Deliverable 1 - Project SOPHYA - Sustainable Optimised PHYsics Algorithms: fundamental physics to build an advanced society (P2022Z4P4B)

Results and activities put forward by the units for M1 in the first six months (december 2023-may 2024)

M1: identification of the main limitations of the current evolution algorithms, focusing on computing costs in terms of energy power and selection of the most convenient ones based also on the criterion of energy saving (december 2023-november 2024)

In this period some numerical methods for solving evolution, deconvolution and boundary value problems have been examined and developed. The considered numerical problems arise in the study of the features of the quark-gluon plasma. In the following months the algorithms and the programs will be evaluated according to their use of computing resources.

The following achievements have been accomplished, and a detailed discussion related to the project tasks can be found in next sections.

1. Development of algorithms and programs based on pseudospectral methods for partial differential equations.
2. Development of algorithms and programs based on the Crank-Nicolson method for partial differential equations using the tridiagonal matrix algorithm to solve linear systems of equations.
3. Development of algorithms and programs using the Newton-Raphson iteration algorithm to solve linear and nonlinear systems of equations.
4. Development of algorithms and programs based on the Crank-Nicolson method for partial differential equations using the Newton-Raphson iteration algorithm.
5. Development of algorithms and programs based on the Kurganov-Tadmor scheme for solving the advection-diffusion equation in the framework of the functional renormalization group.
6. Development of algorithms and programs to solve classical Yang-Mills equations on a real-time lattice.
7. Development of algorithms and programs using Runge-Kutta methods to solve ordinary differential equations.
8. Development of algorithms and programs based on Feedforward Neural Networks neural network model to reconstruct spectral functions in Quantum Chromodynamics with and without noise.
9. Development of algorithms and programs based on Convolutional Neural Networks neural network model to reconstruct spectral functions in Quantum Chromodynamics with and without noise.
10. Development of algorithms and programs based on Deep Learning Architectures neural network models to reconstruct spectral functions in Quantum Chromodynamics with and without noise.

The work is progressing in multifaceted directions: improving the algorithms to gain more efficiency; developing them in different languages to finally choose the most efficient one according to energy power use; establishing in which cases the use of parallel computation should be implemented to further optimize efficiency; comparing models and methods.

A1.1 - time-dependent PDEs

A1.3 - boundary value problems

A1.4 - PIC algorithms and gauge invariant formulation of real time lattice simulations

For these tasks, we have obtained the results 1-7.

Numerical algorithms and programs for partial differential equations have been developed in order to solve the evolution problem of time-dependent Einstein equations and the boundary value problem of a scalar field in a hydrodynamical system with an AdS/QCD model. These studies aim at finding the properties of the quark-gluon plasma, a strongly coupled nearly perfect fluid produced in the early universe, as well as in the early stage of ultrarelativistic nuclear collisions.

The examined numerical methods include the pseudospectral and the Crank-Nicolson ones. In the former case, the functions are written as linear combinations of a truncated set of basis functions. A convenient choice is Chebyshev polynomials. The coefficients are determined by inserting the truncated expansion into the differential equation and demanding that the residual vanishes exactly at a selected set of points, called collocation points. For sufficiently well-behaved functions, accuracy improves exponentially with the dimension of the basis. For partial differential equations, the coefficients are time dependent, and one is left with a system of ordinary differential equations that can be solved with, e.g., Runge-Kutta methods. A key advantage of spectral methods is improved convergence. The Crank-Nicolson method is a finite difference method implicit in time. When implementing pseudospectral methods and the Crank-Nicolson scheme, a linear or nonlinear system of equations must be solved to compute each update. This can be done using the tridiagonal matrix algorithm in the simplest cases, or the Newton-Raphson iteration algorithm for nonlinear systems. Therefore, Runge Kutta and Newton methods have been developed for a particular use-case, i.e. to study pseudoscalar and axial-vector mesons in an AdS/QCD model with the aim of computing their contribution to the anomalous magnetic moment of the muon, a quantity that is challenging the Standard Model (SM) of fundamental interactions given the actual discrepancy of about 5 standard deviations between the theoretical and experimental values [1]. The numerical problem that has been studied was a boundary value problem characterized by a system of differential equations for pseudoscalar mesons and an ordinary differential equation for axial-vector mesons.

A preliminary comparison between the programs based on the pseudospectral and the Crank-Nicolson method developed for the mentioned use cases has shown that the former uses less machine time than the latter, producing results with similar accuracy.

Another study examines the behavior of gluons and quarks, along with their strong interactions, during a first-order phase transition in the early universe [2-3]. The transition occurs through the nucleation of bubbles, which are surfaces separating the plasma into two distinct phases. A framework to investigate the equilibrium properties of plasma in the presence of a traveling domain wall, in the context of a cosmological phase transition, has been developed. This study serves as groundwork for analyzing the non-equilibrium effects. Within this framework, the system of partial differential equations governing the temperature and velocity distributions has been identified, as well as the equation of motion for the bubble wall in a steady-state regime. The system is further defined by appropriate boundary conditions, corresponding to three hydrodynamic regimes commonly referred to as detonation, deflagration and hybrid. The latter two regimes are also characterized by a traveling shock wave, for which the equation of motion has been determined. Solving the equations requires the computation of the free-energy, which has been derived using perturbation theory based on a chosen Beyond Standard Model scenario providing a phase transition in the early universe. To simplify the implementation, a scalar singlet extension of the Standard Model has been selected. A Python program has been implemented for the numerical calculation of the free-energy, validated by comparison with an independent Wolfram Mathematica implementation. Additionally, available tools in the literature [4,5] were utilized to map out regions in the parameter space in which a cosmological first-order phase transition may occur. These regions have been fully analyzed and the thermal-equilibrium observables that characterize them (such as the nucleation temperature, the location of the minima of the free-energy, the latent heat and inverse-time duration of the transition) have been computed. This has finalized the calculation of all inputs necessary to solve the differential equations governing the wall dynamics.

A numerical study of the functional renormalization group (FRG) has been put forward with a Kurganov-Tadmor algorithm, identified as the best algorithm for the implementation of the FRG flow equation in simple models of Quantum Chromodynamics (QCD) [6]. The flow of the effective action with the energy scale can be formally expressed as a time-dependent advection-diffusion equation, in which the role of time is (roughly) taken by the log of the energy.

Gauge-invariant and non gauge-invariant algorithms for the solution of the classical Yang-Mills equations on a real-time lattice have been implemented and compared, in order to model the early stage of the high energy nuclear collision processes at the Relativistic Heavy Ion Collider at Brookhaven and the Large Hadron Collider at the CERN. The developed algorithms use fast Fourier transforms and a leapfrog scheme. In this early stage, the gluon fields form a set of colored filaments that connect the two colliding objects known as the glasma. At the leading order in the coupling, the glasma is made of purely longitudinal, and boost-invariant, gluon fields. The glasma produced in proton-nucleus (pA) and nucleus-nucleus (AA) collisions has been considered. Focus has been put on a gauge-invariant formulation of the problem on the lattice, which results in the most efficient way to implement the evolution of strong gluon fields produced in the pre-equilibrium stage.
A realistic initialization for both AA and pA collisions has been implemented. This new initialization takes into account event-by-event fluctuations, both for the distribution of the color charges in the configuration space at the initial time, that are the sources of the glasma

fields, and of the next-to-leading order corrections to the glasma that lead at the breaking of the longitudinal boost invariance.
The gauge-invariant formulation has then been coupled to the evolution of heavy quarks (HQs), charm and beauty, in the pre-equilibrium stage. The dynamics of the HQs in this stage has been modeled via relativistic kinetic equations, and solved on the lattice in a gauge-invariant fashion developing algorithms based on Runge-Kutta methods. As a preliminary problem, the large-mass limit has been considered, in which HQs are frozen in the configuration space, and their dynamics can be computed by analyzing the time-correlators of the gluon fields. The gauge-invariant formulation of the problem has proven to be suitable for parallelization and implementation on GPUs.

A1.2 - deconvolution

For these tasks, we have obtained results 8-10.

Artificial intelligence (AI) methods, particularly neural networks, have been applied to the reconstruction of spectral functions in Quantum Chromodynamics (QCD). The reconstruction of spectral functions is a fundamental problem in QCD, as it provides insight into the dynamics of strongly interacting particles [7-8]. However, the problem is made challenging by the inherent difficulty in inverting the mathematical relations involved, particularly in the presence of noise. Several types of AI-based models have been developed and tests, including:
1. Feedforward Neural Networks (FNNs): basic neural networks with fully connected layers, trained to predict the spectral function from input data.
2. Convolutional Neural Networks (CNNs): networks designed to capture local structures in the input data, potentially enhancing the model's ability to handle noisy data.
3. Deep Learning Architectures: more complex neural networks with multiple hidden layers, capable of learning hierarchical features and representations from the input data.

Extensive experimentation with diverse neural network models has demonstrated that model complexity, as measured by the number of parameters, is not a definitive predictor of performance, with architecture playing a definitely crucial role. This observation has initiated a preliminary analysis, which will be further developed in the next period, aimed at identifying models that balance accuracy with computational efficiency, that are thus not only effective but also energy-efficient. This effort is particularly focused on minimizing environmental impact by reducing the models’ carbon footprint.

References

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