WP1@Spoke 2: summary & status

Leonardo Cosmai and Leonardo Giusti

INFN & Università di Milano Bicocca

Kick-off meeting Spoke 2 Centro HPC – Virtual - 14.10.2022

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

New Hiring: ~5 RTDA

New PhD : ~4 PhD

People:

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

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) [A. Suma, G. Gonella]

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

WP1 - Lattice Field Theories

I ricercatori coinvolti in WP1 - Lattice QCD

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

Use Cases

Studio della QCD a temperatura finita da principi primi
- Strategia computazionale e algoritmo per simulazione di QCD su reticolo ad alta temperatura
- Simulazioni Monte Carlo su architetture fino a exascale
- ***Interazione con WP5***: creazione di un repository di configurazioni gauge

Multi level Monte Carlo per Lattice QCD
- Strategia numerica per il calcolo di quantità adroniche con altissima precisione
- Simulazioni Monte Carlo su architetture fino a exascale
- ***Interazione con WP5***: creazione di un repository di configurazioni gauge

Simulazione di sistemi di spin come modelli efficaci di teorie di gauge su reticolo a temperatura finita
- Algoritmi e codici per la simulazione
- Tools per l'analisi statistica e la visualizzazione dei dati

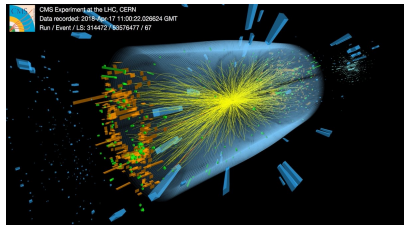
Isospin breaking in Lattice QCD
- Sviluppo di strategie numeriche e codici ottimizzati
- ***Sinergia con WP4*** (porting su GPU)
- ***Sinergia con WP5*** (repository di configurazioni)

Dinamica del confinamento in QCD
- Strategia numerica per il calcolo del tensore cromoelettromagnetico su configurazioni di gauge
- Modulo per algoritmi di smoothing delle configurazioni
- ***Interazione con WP4***: porting su GPU del calcolo del tensore cromoelettromagnetico

Risorse di calcolo

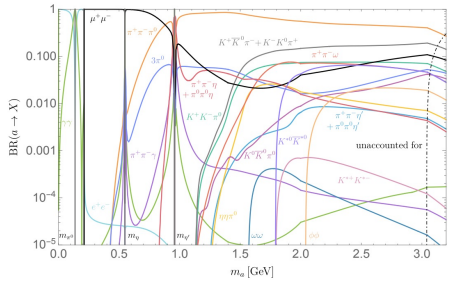
- Cluster CPU/GPU con rete Infiniband
- Accordo Cineca-INFN
- Call competitive (ISCRA, Prace EuroHPC JU)

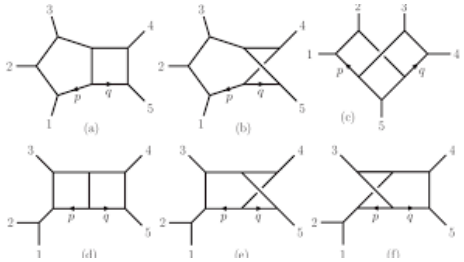
Collider Phenomenology

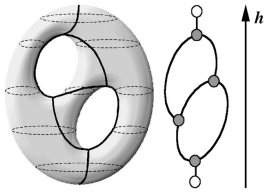


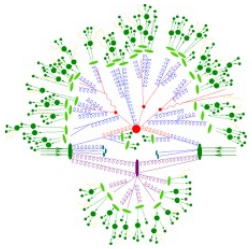
Use cases (a synthesis)

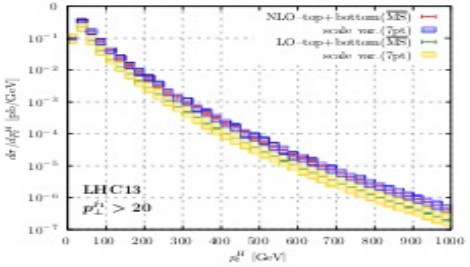
- Fast and accurate predictions for Collider Phenomenology
- Cross Sections and Partonic Distributions
- Accelerating Event Generation
- Scalable numerical evaluation of Feynman integrals
- Advanced Computational Tools for Scattering Amplitudes
- Optimized Strategies for new Particles and Couplings
-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

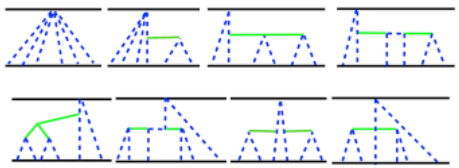


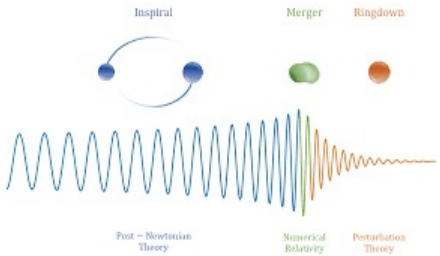












Interaction with WP4

- Porting Parallel CPU codes to GPUs

Interaction with WP5

N/A

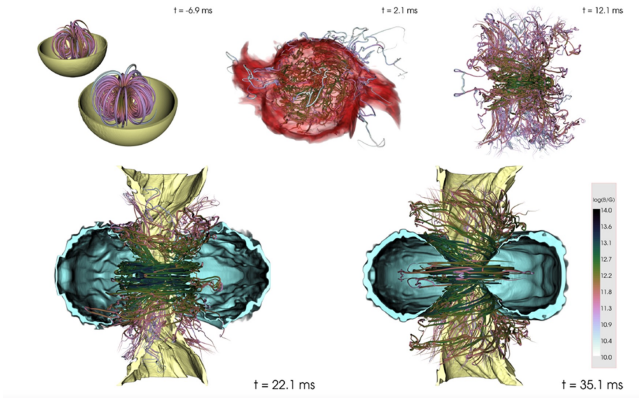
Institutions

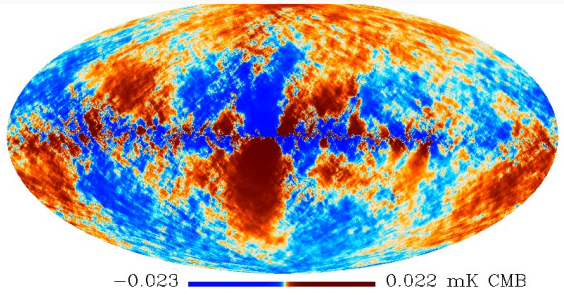
UNIBO, UNICAL, UNIMIB, UNINA, UNIPD

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

Interaction with WP5

N/A

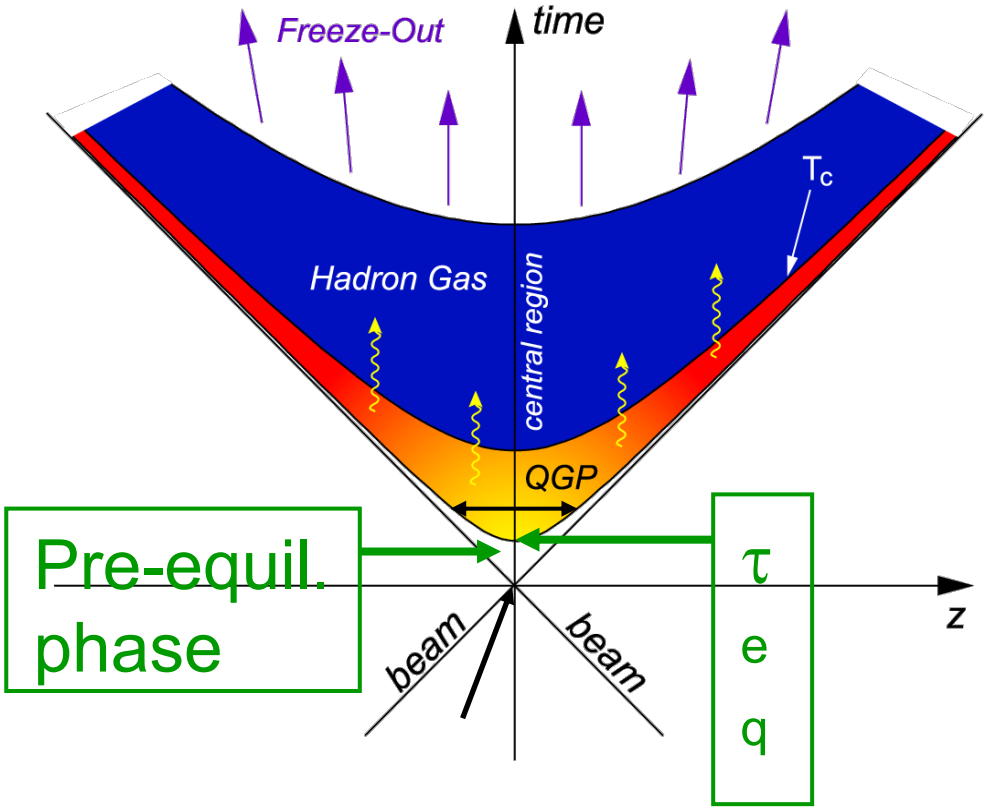
Institutions

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.

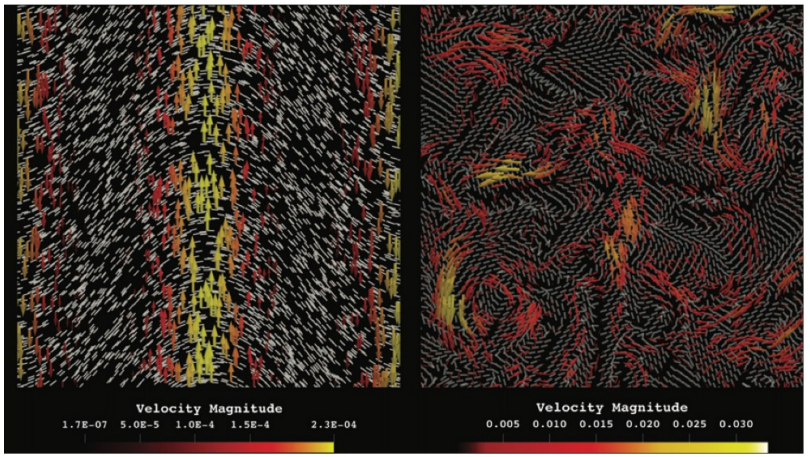


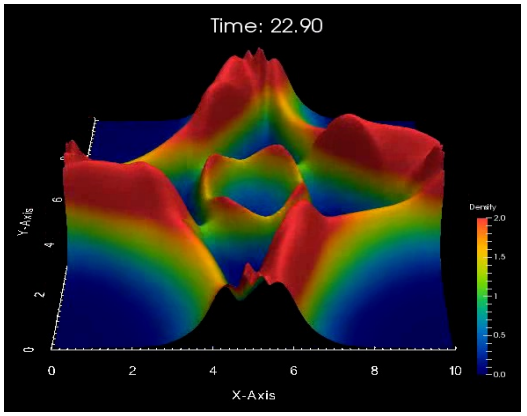
Institutions
UNIFI, UNICT

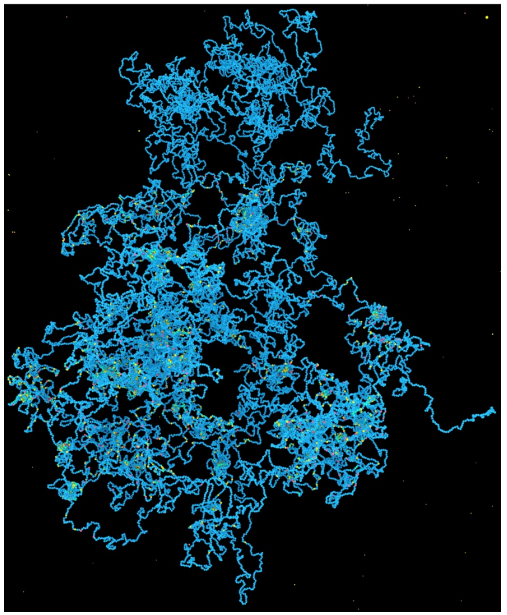
Physics of complex systems

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

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

Conclusions and outlook

Research topics:

Development of algorithms for pre-exascale and exascale architectures.
Lattice field theory
Collider physics phenomenology
Gravitational waves, cosmology and astroparticle physics
High energy nuclear physics
Physics of complex systems
Condensed matter in low dimensional systems

Possible interaction with WP4

Porting Parallel CPU codes to GPUs

Possible interaction with WP5

Data repositories (available to the public ?), and disk storage

Resources (to be quantified better)

HW, computing time: order of 20-30 Mcore-hours/year on HPC CPU/GPU ?
HW, disk space: several Petabytes ?
SW, software: Fortran, C, C++, Mathematica, Maple, MATLAB, Phyton,….