



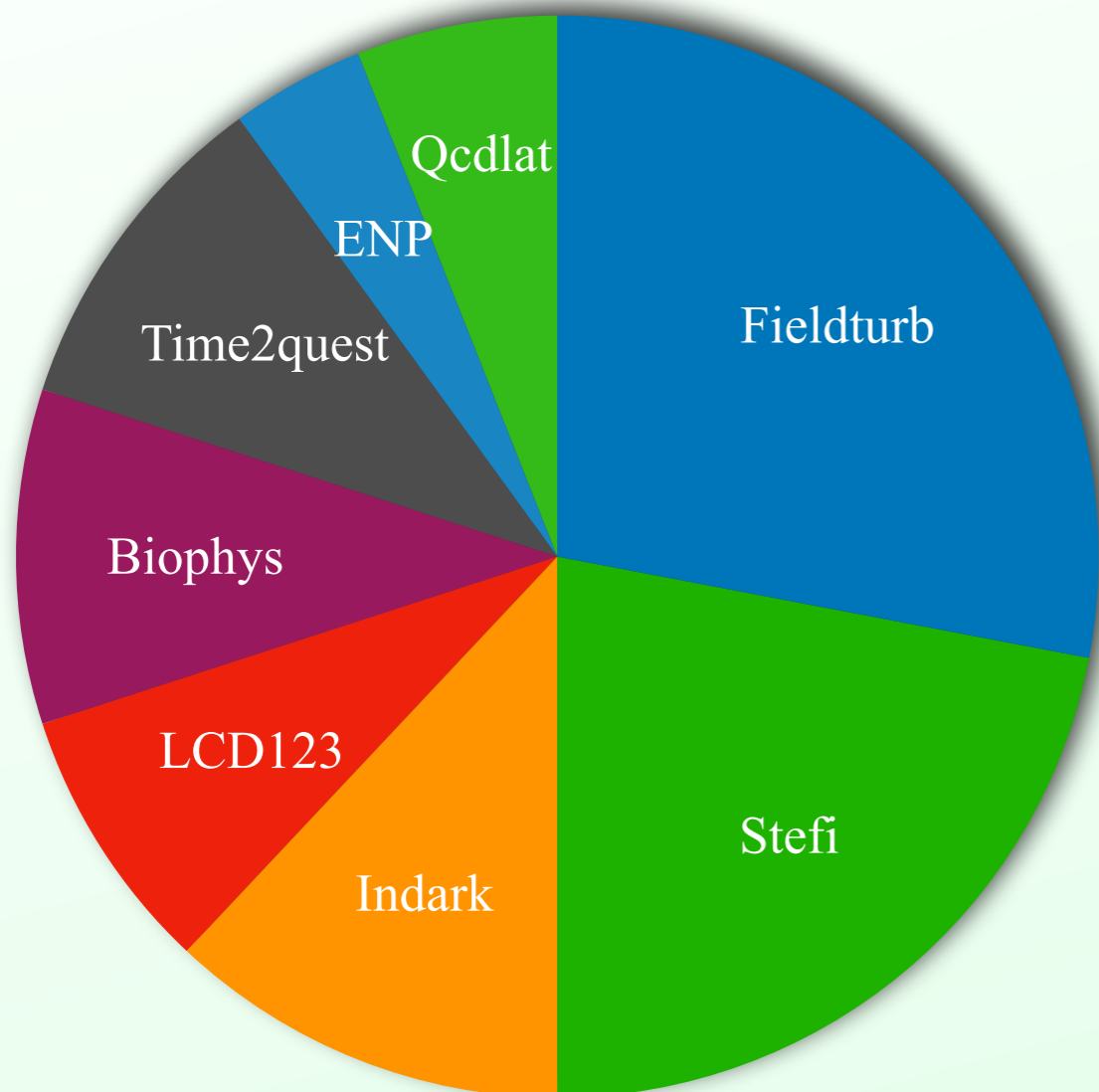
Istituto Nazionale di Fisica Nucleare  
SEZIONE DI ROMA TOR VERGATA

# Preventivi 2023

## Gruppo IV

# Iniziative Specifiche

- FTE:



- ▶ **FIELDTURB:** Sistemi complessi, turbolenza  
Massimo Cencini, **ricercatori: 15, FTE 14**
- ▶ **STEFI:** Teoria di stringa, gauge e gravita  
Gianfranco Pradisi **ricercatori: 12, FTE 10.75**
- ▶ **LQCD123:** Teorie di gauge sul reticolo  
Nazario Tantalò **ricercatori: 4, FTE 3.5**
- ▶ **BIOPHYS:** Biofisica  
Silvia Morante **ricercatori: 7, FTE 4.75**
- ▶ **INDARK:** Cosmologia  
Marina Migliaccio **ricercatori: 11, FTE 6.7**
- ▶ **Time2quest:** Struttura della materia  
Gianluca Stefanucci **ricercatori: 6, FTE 5**
- ▶ **ENP:** Fisica standard model e beyond  
Giulia Maria de Divitiis **ricercatori: 4, FTE 1.75**
- ▶ **QCGLAT:** QCD sul reticolo  
Tassos Vladikas **ricercatori: 4, FTE 3**

**Responsabile locale:** Massimo Cencini  
**Nazionale:** Guido Boffetta (To)

# FieldTurb

1 Benzi Roberto PO 100  
2 Biferale Luca PO 100  
3 Bonaccorso Fabio PHD 100  
4 Buzzicotti Michele RTDA 100  
5 Calascibetta Chiara PHD 100  
6 Capocci Damiano PHD 100  
7 Cencini Massimo CNR 50  
8 Cimini Giulio RTDB 100  
9 Heinonen Robin AR 100  
10 Li Tianyi AR 100  
11 Marra Rossana PO 100  
12 Puglisi Andrea Primo Ricercatore 50  
13 Sbragaglia Mauro PO 100  
14 Taglienti Diego PHD 100  
15 Simeonni Daniele AR 100

**Numero Totale Ricercatori** 15 FTE: 14

## Attività:

In the context of complex fluids we studied how an emulsion with a finite yield stress can be built via large-scale stirring [BGSSST22], developed a thermal lattice Boltzmann model (LBM) for concentrated emulsions with finite-size droplets [PLSB22], and studied via LBM plasma wakefield acceleration [PCDGRS22] and fluctuating multicomponent systems with a wetted finite-size particle model [XBST21]. We also studied the dynamics of confined soft granular flows [BMTBLJSG22], the difference in spatial correlations between boundary- and bulk-driven granular systems [PP21], and the interplay between structural symmetry breaking and frictional forces transmitted by the vibrating plate [PP22]. Finally we studied the statistics and scaling invariance of systems characterized by avalanches in simplified systems [BCTT22].

In the context of particles in turbulence we studied acceleration in compressible turbulence [WWB22] studied the effect of inertial particles on the instabilities of a channel flow [SCMB22] and explored the instabilities in convective flow due to non-isothermal particles [[ABBET22]]. We also studied the alignment of active (self-propelled) particles in turbulent flows with a mean flow [BBCDG22].

In the context of Machine Learning applications we applied nudging to reconstruct Rayleigh-Benard flows [ACB22] and Deep Learning to infer parameters of turbulent flows [BBB22].

We studied the effect of modifications of the Navier-Stokes equation (NSE) considering a reversible dissipative term [MBCGL22] showing in which conditions the statistics match that of the standard NSE.

2023

In the context of Machine Learning applications we plan to use optimal control and Reinforcement Learning to the navigation and accomplishment of other tasks by active swimmers in complex flows. To study new strategies for searching a (or multiple) source emitting signals (particles or odors) in turbulent flows.

We shall continue our exploration on the interplay between fluid transport and self-propulsion in different flow and swimming configurations.

We shall continue our research of complex fluids, emulsions, droplets and granular matter exploring their glassy behavior with multiphase LBM. We also plan to expand the use of relativistic LBM to study plasma wakefield acceleration processes.

**Richiesta:** 24KE

Anagrafica:

1. Massimo Bianchi, PO, Dip. Fisica, Universita' di Roma "Tor Vergata" (100%)
2. Giuseppe D'Appollonio, RTI, Dip. Fisica, Universita' di Cagliari (100%)
3. Giuseppe Dibitetto, RTDB, Dip. Fisica, Universita' di Roma "Tor Vergata" (100%)
4. Giorgio di Russo, PhD, Universita' di Roma "Tor Vergata" (100%)
5. Francesco Fucito, DdR INFN, Sezione di Roma "Tor Vergata" (100%)
6. Francisco Morales, PR INFN, Sezione di Roma "Tor Vergata" (100%)
7. Gianfranco Pradisi, PA, Dip. Fisica, Universita' di Roma "Tor Vergata" (100%)
8. Fabio Riccioni, Dip. Fisica, Universita' di Roma "Sapienza" (100%)
10. Alberto Salvio, RTD B, Dip. Fisica, Universita' di Roma "Tor Vergata" (25%)
11. Raffaele Savelli, PA, Dip. Fisica, Universita' di Roma "Tor Vergata" (100%)
12. Gianluca Zoccarato, RTDB, Dip. Fisica, Universita' di Roma "Tor Vergata" (100%)

Numero ricercatori: 12, FTE: 10.75

The activity of the String Theory group has been focussed on the following topics:

- Application of localization techniques to the study of  $N=2$  supersymmetric gauge theories and black hole physics.
  - Computation of instanton corrections in four and eight dimensional gauge theories and correlators in strongly interacting superconformal theories.
  - Study of the gravitational wave response of black hole and fuzzballs, their spectrum of QNMs, the multipolar structure and echo signals.
  - Study of aspects of beyond-the-Standard-Model physics and its relation with gravity and cosmology. In particular: the study of inflation in modified gravity models, metric-affine theories of gravity and axion-flavour connections.
  - In the framework of  $N=2$  supersymmetric gauge theories, computation of the OPE coefficients for conformal theories which are called of the Argyres-Douglas type. This computation was done keeping only the first two gravitational corrections and the results were shown to be in very good agreement with the conformal bootstrap.
  - Determination of the field theory living on probe D3-branes of general 7-brane stacks wrapped on Abelian orbifolds;
  - Determination of certain flux-dependent 8-derivative couplings in 10-dimensional Type IIB supergravity.
  - Computation of loop amplitudes containing gravitons.
  - Investigation of fuzz-ball phenomenology by exploiting the connection between BH, D-brane and fuzz-ball perturbation theory and  $N=2$  SYM theories in the Nekrasov-Shatavili approach.
  - Study of generalised Couch-Torrence inversions, stringy memories, absorption cross-sections, (near) super-radiant modes and tidal Love numbers.
  - Investigation of holography-inspired models for meson and glue-ball scattering.
  - Computation of higher derivative corrections in  $N=6$  supergravity from strings on asymmetric orbifolds.
  - Study non-perturbative aspects of gauge theories on curved manifolds.
  - Study of the leptogenesis in post-inflationary models with additional dominating scalar fields.
  - Study of Metric-Affine theories of gravity with dynamical torsion. The case of Weyl gauging.

Richiesta: 21.5 KE

# INDARK

**Title:** Inflation, Dark Matter and the Large-Scale Structure of the Universe

**Responsabile Nazionale:** Massimiliano Lattanzi (INFN Ferrara)

**Responsabile Locale:** Marina Migliaccio

**Anagrafica:**

1) Hervé Bourdin (RTD-B UniRM2)	50%
2) Giancarlo De Gasperis (Ric. Univ UniRM2)	20%
3) Pasquale Mazzotta (PO UniRM2)	50%
4) Marina Migliaccio (Coord., RTD-B UniRM2)	50%
5) Nicola Vittorio (PO UniRM2)	50%
6) Giuseppe Puglisi	30%
7) Javier Carron Duque (INFN postdoc )	100%
8) Viviana Cuzzo (Ph.D. student UniRM2)	100%
9) Adria Gomez Valent (INFN Post)	100%
10) Giacomo Galoni (PHD)	60%
11) Giulia Piccirilli (PHD)	60%

Ricercatori 11, FTE 6.7

**Attività' scientifiche:**

The InDark project aims to investigate crucial aspects of the standard cosmological model and its extensions, together with their connection with particle physics. The main contributions of the Roma2 RU include:

- i) Late-time Cosmology. Constrain models of Dark Energy and Modified Gravity with current cosmological datasets and derive forecasts for the combination of future observations of the Cosmic Microwave Background (from LiteBIRD, Simons Observatory, CMB-S4) and the Large-Scale Structure (LSS) of the Universe (e. g. from the Euclid galaxy survey). Investigate viable solutions to the recently found tensions between measurements of the Hubble constant from early- and late-time Universe observations. The plan is to both assess the impact of data analysis methodological choices and approximations on the tensions, and develop new approaches that use galaxy clusters observations to measure the Universe expansion rate.
- ii) Dark Matter. Develop estimators for measuring the correlation of CMB lensing with tracers of the LSS, such as galaxy counts, cosmic shear and cosmic filaments, in order to map the distribution of Dark Matter in the Universe and constrain models for the growth of structures.
- iii) Inflation and the primordial universe. Assess the capability to constrain models of cosmic inflation from the combination of current and future CMB polarization data and Gravitational Wave measurements.

Richiesta in KE: 12 KE

# LQCD123

## Phenomenology with Lattice QCD in Roma123

Responsabile nazionale: Vittorio Lubicz (Roma Tre)

Responsabile locale: Nazario Tantalo

### Anagrafica

- 1) Roberto Frezzotti (PO 50%)
- 2) Marco Guagnelli (R INFN 100%)
- 3) Giancarlo Rossi (PO 0%),
- 4) Nazario Tantalo (PA 100%)
- 5) Alessandro de Santis (PhD, D)

Ricercatori: 5, FTE: 3.5

### Attività' scientifica

The activity of our group is focused on challenging non-perturbative lattice computations. In particular, we are leading experts in non-perturbative calculations of isospin breaking and QED radiative corrections to hadronic observables and of inclusive hadronic decay rates. Part of our activity is also focused on investigations of new physics models with new strong interactions.

We have proposed a scheme of lattice twisted-mass fermion regularization which is particularly convenient for application to isospin breaking (IB) QCD and QED calculations. We performed the first direct lattice calculation of the chiral perturbation theory low-energy constant  $l_7$  which parametrizes strong isospin effects at next-to-leading order (NLO) in SU(2) chiral perturbation theory.

We performed a determination of the gradient flow scales  $w_0$  and  $t_0$  in isosymmetric QCD, a calculation of the Mellin moments of the transverse quark spin densities in the nucleon using lattice QCD, a first-principles lattice calculation of the charged/neutral pion mass  $M_{\pi^+} - M_{\pi^0}$  difference at  $O(\alpha_{em})$ .

a lattice determination of the leading-order hadronic vacuum polarization (HVP) contribution to the muon anomalous magnetic moment

an extensive test in the 1+1 dimensional O(3) sigma model of a recently proposed method to extract hadronic spectral densities from euclidean lattice correlators.

We performed a first-principles lattice calculation of the radiative leptonic decay rates  $P \rightarrow l \nu l'$ , where P is a light pseudoscalar meson and l and l' are charged leptons.

We performed an ab initio study of inclusive semileptonic decays of heavy mesons from lattice QCD. Our approach is based on a recently proposed method, that allows one to address the study of these decays from the analysis of smeared spectral functions extracted from euclidean lattice correlators.

accepted on JHEP

2023 We plan to:

- determine the QED and isospin breaking corrections to the neutron beta decay, which, once combined with the measured value of the neutron's lifetime, allows a precise determination of  $V_{ud}$ . We will also compute the rate for the semileptonic charged pion decay including QED radiative corrections;
- to extend the computation of the form factors for the radiative and virtual leptonic decays of pseudoscalar mesons to the case of heavy mesons;
- generate configurations of non-perturbative QCD+QED with C-parity boundary conditions. These simulations, performed with the openQ\*D code, include the QED radiative effects associated to electrically charged sea-quarks loops;
- to apply the techniques introduced by our group to extract hadronic spectral densities from euclidean correlators in order to: -- perform an extensive first-principles study of the R-ratio on the lattice, smeared with functions having support in different energy ranges, and compare the theory results with the corresponding experimental determinations;
- perform the first direct lattice calculation of inclusive hadronic tau decay rates and extract, from the comparison with the corresponding experimental data in these channels, the CKM matrix elements  $V_{ud}$  and  $V_{us}$ ;
- extend our calculation of inclusive decay rates of heavy mesons to the phenomenologically relevant cases of B(s) and D(s) decays;
- generalize the techniques for the extraction of hadronic spectral densities in order to compute generic scattering amplitudes

RICHIESTA: 9 KE

# Biophys

**Title:** Intrinsically disordered proteins: multi-level computational approaches

**Responsabile Nazionale:** Mario Nicodemi

**Responsabile Locale:** Silvia Morante

**Anagrafica:**

- 1) Simone Botticelli, assegnista, 100%
- 2) La Penna Giovanni, PR, 50%
- 3) Minicozzi Velia, R 100%
- 4) Morante Silvia, PO, 100%
- 5) Nobili Germano, PhD, 100%
- 6) Rossi Giancarlo, PO
- 7) Stellato Francesco, R, 100%

**Ricercatori** 7 FTE 4.75 (totale)

**Attività' scientifiche:**

The main objective of this project is the development and application of computational methods to determine the structure and the dynamics of biologically relevant molecules. To this end, we employ different molecular dynamics approaches, ranging from classical molecular dynamics simulations to *ab initio* calculations by means of HPC resources. The computational strategy is also applied to analyse experimental results obtained exploiting Large Scale facilities such as synchrotrons and Free Electron Lasers.

The principal lines of research we intend to pursue in 2023 are:

- the optimization, via computer simulations, of the hydrogenase enzyme in selected microalgae strains for the sustainable production of hydrogen
- the role of Zn ions in the SARS-CoV-2 virus strategy to escape the immune response mediated by the BST2 host protein
- the behaviour of trimeric proteins, like TRAF2 and spike protein

Richiesta in KE: 9 KE

# TIME2QUEST

Title: Advanced Theoretical methods for emerging 2D materials in Quantum Information Technology Studies

**Responsabile Nazionale:** Stefano Bellucci

**Responsabile Locale:** Gianluca STEFANUCCI

## **Anagrafica:**

- 1) Gianluca Stefanucci (PA) - 100%
- 2) Enrico Perfetto (RTDB) - 100%
- 3) Olivia Pulci (PA) - 100%
- 4) Maurizia Palumbo (PA) - 100%
- 5) Simone Grillo (PhD) - 100%
- 6) Simone Brozzesi (PhD) - 100%

**Ricercatori** 6, **FTE** 5.0

## **Attività' scientifiche:**

Investigation of the ultrafast electronic and nuclear dynamics of photoionized organic molecules and low dimensional semiconductors using the novel Nonequilibrium Green's function time-linear scheme, which allows for a selective inclusion of correlation mechanisms. We will consider the role of nuclear-induced decoherence and non-perturbative electronic correlation mechanisms on the charge migration processes activated by the ionization of organic molecules with sub-fs laser pulses. We will also study the formation of coherent excitonic condensates in 2D semiconductors and the subsequent evolution toward a mixed phase where a plasma and an excitonic fluid coexists.

The aim is to continue to investigate theoretically in a fully ab-initio computational framework, the electronic and optical properties of suitably combined and functionalized classes of two-dimensional and layered materials that may have an impact in quantum technology and quantum information processing. The main focus will remain on chalcogen-based 2D/layered materials and on a novel class of 2D kagome lattices which interestingly present bands flat and with a typical Dirac like linear dispersion. Both classes of materials, in these last years, show enhanced many-body effects due to low-dielectric screening and peculiar, often topological, quasi-particles and strongly bound excitons.

**Richiesta in KE:** 9 KE



**Title:** Exploring New Physics

**Responsabile Nazionale:** Giancarlo D'Ambrosio (Napoli)

**Responsabile Locale:** Giulia Maria de Divitiis

**Anagrafica:**

- 1) Giulia Maria de Divitiis (RU 50%)
- 2) Roberto Frezzotti (PA 50%)
- 3) Alberto Salvio (RTDB 75%)
- 4) Antonio Evangelista ( studente laurea magistrale 0%)

**Ricercatori** 4, **FTE** 1.75

**Attività' scientifiche:**

Research activity

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— Proposals of BSM models valid over a vast energy range

-- Numerical and theoretical investigation of the mounting strong tension (4.2 sigmas) between SM lattice predictions and e+e- experiment data-driven values for the photon HVP

-- First-principle computation in Lattice QCD of hadronic matrix elements and other observables (e.g. related to the muon g-2) that are relevant to constrain various possible extensions of the Standard Model

-- A non-perturbative approach to the origin of the masses of elementary fermions and the dynamical generation of the electroweak scale: universality and predictive power limitations.

**Richiesta:** 4.5 KE

# QC DLAT

**Title:** Next generation lattice field theory for searching new phenomena in particle physics

**Responsabile Nazionale:** Leonardo Giusti

**Responsabile Locale:** Tassos Vladikas

## Anagrafica:

- 1) Giulia Maria de Divitiis 50%
- 2) Mauro Lucio Papinutto 50%
- 3) Anastassios Vladikas 100%
- 4) Ludovica Pirelli 100%

**Ricercatori** 4, **FTE** 3

## Attività' scientifiche:

We will evaluate  $b_g$ , the Symanzik improvement coefficient of the gauge coupling in lattice QCD with Wilson fermions. This is achieved through the computation of  $g_S$ , the Symanzik improvement coefficient of the singlet scalar density. The two quantities are related, and the latter is computed using a chiral Ward identity which relates correlation functions of singlet scalar and non-singlet pseudoscalar densities. The setup is that of finite-volume lattice QCD with the tree-level Symanzik-improved gauge action,  $N_f=3$  mass-degenerate  $O(a)$  improved Wilson fermions close to the chiral limit and Schrödinger functional boundary conditions. Our result will be used in  $N_f=2+1$  QCD simulations in large volumes by the CLS collaboration.

We will also conclude our study of the Renormalisation Group (RG) running of the tensor operator, for  $N_f=3$  QCD with Wilson fermions in a mixed action setup, with standard Schrödinger Functional (SF) boundary conditions for sea quarks and chirally rotated Schrödinger Functional (chiSF) boundary conditions for valence quarks. All necessary tunings have been performed, the recovery of chiral symmetry has been tested and the step scaling functions of the pseudoscalar and tensor operators have been measured. We are implementing a novel renormalisation scheme for the computation of the renormalisation parameter of the tensor operator and its step scaling function, in which the cancellation of the renormalisation parameter of the Schrödinger functional boundary fields is based on the conserved vector current. This is expected to improve the signal to noise ratio of these quantities, and preliminary analyses confirm this expectation. In the case of  $\Delta S = 2$  four-fermion operators, the  $O(a)$  improvement of the correlation functions obtained through the use of the chiral Schrödinger functional (xSF) scheme together with twisted mass QCD would not be achievable at present in other ways. These two tools also allow the development of a strategy to remove the additional mixing present with Wilson-like regularisations. We are currently computing, in the high energy regime, the xSF correlation functions from which the renormalisation constants of the four-fermion operators are extracted. We are also performing a preliminary analysis of the RG-running of these operators. The analysis in the low energy regime is also under way. We are planning to start the computation of the bare matrix elements using twisted mass valence quarks on gauge configurations with Wilson sea quarks.

**Richiesta in KE:** 6 KE