECA consortium. The requested CPU time can be barely used to set up one of the applications proposed in the research program of the present IS for 2023.

[1] K. Novoselov et. al., Science 353, aac9439 (2016)
[2] M. Palummo, K. Yamashita, G. Giorgi, Sustainable Strategies in Organic Electronics, 391-4224 (2022)
[3] L. Bastonero, G. Cicero, M. Palummo, M. Re Fiorentin, ACS applied materials & interfaces 36 2021
[4] X. Gonze, et. al., Comput. Phys. Commun. 180, 2582 (2009)
[5] Giannozzi et. al., J. Phys.: Condens. Matter 2009, 21, 395507
[6] Sangalli et al., J. Phys Condens. Matter 2019, 31, 325902
[7] C. Vacacela Gomez, M. Pisarra, M. Gravina, J. M. Pitarke, and A. Sindona, Phys. Rev. Lett. 117, 116801 (2016)
[8] M. Palummo et al., Nano Lett. 15, no. (May 13, 2015): 2794–2800
[9] Molina-Sánchez et al, Phys. Rev. B 93, 155435 (2016)

LE RICHIESTE DI

RISORSE DI CALCOLO

Il consumo delle risorse di calcolo CPU al CINECA nel 2020 (*)

(*) ultimo anno con risorse MARCONI-A3 come da accordo attuativo per cofinanziamento da fondi HPC_HTC (CIPE)

CPU (MARCONI + GALILEO)	
account	consumo (corehours)
INF20_FBS	1,930,453
INF20_biophys	2,195,372
INF20_disorder	9
INF20_fldturb	10,176,062
INF20_indark	1,452,919
INF20_lqcd123	35,895,679
INF20_manybody	1,798,454
INF20_nemesys	528,331
INF20_neumatt	10,394,869
INF20_npqcd	35,990,061
INF20_qcdlat	35,383,721
INF20_qftatcol	0
INF20_quantum	516,347
INF20_sft	3,096,754
INF20_sim	5,987,693
INF20_strength	534,739
INF20_teongrav	13,574,603
INF20_test	551,823
TOTALE	***160,007,889***

Il 35% delle risorse può essere spostato su GPU nel 2023

intervista alle sigle sulla transizione alle GPU

sigla	GPU 2023
LQCD123	60% [1]
SIM	100%
ENESMA	0
BIOPHYS	70%
QFTATCOL	5%
TEONGRAV	0
NUCSYS	50%
FIELDTURB	0%
QCDLAT	15%
MONSTRE	15%
INDARK	1.5
NPQCD	60%
FIELDTURB	20%

Richieste fatte e proposte di assegnazione 2023 (CPU e GPU)

sigla	richieste 2023 per CPU (corehours)	proposta di assegnazione per CPU 2023 (corehours)	richieste 2023 per GPU (nodehours)	proposta di assegnazione per GPU 2023 (nodehours)
BIOPHYS	2,125,000	800,000	675,000	200,000
ENESMA	50,000	50,000	0	0
FIELDTURB	14,000,000	6,000,000	250,000	150,000
GAGRA	250,000	250,000	0	0
INDARK	2,400,000	1,500,000	1,600	5,000
LQCD123	15,000,000	12,000,000	600,000	520,000
MONSTRE	2,600,000	1,500,000	20,000	20,000
NEMESYS	1,200,000	400,000	600,000	20,000
NEUMATT	9,000,000	4,500,000	50,000	50,000
NPQCD	15,000,000	12,000,000	800,000	520,000
NUCSYS	1,000,000	350,000	200,000	100,000
QCDLAT	30,000,000	25,000,000	250,000	120,000
QFTATCOL	3,000,000	1,800,000	0	0
QUANTUM	300,000	300,000	25,000	25,000
SFT	4,500,000	2,800,000	4,000	20,000
SIM	4,500,000	1,000,000	3,000	100,000
TEONGRAV	15,000,000	9,750,000	100,000	150,000
TEST	0	0	0	0
Totale	**119,925,000**	***80,000,000***	**3,578,600**	***2,000,000***

- **Richiesta CPU 2023**

  (massima riduzione che riteniamo possibile in base alla previsione di attività dei gruppi, ma saremmo in grado, in base allo storico, di usare più risorse CPU)

- **Possiamo usare più risorse GPU di quante indicate nella proposta di assegnazione**

Risorse Accordo Attuativo Cineca-INFN 2023

	CPU	GPU	CPU (corehours)	GPU (corehours)	*GPU (nodehours)*
MARCONI-A3	Intel SkyLake (48 core/nodo)		60,000,000		
MARCONI100	IBM Power9 (32 cores/nodo)	4xNVIDIA Volta per nodo		15,000,000	*468,750*
GALILEO100	Intel CascadeLake (48 core/nodo)		6,000,000		
LEONARDO (General Purpose)	Intel Sapphire Rapids (48 core/nodo)		70,000,000		
LEONARDO (Booster)	Intel Ice-Lake (32 cores/nodo)	4xNVIDIA Ampére per nodo		96,000,000	*3,000,000*

ALTRE RICHIESTE

Richieste per piccoli sistemi CPU e GPU per attività di R&D

- 16 nodi di calcolo con 128 cores/nodo connessi con rete InfiniBand 200Gb/s bidirezionale
- 4 nodi di calcolo con 4 GPU/nodo

Richieste per storage su nastro al CNAF

- 850 TB

BACKUP SLIDES

Le risorse di calcolo HPC

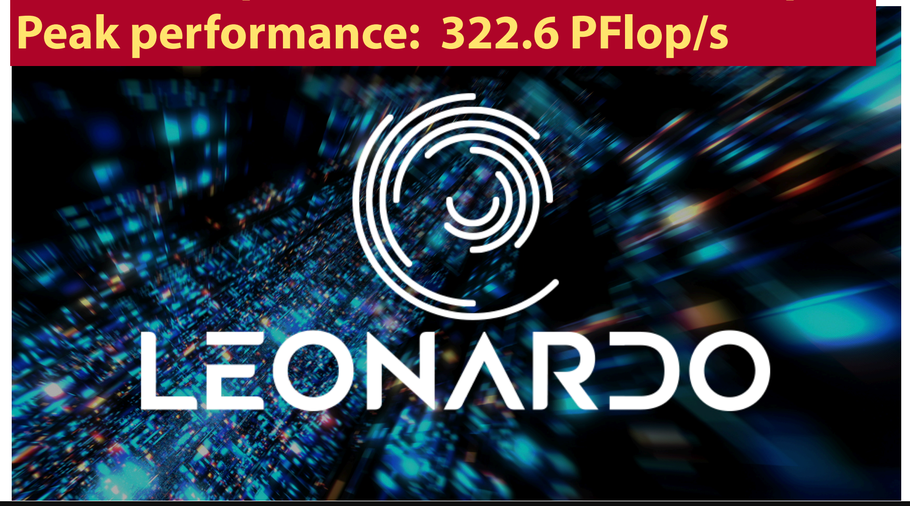
- **Accordo Quadro CINECA-INFN 2022-2026**
- **Accordo Attuativo dell'Accordo Quadro CINECA-INFN**

- **MARCONI-A3**
- **MARCONI100**
- **GALILEO100**

	CPU (mhz,core, ...)	Total cores / Total Nodes	Memory per node	Accelerator
MARCONI-A3	Intel SkyLake 2x Intel Xeon 8160 @2.1GHz 24 cores each	48*3216 / 3216	192 GB	-
MARCONI100	IBM Power9 AC922 @3.1GHz 32 cores HT 4 each	32*980 / 980	256 GB	4x NVIDIA Volta V100 GPUs per node, NVlink 2.0 16 GB
GALILEO100	2 x Intel CascadeLake 8260 @2.4 GHz 24 cores each,	48*554 / 554	384 GB 3.0 TB	34 nodes with 2x NVIDIA V100 per node, PCIe3

LEONARDO

Sustained performance: 249.4 PFlop/s
Peak performance: 322.6 PFlop/s



Specifiche tecniche

Il supercomputer Leonardo è costituito da 3 parti:

- La prima, chiamata Booster, è formata da oltre 3.000 nodi basati sui sistemi a raffreddamento diretto a liquido BullSequana XH2000, che integrano una CPU Intel Xeon SP di terza generazione e quattro GPU Nvidia Ampère A100, per un totale di quasi 14.000 acceleratori;
- La seconda, chiamata Data Centric Partition, è formata da oltre 1.500 nodi basati sugli stessi BullSequana XH2000, ma che ospitano processori Intel Xeon di generazione futura.
- L'intero sistema è collegato ad un terzo modulo di servizio e visualizzazione, ed ad un'area di archiviazione multi-tier ad alte performance, con una capienza aggregata di olte 100 PetaByte, basata sui prodotti DDN. Tutte le parti del sistema comunicano tra di loro grazie un'interconnessione a bassa latenza InfiniBand HDR a 200Gb/s per collegamento, allocata su tecnologia Nvidia Networking.

I processori Intel Xeon di generazione futura sono ottimizzati per eseguire carichi di lavoro computazionalmente intensi in sistemi di calcolo ad alte prestazioni consentendo computing con avanzate capacità di accelerazione AI integrate.

- Più di 136 BullSequana XH2000 rack di raffreddamento diretto a liquido
- 250 PFLOPs HPL Linpack Performance (Rmax) aggregata
- 3+PB RAM
- 10 ExaFLOPs di prestazioni FP16 AI
- 3456 server equipaggiati con Intel Xeon Ice Lake e GPU con architettura Nvidia Ampère
- 1536 server con processori Intel Xeon SP di prossima generazione
- 5PB di storage ad alte prestazioni
- 100PB di storage a grande capacità
- Larghezza di banda di interconnessione minima di 200Gb/s per singolo link InfiniBand HDR
- 9MW di Potenza elettrica aggregate
- Oltre 140 km di cablaggi in fibra ottica

Le risorse di calcolo HPC

- **Accordo Quadro CINECA-INFN 2022-2026**

ACCORDO QUADRO DI COLLABORAZIONE PER LO SVOLGIMENTO DI ATTIVITÀ DI RICERCA E SVILUPPO NEL SETTORE DEL CALCOLO SCIENTIFICO AD ALTE PRESTAZIONI (HPC) IN AMBITO DI FISICA DELLE ALTE ENERGIE, FISICA ASTROPARTICELLARE, FISICA NUCLEARE

Art. 2 – Oggetto e finalità dell'Accordo

Con il presente Accordo Quadro, le Parti instaurano una collaborazione rivolta allo

- sviluppo e sperimentazione di sistemi di calcolo ad alte prestazioni e ad alta capacità;
- sviluppo di algoritmi e applicazioni relative all'ambito della modellazione e della simulazione numerica e dell'analisi dei dati in aree di interesse della fisica fondamentale, in particolare utilizzando architetture innovative dei processori, delle reti d'interconnessione e delle strutture di input-output;

- **Accordo Attuativo dell'Accordo Quadro CINECA-INFN**

ACCORDO ATTUATIVO DELL'ACCORDO QUADRO DI COLLABORAZIONE PER LO SVOLGIMENTO DI ATTIVITÀ DI RICERCA E SVILUPPO NEL SETTORE DEL CALCOLO SCIENTIFICO AD ALTE PRESTAZIONI (HPC) IN AMBITO DI FISICA DELLE ALTE ENERGIE, FISICA ASTROPARTICELLARE, FISICA NUCLEARE

- **MARCONI-A3:** 60 Mcorehours/anno fino a dismissione
- **MARCONI100:** 15 Mcorehours/anno fino a dismissione
- **GALILEO100:** 6 Mcorehours/anno fino a dismissione
- **LEONARDO**

PARTIZIONE	2023	2024	2025	2026		
General Purpose (CPU)	165 nodi	300 nodi	300 nodi	300 nodi	su 1536 nodi	*Intel Sapphire Rapids (48 cores)*
Booster (GPU)	3 Mnodehours	3 Mnodehours	3 Mnodehours	3 Mnodehours	su 3456 nodi	*Intel Ice-Lake (32 cores)*

Le risorse di calcolo HPC

ISCRA: Italian SuperComputing Resource Allocation

CINECA, through the **Italian SuperComputing Resource Allocation - ISCRA**, releases Call for Proposals.

CINECA, the Italian most powerful HPC center, twice a year **will directly award in excess of 100 millions core hours**, to ensure an adequate supply to scientists and engineers for HPC-related research.

CINECA infrastructure offers different HPC resources to its users. The available resources are divided in three categories:

- The TIER-0, top level computing resources, which is the new **MARCONI100** machine and can be accessed trough class B and C projects.
- The TIER-1 level, is **GALILEO100** (BROADWELL) and can be accessed trough class C and B projects.
  The Big Data resources and new state-of-the-art public CLOUD.
  The data infrastructure is available for data analysis, visualization, post-processing, bio-informatics applications.
  The **CLOUD** infrastructure integrates and completes the HPC ecosystem, providing a tightly-integrated infrastructure that covers both high performance and high flexible computing. The flexibility of the CLOUD will better adapt to the diversity of user workloads, while still providing high-end computing power.
- The DGX resources:
  Available through ISCRA-C: these projects aim to support researchers in the domain of Machine Learning and Artificial Intelligence and their applications.
- The Quantum Computing Resources.
  Available through ISCRA-C, CINECA makes quantum computing resources of various kinds available to its users. It will be possible to request machine time on our Tier-0 system to emulate complex quantum circuits (both general purpose and special purpose type) and directly request quantum computing resources (currently of quantum annealing type).

Class B projects are received twice a year. They go under peer-review evaulation and a 3 month delay is expected before your project gets access to HPC resources. For each user it is allowed to have only one class B project each 6 months as Project Investigator.

Class C projects are received through continuous submission and reviewed once per month. An average period of about 15 days is required for activating the project. For each user it is allowed to have only one class C project each 6 months as Project Investigator.

Le risorse di calcolo HPC

PRACE, EuroHPC JU (Joint Undertaking)

PRACE PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

- International, not-for-profit
- 25 member countries - pan-European supercomputing infrastructure enabled by 5 Hosting Members
  - BSC (Spain), CINECA (Italy), ETH/CSCS (Switzerland), GSC (Germany), GENCI (France)
- Access on basis of peer-reviewed (open) science & industry proposals
- Additionally, schools, workshops, PRACE IP …

- Enable high-impact scientific & engineering discovery and R&D.
- Tier-0 computing and data management resources and services through **competitive peer review.**
- Training & education via schools, workshops, seminars.
- Enabled by 5 Hosting Centres.
- **No procurement, no technology development.**

EuroHPC Joint Undertaking

- Based on 2 EU Council Regulations (2018 & 2021)

Objectives

- Build and operate a world class integrated HPC and data infrastructure
- Enable member states to improve HPC competency
- Foster HPC skills, education and training
- Develop HPC core technology
  - *European Processor Initiative (EPI)*
  - *Energy efficient HPC*
  - *Quantum Computing*

In 2021 EuroHPC planned resources and timelines

Infrastructure and Operations

- 5 x petascale machines @ 15-30 petaflops. In operation by Q1 2021. Bulgaria, Czech Republic, Luxembourg, Portugal, Slovenia.
- 3 x pre-exascale machines. In operation Q2/3 2021:
  - CSC - Finland *Cray: 375PF sustained, 552PF peak; GPU, x86, data analytics, cloud container partitions*
  - Cineca - Italy *ATOS-Bull Sequana 249PF sustained, CPU-GPU, DDR5 & local NVM for data analysis*
  - BSC - Spain
- 2 x exascale in operation by 2022-2023. In coordination with EPI (European-based technology) for at least one machine?
- Data I/O, management, storage and security federation for impact: GEANT, EOSC etc

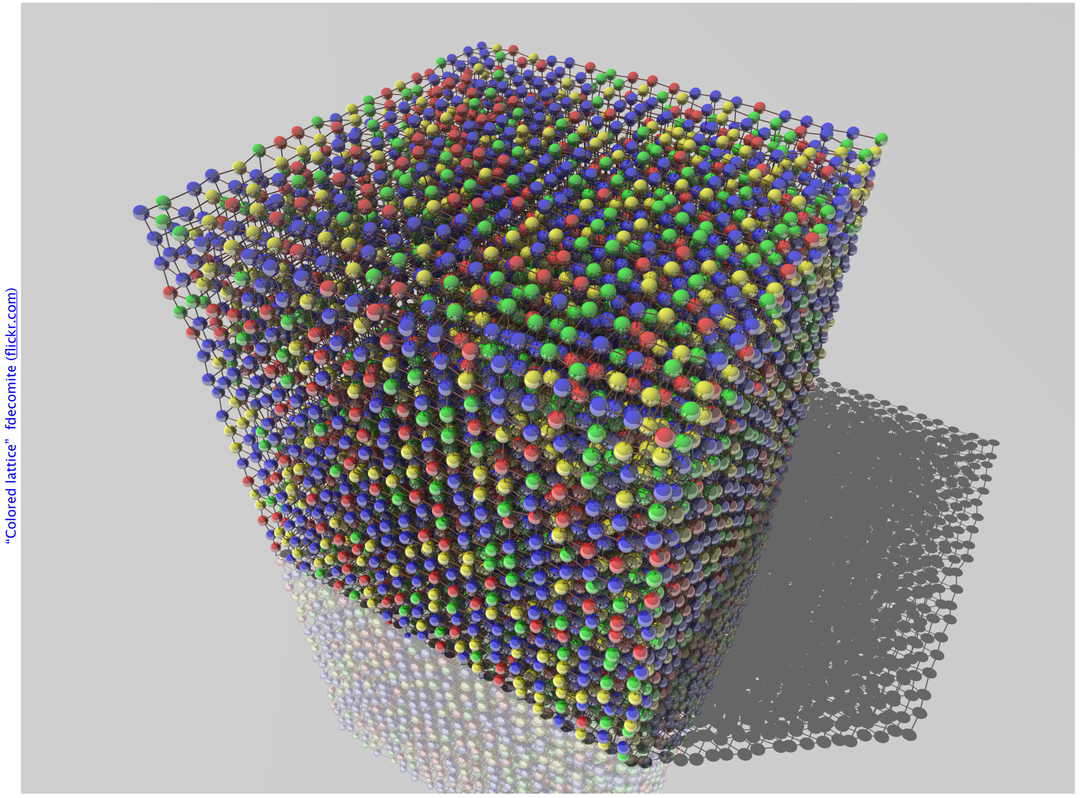
Access

There is an access policy at https://eurohpc-ju.europa.eu/access-our-supercomputers

Talk S. Ryan @ GGI Mini Workshop "Phase transitions in particle physics"

HIGH PERFORMANCE COMPUTING & LQCD: a paradigmatic use case

Lattice QCD calculations typically require multidimensional integration over the gauge fields



"Colored lattice" fdecomite (flickr.com)

The integration dimension in state-of-the-art calculations is $\mathcal{O}(10^{10})$

Markov Chain Monte Carlo methods are used to perform the multidimensional integrations

Generation of ensembles of configurations with importance sampling via Monte Carlo methods is an essential step in numerical simulations of the path-integral of statistical mechanics systems and field theories.

The development of numerical algorithms is crucial: over the history of lattice gauge theory calculations, the improvement from algorithm development has been similar to the gain from Moore's law.

HIGH PERFORMANCE COMPUTING & LQCD: a paradigmatic use case

The Lattice QCD workflow

Monte Carlo sampling phase

$$P_{\text{eq}}(U) = \frac{1}{\mathcal{Z}} \text{Det}(M^\dagger M) e^{-S(U)}$$

- Generates an ensemble of gluon field configurations U distributed according to the QCD action (using the hybrid Monte Carlo algorithm): $\text{Cost} \propto V^{9/8} a^{-2}$
- This ensemble generation is serially dependent and represents a **strong scaling computational problem**.
- A large number of computing nodes is required. On the largest scales this becomes a **halo-exchange communication problem** since the local data bandwidths vastly exceed those of inter-node communication.

Hadronic observables are calculated on each sampled configuration U:

$$\langle \mathcal{O} \rangle \approx \overline{\mathcal{O}} = \frac{1}{N} \sum_U \mathcal{O}(U)$$

- High degree of trivial parallelism: computer interconnect limitations are more easily avoided by exploiting this trivial parallelism.

Physics goals:
calculations with ensembles of gauge fields with physical volumes V large enough to ensure that finite-volume effects are under control.

- Example at the ***exascale frontier:***

  Simulation with up/down, strange, charm and bottom quarks at their physical masses with physical volume $V = (10\,\text{fm})^4$ at a lattice spacing $a = 0.04\,\text{fm}$ ($a^{-1} \sim 5\,\text{GeV}$) (lattice size $256^3 \times 512$)

  $\sim 12{,}000$ Exaflop hours $= 12{,}000 \times (3600 \times 10^{18})$ floating-point operations