Deliverable 3 - Project SOPHYA - Sustainable Optimised PHYsics Algorithms: fundamental physics to build an advanced society (P2022Z4P4B)

Results and activities put forward by the units for M2 and M3 , also indicating the published papers at month 18 (May 2025)

M2: development and test of the algorithms on problems in fundamental physics
M3: algorithms at work in physics

Activity A2.3 has been accomplished by the INFN unit. Algorithms for the solution of boundary value problems (Activity A2.3) and of time-dependent partial differential equations (Activity A2.1) have been developed and tested to study the evolution of the chiral condensate in a time-dependent setup, in which the temperature of the system varies with time. The model in which the computation has been put forward is the soft-wall model, an AdS/QCD model with static dilaton, in which the position of the black-hole horizon changes with time, producing an increasing or decreasing temperature. Two different scenarios have been analysed: in the first a general power-law time dependence is assumed, while in the second the energy-momentum tensor at late times reproduces the one found in viscous hydrodynamics. We have found that, depending on the rate at which the system evolves, the chiral phase transition shifts toward lower temperatures. If the chiral condensate is far from equilibrium at low temperatures, oscillations around its equilibrium value have been observed before thermalization. A prethermalization stage has been found in the chiral limit if the initial condition is set at a temperature close to the critical one. In the hydrodynamic setup the evolution of the medium is slow enough, and the chiral condensate soon matches the equilibrium curve. These results have been obtained using the Chebyshev pseudospectral method. The general solution has been expanded in a truncated series of N Chebyshev polynomials depending on the spatial variable with coefficients depending on time. By requiring the equation to be satisfied in N Gauss-Lobatto collocation points, one is left with a system of N (nonlinear) ordinary differential equations in time, which have been solved using a standard Runge-Kutta algorithm. N = 30 has been used, and we have checked the final results do not change for higher values of N. After an initial implementation of the algorithms in Mathematica, in order to accomplish the final goal of the project and enhance efficiency and reduce our environmental footprint, we opted for easily reusable scripts written in an open-source language, Python, designed for execution on an HTC/HPC cluster, which significantly lowers energy consumption and pollution compared to running standalone programs on personal computers. This has also helped us in the cases in which the execution time was longer, i.e. when the temperature varies slowly over time.

For activities A3.1 and A3.4, we have started using these algorithms for different problems concerning finite temperature QCD at equilibrium and out of equilibrium. The preliminary studies have been devoted to the framework we already developed for the chiral condensate.

For activities A2.2 and A3.2, after developing some reconstruction algorithms based on neural networks, particularly deep learning models, we have selected the optimal holographic model in which the spectral functions will be computed, in order to obtain data to train the model. We have also started developing algorithms to get a best fit of the model parameters. The neural network previously developed for reconstructing spectral functions has been trained using data extracted from a holographic model. Preliminary results suggest that the input data require refinement, such as selecting appropriate energy intervals or applying a standardization procedure, to achieve more accurate and reliable outcomes.

Algorithms for the solution of time-dependent partial differential equations (Activity A2.1) have been developed and tested to study a first-order phase transition far from equilibrium. For activities A3.1 and A3.4, the INFN unit has developed and begun analyzing a model that reproduces the first-order chiral phase transition in QCD, which is expected to occur in the three-flavour case for small quark masses. To capture this first-order transition, a different potential is required compared to the one used in the previous study. Specifically, the new potential includes a cubic term arising from the determinant of the scalar field, which, in this case, is represented by a 3x3 matrix.

As part of activities A3.1 and A3.4, neural network-based algorithms have been developed to numerically study an Einstein-dilaton holographic model, which is governed by a system of differential equations. These algorithms enable the use of lattice QCD data to constrain the geometry underlying the model. Input data include lattice results for the entropy density above the deconfinement transition, as well as the masses of the glueball ground state and first excited state. The novelty of this approach lies in the unified description of both thermodynamic quantities and the hadron spectrum, which are jointly used to construct the model. The resulting model has then been employed to compute additional thermodynamic observables, such as pressure, energy density, and the trace anomaly, above the deconfinement temperature, along with the masses of higher excited states in the glueball spectrum.

Regarding activities A2.1 and A3.3, the Cosenza unit has improved the algorithmic efficiency for computing bubble wall dynamics in the hydrodynamical regime during first-order phase transitions in the early universe. The main objective has been to enhance the performance and scalability of the numerical tools used to model these dynamics across a broad class of beyond the Standard Model scenarios.

Key advancements include the identification of optimized initial conditions for root-finding algorithms, informed by physical insights into the system, as well as the refinement of Jouguet velocity calculations. In addition, significant improvements were made to the Python code responsible for computing equilibrium quantities that characterize first-order phase transitions and for managing efficient parameter space scans of the models under study.

The core algorithm was implemented in C++ and benchmarked on a computing cluster, allowing for parallel exploration of extensive parameter spaces. The considered models involve Standard Model extensions with scalar fields that can trigger a first-order phase transition.

Preliminary estimates of the resulting gravitational wave spectra were obtained and the impact of bubble wall velocity was assessed, providing insights into potential observational signatures. The accuracy of the numerical results was assessed through comparisons with theoretical expectations wherever feasible, and the uncertainties associated with the numerical algorithms were also estimated.

In parallel, the unit progressed in extending the core algorithm to incorporate out-of-equilibrium plasma effects. The computation of the kernel functions for collision integrals were performed using Wolfram Mathematica. These kernels were evaluated by

decomposing them onto their eigenfunction basis, a method found to be more efficient than expanding in Chebyshev polynomials. The analysis focused on 2-to-2 annihilation and scattering processes in QCD involving the top quark, which is the heaviest particle in the broken phase and therefore plays a dominant role.
An iterative numerical approach has been developed by the Cosenza unit for the solution of the Boltzmann equation for the distribution functions of particle species in a high-temperature plasma during a first-order phase transition in the early Universe. By splitting the distribution function for each species into the sum of the local thermal equilibrium (LTE) contribution and its out-of-equilibrium deviation, the problem is solved through successive approximations until convergence is reached. The iterative approach has been implemented to solve the Boltzmann equation for the top quark species, taking into account 2-to-2 annihilation and scattering processes in QCD. While the working unit has so far focused on the solution of the Boltzmann equation for fermions, the algorithm has been developed in such a way that it can also address bosonic species. The whole framework relies on the computation of the kernel functions (also known as collision integrals), specific to the relevant collision processes, which had been previously calculated with Wolfram Mathematica. The numerical evaluation of the kernels can be performed very efficiently and with high accuracy by decomposing them into Legendre polynomials. The remaining angular-independent blocks are then decomposed into the eigenfunction basis. This set of eigenfunctions constitutes the natural basis for the decomposition of the collision integral and allows control over the accuracy of its evaluation by exploiting the hierarchy of the eigenvalues. For instance, it was found that for the first Legendre block, all the eigenvalues except the first four are suppressed by a factor of about 10^{-4}, with the suppression even stronger for higher modes. Consequently, to reconstruct the kernel with, for example, an accuracy of order 1%, only a few eigenvectors belonging to the lowest modes are sufficient. Moreover, the kernels depend solely on the scattering processes considered; therefore, when performing a survey of a model, they only need to be computed once. The algorithm has been implemented in a C++ program. The resulting algorithm has been successfully tested to scan the entire parameter space of specific benchmark models. The results obtained, particularly the bubble wall velocity and the bubble width, in one of the selected benchmark models (the singlet-extended Standard Model) were then used as input to numerically solve the set of differential equations for the transport equations within models of electroweak baryogenesis. These solutions were subsequently employed to compute the matter–antimatter asymmetry. The results show a very significant dependence on the inclusion of out-of-equilibrium effects.

For what concerns A3.4, the Catania unit has worked on the thermodynamic quantities in the cold-and-dense QGP phase relevant for the physics of compact stellar objects. The object of the physical investigation has been the topological susceptibility and the low-energy axion properties in the superdense QCD matter. An algorithm that solves a Dyson-Schwinger equation for the full quark propagator in these phases has been implemented, coupling it to a resummed gluon propagator that takes into account medium effects non-perturbatively, and in the rainbow approximation for the quark-gluon vertex. The Dyson-Schwinger equation, that in this context is called the gap equation, has been solved within the high density effective theory, which has never been used before for this type of problem. The scheme adopted corresponds to a standard self-consistent solution of a non-linear integral equation, completed by Montecarlo integrations to compute the topological susceptibility and the axion mass and self-coupling from the solution of the gap equation.

In addition to this, the unit has applied the techniques of the functional renormalization group to the study of the chiral phase transition in QCD, investigating the theory at imaginary chemical potential μ and checking the effective convergence radius of the small-μ expansion centered at $\mu=0$. For this part of the work, the unit has implemented a Kurganov-Tadmore algorithm at finite (both real and imaginary) chemical potential. The unit has studied the behavior of the critical line versus imaginary μ, similarly to what has been done in Lattice QCD; then, the critical curvature at finite and real μ has been extrapolated by analyzing the data at imaginary μ, and the results have been compared with the actual calculations at real μ. This type of analysis has been then used to measure an effective convergence radius of the small-μ expansion, improved by the imaginary chemical potential data.

Still within A3.4, the unit has started an investigation of Dyson-Schwinger equation in the superfluid phase of superdense QCD with two colors. For this, the unit has improved the previous algorithm used for the solution of the gap equation for dense QCD, and started a detailed study of the poles of the quark propagator. For this part of the work, besides the algorithm for the solution of the integral gap equation, multiple numerical techniques have been adopted to diagonalize large matrices and perform analytic continuation from imaginary to real frequencies.

Regarding A3.2, the Catania unit has implemented an algorithm to follow the evolution of the density matrix of J/ψ and Y in the pre-equilibrium stage of the proton-nucleus collisions, and analyze their survival probability as well as their melting into color-octet states. The formalism is similar to that of open quantum systems, in which however the quantum system, in this case the hadron state, is coupled to an environment of strong random fields, whose fluctuations force the singlet-to-octet transitions. Similarly to A3.4, the implemented algorithm is that of the solution of an integral equation for the density matrix of the octet states, while the fluctuations of the background have been computed within statistical classical simulations of the gluon field in real time.

Within A3.2, the same problem has also been approached from the point of view of relativistic transport theory coupled to the external random gluon fields. The unit adopted a particle-in-cell algorithm to solve the relativistic kinetic equation of the heavy quarks in the c-cbar and b-bbar pairs coupled to the external fields, which run on HPC clusters.

Within A3.1, the unit has analyzed the energy loss and the momentum broadening of heavy quarks in the pre-equilibrium stage of high-energy proton-nucleus and nucleus-nucleus collisions. In particular, the momentum and coordinate broadenings allow for the estimate of the diffusion coefficient in coordinate and momentum spaces. The same approach allows for the calculation of the energy loss of the heavy quarks. Also for this part of the work, the unit has used a particle-in-cell algorithm, run on an HPC cluster.

Within A2.4, the particle-in-cell algorithm for the evolution of colored particles in a set of random gluon fields has been stabilized, as well as the real-time lattice simulation code that is used to study the dynamics of the gluon fields in the early stage of high-energy nuclear collisions.

After an initial implementation of the algorithms in Mathematica, Fortran and C++, in order to accomplish the final goal of the project and enhance efficiency and reduce our environmental footprint, we opted for easily reusable scripts written in an open-source language, Python, designed for execution on an HTC/HPC cluster, which significantly lowers energy consumption and pollution compared to running standalone programs on personal computers.

In addition to this, the unit has produced a calculation of the critical temperature of QCD using techniques based on the functional renormalization group combined with analytical continuations from imaginary chemical potential. The unit has analyzed in detail a few interpolation schemes that allow for the calculation of the critical line of the QCD phase diagram at finite chemical potential starting from data computed at imaginary chemical potential, using them to estimate an uncertainty on the curvature of the critical line at small real chemical potential. Even more, the unit has analyzed in detail within QCD effective models the predictions on the location of critical endpoint coming from continuation techniques, and compared them with the actual, computed location of the endpoint. The unit has found that while the analytical continuation from imaginary chemical potential gives reliable results at small real chemical potential, the predictions of the location of the critical endpoint are subject to severe uncertainties.

Published papers

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10. P. Colangelo, F. De Fazio and G. Roselli, Charming case of $X(3872)$ and $\chi c1(2P)$, Phys. Rev. D 111, 074014 (2025), doi:10.1103/PhysRevD.111.074014
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