UNIVERSITY OF SÃO PAULO

INSTITUTE OF PHYSICS
Campus Butantã, São Paulo

Master's Project

Study of the effect of correlated experimental uncertainty on Bayesian Inference of quark–gluon plasma properties

Proponent

NARA ÁVILA MORAES

Advisor

Prof. Dr. Matthew William Luzum

To

GRADUATE STUDIES COMMITTEE - CPG/IFUSP
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Nara Ávila Moraes
Bch. Computer Engineer

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General Information about the Project

Title:

Study of the effect of correlated experimental uncertainty on Bayesian Inference of quark–gluon plasma properties

Researcher in charge:

Nara Ávila Moraes, Bch. Computer Engineer

Advisor:

Prof. Dr. Matthew William Luzum

Host institution:

Institute of Physics
at the University of São Paulo

Major Area of Physics and Subareas:

High Energy Physics, Nuclear Physics

Project proposed term:

Jun 1, 2025 to May 31, 2027

Informações Gerais do Projeto

Título:

Estudo do efeito das incertezas experimentais correlacionadas na inferência bayesiana das propriedades do plasma de quarks e glúons

Pesquisador responsável:

Nara Ávila Moraes, Bch. Eng. Computação

Orientação:

Prof. Dr. Matthew William Luzum

Instituição sede:

Instituto de Física
Universidade de São Paulo

Grande Área da Física e Sub Áreas:

Física de Altas Energias, Física Nuclear

Período de vigência proposto:

1 de Junho de 2025 a 31 de Maio de 2027

Abstract

In nuclear theory, the characterization of transport parameters and phase transition properties of a new state of matter — the quark–gluon plasma (QGP), believed to have existed only in the earliest moments after the Big Bang — has been a central objective of scientists since the 1980s, when the development of quantum chromodynamics (QCD) predicted its existence. Since then, scientists have sought to reproduce the conditions necessary for its formation in large heavy-ion collision facilities, such as the LHC and RHIC. According to QCD, a smooth transition is expected to occur at energy densities of $1\,\mathrm{GeV/fm^3}$. More recent experiments reach center-of-mass energies of up to $5.2\,\mathrm{TeV}$, sufficient to produce the conditions required for QGP formation. This state is estimated to last on the order of $10^{-23}\,\mathrm{s}$, and therefore analyses of particle collision detector data can only probe properties of the matter after hadronization. The extraction of the physical parameters of the QGP is performed through the model-to-data comparison methodology, in which simulations of heavy-ion collisions are confronted with measured observables. Recent studies have achieved precise estimates of parameters such as the shear viscosity η/s using Bayesian inference, combined with Gaussian process emulators to efficiently explore the model parameter space. This approach accounts for multiple sources of uncertainty, including statistical and systematic uncertainties in the experimental data, uncertainties associated with the physical model and the emulation process, as well as correlations between different experimental observables. However, the correlation structure of these uncertainties has often been treated in a simplified manner, typically assuming independence between bins or employing limited approximations. In this work, we propose a systematic analysis of the impact of correlations in experimental uncertainties on the Bayesian inference of QGP parameters. In particular, we investigate how different structures of the covariance matrix of observables — including correlations between adjacent bins, global systematic effects, and varying correlation lengths — affect the shape of the posterior distribution, the width of marginal parameter distributions, and the correlation structure among them, with the aim of achieving a more robust and accurate characterization of the properties of the quark–gluon plasma.

Keywords: Quark-Gluon Plasma, Heavy-Ion Collisions, Bayesian Inference, Gaussian Processes, Correlated Experimental Uncertainties.

Resumo

Em teoria nuclear, a caracterização de parametros de transporte e transição de fase de um novo estado da matéria, o plasma de quarks e gluons, suposto existir apenas nos primeiros momentos após o Big Bang, tem sido objetivo de cientistas desde a década de 80, quando o desenvolvimento da teoria quantum chromodynamics previu a sua existencia. Desde então cientistas tentam reproduzir as condições para sua formação em grandes laboratórios de colisão de íons, como LHC e RHIC. De acordo com a teoria QCD uma transição suave ocorreria a densidades de $1GeV/fm^3$. Experimentos mais recentes alcançam energias de até $5,2TeV$, suficientes para a formação do QGP. Estima-se que este estado tenha duração de $10^{-23}s$, e por isso análises de dados dos detectores de colisões de partículas podem apenas analisar caracteristicas da matéria após a hadronização. A extração dos parâmetros físicos do QGP é realizada através da metodologia de comparação entre modelo e dados experimentais (*model-to-data comparison*), na qual simulações de colisões são confrontadas com observáveis medidos. Trabalhos recentes alcançaram estimativas precisas de parâmetros como a viscosidade de cisalhamento η/s utilizando inferência Bayesiana, combinada com emuladores baseados em processos gaussianos para explorar eficientemente o espaço de parâmetros do modelo. Essa abordagem leva em consideração diversas fontes de incerteza, incluindo incertezas estatísticas e sistemáticas dos dados experimentais, incertezas associadas ao modelo físico e ao processo de emulação, bem como correlações entre diferentes observáveis experimentais. Entretanto, a estrutura de correlação dessas incertezas até então tem sido tratadas de forma simplificada, assumindo independência entre bins ou utilizando aproximações limitadas. Neste trabalho, propõe-se uma análise sistemática do impacto das correlações nas incertezas dos dados experimentais sobre a inferência Bayesiana dos parâmetros do QGP. Em particular, investigamos como diferentes estruturas para a matriz de covariância dos observáveis — incluindo correlações entre bins adjacentes, efeitos sistemáticos globais e diferentes comprimentos de correlação — afetam a forma da distribuição a posteriori, a largura das distribuições marginais dos parâmetros e a estrutura de correlação entre eles, com o objetivo de obter uma caracterização mais robusta e acurada das propriedades do plasma de quarks e glúons.

Palavras-chave: Plasma de Quarks e Glúons, Colisões de Íons Pesados, Inferência Bayesiana, Processos Gaussianos, Incertezas Experimentais Correlacionadas.

Contents

1 Introduction

As a result of a heavy-ion collision research program initiated at CERN in the 1980s, aimed at studying matter at high densities and temperatures, the first experimental evidence for the production—within particle accelerator experiments—of a state of matter previously predicted to exist only in the earliest moments after the Big Bang was announced in 2000: the quark–gluon plasma (QGP) (Ulrich Heinz, 2000). Since the earliest theoretical proposals, heavy-ion collisions have been identified as a viable experimental approach to achieve the energy densities required for QGP formation. In that same year, the Relativistic Heavy Ion Collider (RHIC) in the United States was inaugurated, featuring the STAR, PHENIX, PHOBOS, and BRAHMS detectors. A few years later, the Large Hadron Collider (LHC)—the largest accelerator dedicated to hadron collisions—began operations at CERN, with the ALICE detector specifically designed for heavy-ion physics. The study of heavy-ion collisions, in conjunction with theoretical models, remains to this day the primary tool for investigating the quark–gluon plasma.

Heavy-ion collision experiments reach some of the highest temperatures and energy densities achieved in later stages of the Universe's evolution—exceeding, for example, those of any currently known astrophysical object. Lattice QCD calculations estimate that the QGP is formed at energy densities on the order of $1\,\text{GeV/fm}^3$. Such conditions were initially achieved in lead–lead collisions, but today the QGP is also studied in collisions involving lighter systems such as gold (Nagle; Zajc, 2018), and more recently oxygen (Behera *et al.*, 2022).

In this state, quarks and gluons—which constitute hadrons, the fundamental building blocks of all known matter—become deconfined due to the strong coupling constant decreasing significantly at high temperatures and energy densities, and are therefore expected to exhibit collective fluid-like behavior consistent with a hydrodynamic description. QCD calculations for these temperature regimes indicate that the QGP exists for a timescale on the order of 10^{-23} seconds (Bernhard; Moreland; Bass, 2019). This extremely short lifetime imposes fundamental limitations on the direct observation of QGP properties, requiring indirect inference strategies based on the analysis of final-state observables, such as hadrons, direct photons, and other electromagnetically interacting particles. The final state consists of thousands of produced particles, of which approximately 99% are hadrons.

The observables accessible in heavy-ion collision experiments thus emerge only from the final stage of the system evolution, known as freeze-out. As the system cools to temperatures of approximately $170\,\text{MeV}$, confinement due to the strong interaction becomes dominant again, and quarks and gluons recombine into a dense hadron gas in a process known as hadronization. The newly formed hadrons still overlap for a brief period until the energy density decreases to around $50\,\text{MeV}$, at which point they cease interacting and undergo a collective expansion resembling a small explosion, reaching velocities of about $0.5\,c$ (Ulrich Heinz, 2000). Detectors are then sensitive to the resulting hadronic jets, including the multiplicities of different hadron species—for example K/π, p/π, or Ω/π—which are fixed at the moment of hadronization and provide information about the freeze-out temperature and chemical potential (Tiwari; Singh, 2013).

Among the theoretical predictions whose early experimental observations provided indirect evidence for a deconfined phase are the enhanced production of strange quarks relative to proton–proton collisions—predicted two decades earlier by quantum chromodynamics as a signature of the QGP—as well as a fifteenfold increase in the production of multi-strange hadrons, such as the Ω particle, composed of three strange quarks. Additional signatures include a broader mass spectrum of produced hadrons and the anomalous suppression of charmonium states (J/ψ), consistent with the dissociation of bound states (Ulrich Heinz, 2000).

Subsequently, the experimental scope was significantly expanded with the operation of the Large Hadron Collider (LHC) at CERN, which enabled collisions at much higher center-of-mass energies. This led not only to a substantial increase in the statistical precision of the data but also to an expansion of the accessible set of observables, including more detailed measurements of collective flow and electromagnetic probes. These advances have established the study of the QGP as a mature field within high-energy physics, characterized by extensive datasets and a rich phenomenology.

2 Motivation

In the *model-to-data comparison* stage, the quantitative characterization of the quark–gluon plasma (QGP) produced in relativistic heavy-ion collisions requires inferring model parameters from experimental observables. Bayesian analyses in heavy-ion physics have proven highly effective in constraining QGP properties (Bernhard; Moreland; Bass, 2019).

In this context, model parameters are constrained by statistically comparing theoretical predictions with experimental observables, a strategy employed in frameworks such as JETSCAPE and related analyses (Bernhard, 2018; Ehlers *et al.*, 2026). This comparison is encoded through a likelihood function that depends explicitly on the covariance matrix of experimental uncertainties.

The covariance matrix can be written as (Bernhard, 2018):

$$\Sigma_{ij} = \rho_{ij}\,\sigma_i \sigma_j. \tag{1}$$

where, σ_i are the uncertainties associated with individual observables and ρ_{ij} represents their correlation structure. A limitation arises from the fact that experimental collaborations do not provide the covariance matrix, specially the off-diagonal components encoding correlations between observables. The absence of reported correlation structures requires the introduction of assumed models for ρ_{ij} (Bernhard, 2018).

More recent work further emphasizes this limitation, explicitly stating that only individual uncertainties are typically available, while the full error covariance matrix remains unknown (Ehlers *et al.*, 2026). As a consequence, many analyses adopt a diagonal covariance matrix, effectively assuming independence between observables (Ehlers *et al.*, 2026).

However, it is well established that systematic uncertainties introduce nontrivial correlations across measurements, making this assumption physically incomplete (Ehlers *et al.*, 2026). Furthermore, different prescriptions for the non-diagonal components of the covariance matrix can lead to nontrivial and even counterintuitive effects on the inferred posterior distributions (Ehlers *et al.*, 2026). This observation highlights the sensitivity of Bayesian parameter estimation to the assumed structure of experimental uncertainties, and indicates that the covariance matrix plays an active role in shaping the geometry of the posterior distribution.

3 Objectives

The present work aims to systematically investigate the impact of different covariance structures on Bayesian inference of QGP parameters. By that we expect the following:

1. Recompute posterior distributions from previously published Bayesian analyses - JETSCAPE calibrations from Everett et al. (Everett *et al.*, 2020) and Mankolli et al. (Mankolli; Shen; Luzum, 2026), using identical simulation data and emulator configurations, while varying the assumed covariance matrix;

2. Quantify the impact of covariance assumptions on:

    (i) the width of marginal posterior distributions;

    (ii) the strength and structure of parameter correlations;

    (iii) the emergence or resolution of degeneracies in parameter space;

    (iv) and shifts in the most probable values of QGP transport parameters;

3. Compare baseline analyses (assuming independent uncertainties) with extended covariance models incorporating bin-to-bin correlations and global systematic effects;

4. Develop a methodology to infer covariance structures from synthetic datasets with controlled correlations, such that it can be applyed into Bayesian analyses of heavy-ion collision observables.

4 Methodology

4.1 Bayesian Inference in Heavy-Ion Collisions

Within the Bayesian framework, the goal is to determine the posterior distribution of the model parameters θ, conditioned on the experimental data y_{exp}. This is achieved via Bayes' theorem (Bernhard, 2018):

$$P(\theta \mid y) \propto P(y \mid \theta)\, P(\theta), \tag{2}$$

where $P(\theta)$ represents prior knowledge about the parameters, and $P(y \mid \theta)$ is the likelihood function, which quantifies the agreement between model predictions and experimental data.

The likelihood function is constructed as:

$$\mathcal{L}(\theta) \propto \exp\left[-\frac{1}{2}\left(y_{\text{exp}} - y_{\text{model}}(\theta)\right)^T \Sigma^{-1} \left(y_{\text{exp}} - y_{\text{model}}(\theta)\right)\right], \tag{3}$$

where Σ is the covariance matrix encoding the uncertainties associated with the experimental data.

Sources of uncertainty include experimental uncertainties, model uncertainties, and correlations between parameters (Bernhard, 2018). The posterior distribution provides estimates of the parameters while also quantifying their uncertainties and correlations.

Gaussian process emulators enable interpolation of model predictions across the parameter space, making it feasible to efficiently explore the posterior distribution using Markov Chain Monte Carlo (MCMC) methods.

Marginal distributions for each parameter are obtained by integrating over the remaining parameters, allowing the determination of credible intervals.

4.2 Gaussian Processes

A Gaussian Process (GP) is a collection of random variables such that any finite subset follows a multivariate Gaussian distribution (Rasmussen; Williams, 2008). It is fully specified by a mean function and a covariance function:

$$m(\mathbf{x}) = \mathbb{E}[f(\mathbf{x})], \tag{4}$$

$$k(\mathbf{x}, \mathbf{x}') = \mathbb{E}\Big[(f(\mathbf{x}) - m(\mathbf{x}))(f(\mathbf{x}') - m(\mathbf{x}'))\Big], \tag{5}$$

so that:

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')). \tag{6}$$

Within this work, Gaussian processes are employed as statistical emulators of the underlying physical model, enabling the interpolation of observables across the parameter space with a well-defined quantification of predictive uncertainty. Owing to their intrinsic multivariate Gaussian formulation, they also provide a principled framework for modeling and characterizing correlations among observables through their covariance structure.

This latter aspect is particularly relevant for the present study, where the inference of covariance structures and their impact on Bayesian parameter estimation are central objectives.

5 Expected Results

This work is expected to deliver a systematic quantitative and qualitative analysis of the impact of experimental covariance structures on Bayesian inference of quark–gluon plasma (QGP) transport parameters in relativistic heavy-ion collisions, presenting the following:

1. **Quantitative analysis:**

   (i) Controlled reanalyses of previously published Bayesian studies (e.g., JETSCAPE calibrations), in which posterior distributions are recomputed using identical simulation data and emulator configurations, while varying the assumed covariance matrix;

   (ii) Quantification of how different covariance assumptions affect:

   (a) the width of marginal posterior distributions, reflecting changes in uncertainty quantification;

   (b) the strength and structure of correlations between inferred parameters;

   (c) shifts in the most probable values of QGP transport coefficients;

   (iii) Systematic comparison between baseline configurations, typically assuming uncorrelated uncertainties, and extended covariance models incorporating bin-to-bin correlations and global systematic effects;

2. **Qualitative analysis:**

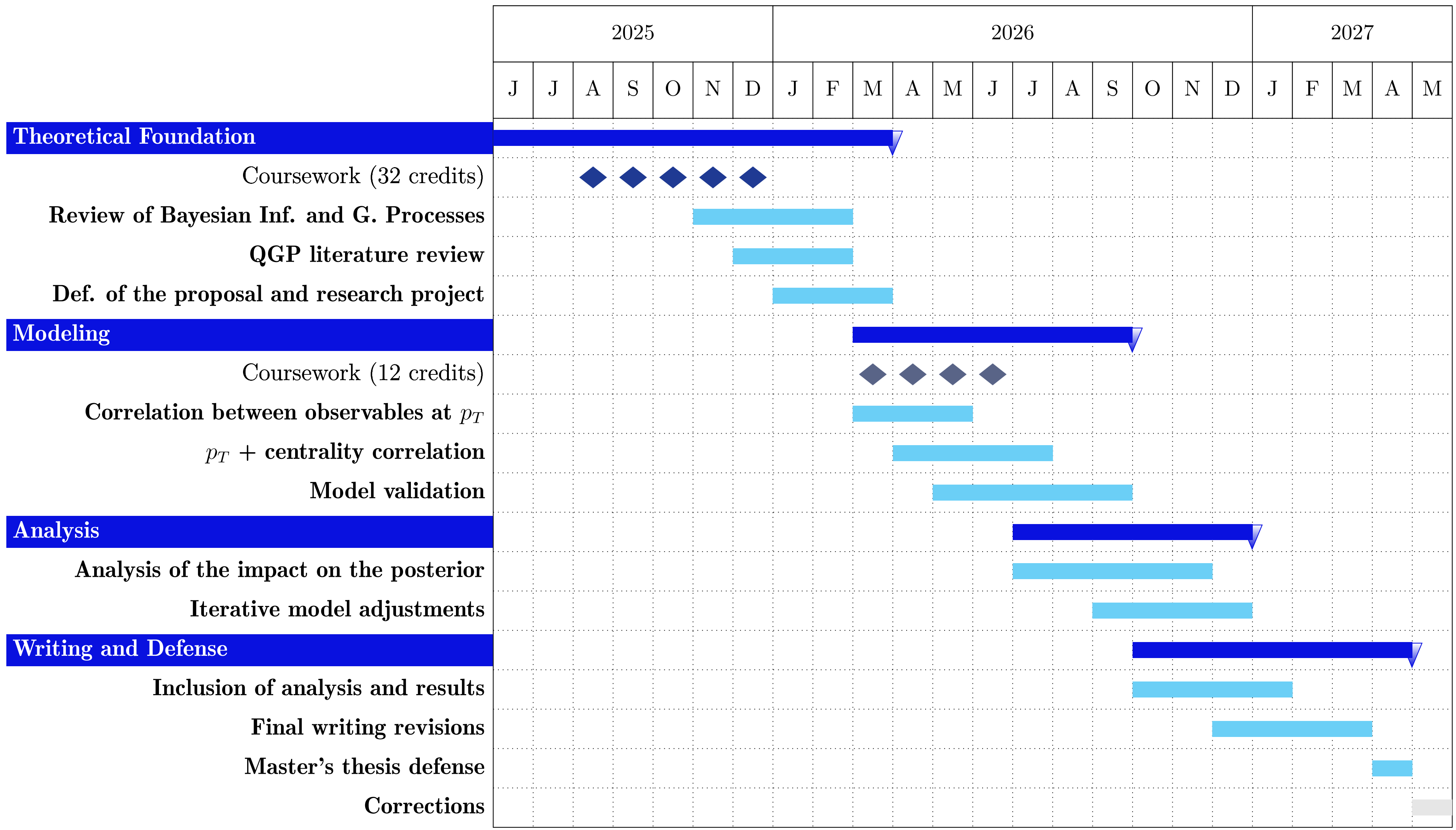
   (i) Interpretation of the quantitative results to assess the relevance of experimental correlations in Bayesian parameter inference;

   (ii) Identification of regimes in which covariance assumptions significantly affect the inferred QGP properties, versus regimes in which their impact is negligible.

In addition, the project is expected to establish and validate a methodology to infer aspects of the experimental covariance structure using synthetic datasets with controlled correlations, and to apply this methodology within the quantitative analysis.

Overall, the results are expected to clarify the role of covariance modeling in shaping posterior distributions and to assess the extent to which neglecting correlations may affect the inferred properties of the QGP.

6 Timeline



2025
2026
2027
J J A S O N D J F M A M J J A S O N D J F M A M
Theoretical Foundation
Coursework (32 credits)
Review of Bayesian Inf. and G. Processes
QGP literature review
Def. of the proposal and research project
Modeling
Coursework (12 credits)
Correlation between observables at p_T
p_T + centrality correlation
Model validation
Analysis
Analysis of the impact on the posterior
Iterative model adjustments
Writing and Defense
Inclusion of analysis and results
Final writing revisions
Master's thesis defense
Corrections

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