Deliverable 2 - Project SOPHYA - Sustainable Optimised PHYsics Algorithms: fundamental physics to build an advanced society (P2022Z4P4B)

Results and activities put forward by the units for M2 in the first year (december 2023-november 2024)

M2: development and test of the algorithms on problems in fundamental physics (december 2023-november 2024)

Some numerical methods for solving evolution, deconvolution and boundary value problems have been developed and tested for problems in fundamental physics, in particular for studying the features of high-temperature plasma in the early universe.
A detailed discussion on the achievements related to the project tasks is reported in the following.

Algorithms and programs based on pseudospectral methods have been developed using Wolfram Mathematica, at first, and then Python to numerically solve partial differential equations and study the chiral transition in a holographic model with a time-dependent metric. Pseudospectral methods are particularly useful in the considered physical problem characterised by nonlinear equations, and in which boundary conditions should be imposed in points for which singularities of the equations of motion can arise. A scalar field containing the quark mass and the chiral condensate has been introduced in the model. The nonlinear term in the equation of motion comes from the quartic potential chosen for the scalar field in the action, which allows to describe both explicit and spontaneous chiral symmetry breaking. A static dilaton and an anomalous dimension in the five-dimensional mass of the scalar field have been introduced as well. Various time-dependent metrics have been considered, in which the position of the black-hole horizon varies with time, one of them describing a hydrodynamic setup with small viscosity. Preliminary results show that, in a simple model with fixed dilaton, a time-dependent metric changes the transition from first order to crossover for a vanishing quark mass, independently of the functional form of the time dependence, and the transition gets slower when the quark mass is different from zero. When the metric rapidly changes with time, instabilities occur which need further investigations.

Algorithms based on neural networks, particularly deep learning models, have been further developed and optimized, showing promising performance in reconstructing spectral functions from clean data. The presence of noise significantly degrades the reconstruction quality, as expected. In these problems one has also to care about overfitting, especially when training on noisy data, and strategies such as dropout and regularization are being explored to mitigate this issue. Optimization techniques, including hyperparameter tuning and regularization methods, have been applied to improve the model robustness, particularly in noisy environments. More extensive tests on noisy datasets, also changing the noise form, have been conducted to assess the capabilities of the models in real-world scenarios where noise is a significant factor. Convolutional architectures seem to outperform feedforward models when noise is present, suggesting that Convolutional Neural Networks can better capture relevant features in noisy data.

Algorithms for studying the dynamics of domain walls in the high-temperature plasma of the early universe have been developed and implemented in C++ codes. They aim at solving the system of integro-partial differential equations that govern hydrodynamics and out-of-equilibrium effects. Efforts have been concentrated on enhancing the efficiency of the solution strategy, with a particular emphasis on reducing code execution time.

The complexity of the hydrodynamic system of differential equations has been significantly reduced by reformulating them as moment equations. These were solved using a combination of minimization and root-finding algorithms, resulting in a substantial decrease in computational complexity and resource requirements. Additionally, parallelization techniques were employed to efficiently compute equilibrium quantities, which serve as input data for solving the hydrodynamic equations. These equations were solved across the entire parameter space via a diffusion process.

The algorithms were initially tested on specific benchmark points of the singlet-extended Standard Model and subsequently applied to its full parameter space. In particular they have been used in cosmological scenarios relevant to physics beyond the Standard Model, specifically those in which the electroweak phase transition can be first-order. Such scenarios are of interest due to their potential to produce observable gravitational wave signatures, which could be detected by future interferometers. Further tests were conducted on models involving additional electroweak doublets and triplets to validate the tools' usability. The convergence properties and robustness of the results were also rigorously verified.

Algorithms for solving the Yang-Mills equations and simulating the glasma dynamics have been developed and optimized. Specifically, they worked on two approaches: solving the equations in the continuum limit and implementing real-time dynamics on a lattice. These advancements allowed them to achieve greater precision in modeling the evolution of classical color fields, ensuring a more reliable description of the pre-equilibrium stage in high-energy nuclear collisions. The stability of the algorithms has been tested also after the inclusion of initial-state fluctuations of the gluon fields that are known to trigger plasma-like instabilities in the evolving gluon fields. Numerical stress-tests have been performed to check that the plasma instabilities do not alter the quality of the output of the calculation, by finding a good balance between the parameters of the lattice (lattice spacing, lattice size) and the efficiency of the code (like numerical time steps, sheets of color charges, ensemble average and so on).

A particle-in-cell algorithm has been implemented and tested to solve the relativistic Wong equations in the background fields of the evolving glasma to describe the diffusion of heavy quarks within the medium. A key focus was on validating the convergence of the algorithm and optimizing its performance. Through systematic tests, the optimal parameters for efficient operation have been identified, including the number of test particles required to balance computational cost and accuracy. The algorithm was applied to both nucleus-nucleus and proton-nucleus initializations, demonstrating its flexibility and robustness in modeling heavy quark dynamics across different collision environments. Effort has been made on understanding the evolution of heavy quarks and their dissociation under

the influence of both a strong-force potential, combining Coulomb-like and confining terms, and the classical glasma fields.
The codes have been written in Julia and Python, while Mathematica codes have been used to test the output of the main codes. Their findings highlighted the dominant role of the glasma fields in increasing pair separation and enhancing dissociation probabilities. The dissociation process revealed differences tied to quark flavor, with c-cbar and b-bbar pairs exhibiting distinct behaviors. Additionally, analysis of dissociation spectra showed a momentum shift, suggesting an energy gain during interaction. These results provide valuable insights into the interplay of QCD dynamics during the early stages of nuclear collisions, with potential implications for interpreting experimental data.

A particle-in-cell algorithm has been coupled to the evolving SU(3)-glasma framework, and to a Monte Carlo generator for the preparation of the correct initialization for proton-nucleus collisions. The aim was studying the melting of heavy quark pairs during the early stage of high-energy proton-nucleus collisions. The results showed that color charge fluctuations of the heavy quarks significantly enhance the melting of the pairs, with approximately 50% of heavy quark pairs dissociating within 0.2 fm/c. Neglecting color fluctuations doubles this timescale, highlighting their critical role in the process. The algorithms have also been applied to the calculation of the energy loss of heavy quarks in the early stage of proton-nucleus collisions.