

Deliverable 4 - Project SOPHYA - Sustainable Optimised PHYsics Algorithms: fundamental physics to build an advanced society (P2022Z4P4B)

Results and activities put forward by the units for M2, M3, M4, also indicating the published papers, publication of algorithms optimised in efficiency and portability (February 2026)

M2: development and test of the algorithms on problems in fundamental physics

M3: algorithms at work in physics

M4: generalisation and publication of algorithms optimised in efficiency and portability

The milestone M2 (development and test of the algorithms on problems in fundamental physics) was completed in May 2025 (bimester 9).

The milestone M3 (algorithms at work in physics) and the milestone M4 (generalisation and publication of algorithms optimised in efficiency and portability) have been completed at the end of the project.

In compliance with the stated project objectives O1 (development of optimised numerical algorithms to solve PDEs showing different critical issues, and PIC algorithms, comparing the outcomes and performances to standard numerical techniques) and O3 (availability of computational procedures and codes as FOSS in public repositories), some numerical codes have been produced and published in the public repositories at <https://github.com/PRIN-SOPHYA>. Four repositories have been created, one for each activity in milestone M4. For each code, a README file, containing information about the aim of the code and instructions on how to use it, has been produced and published in the repositories, in order to facilitate third-party usage.

In addition, in the following the results obtained by the units, fulfilling the goals established in objective O2 (computation of physical quantities of interest for QGP physics via the algorithms of O1, and comparison of results), are also described.

The behavior of thermodynamic quantities in the QGP phase at finite temperature (T) and baryon chemical potential (μ_B) - specifically pressure, entropy, baryon number density, baryon number susceptibility, and speed of sound - has been investigated by the INFN unit by means of an AdS/QCD model. Furthermore, the critical endpoint (CEP) in the μ_B - T plane, which separates the crossover region from the first-order phase transition, was identified at $\mu_B = 0.678$ GeV, $T = 0.110$ GeV.

The model has also been used to study some features of light vector mesons at zero and finite temperature and density. This requires introducing a new gauge field, describing vector mesons, and a new gauge kinetic function. An algorithm utilizing automatic differentiation and the Adam optimizer was developed to optimize model parameters. The procedure identifies the specific gauge kinetic function that best fits the masses of the first four vector meson resonances. The mass of the subsequent resonance was then calculated, showing

good agreement with experimental data. Furthermore, the INFN unit extracted the hadronic spectral functions for vector mesons at finite temperature and chemical potential, observing the characteristic thermal broadening of the peaks. Notably, the ρ meson was found to dissociate (melt) in the QGP near the deconfinement transition temperature, a phenomenon occurring consistently across both crossover and first-order phase transitions. From these spectral functions, the electrical conductivity σ was derived. The ratio σ/T increases with temperature, peaking just above the critical point before entering a decreasing regime; at high temperatures, the conductivity becomes independent of μ_B , converging to a constant value of $\sigma/(C_{em}T) \sim 0.3$. Finally, the INFN unit investigated the transport properties of heavy quarks moving through the QGP. The drag force and energy loss were analyzed as a function of temperature and velocity at fixed chemical potentials. The diffusion coefficient was found to be consistent with existing theoretical studies, particularly lattice QCD, and aligned with ALICE experiment data.

The Cosenza unit has mainly contributed to activities A3.3 and A4.1, focusing on the numerical study of non-equilibrium dynamics in a high-temperature plasma during a first-order phase transition in the early Universe. In particular, the unit has developed and refined an iterative numerical strategy to solve the Boltzmann equation governing the distribution functions of particle species interacting with an expanding bubble wall. The method is based on decomposing the distribution function of each species into a local thermal equilibrium component and a perturbative out-of-equilibrium correction, which is determined through successive iterations until convergence is achieved.

The iterative framework, developed in the previous months for the solution of the Boltzmann equations for fermionic degrees of freedom, has now been extended to include bosonic states, in particular, the electroweak gauge bosons. To this end, the relevant electroweak 2-to-2 scattering and annihilation processes have been computed and incorporated into the numerical implementation. This extension represents a significant step toward a more complete description of the plasma dynamics beyond the fermionic sector.

Qualitative and quantitative comparisons of the state-of-the-art results achieved by the unit and similar studies in the literature have been thoroughly addressed.

Furthermore, we have started investigating the incorporation of thermal masses for both fermions and bosons directly within the collision integrals, with the aim of achieving a more accurate treatment of medium effects in the high-temperature regime.

The full algorithm has been implemented in a C++ code and integrated with the LTE-based framework and the solver of the Boltzmann equations for the fermionic sector developed during the previous phases of the project. The numerical stability has been explored in detail to ensure robustness across different regimes of interest. In particular, special attention has been paid to the convergence properties of the iterative solution and to the impact of newly introduced effects, such as thermal masses, on the stability of the computation. In this context, it has been found that, in the diagonalization of the collision operator, enhanced numerical precision is required in the computation of the eigenvectors in order to avoid the onset of propagating instabilities at large iteration numbers.

The Catania unit focused on Activity 3.2, specifically analyzing the spectral properties of quarkonia during the early stages of heavy-ion collisions. The unit implemented an approach that mimics the formalism of the open quantum systems, treating the quarkonium as the quantum system and the strong gluon fields produced in the pre-equilibrium stage as the environment. The basic interaction Hamiltonian is a color-dipole interaction with the electric

part of the gluon fields. By tracing over the environmental degrees of freedom and performing an ensemble average, an evolution equation has been derived for the density operator of the quarkonium states in the singlet-octet color space. In this framework, the color-projected density matrix couples to gauge-invariant field correlators that measure the fluctuations of the gluon fields in the environment. Using this approach, singlet-to-octet transitions in the pre-equilibrium stage were quantitatively investigated to analyze the melting of the pairs. Calculations were specialized to the cases of J/Psi and Ypsilon states in both nucleus-nucleus (A-A) and proton-nucleus (p-A) collisions. The results indicate that in A-A collisions, the strength of the gluon fields is sufficient to melt a substantial fraction of quarkonia; conversely, in p-A collisions, the strength of the fields is not enough to cause significant melting. These results shed light on the role of the pre-equilibrium stage on the melting of the quarkonium states in heavy ion collisions, and allow to quantify how many bound pairs have to be expected in the quark-gluon plasma compared to those produced by hard QCD processes in the very early stage of the collisions.

Published papers

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