# WP1@Spoke 2: status report

Leonardo Cosmai (INFN BA) and Leonardo Giusti (UNIMIB & INFN)




Spoke2 Annual Meeting – Bologna- 19.12.2023

# WP1@Spoke2: Research topics

a) Development of algorithms, codes and computational strategies for the simulation of physical theories and models, towards pre-Exascale and Exascale architectures. [L. Cosmai, L. Giusti]

b) Theoretical research projects in domains already using HPC solutions, such as:

b1) **Lattice field theory** (flavour physics, QCD phase diagrams, hadronic physics, interactions beyond the Standard Model, machine learning in quantum field theories, electromagnetic effects in hadronic processes) [L. Cosmai, L. Giusti]

b2) **Collider physics phenomenology** [P. Mastrolia]

b3) **Gravitational waves, cosmology and astroparticle physics** (neutron-star physics, primordial universe, dark matter and energy, neutrino physics) [B. Giacomazzo]

b4) **High energy nuclear physics** [F. Becattini]

b5) **Physics of complex systems** (fluid dynamics, disordered systems, quantitative biology) [G. Gonella]

b6) **Condensed matter in low dimensional systems** [D. Giuliano]

# WP1@Spoke2: The Group

**Institutions & contacts:**

| | |
|---|---|
| INFN | Leonardo Cosmai |
| SALENTO | Daniele Montanino |
| SAPIENZA | Alessandro Melchiorri |
| UNIBA | Alessandro Mirizzi |
| UNIBO | Daniele Bonacorsi |
| UNICAL | Alessandro Papa |
| UNICT | Salvatore Plumari |
| UNIFI | Francesco Becattini |
| UNIFE | Walter Boscheri |
| UNIMIB | Leonardo Giusti |
| UNINA | Costantinos Siettos |
| UNIPD | Pierpaolo Mastrolia |

**People:**

| | |
|---|---|
| Staff | 66 (60+6) |
| RTDA | 7 |
| PhD | 9 |
| --- | --- |
| Total | 82 (~288 months committed) |

**New Hiring as RTDA:**

| | |
|---|---|
| Mitsuaki Hirasawa | UNIMIB |
| Mandal Manoj Kumar | UNIPD |
| Giuseppe Negro | UNIBA |
| Luca Panizzi | UNICAL |

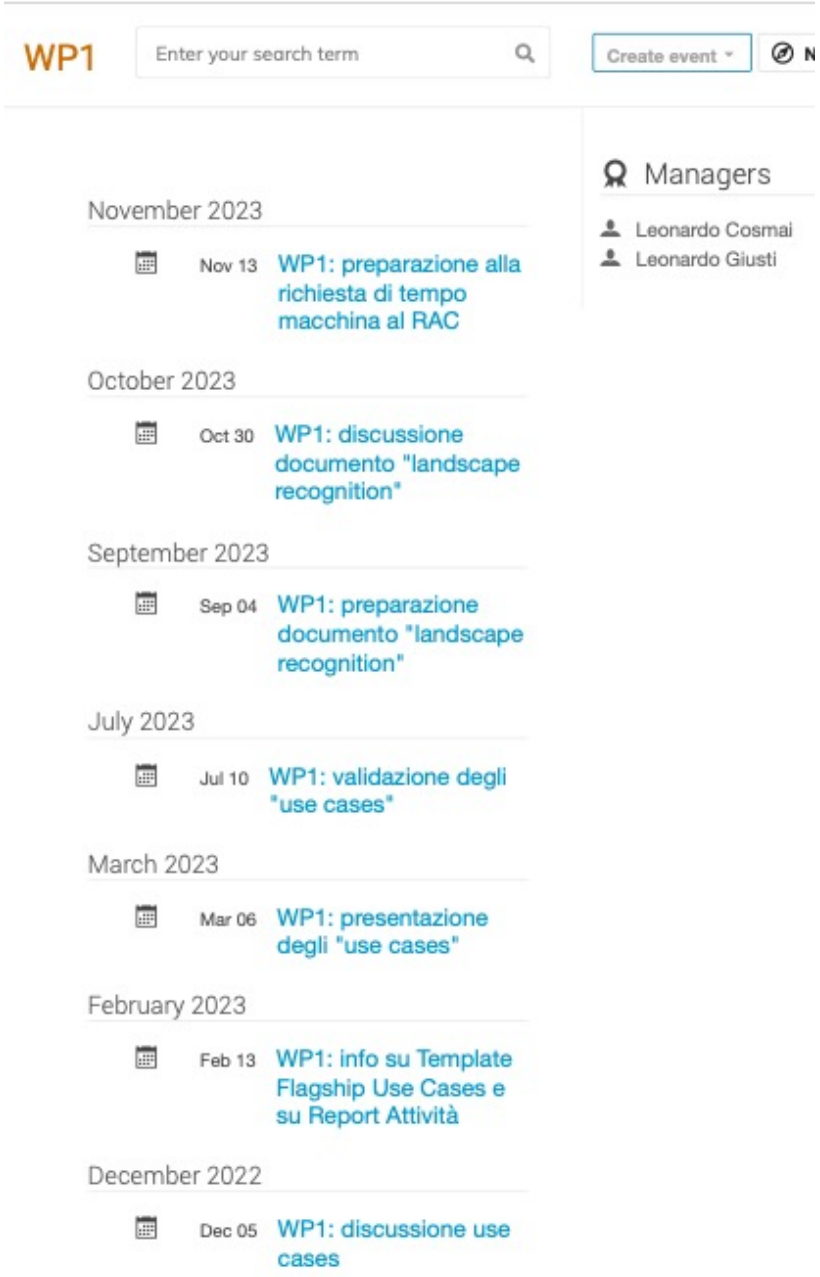
**New Hiring as Postdoc (assegni):**

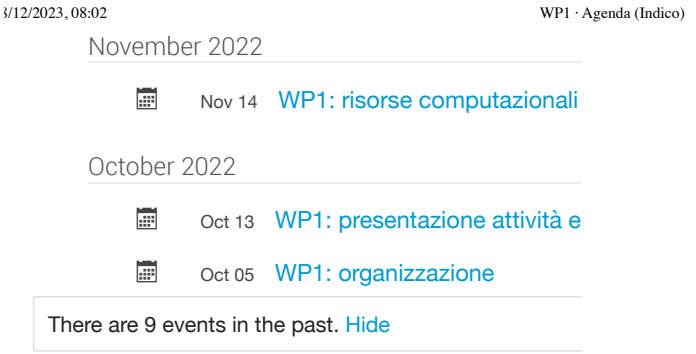
| | |
|---|---|
| Federico Cattorini | UNIMIB |
| Juri Fiaschi | UNIMIB |
| Sushant Kumar Singh | UNIFI |

**New Hiring as PhD :**

| | |
|---|---|
| Muhammad Ammar | UNIMIB |
| Emmanuele Cinnirella | UNICAL |
| Mauro Giliberti | UNIFI |
| Dario Melle | UNISALENTO |
| Pietro Rescigno | UNIMIB |
| Alice Spadaro | UNIMIB |
| Natascia Vignaroli | UNISALENTO |

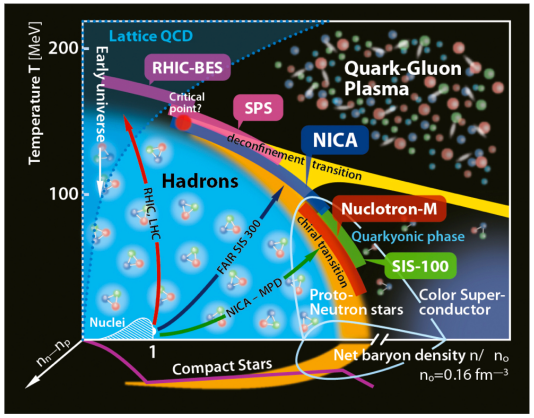
# WP1@Spoke2: Meetings



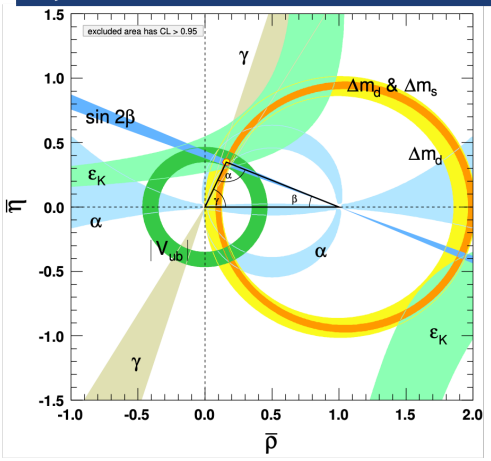



# WP1 - Lattice Field Theories

## Study of QCD in extreme conditions




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




# Use Cases

**Study of QCD at finite temperature from first principles:**
- Computational strategy and algorithm for simulating QCD on a lattice at high temperature
- Monte Carlo simulations on architectures up to exascale
- ***Interaction with WP5***: creation of a gauge configuration repository

**Dynamics of confinement in QCD:**
- Numerical strategy for the calculation of the chromoelectromagnetic tensor on gauge configurations
- Module for configuration smoothing algorithms
- ***Interaction with WP4***: porting of the calculation of the chromoelectromagnetic tensor to GPU

**Simulation of spin systems as effective models of gauge theories on a lattice at finite temperature:**
- Algorithms and codes for the simulation
- Tools for statistical analysis and data visualization

**Multi level Monte Carlo for Lattice QCD:**
- Numerical strategy for the calculation of hadronic quantities with very high precision
- Monte Carlo simulations on architectures up to exascale
- ***Interaction with WP5***: creation of a gauge configuration repository

**Isospin breaking in Lattice QCD:**
- Development of numerical strategies and optimized codes
- ***Synergy with WP4*** (porting to GPU)
- ***Synergy with WP5*** (configuration repository)

## The researchers involved in WP1 - Lattice

Mattia Bruno (UniMiB),
Leonardo Cosmai (INFN),
Leonardo Giusti (UniMiB),
Alessandro Papa (UniCal),
Michele Pepe (INFN),
Francesco Sanfilippo (INFN)

# UC2.1.1: Multilevel Hybrid Monte Carlo for lattice QCD

**Goal:** Develop, test and validate a numerical strategy and a fully optimized parallel code for simulating QCD with a multilevel Monte Carlo. Final code will implement an MPI+openMP parallelization so to run efficiently up to approximately 100,000 cores

**Status of advancement:** In this first year of activity the theoretical (Domain Decomposition for fermion factorization) and the algorithmic (Domain-Decomposed Hybrid Monte Carlo) strategies have been defined. The development of a first Monte Carlo code (MPI only) started from the open source OpenQCD code.

**PI:** L. Giusti (UNIMIB)

**Personnel Hired:** Mitsuaki Hirasawa (RTDA, UNIMIB), Pietro Rescigno (PhD, UNIMIB)

**Computing Resources:** Application for computer time submitted to ICSC

# UC2.1.2: QCD under extreme conditions

**Goal:** Develop, test and validate a numerical strategy and a fully optimized parallel code for simulating thermal QCD up to temperatures of the order of the electroweak scale. Final code will implement an MPI parallelization so to run efficiently up to  run approximately 10,000 cores

**Status of advancement:** In this first year of activity the theoretical (shifted boundary conditions) and the algorithmic (Hybrid Monte Carlo) strategies have been defined. The development of a first Monte Carlo code started from the open source OpenQCD code.

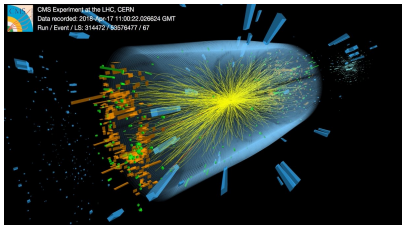
**PI:** M. Pepe (INFN)

**Personnel Hired:** Mitsuaki Hirasawa (RTDA, UNIMIB), Pietro Rescigno (PhD, UNIMIB)

Lightning talk: P. Rescigno Tue 19/12 18:15

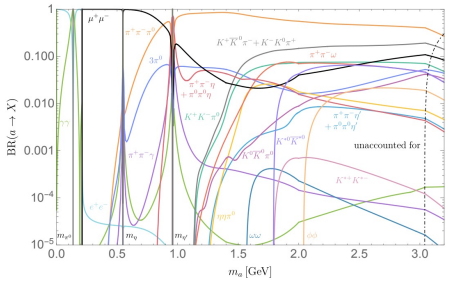
**Computing Resources:** Application for computer time submitted to ICSC

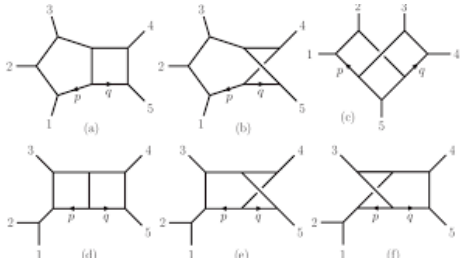
# Collider Phenomenology

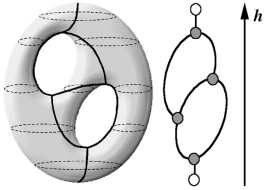


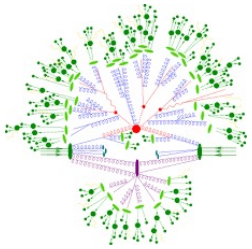
**Use cases** (a synthesis)

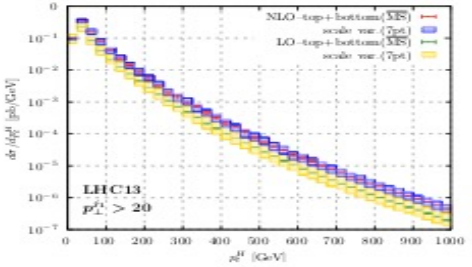
- Fast and accurate predictions for Collider Phenomenology
- Cross Sections and Partonic Distributions
- Accelerating Event Generation
- Scalable numerical evaluation of Feynman integrals
- Advanced Computational Tools for Scattering Amplitudes
- Optimized Strategies for new Particles and Couplings
- EFT Diagrammatic Approach to Gravitational Wave Physics
- Improved Methods for New Physics from Large Scale Structure observables

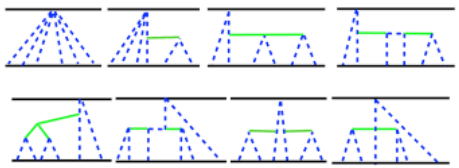


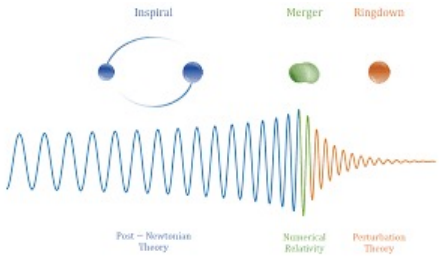










**Interaction with WP4**

- Porting Parallel CPU codes to GPUs

**Interaction with WP5**

N/A

**Institutions**

UNIBO, UNICAL, UNIMIB, UNIPD

# UC2.1.3: Advanced Calculus for Precision Physics (ACPP)

**Goal:** Develop computational strategies and software for phenomenology analyses which aim at detection and observations of new physics events or weak signals within the advanced collider physics programs (CERN, Fermilab, etc.)

**Status of advancement:** In this first year of activity three directions of research have been identified: Amplitudes, Event Generators, Monte Carlo Sample deconstruction. In all these areas the design of the computational strategies and the writing of the corresponding codes started.

**PI:** P. Mastrolia (UNIPD)

**Personnel Hired:** Juri Fiaschi (Postdoc, UNIMIB), Mandal Manoj Kumar (RTDA, UNIPD), Luca Panizzi (RTDA, UNICAL)

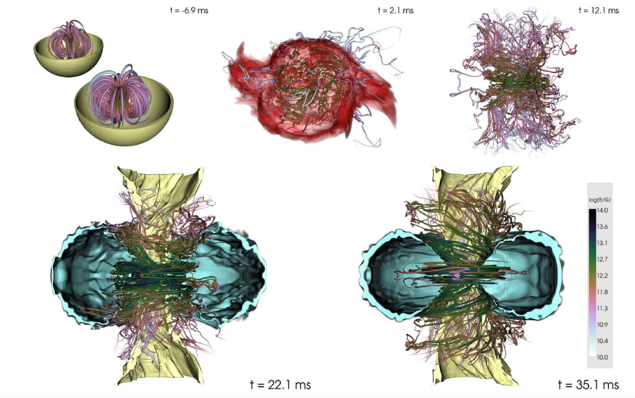
Lightning talk: M. Manoj Kumar Wed 20/12 10:20

**Computing Resources:** Application for computer time submitted to ICSC

# GW, Cosmology, and Astroparticle

**Use cases** (a synthesis)

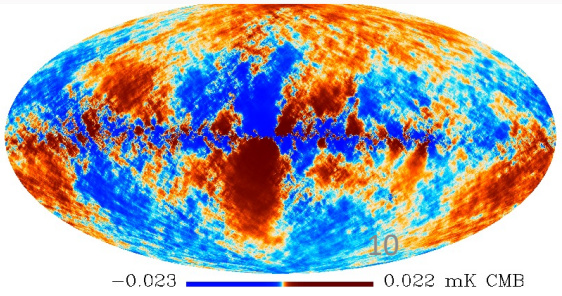
- Numerical Codes to study plasma in early universe
- Lattice and Markov Chain Monte Carlo Simulations of phase transitions
- Numerical Relativity Simulations of Compact Objects (including GRMHD, neutrinos, alternative gravity models)
- Numerical Algorithms to study neutrino oscillations and axion-photon conversions
- Cosmological simulations of the dynamics of bubbles of true vacua
- Computing the spectrum of gravitational waves in transplanckian collisions
- Simulating black hole formation environment (via SPH and N-body codes)
- Improving theoretical modelling in data analysis of large cosmological datasets
- Cosmological codes to calculate Large Scale Structure observables




**Interaction with WP4**

- Porting Parallel CPU codes to GPUs

Lightning talk: A. Spadaro Tue 19/12 17:25



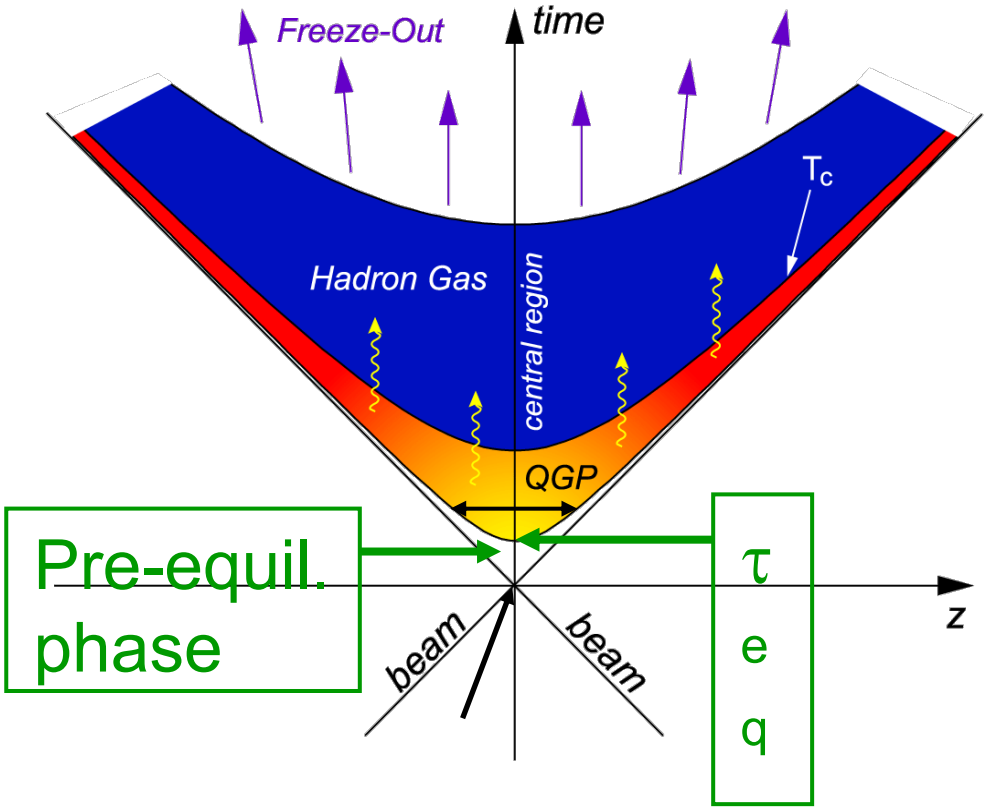

**Institutions**

UNICAL, UNIMIB, UNIBA, UNIFI, UNIFE, UNISAPIENZA, SALENTO, UNIPD

# High energy nuclear physics

**Use cases** (a synthesis)

- Advanced relativistic hydrodynamics numerical codes including viscous terms to simulate QCD plasma formed in relativistic nuclear collisions;
- Relativistic kinetics numerical codes to study transport phenomena: heavy quark diffusion in the plasma etc.

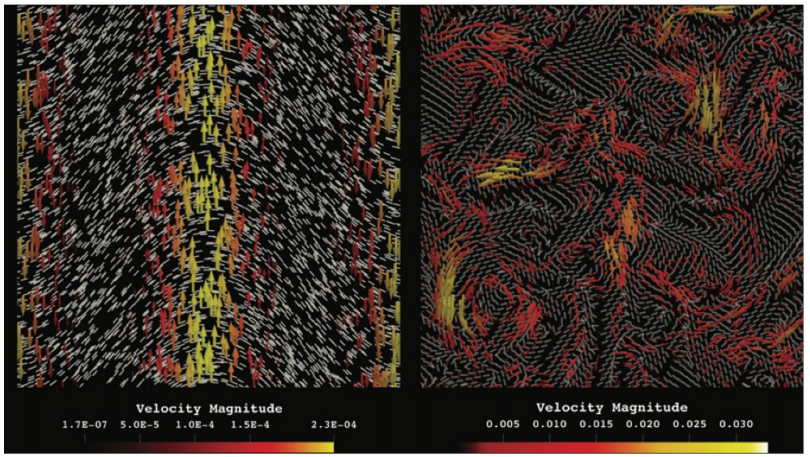


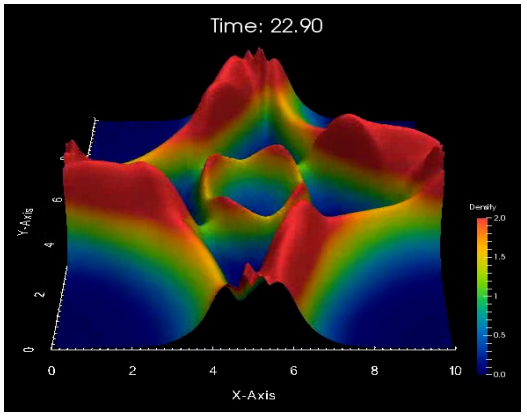

**Institutions**
UNIFI, UNICT

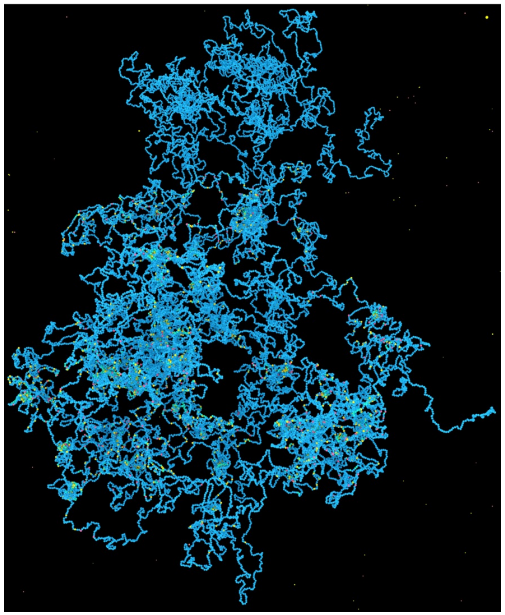
# Physics of complex systems

**Use cases**

-Complex  and active fluids
-Emergence behavior in living biological systems
-Fluid dynamics and rarefied flows
-Medical applications
-Non-equilibrium statistical mechanics
-Model for lipid bilayers and ion channels
-Bridging micro and macro scales
-Development of coarse-grained models based on Field Theory for soft matter simulations
-Model for chromatin



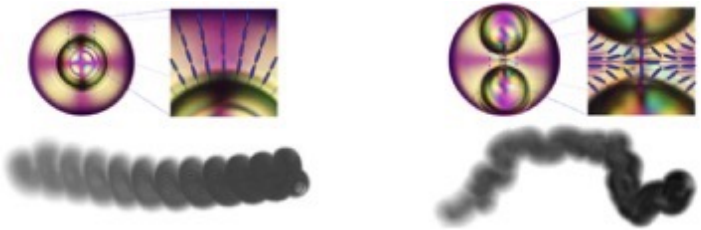



**Institutions**

UNIBA
UNIFE
UNINA

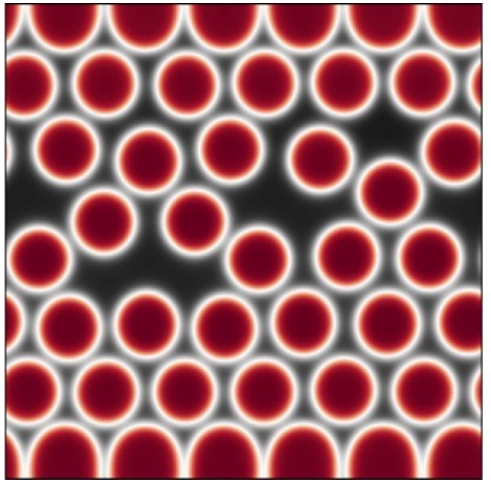
# UC2.1.4: Large Scale Simulations of Complex Systems

**Goal:** We aim to develop, test, and validate an optimized parallel Lattice Boltzmann (LB) solver specifically designed for simulating 3D multiphase active droplets (dense suspensions of biological extracts confined in droplets).



B. V. Hokmabad *et al. PRL 2021*

**Status of advancement:** In this first year of activity the lattice Boltzmann model have been
Identified (D3Q15, 3 spatial dimensions, 15 lattice velocities). The development/adaptation of a first 3D code started from a 2D (D2Q9) code for droplets suspensions.



G. Negro et al. Science Advances 2023

**PI:** G. Gonnella (UNIBA)

**Personnel Hired:** Giuseppe Negro (UNIBA)

Lightning talk: G. Negro Wed 20/12 9:30

**Computing Resources:** Application for computer time submitted to ICSC

# Condensed Matter and Low-dimensional systems

**Use cases**

- Numerical simulation of numerical effects of disorder on topological systems: stability of the topological phase, phase diagram and disorder-induced phase transitions.
- Open- and out-of-equilbrium topological systems: analysis and numerical characterization of the non-equilibrium steady states, of their properties and of their practical implementation.
- Phase diagram and phase transitions in open topological systems with various types of disorder.
- Numerical solution of Non-Linear Integral Equations and Thermodynamic Bethe Ansatz equations, with applications to computations of observables (especially energy levels, free energy) at zero and finite temperature in integrable models in 1+1 dimensions.
- Study/simulation of topological materials for joint applications in field theory and condensed matter. Application of effective field theory methodologies in the equations of transport and numerical studies of response functions in anomalous transport.
- Study and modeling of gravitational waves in strongly first order phase transitions with physics beyond the Standard model. Study of models of modified gravity with quadratic corrections in the curvature and conformal signatures in gravitational wave production.
- Battery modeling; Bulk-surface PDE systems; Finite and Virtual element methods; Matrix oriented techniques; Parameter estimation; Convolutional Neural Networks

**Institutions**

SALENTO, UNICAL

# IG2.3: Enabling scientific research and technology innovation on the Tier1 of the ENI green data center in Ferrera Erbognone

**Goal:** Install and manage of a HPC system of several PetaFlops (Tier1), with a mixed architecture based on CPUs and GPUs, at the ENI site of Ferrera Erbognone in the second half of the year 2024. Enable the research and innovation use cases of common interest among CINECA, ENI and UNIMIB in the areas of nuclear fusion and on algorithms with extreme parallelization so to run efficiently on pre-Exascale and Exascale architectures.

**Status of advancement:** Final phase for the preparation of the agreements/contracts among UNIMIB, CINECA and ENI for the acquisition and installation of the machine. Hiring of the 3 technicians in progress.

**PI:** A. Amendola (ENI)

**Personnel to be hired:** 3 Technicians (1 UNIMIB, 1 CINECA, 1 ENI)

**Computing Resources:** Application for computer time submitted to ICSC

# Conclusions and outlook

**Hiring:** All RTDA, Postdocs and PhD students hired

**Use case flagship selected :**
UC2.1.1: Multilevel Hybrid Monte Carlo for lattice QCD
UC2.1.2: QCD under extreme conditions
UC2.1.3: Advanced Calculus for Precision Physics (ACPP)
UC2.1.4: Large Scale Simulations of Complex Systems

**Possible interaction with WP5:**
Data repositories in UC2.1.1 and UC2.1.2

**Possible interaction with WP4:**
Porting CPU codes to GPUs in UC2.1.3

**Numerical resources requested for use cases flagship + IG:**
- 33.1 Mcoreshours/year - CPU (Galileo100 or Leonardo GP)
- 165kGPUhours/year - GPU (Leonardo Booster)
- 8x192=1536 cores for 2.5 months/year (INFN HPC Bubbles)
- 4 GPUs for 1 month/year (INFN HPC Bubbles)
- 350 TB on disk,
- 4 PB on tape

**Numerical resources requested for other use cases:**
- 1.1 Mcoreshours/year - CPU (Galileo100 or Leonardo GP)
- 300 kGPUhours/year - GPU (Leonardo Booster)
- 70 TB on disk

**Critical aspects:**
- Computer time for all activities still not allocated
- Funds for travelling not given to many of us
- Open calls