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Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA
ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

WP1@Spoke2: status report

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

INFN

UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA

ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

"ICSC and Spoke2 - Where Are We Now?" - Physics Dept and INFN, Catania - 11 Dec 2024

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
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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

October 2024

- 28 Oct WP1: informazioni e preparazione report MS9 per gli use case
- 21 Oct WP1: informazioni e preparazione report MS9 per gli use case

February 2024

- 26 Feb WP1: meeting use cases
- 05 Feb WP1: informazioni e preparazione "intermediate report" per gli use case

November 2023

- 13 Nov WP1: preparazione alla richiesta di tempo macchina al RAC

October 2023

- 30 Oct WP1: discussione documento "landscape recognition"

September 2023

- 04 Sept WP1: preparazione documento "landscape recognition"

July 2023

- 10 Jul WP1: validazione degli "use cases"

March 2023

- 06 Mar WP1: presentazione degli "use cases"

February 2023

- 13 Feb WP1: info su Template Flagship Use Cases e su Report Attività

December 2022

- 05 Dec WP1: discussione use cases

November 2022

- 14 Nov WP1: risorse computazionali e flagship use cases

October 2022

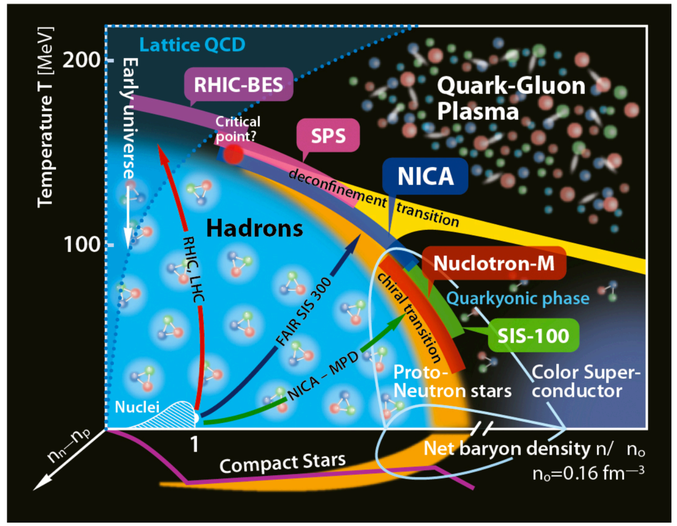
- 13 Oct WP1: presentazione attività e tavola rotonda
- 05 Oct WP1: organizzazione

WP1@Spoke2: Theoretical Physics

- Development of algorithms, codes and computational strategies for the simulation of physical theories and models, towards pre-Exascale and Exascale architectures.

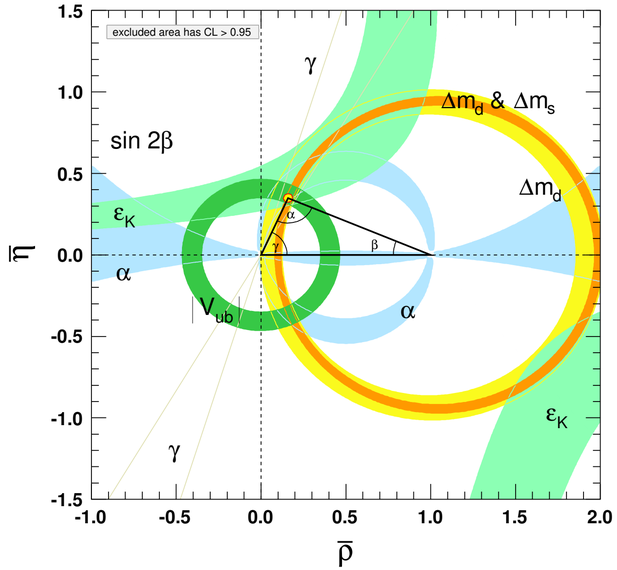
- Theoretical research projects in domains already using HPC solutions, such as:
  i. **lattice field theory** (flavour physics, QCD phase diagrams, hadronic physics, interactions beyond the Standard Model, machine learning in quantum field theories, electromagnetic effects in hadronic processes);
  ii. **collider physics phenomenology**;
  iii. **gravitational waves, cosmology and astroparticle physics** (neutron-star physics, primordial universe, dark matter and energy, neutrino physics);
  iv. **nuclear physics**;
  v. **physics of complex systems** (fluid dynamics, disordered systems, quantitative biology);
  vi. **condensed matter in low dimensional systems**.

Study of QCD in extreme conditions



Lattice Field Theory

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



Use cases:

- UC2.1.1: Multilevel Hybrid Monte Carlo for lattice QCD *(Leonardo Giusti)*
- UC2.1.2: QCD under extreme conditions (*Michele Pepe*)

Open calls:

- Development of a GPU library for massively parallelized simulations of QCD and QCD+QED on the lattice in the context of the activities of the Spoke2 in ICSC (*Vittorio Lubicz*)

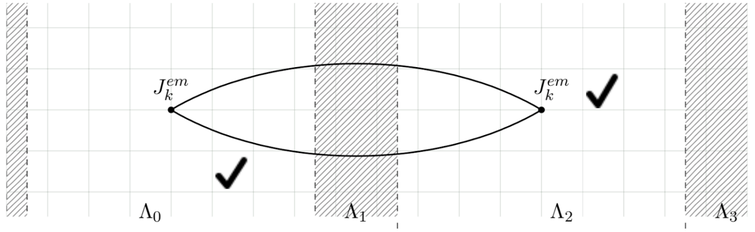
Lattice Field Theory

UC2.1.1: Multilevel Hybrid Monte Carlo for lattice QCD *(Leonardo Giusti)*

from the MS report

- During the last year (MS7, MS8 and MS9) we have developed, tested and validate a **fully optimized parallel code for simulating QCD with a multi-level Hybrid Monte Carlo (HMC)**. Lattice QCD computations are numerically very demanding, and this first version of the code implements an MPI parallelization **to run efficiently up to approximately 10,000 cores or more simultaneously** (KPI2.1.1.2).

- The implemented multi-level integration strategy is based on the decomposition of the lattice into domains.



- The **Multi-boson Domain-Decomposition HMC** (MB-DD-HMC) has been implemented starting from the publicly available code openQCD-1.6 (https://luscher.web.cern.ch/luscher/openQCD/) which implements a standard non-factorized HMC.

- **with the MB-DD-HMC the reduction of the number of Monte Carlo field configurations needed for a given precision with respect to the standard HMC is more than a factor 3**

- **The code is highly optimized to run with Intel or AMD processors** but it works correctly on any system that complies with the ISO C89 and the MPI 1.2 standards.

Marco Cè, Lightning Talk: *Lattice QCD in the exascale computing era*

Lattice Field Theory

UC2.1.2: QCD under extreme conditions (*Michele Pepe*)

from the MS report

- **During the last year** (MS7, MS8 and MS9) we have been working on the first version of a **code for measuring baryonic screening masses.** The project focuses on the development of a new code implementing the framework of **shifted boundary conditions starting from the publicly available code OpenQCD**. This is a parallel program for the Monte Carlo simulation of QCD on the lattice based on the Wilson formulation of the quark fields.

- In parallel, we have also been working on **modifying the MILC code to introduce an external chromomagnetic background field**. The MILC code is another publicly available program for simulating QCD on the lattice but based on the staggered formulation of the quark fields.

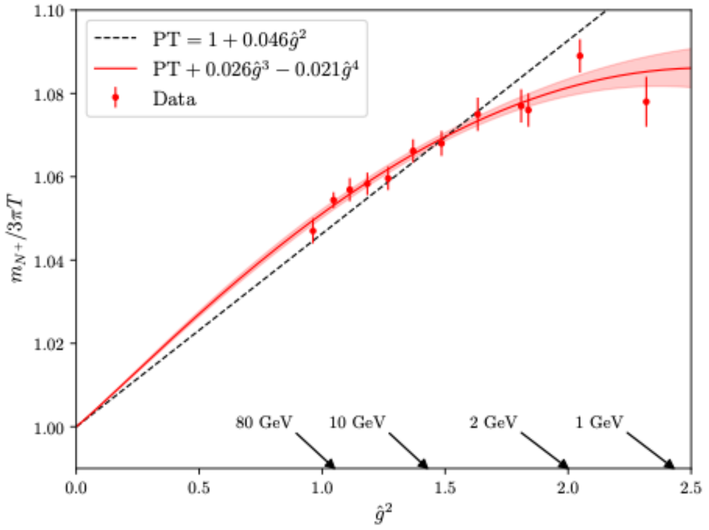
- **From January to February 2024**, further progress was made on the first versions of the codes. This phase involved completing tests that checked the correct **implementation of shifted boundary conditions within MPI communications** and extending these checks to include their implementation in Hybrid Monte Carlo simulations.
- During this time, **the MILC code was also tested in two important cases: pure gauge dynamics and QCD which involves dynamical fermions**, both of which used the Hybrid Monte Carlo algorithm.
- During the following two months we completed the **tests to confirm the proper update of the gauge field by the Hybrid Monte Carlo algorithm both with shifted boundary conditions and with a chromomagnetic background field.** Furthermore, we began to optimize the codes, improving the overall performance; initial scaling tests were carried out to evaluate how the codes perform on large system sizes.

Lattice Field Theory

UC2.1.2: QCD under extreme conditions (*Michele Pepe*) from the MS report (cont'd)

- Next, we started working to perform **measurements of observables**. Specifically, we implemented routines to compute the correlation function of baryonic operators in order to measure **baryonic screening masses with the target accuracy of 1%** (KPI2.1.2.3).

- **Measurement of baryonic screening masses** with nucleon quantum numbers and its negative parity partner in thermal QCD with 3 flavours of massless quarks for a wide range of temperatures, from T ~ 1 GeV up to ~ 160 GeV. Very large spatial extensions have been considered in order to have negligible finite volume effects.



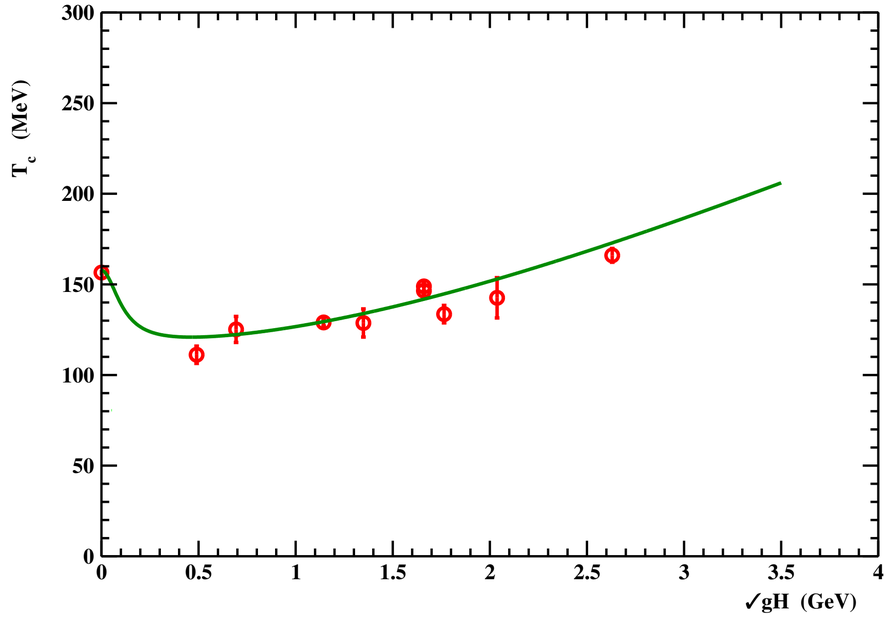
the nucleon screening mass is plotted as a function of the temperature T (g2is a function of T). The label PT refers to the prediction of 1-loop Perturbation Theory (dashed line) and the red band represents the best fit to the data.

Lattice Field Theory

UC2.1.2: QCD under extreme conditions (*Michele Pepe*)

from the MS report (cont'd)

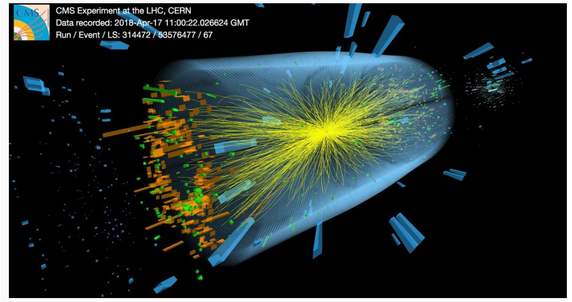
- We have used the **MILC code integrated with the modified routines described above** to investigate **QCD with (2+1)-flavour of HISQ fermions** at the physical point in the presence of a uniform Abelian chromomagnetic background field H. In particular, we have studied **the effect of the chromomagnetic background field on the crossover temperature T_c.**

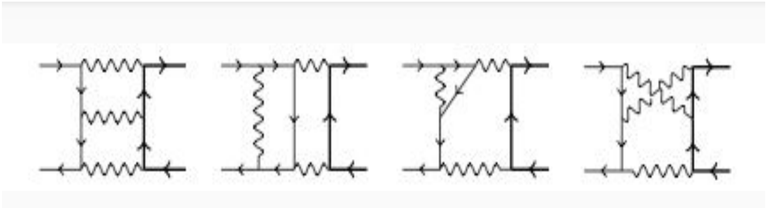


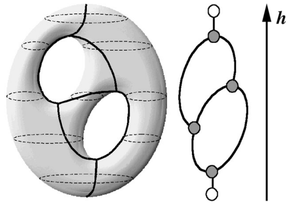
the results of our Monte Carlo simulations on the lattice: the data indicate that Tc begins to decrease in the small field region, soon after it seems to saturate and finally it increases with the strength of the chromomagnetic field.

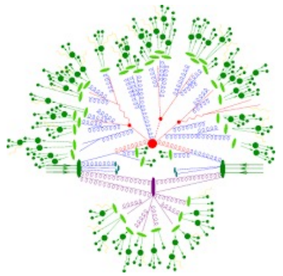
Collider Phenomenology

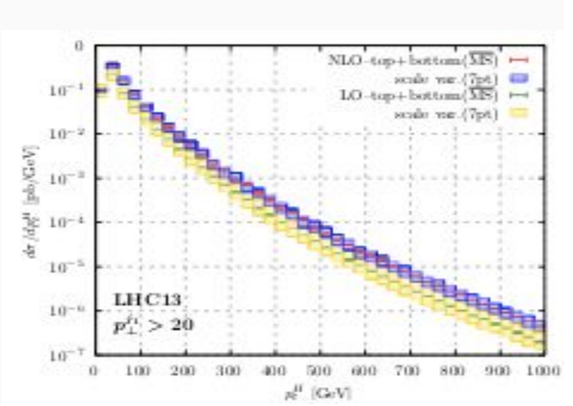
- Standard Model Physics
- Beyond Standard Model Physics
- Parton Distributions Functions
- Higgs boson and Heavy Particles Physics
- Anomalous magnetic moment (g-2) of muon and electron
- Effective Field Theories for Quantum and Classical Physics
- Scattering Amplitudes
- Physics of the Universe and Gravitational Waves Physics
- Computational Algebraic Geometry











Use cases:

UC2.1.3: Advanced Calculus for Precision Physics (ACPP) (*Pierpaolo Mastrolia*)

Institutions

UNIBO, UNICAL, UNIMIB, UNIPD

Collider Phenomenology

UC2.1.3: Advanced Calculus for Precision Physics (ACPP) (*Pierpaolo Mastrolia*)

- We developed **LoopIn**, **a software dedicated to the automatic evaluation of scattering amplitudes**, which has been conceived as a tool to support physicists in the study of perturbative corrections to scattering processes, whose Leading-Order (LO) diagrams are tree-level graphs

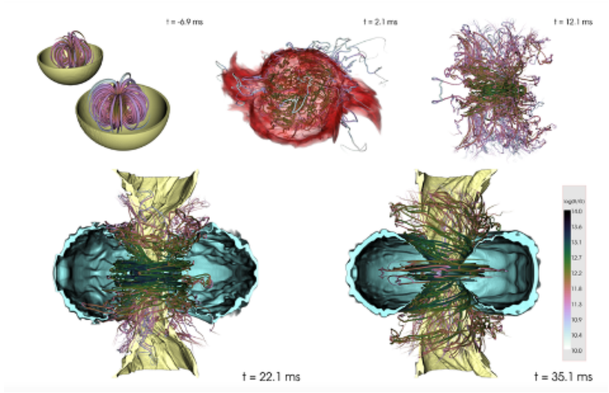
- **LoopIn is written in Mathematica** and its main task is to combine:
  1. Feynman diagrams' generation;
  2. Amplitude's integrand algebraic manipulation;
  3. Amplitude's decomposition in terms of Master Integrals;
  4. Master Integrals' (numerical) evaluation;

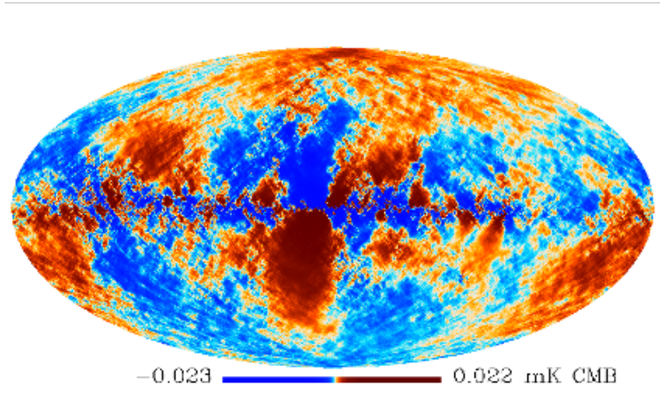
- The code has been tested on a virtual machine (CPU – 32 cores, Memory – 128 GB, DiskSpace – 1.5 TB) set on the VenetoCloud infrastructure.

- For the most time consuming phases, for which the use of the **Leonardo HPC and parallelization** would be significantly helpful.

→ **Jonathan Ronca, Lightning Talk: *LoopIn: a code for automating scattering amplitudes calculations***

Gravitational waves, cosmology and astroparticle physics





- 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

Institutions

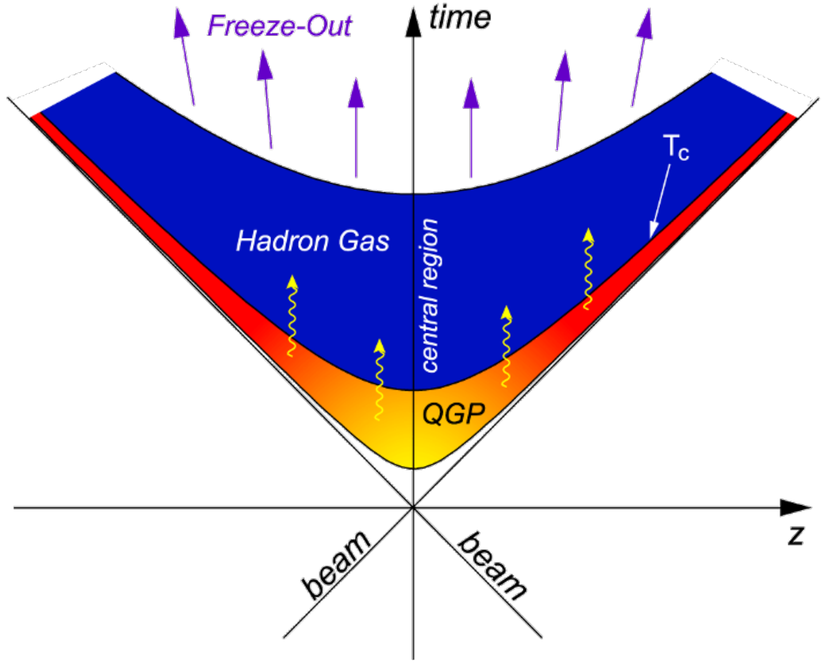
UNICAL, UNIMIB, UNIBA, UNIFI, UNIFE, UNISAPIENZA, SALENTO, UNIPD

High energy nuclear physics

- 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.

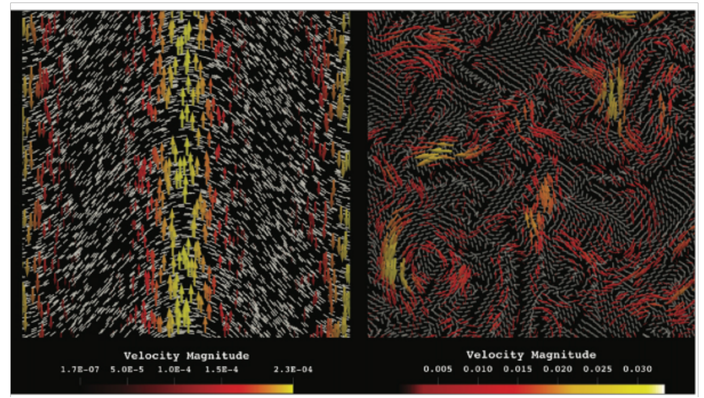
Institutions

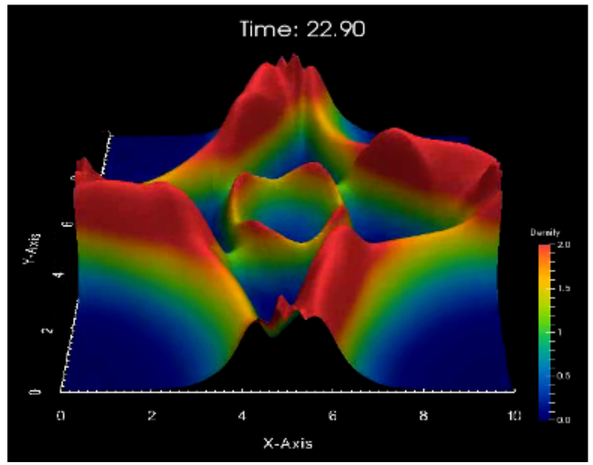
UNIFI, UNICT

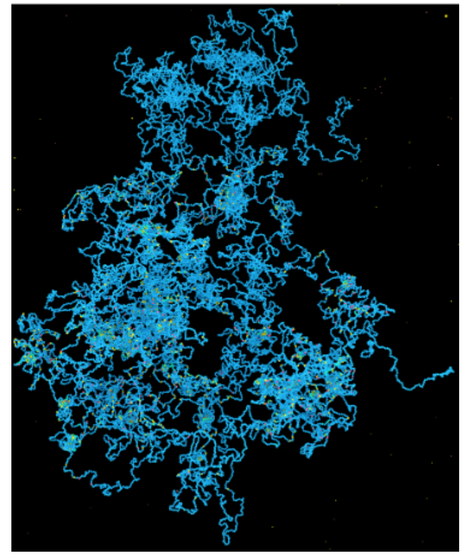


Physics of Complex Systems

- 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







Use cases:

- UC2.1.4: Large Scale Simulations of Complex Systems *(Giuseppe Gonnella)*

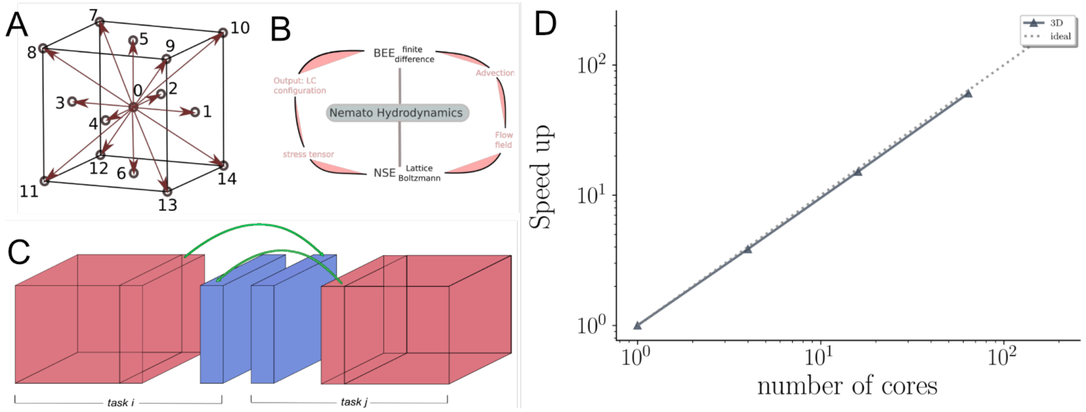
Physics of Complex Systems

UC2.1.4: Large Scale Simulations of Complex Systems *(Giuseppe Gonnella)*

- During the last year (MS7, MS8 and MS9), we have been working on the first version of a parallel code to simulate out of equilibrium complex fluids in 3D, and a routine to track topological defects and their dynamics in these systems: we developed and implemented **a parallel Lattice Boltzmann (LB) solver coupled with a finite difference method for simulating complex emulsions composed of active nematic liquid crystals with immersed passive inclusions.**

- We have developed a parallel numerical framework based on the Lattice Boltzmann Method (LBM) to solve the active fluid dynamics, coupled with finite difference schemes to solve the scalar and tensorial order parameter dynamics

- **The code was parallelised using domain decomposition, distributing the computational domain across multiple processors**. Process communication was handled via MPI (Message Passing Interface), ensuring efficient data exchange at domain boundaries. We divided the physical grid in subdomains, each assigned to a different computational unit in the MPI communicator.



Giuseppe Negro, Lightning Talk: ***A numerical framework to study topologically induced flow patterns in active emulsions***

Condensed Matter in Low Dimensional Systems

- 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

PI: A. Amendola (ENI)

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.

Personnel to be hired:

3 Technicians (1 UNIMIB, 1 CINECA, 1 ENI)

Conclusions

- MS9 reports for the Use case flagship selected:

  UC2.1.1: Multilevel Hybrid Monte Carlo for lattice QCD *(Leonardo Giusti)*
  UC2.1.2: QCD under extreme conditions *(Michele Pepe)*
  UC2.1.3: Advanced Calculus for Precision Physics *(Pierpaolo Mastrolia)*
  UC2.1.4: Large Scale Simulations of Complex Systems *(Giuseppe Gonnella)*

- WP1: 66 papers, 41 talks

- Numerical resources requested have been allocated.

- Additional numerical resources could be effectively employed during the final stages of the projects.