

Pre-equilibrium evolution effects on relativistic heavy-ion
collision observables

Dissertation

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Jia Liu, B.S.

Graduate Program in Physics

The Ohio State University

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Dissertation Committee:

Professor Ulrich Heinz, Advisor

Professor Michael Lisa

Professor Robert Perry

Professor Junko Shigemitsu

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Abstract

In this thesis, we improve several aspects of the standard model of relativistic heavy-ion collisions. We include a pre-equilibrium dynamical stage and study it in the strong and weak coupling limits. We stress the importance of this stage on the later hydrodynamic evolution as well as on the mean transverse momenta, transverse momentum distributions and anisotropic flow coefficients of directly emitted hadrons. In order to properly address the bulk viscosity, we update the hydrodynamic equations within the boost-invariant viscous hydrodynamic simulation program VISH2+1 to a more complete set of equations that includes non-linear terms related to the shear stress tensor and bulk pressure. The importance of each non-linear term is discussed.

With the understanding that the effects of tunable parameters in the heavy-ion simulation model on physical observables are entangled, we optimize them simultaneously. We perform such optimizations for Pb + Pb collisions at the Large Hadron Collider (LHC) for both Monte Carlo Kharzeev-Levin-Nardi (MC-KLN) and Monte Carlo Glauber (MC-Glb) initial-state models. In a first stage we test the parameter optimization routine with zero bulk viscosity and without the hadronic after-burner. This sets the baseline for subsequent searches including the hadronic after-burner and a non-zero bulk viscosity. We report the preferred parameter ranges and compare them across different initial-state models, with and without pre-equilibrium dynamics. The parameter space for the runs with hadronic after-burner is further explored

within a Bayesian approach. Using a Markov Chain Monte Carlo routine we determine the posterior probability distribution of each parameter and assign quantitative uncertainty ranges to them.

To my parents

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Vita

September 2004 - June 2008 Bachelor of Science in physics,
Central China Normal University
September 2011 - Present Graduate Supplement Fellow, Research
Associate
Art and Science College
The Ohio State University

Publications

Research Publications

J. Liu, C. Shen and U. W. Heinz, “*Pre-equilibrium evolution effects on heavy-ion collision observables*’, Phys. Rev. C **91**, no. 6, 064906 (2015)

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Major Field: Physics

Studies in relativistic heavy-ion collisions: Professor Ulrich Heinz

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Chapter 1: Introduction

1.1 Relativistic heavy-ion collisions

It has been a long history for mankind to reveal the building blocks of matter. The ancient Greek philosophers suggested that matter is built from atoms, individual particles that cannot be divided further. Support for this theory came after two thousand years with John Dalton's view on chemical reaction and the observation of Brownian motion. But the indivisible property of atoms was overthrown early in the twentieth century by the collision experiments conducted by Rutherford and his collaborators, who pointed out that atoms have internal structure. Ever since, collision experiments have become an indispensable tool to study atomic and subatomic physics, where the human eye and optical and electronic microscopes cannot reach. After identifying the proton and neutrons as the building blocks for the nucleus, together with the discovery of a large number of additional unstable particles (collectively called hadrons) from radioactive decays and in cosmic rays colliding with atmospheric molecules, people were wondering if even these hadrons have internal structure. The quark model, independently proposed by M. Gell-Mann [1] and G. Zweig [2, 3], pointed out that hadrons consist of quarks, with gluons as carriers of the strong force acting between them [4]. This theory successfully explains the experimental results of deep inelastic

scattering between high energy electrons and protons [5]. The dynamics between quarks and gluons are described by the non-abelian gauge theory Quantum Chromodynamics (QCD), which states that the interactions between quarks and gluons are different than all other kinds of interactions. The potential between quarks increases linearly when their distance becomes large, preventing the possibility to isolate a quark from other quarks; on the other hand, the effective coupling constant describing the potential at short distance becomes small. This is the so-called “asymptotic freedom” [6, 7]. Therefore, quarks are confined in hadrons and only free at extremely high energy and temperature.

Quarks, if deconfined, together with gluons form a state of matter which, when it reaches a state of thermodynamic equilibrium, is called quark-gluon plasma (QGP). This exotic state of matter existed for a few microseconds in the early universe, and a low temperature form of it may still exist in the core of neutron stars. Lattice QCD suggests that, at zero net baryon number density, this deconfinement can happen when the system reaches the hadronic matter - QGP phase transition temperature of about 155 MeV [8, 9], corresponding to several trillion Kelvin. Experimentalists strive to reach this temperature in the lab by conducting relativistic heavy-ion collision experiments, in which atoms with high atom numbers are fully ionized, accelerated to nearly the speed of light, and led to collide with each other. Such collision experiments started in the late 1970s at Lawrence Berkeley National Laboratory [10], where the maximum center of mass energy per nucleon was $\sqrt{s_{NN}} \approx 1 - 2$ GeV. With time experimentalists kept increasing the collision energy in order to find signatures of the deconfinement. Although tantalizing hints were seen in Pb + Pb collision at

$\sqrt{s_{NN}}=17$ GeV at the CERN SPS [11], it was not until the Relativistic Heavy-ion Collider (RHIC) in Brookhaven National Laboratory (BNL) started Au + Au collisions with $\sqrt{s_{NN}} = 200$ GeV, creating temperatures of about 2 times the phase transition temperature, that unambiguous signals of the QGP were observed [12–14], including strong collective flow, strangeness enhancement and jet quenching. The RHIC data also suggested that, contrary to most scientists' expectations, the QGP behaves like a strongly coupled liquid with nearly zero viscosity, and not as a weakly coupled quark-gluon gas. The experimentally observed hadron spectra and elliptic flow were very well (although not perfectly) described by the ideal relativistic hydrodynamics calculations [15, 16]. Quantitatively, however, ideal hydrodynamics disagrees with some of the experimental observables (especially with the elliptic flow data) at the level of 20% - 30%, indicating that the QGP is close to but not perfectly in local thermal equilibrium. Deviations from local equilibrium, driven by the rapid dynamical evolution of the QGP fireball created in the collision, manifest themselves in viscous corrections to the ideal fluid behavior. Pinning down the shear and bulk viscosity of the QGP has since then drawn a lot of attention. Starting in 2010, the Large Hadron Collider (LHC) has increased the maximum available collision energies by another factor of 25. Pb + Pb collisions were studied 2010 - 2012 at $\sqrt{s_{NN}} = 2760$ GeV, with initial temperatures estimated close to 3 times the transition temperature, while RHIC continues to operate at collision energies between $\sqrt{s_{NN}} = 5$ GeV and 200 GeV. The two combined programs enable a detailed study of the properties of QGP. With RHIC and LHC data and recent theoretical developments in viscous hydrodynamic simulations, huge progress has been made in the past decade. The clarification of a few remaining uncertainties and the desire to arrive at a quantitatively precise,

complete understanding of QGP dynamics drive the experimental programs at RHIC and LHC for the coming decade [17].

1.2 Evolution stages of relativistic heavy-ion collisions

As shown in Fig. 1.1, relativistic heavy-ion collisions have three evolution stages, associated with characteristic time scales. In this section we give a brief introduction to these stages. Different theoretical frameworks are used to describe different stages because each stage is controlled by different physics and described by different effective degrees of freedom that come with different theoretical disciplines. These different theoretical approaches have limited regions of validity and thus must be studied together in order to arrive at a complete dynamical framework, known as the “standard model of the Little Bang” [19].

The first stage is the pre-equilibrium stage which ranges from the first impact at $\tau = 0^+$ fm/ c to $\tau \lesssim 1$ fm/ c . During this stage the system evolves from a locally highly anisotropic state towards a state of approximate local thermal equilibrium. The central issue is how such a short local thermal equilibration time is achieved. During this stage the system is characterized by a very high energy density near mid-rapidity which is dominated by small- x gluons with a large occupation number (of the order of $\frac{1}{\alpha} \gtrsim 1$). The large gluon occupation number allows the system to be described by classical SU(3) Yang-Mills theory [20, 21], supplemented by quantum corrections [22]. However, a purely classical mean field theory does not lead to thermalization. Significant amount of work has been done to elucidate the role of quantum corrections in the equilibration process [23–30]. However, these studies have not yet fully explained the rapid thermalization; faced with poor knowledge of the pre-equilibrium

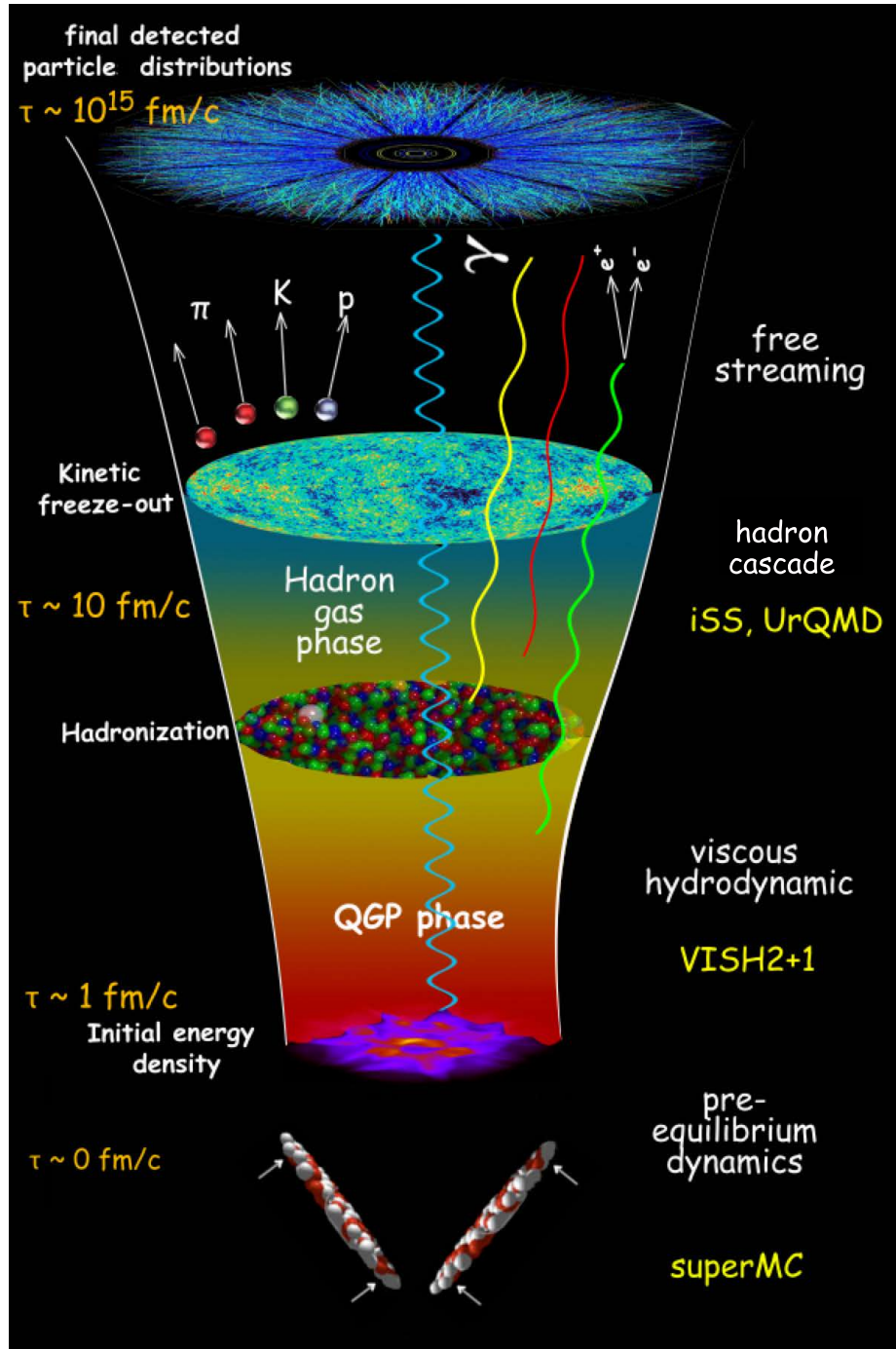


Figure 1.1: A sketch of the time line (left side) and a list of the corresponding simulation codes (right side) for a relativistic heavy-ion collision. This plot was created by Chun Shen and is taken from Ref. [18].

stage, most researchers therefore ignored this stage in the numerical simulations of heavy-ion collisions. To change this is one of the primary goals of this thesis.

After the matter has thermalized, the system expands in response to large pressure gradients. This stage can be described by relativistic hydrodynamics. Hydrodynamics solves for the time evolution of macroscopic quantities, such as the energy density, pressure, and temperature, instead of following individual particles microscopically. The validity of hydrodynamics relies only on whether the system is in or near local thermal equilibrium, not on the details of the microscopic structure of the fluid (it does not even need to consist of particles and can be a complicated state of quantum fields). The assumption of local thermal equilibrium is justified if the mean free path (or the mean microscopic interaction time) in the hydrodynamic stage is much smaller than any macroscopic length or time scale associated with the expansion of fireball. If we ignore any deviation from local equilibrium and thus assume the system is able to restore local equilibrium instantaneously after any perturbation, we can describe the matter evolution by ideal hydrodynamics. This ideal theory can qualitatively explain the flow observed in RHIC experiments [15, 16]. However, ideal hydrodynamics, which is the zeroth order of an expansion around local thermal equilibrium, does not take into account any deviations from local equilibrium; it also fails to explain the experimental data quantitatively, especially at high transverse momenta or in peripheral collisions [31]. In order to account for these deviations one needs a hydrodynamic theory which properly includes the viscous effects induced by such deviations. A viscous hydrodynamic framework containing only the first order of gradients of the hydrodynamic flow velocity and temperature, the Navier-Stokes

theory [32, 33], is not practical because it violates causality [34, 35]. The heavy-ion community therefore adopted a second-order viscous hydrodynamic approach to describe the QGP evolution. This framework was first proposed by Müller [36] and Israel and Stewart [37] and further developed in the recent decade [38–43]. This formalism includes second order derivatives of the gradients of thermal quantities to account for the deviation from the local thermal equilibrium, and restores causality by taking into account the non-zero microscopic relaxation time which characterizes the time the system needs to restore equilibrium. Nowadays, viscous hydrodynamics serves as a crucial component of any quantitative description of QGP evolution.

Partons hadronize when the system reaches the transition temperature $T_c \sim 155$ MeV [9] after about 10 fm/ c (depending on collision centrality). After hadronization, elastic collisions between hadrons are still on-going for some period (lasting a few additional fm/ c). Except for occasional baryon - antibaryon annihilation processes, inelastic collisions cease almost immediately after hadronization, and the chemical composition of the hadronic system is frozen out, reflecting the quark - hadron transition temperature [44, 45]. Subsequent quasi-elastic collisions, mostly proceeding through short-lived resonances, continue to cool the hadron gas and build additional radial flow. As the hadrons move farther away from each other and the interactions become weaker, the elastic and quasi-elastic collisions finally stop and the hadrons undergo the kinetic freeze-out, after which they stream freely to the detectors. During the hadronic stage, the mean free path between hadrons becomes so large that local thermal equilibrium can no longer be well-maintained. So one can cast doubt on the validity of hydrodynamics during this stage. Still, many studies continue to use hydrodynamics until the kinetic freeze-out. A more robust approach, applied in

many recent works and also in the last part of this thesis, switches at $T \approx 155$ MeV to a microscopic description in terms of individually colliding hadrons and resonances.

1.3 Numerical simulation of relativistic heavy-ion collisions

In this thesis, the iEBE-VISHNU package [18], developed in Prof. Heinz's group at The Ohio State University, is employed to simulate the evolution of heavy-ion collisions. iEBE-VISHNU (<http://u.osu.edu/vishnu/>) is a comprehensive open source relativistic heavy-ion collision simulation program. The rightmost column of Fig. 1.1 shows its components for each of the stages of a heavy-ion collision. In this section, we give a brief introduction to the iEBE-VISHNU package, and also mention a few other commonly used numerical codes for heavy-ion collisions.

The initial conditions are generated by the code **superMC**. This code gives the entropy (or energy) density distribution in the transverse plane at the beginning of the hydrodynamic evolution, using the Monte Carlo Kharzeev-Levin-Nardi (MC-KLN) [46–48] or Monte Carlo Glauber (MC-Glb) [49] models (This part of the code will be supplemented in this thesis by a pre-equilibrium evolution model which accounts for the evolution of the collision zone between the time of nuclear impact and the beginning of the hydrodynamic stage). Both models sample positions of nucleons from a Woods-Saxon distribution for the colliding nuclei and project them on the transverse plane. This is justified by the fact that the nuclei are highly Lorentz contracted along the beam direction. In the version of **superMC** used in this thesis, a collision between two nucleons happens if their distance is smaller than a threshold value calculated from the inelastic nucleon - nucleon collision cross-section [50]. In the MC-Glb model the entropy generated from any nucleon collision is assumed to

have a cylindrical shape with a gaussian profile in the transverse plane, centered in the middle of a binary collision or at the center of the so called wounded nucleons of the two participating nuclei. The final entropy density profile is parameterized as a linear combination of entropies from wounded nucleons and binary collisions, with a mixing parameter adjusted to describe the measured centrality dependence of particle production.

MC-KLN is a saturation physics inspired model. It models produced gluons through the fusion of two colliding gluons from the incoming heavy nuclei, and calculates the gluon density distribution within the k_T -factorization approach [48]. The resulting gluon distribution depends on the gluon saturation scale, which in turn depends on the thickness function of the nuclei, which is calculated from the densities of the wounded nucleons. Moreover, the MC-KLN model predicts the initial parton momentum distribution, which makes it useful for a detailed study of the pre-equilibrium phase-space evolution. The MC-Glb model makes no prediction for that distribution. There are other codes that can provide initial conditions, such as HIJING [51], NeXuS [52], AMPT [53–55], GLISSANDO [56], EPOS [57, 58], IP-Glassma [59, 60], Trento [61], etc., which we mention here only for completeness.

Pre-equilibrium dynamics has long been ignored in the heavy-ion collisions because of the lack of a model which can properly thermalize the post collision system. In order to explore the possible importance of this stage, we here include (for the first time) the pre-equilibrium dynamics, using an extreme simplification: we treat the pre-equilibrium as free-streaming partons. The motivation for doing so will be explained in Chapter 2. The free-streaming stage is implemented into the iEBE-VISHNU code package as a module called **fs**. **fs** solves the collisionless Boltzmann equation for the

early phase-space distribution analytically, allowing for the calculation of the energy momentum tensor at any point and any time, if the initial parton configuration in phase-space is given at an initial parton formation time τ_0 . In our study, we stop the pre-equilibrium evolution at a longitudinal proper “switching time” τ_s , when the system switches from the pre-equilibrium stage to the hydrodynamic stage. (You can also think of τ_s as the “starting” time for the subsequent hydrodynamic evolution.) **fs** contains a general interface that converts the energy momentum tensor resulting from pre-equilibrium evolution to the initial conditions required by the hydrodynamic code. We note that this stage has also been alternatively modeled by colliding shock waves in anti-de Sitter space [62], using the code available in [63]. This approach implements the opposite assumption of ours, namely that the pre-equilibrium is coupled infinitely strongly, rather than not at all. Reality is expected to lie between these two approaches.

The hydrodynamic stage is simulated by **VISHNew**. **VISHNew** is a more robust version of **VISH2+1**, originally developed by H. Song [64] and recently improved by Chun Shen and Zhi Qiu [18]. It is a longitudinally boost-invariant (2+1)D viscous hydrodynamic simulation program, which solves the 2nd order Israel-Stewart equations [40, 65]. This program employs the UPSHASTA algorithm [66] to solve the evolution equations, with the advantage of effectively reducing shock instabilities. Given the initial entropy/energy density in the transverse plane, it outputs the energy momentum tensor on the freeze-out surface (current implementation defines the freeze-out surface as a hypersurface of constant energy density). There are other hydrodynamic codes, such as the (2+1)D viscous code VH2+1 [67], the (3+1)D

ideal hydrodynamic code NeXSPheRIO [68], the (3+1)D viscous hydrodynamic code MUSIC [69, 70], as well as several others.

The hadronization process is taken care of by the code **iS**, which implements the Cooper-Frye algorithm [71]. With the energy momentum tensor on the freeze-out surface output by the hydrodynamic code, it gives the directly emitted hadron spectra and flow anisotropy coefficients. These directly emitted particles are still in an (approximately) thermal distribution, so they are often called thermal particles. Decay of unstable heavy resonances is implemented in the code **resonance8**. After the decays, the code **iInteSp** recalculates the final stable particle spectra and their anisotropic flow coefficients, by adding the contributions from resonance decay products to the thermal stable particles.

If one assumes that hydrodynamics is still valid during the hadronic stage and runs it all the way down to kinetic freeze-out, we call this the “pure hydro” run mode. A more realistic approach employs a hadronic after-burner after hadronization. This run mode is called “hybrid” [72], because this type of simulation couples macroscopic hydrodynamics with a microscopic hadron cascade. The iEBE-VISHNU package uses **UrQMD** (The Ultrarelativistic Quantum Molecular Dynamics model) [73, 74] as the hadronic after-burner. There are other hadronic cascade codes available, for example B3D [75]. In order to connect the hydrodynamic code and the hadron cascade code, the iEBE-VISHNU package provides the particle sampling code **iSS** for Monte-Carlo sampling the hadrons from the freeze-out surface, using the Cooper-Frye distribution as weight. These sampled particles are then fed into **UrQMD** for further hadronic evolution. Both pure hydro and hybrid run modes are supported by the

iEBE-VISHNU package. A list of other hybrid simulation programs can be found in [18, 76].

After the end of the hadronic stage, the particles need to be captured and processed to generate final observables. In the iEBE-VISHNU package, **EbeCollector** serves the role of detector: it collects and stores the hadron information for further processing. **binUtilities** calculates the final observables such as hadron spectra and anisotropic flow coefficients. While these Python scripts are light-weight and convenient to use, they are rather slow when dealing with large numbers of events ($\sim \mathcal{O}(10^6)$). Alternatively, one can use C++ written tools to collect and process **UrQMD** data [77] if speed is important.

1.4 Conventions and Notations

In this thesis, we employ natural units $\hbar = k_B = c = 1$. The metric for Cartesian coordinates (t, x, y, z) is $g^{\mu\nu} = \text{diag}(1, -1, -1, -1)$. We also use Milne coordinates (τ, x, y, η_s) , where $\tau = \sqrt{t^2 - z^2}$ is the proper time and $\eta_s = \frac{1}{2} \ln[(t+z)/(t-z)]$ is the space-time rapidity. The metric for this coordinate system is

$$g^{\mu\nu} = \text{diag}(1, -1, -1, -1/\tau^2), \quad (1.1)$$

$$g_{\mu\nu} = \text{diag}(1, -1, -1, -\tau^2). \quad (1.2)$$

In this curvilinear space, the partial derivatives in Cartesian coordinate need to be replaced by covariant derivatives:

$$\partial_\mu A^\nu \rightarrow d_\mu A^\nu = \partial_\mu A^\nu + \Gamma_{\mu\rho}^\nu A^\rho, \quad (1.3)$$

$$\partial_\mu B^{\nu\lambda} \rightarrow d_\mu B^{\nu\lambda} = \partial_\mu B^{\nu\lambda} + \Gamma_{\mu\rho}^\nu B^{\rho\lambda} + B^{\nu\rho} \Gamma_{\rho\mu}^\lambda, \quad (1.4)$$

where $\Gamma_{\mu\rho}^{\nu} = \frac{1}{2}g^{\nu\sigma}(\partial_{\mu}g_{\rho\sigma} + \partial_{\rho}g_{\sigma\mu} - \partial_{\sigma}g_{\mu\rho})$ are the Christoffel symbols, whose non-zero components in Milne coordinates are

$$\Gamma_{\eta\tau}^{\eta} = \Gamma_{\tau\eta}^{\eta} = \frac{1}{\tau}, \quad (1.5)$$

$$\Gamma_{\eta\eta}^{\tau} = \tau. \quad (1.6)$$

The fluid 4-velocity is normalized as $u^{\mu}u_{\mu} = 1$. We define the projection operator $\Delta^{\mu\nu} \equiv g^{\mu\nu} - u^{\mu}u^{\nu}$, which is orthogonal to the fluid velocity u^{μ} and thus projection on the spatial direction is the fluid rest frame. Partial derivative can be decomposed into “transverse” and “longitudinal” components:

$$\partial^{\mu} = \nabla^{\mu} + u^{\mu}D. \quad (1.7)$$

The transverse component, given by the first term on the right hand side, is

$$\nabla^{\mu} = \Delta^{\mu\nu}\partial_{\nu}, \quad (1.8)$$

and it is orthogonal to u^{μ} ; it represents the spatial gradient in the local rest frame and express it covariantly. The longitudinal component $D = u^{\mu}\partial_{\mu}$ is the covariant expression for the time derivation in the local rest frame.

We also define the double projection operator

$$\Delta_{\alpha\beta}^{\mu\nu} \equiv \frac{1}{2}(\Delta_{\alpha}^{\mu}\Delta_{\beta}^{\nu} + \Delta_{\beta}^{\mu}\Delta_{\alpha}^{\nu}) - \frac{1}{3}\Delta^{\mu\nu}\Delta_{\alpha\beta}, \quad (1.9)$$

which can project any rank-2 Lorentz tensor onto its transverse (to u^{μ}) and traceless part.

1.5 Outline

In this thesis, we improve several aspects of the phenomenological description of heavy-ion collisions. We discuss the effects and consequences brought by non-linear terms in the hydrodynamic equation. In Chapter 2, we include a dynamic

pre-equilibrium in the evolution model for heavy-ion collisions. We discuss the importance of this initial stage evolution to the subsequent hydrodynamic evolution and the final observed hadron mean transverse momentum and anisotropic flow coefficients. Moreover, we also explore different methods to constrain the length of the pre-equilibrium stage. In Chapter 3, we complete the hydrodynamic evolution equations by including the non-linear terms derived from the kinetic theory, and analyze the importance of each newly added term. The effect of bulk viscosity is stressed in this chapter. In Chapter 4, we optimize the free parameters in our model by implementing a parameter search, and further explore the parameter space to study the distribution of each parameter. After optimizing the model parameters, we utilize these optimal parameters found in Chapter 4 to resolve the elliptic flow mass-ordering problem. Our findings are summarized in Chapter 5.

Chapter 2: Pre-equilibrium evolution effects on heavy-ion collision observables

The material presented in this chapter draws heavily on Ref. [78] where these results were first published.

2.1 Chapter introduction

The importance of pre-equilibrium dynamics on relativistic heavy-ion collision observables is investigated in this chapter. We match a highly non-equilibrium early evolution stage, modeled by free-streaming partons generated from the Monte Carlo Kharzeev-Levin-Nardi (MC-KLN) and Monte Carlo Glauber (MC-Glb) models, to a locally approximately thermalized later evolution stage described by viscous hydrodynamics, and study the dependence of final hadronic transverse momentum distributions, in particular their underlying radial and anisotropic flows, on the switching time between these stages.

The validity of hydrodynamics relies on the matter being close to local thermal equilibrium. Within a purely hydrodynamic approach that ignores details about how the system approaches equilibrium, the observed large hadron momentum anisotropy can only be explained if thermalization happens fast and the hydrodynamic expansion does not begin later than about $1\text{fm}/c$ after the two nuclei impact each other [79].

This finding calls for a mechanism to explain how the matter produced in the collision can thermalize so fast. Recently, significant work has been done on modeling the thermalization process during the pre-equilibrium stage [26, 27, 29, 80–82]. While these studies have not yet fully explained the rapid thermalization, some of them have indicated that pre-equilibrium evolution can have a non-negligible influence on the final observables.

In this chapter, we return to the question of how quickly thermalization must happen for a hydrodynamic approach to provide a successful description of experimental data, by studying the weakly interacting limit of pre-equilibrium dynamics. Freely streaming partonic quanta can be considered as the extreme limit of a weakly interacting system and the diametrically opposite to a fluid dynamical description which requires strong coupling. By coupling a free-streaming pre-equilibrium stage to hydrodynamics and varying the switching time τ_s one can smoothly interpolate between a very strongly coupled (small τ_s , early transition to hydrodynamics) and weakly coupled (large τ_s , late transition to hydrodynamic behavior) early evolution stage. We are interested in finding the largest τ_s value that is compatible with phenomenology. Replacing the non-interacting free-streaming parton stage in our model by a model in which the matter constituents interact more realistically with modest interaction strength should allow for an earlier transition to hydrodynamic behavior. For this reason we expect our approach to yield a robust upper limit, for a fixed viscosity during the subsequent hydrodynamic stage, for the time at which the matter created in the collision must have reached a sufficient degree of local equilibrium to be described hydrodynamically. The dependence of this upper limit on the viscosity

in the hydrodynamic stage will also be explored. In a realistic treatment of the pre-equilibrium dynamics, the transition from the pre-equilibrium to the hydrodynamic stage should be smooth, and the parameter τ_s does not exist. But the thermalization time, which is also indicated by τ_s in our study, still exists and serves as an important parameter for heavy-ion collisions.

It was initially thought that substituting the earliest stage in a hydrodynamic evolution model by a free-streaming gas would delay the buildup of thermodynamic pressure and thus reduce the finally observed collective flow [79]. This ignored, however, the fact that in a spatially inhomogeneous medium free-streaming (or, for that matter, any kind of pre-equilibrium evolution) generates strong position-momentum correlations which, upon thermalization, lead to strong initial flow in the hydrodynamic stage. We show here that this “pre-flow” actually increases the finally observed radial flow, with consequences that are opposite to the expectations reported in Refs. [79]. Here we explore the evolution of the widely implemented MC-KLN [46,47] and MC-Glauber [49] initial conditions at LHC energies, allowing them to be evolved by free-streaming for a time τ_s before switching to a viscous hydrodynamic description for the rest of the evolution.

Our work focuses on the effects brought by free-streaming on both the hydrodynamic initial conditions and the final observables. We mainly focus on the MC-KLN model which provides a complete prediction for the initial gluon distribution, not only in space but also in momentum. However, we show that for massless partons moving with the speed of light the shape of the initial momentum distribution is irrelevant as long as it is locally isotropic. This allows to apply our description also to MC-Glb initial conditions although that model makes no prediction per se about

the initial parton momentum distribution. Free-streaming evolves the initial conditions from an initial parton formation time τ_0 (which is taken to be very close to zero) to the switching time τ_s when we switch to a near-equilibrium hydrodynamic description. The sudden transition to approximate local equilibrium is implemented by applying the Landau matching procedure. By tuning the switching time, we can enforce fast thermalization by setting $\tau_s \simeq \tau_0$, or slow thermalization by setting $\tau_s \gg \tau_0$. The hydrodynamic initial conditions obtained from the Landau matching procedure vary with the switching time, enabling an investigation of the influence of τ_s on the final observables. The hydrodynamic evolution is performed with the code VISH2+1 [18,65], without hadron cascade afterburner. For the hydrodynamic evolution, we use a constant specific shear viscosity η/s . Freeze-out is implemented at a fixed kinetic freeze-out temperature T_{dec} , followed by a Cooper-Frye procedure with full resonance decay cascade to convert the hydrodynamic output into final stable particle spectra.

In Section 2.2, we outline the free-streaming evolution in the pre-equilibrium stage and describe the Landau matching procedure. Its consequences on the hydrodynamic initial conditions are discussed in Section 2.3. Section 2.4 shows how the hydrodynamical evolution responds to initial conditions generated at different switching times. A difficulty related to the conversion of partons to hadrons that arises from a late switching time τ_s is discussed and resolved in Section 2.5. In Sections 2.6 and 2.7, the energy flow anisotropy and hadron mean transverse momenta are constructed to illustrate how final observables change with switching time. We wrap this chapter up in Section 2.8.

2.2 Formulation of free-streaming and Landau matching

The evolution of partons in the free-streaming model is described by the collisionless Boltzmann equation

$$p^\mu \partial_\mu f(x, p) = 0. \quad (2.1)$$

We work in Milne coordinates and write $f(x, p) = f(\mathbf{x}_\perp, \eta_s, \tau; \mathbf{p}_\perp, y)$, with longitudinal proper time $\tau = \sqrt{t^2 - z^2}$, space-time rapidity $\eta_s = \frac{1}{2} \ln[(t+z)/(t-z)]$, and rapidity $y = \frac{1}{2} \ln[(E+p_z)/(E-p_z)]$. Assuming longitudinal boost-invariance, the dependence of $f(x, p)$ on η_s and y is restricted as follows [83, 84]:

$$f(\mathbf{x}_\perp, \eta_s, \tau; \mathbf{p}_\perp, y) = \frac{\delta(y - \eta_s)}{\tau m_\perp \text{ch}(y - \eta_s)} \tilde{f}(\mathbf{x}_\perp, \tau; \mathbf{p}_\perp, y). \quad (2.2)$$

We assume massless partons for which $E = |\mathbf{p}| = \sqrt{\mathbf{p}_\perp^2 + p_z^2}$ and $m_\perp = \sqrt{m^2 + \mathbf{p}_\perp^2} = p_\perp$. Then the collisionless Boltzmann equation is easily solved analytically, relating the final parton distribution $f(\mathbf{x}_\perp, \eta_s, \tau_s; \mathbf{p}_\perp, y)$ to the $f(\mathbf{x}_\perp, \eta_s, \tau_0; \mathbf{p}_\perp, y)$ by a spatial coordinate shift, keeping the $\mathbf{p}_\perp$ distribution unchanged:

$$f(\mathbf{x}_\perp, \eta_s, \tau_s; \mathbf{p}_\perp, y) = f(\mathbf{x}_\perp - (\tau_s - \tau_0) \hat{\mathbf{p}}_\perp, \eta_s, \tau_0; \mathbf{p}_\perp, y), \quad (2.3)$$

where $\hat{\mathbf{p}}_\perp = \mathbf{p}_\perp / p_\perp = (\cos \phi_p, \sin \phi_p)$, with ϕ_p being the azimuthal angle of $\mathbf{p}_\perp$ in the plane transverse to the beam. The initial distribution $f(\mathbf{x}_\perp, \eta_s, \tau_0; \mathbf{p}_\perp, y)$ is assumed to be locally isotropic in transverse momentum, i.e. independent of ϕ_p : $f_0 = f(\mathbf{x}_\perp, \eta_s, \tau_0; p_\perp, y)$. A general solution to Eq. (2.1) without the assumption of longitudinal boost-invariance can be found in [85].

To initialize the hydrodynamic we must decompose the energy momentum tensor $T^{\mu\nu}$ in hydrodynamic form. In the free-streaming stage $T^{\mu\nu}(x)$ can be obtained from

the solution of Eq. (2.3) for the parton distribution as

$$T^{\mu\nu}(\mathbf{x}_\perp, \eta_s, \tau_s) = \frac{g}{(2\pi)^3} \int \frac{d^3p}{E} p^\mu p^\nu f(\mathbf{x}_\perp, \eta_s, \tau_s; \mathbf{p}_\perp, y), \quad (2.4)$$

where for massless particles $p^0 = E = |\mathbf{p}|$ and g is a degeneracy factor. For a boost-invariant system it is sufficient to know $T^{\mu\nu}$ in the transverse plane at $z = 0$ (i.e. $\eta_s=0$) where

$$\begin{aligned} T^{\mu\nu}(\mathbf{x}_\perp, \eta_s=0, \tau) &= \frac{g}{(2\pi)^3} \frac{1}{\tau} \int_0^\infty dp_\perp \int_{-\pi}^\pi d\phi_p \\ &\times \left[p^\mu p^\nu \tilde{f}(\mathbf{x}_\perp, \tau; \mathbf{p}_\perp, y) \right] \Big|_{y=0}. \end{aligned} \quad (2.5)$$

The factor $1/\tau$ is characteristic for systems with boost-invariant longitudinal expansion.

Inspection of this formula shows that for massless partons the evolution of $T^{\mu\nu}(\mathbf{x}_\perp, \eta_s=0, \tau)$ does not depend on the underlying parton momentum distribution. For massless partons that are initially distributed locally isotropically in $\mathbf{p}_\perp$ the spatial distribution of the energy momentum tensor $T^{\mu\nu}(\mathbf{x}_\perp, \tau)$ at time τ depends only on its initial spatial distribution at time τ_0 , but not on the $p_\perp$ -distribution (which may or may not depend on $\mathbf{x}_\perp$). One sees this by observing that the integral on the right hand side of Eq. (2.5) can be rewritten as

$$\begin{aligned} &\int_0^\infty dp_\perp \int_{-\pi}^\pi d\phi_p \left[p^\mu p^\nu \tilde{f}(\mathbf{x}_\perp, \tau; \mathbf{p}_\perp, y) \right] \Big|_{y=0} \\ &= \int_0^\infty p_\perp^2 dp_\perp \int_{-\pi}^\pi d\phi_p \hat{p}^\mu \hat{p}^\nu \tilde{f}(\mathbf{x}_\perp - (\tau - \tau_0) \hat{\mathbf{p}}_\perp, \tau_0; p_\perp, 0) \end{aligned} \quad (2.6)$$

where $\hat{p}^\mu \equiv \frac{p^\mu}{p_\perp} \Big|_{y=0}$ depends only on ϕ_p . Hence

$$T^{\mu\nu}(\mathbf{x}_\perp, \eta_s=0, \tau) = \frac{1}{\tau} \int_{-\pi}^\pi d\phi_p \hat{p}^\mu \hat{p}^\nu F(\mathbf{x}_\perp, \tau; \phi_p), \quad (2.7)$$

where

$$\begin{aligned}
F(\mathbf{x}_\perp, \tau; \phi_p) &= F_0(\mathbf{x}_\perp - (\tau - \tau_0)\hat{\mathbf{p}}_\perp) \\
&\equiv \frac{g}{(2\pi)^3} \int_0^\infty p_\perp^2 dp_\perp \tilde{f}(\mathbf{x}_\perp - (\tau - \tau_0)\hat{\mathbf{p}}_\perp, \tau_0; p_\perp, 0)
\end{aligned} \tag{2.8}$$

is independent of how f_0 depends on the magnitude of $p_\perp$, and $F_0(\mathbf{x}_\perp)$ denotes the spatial distribution function (integrated over momenta) at $\tau = \tau_0$.

At the switching time τ_s , the solution (2.7) for $T^{\mu\nu}$ is decomposed in viscous hydrodynamic form:

$$T^{\mu\nu} = eu^\mu u^\nu - (\mathcal{P} + \Pi)\Delta^{\mu\nu} + \pi^{\mu\nu}. \tag{2.9}$$

Here e and $\mathcal{P}$ are the energy density and pressure in the local fluid rest frame (LRF), Π is the local bulk viscous pressure, $\pi^{\mu\nu}$ is the shear pressure tensor, and u^μ is the local fluid velocity. The projection operator $\Delta^{\mu\nu} \equiv g^{\mu\nu} - u^\mu u^\nu$ projects on the spatial coordinates in the LRF, and the spacetime metric $g^{\mu\nu}$ in Milne coordinates is given by $g^{\mu\nu} = \text{diag}(1, -1, -1, -1/\tau^2)$.

The Landau matching condition defines the fluid rest frame velocity as the time-like eigenvector of $T^{\mu\nu}$, and the energy density e as its eigenvalue:

$$T^{\mu\nu}u_\nu = eu^\mu, \tag{2.10}$$

with $u^\mu u_\mu = 1$. If such a solution exists [86] it is unique since $T^{\mu\nu}$ has at most one time-like eigenvector.

Landau matching conserves the system's total energy, but not its entropy. Due to the absence of collisions, Eq. (2.1) conserves entropy. The solution (2.3) therefore yields the same entropy at τ_s and τ_0 . After matching, however, the entropy density $s = \partial\mathcal{P}/\partial T$ is related to the energy density e and pressure $\mathcal{P}$ by the thermalized fluid's

equation of state (EOS) $\mathcal{P} = \mathcal{P}(e)$. This implies that in general the total entropy $\mathcal{S}$ of the system increases discontinuously at the switching time τ_s . This sudden increase is the consequence of the assumed sudden thermalization of the system that is implicit in the Landau matching procedure. For successful phenomenology, we have to normalize the entropy density profile after Landau matching such that, upon completion of the dynamical evolution, it correctly reproduces the observed final multiplicity dN_{ch}/dy . This is done for central collisions, and the predicted impact parameter dependence of the final dN_{ch}/dy is then taken as an argument for or against the validity of the initial model used to generate the initial conditions. In spite of the entropy jump at τ_s , the normalization of the entropy density profile after Landau matching has a one-to-one relation with the normalization of the initial distribution function. Since the entropy jump depends on the chosen value of the switching time, this initial normalization also depends on τ_s : to preserve the same dN_{ch}/dy at the end of the hydrodynamic evolution thus requires a renormalization of the initial distribution function when τ_s is varied.

After finding the energy density, the thermodynamic pressure is given by the EOS $\mathcal{P} = \mathcal{P}(e)$ of the thermalized liquid. The dynamically induced bulk viscous pressure is then reconstructed from $T^{\mu\nu}$ by using the identity

$$\Pi = -\frac{1}{3}\text{Tr}(\Delta_{\mu\nu}T^{\mu\nu}) - \mathcal{P}. \quad (2.11)$$

Finally, the shear pressure tensor is obtained by contracting $T^{\mu\nu}$ with the double projection operator $\Delta_{\alpha\beta}^{\mu\nu} \equiv \frac{1}{2}(\Delta_{\alpha}^{\mu}\Delta_{\beta}^{\nu} + \Delta_{\beta}^{\mu}\Delta_{\alpha}^{\nu}) - \frac{1}{3}\Delta^{\mu\nu}\Delta_{\alpha\beta}$,

$$\pi^{\mu\nu} = \Delta_{\alpha\beta}^{\mu\nu}T^{\alpha\beta}. \quad (2.12)$$

Alternatively,

$$\pi^{\mu\nu} = T^{\mu\nu} - eu^\mu u^\nu + (\mathcal{P} + \Pi)\Delta^{\mu\nu}, \quad (2.13)$$

where $T^{\mu\nu}$ is from Eq. (2.7), u^μ and e from Eq. (2.10), $\mathcal{P}$ from EOS and Π from Eq. (2.11).

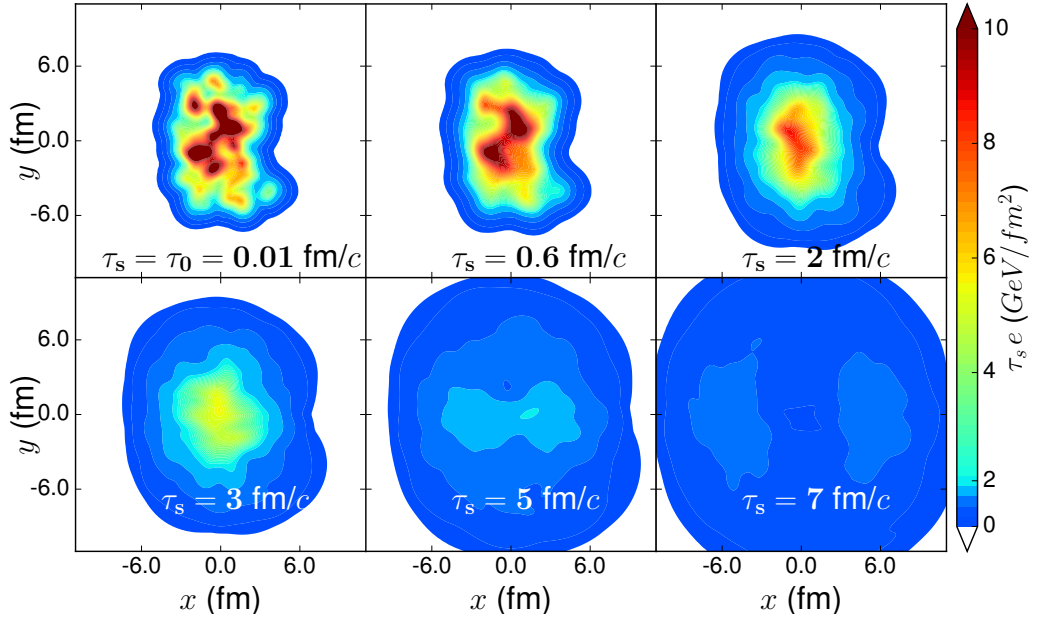


Figure 2.1: Contour plots of the local energy density multiplied by τ_s in the transverse plane, for a single fluctuating Pb+Pb collision event of 10% – 20% centrality at $\sqrt{s} = 2.76$ ATeV. To show the edge of the fireball more clearly, white is used for $\tau_s e$ below 10^{-4} GeV/fm², and dark red is used for $\tau_s e > 10$ GeV/fm².

The initial conditions for u^μ , e , $\mathcal{P}$, Π and $\pi^{\mu\nu}$ obtained from Eqs. (2.10)-(2.12) are more realistic than those used in many recent implementations of hydrodynamics where any evolution of the system of the system between τ_0 and the hydrodynamic starting time τ_s is ignored and the hydrodynamic stage is initialized with zero transverse flow and an ad hoc guess for the viscous pressure components. We will see that

the non-zero flow velocities and well-defined non-zero initial conditions for Π and $\pi^{\mu\nu}$ resulting from the Landau matching procedure (2.10) have important consequences for the subsequent hydrodynamic evolution and final observables. In this work, we focus on the effects of shear viscosity on the evolution of the collision systems. We implement our assumption of vanishing bulk viscosity ζ by setting $\zeta/s = 10^{-6}$ and then using the second order evolution equation [38] ($D \equiv u^\mu \partial_\mu$)

$$D\Pi = -\frac{1}{\tau_\Pi}(\Pi + \zeta\theta) - \frac{1}{2}\Pi\frac{\zeta T}{\tau_\Pi}\partial_\mu\left(\frac{\tau_\Pi}{\zeta T}u^\mu\right) \quad (2.14)$$

to evolve the bulk viscous pressure Π dynamically to zero, on a microscopic time scale given by the bulk relaxation time $\tau_\Pi = \frac{3}{4\pi T}$ [87].

2.3 Hydrodynamic initial conditions after a free-streaming pre-equilibrium stage

In this and the following sections where we investigate the qualitative effects of a free-streaming pre-equilibrium stage on the hydrodynamical evolution and final observables, we focus on MC-KLN initial conditions [46, 47]. We will return to the MC-Glauber model in Sec. 2.7.

Compared to hydrodynamics, free-streaming allows the energy density to spread out in the transverse plane much more rapidly. Because there are no collisions, signals carried by the massless partons move with the speed of light instead of the smaller drift velocity that would characterize an interacting medium (for a thermalized medium this would be the speed of sound). In Fig. 2.1, the local energy density just after switching to hydrodynamics is shown at different switching time τ_s . In the first panel, Landau matching is implemented at the matter formation time τ_0 (taken as $\tau_0=0.01$ fm/c). At this time, the matter distribution features many hot spots in the transverse

plane, reflecting the fluctuating nucleon positions that, through the nuclear thickness function, control the saturation momentum and thus the density of the produced gluons in the MC-KLN model. As the switching time increases, the bumps in the energy density spread and gradually dissolve as a result of the free-streaming of the partons. The initially bumpy energy density profile becomes much smoother and less deformed, resulting in decreasing spatial eccentricity coefficients $\mathcal{E}_n$.

The spatial eccentricity coefficient of harmonic order n at the beginning of hydrodynamical stage is usually defined as [88, 89]

$$\mathcal{E}_n = \epsilon_n e^{in\Phi_n} = -\frac{\int d^2r_\perp r_\perp^n e^{in\phi} e(\mathbf{r}_\perp)}{\int d^2r_\perp r_\perp^n e(\mathbf{r}_\perp)}, \quad n > 1, \quad (2.15)$$

where $e(\mathbf{r}_\perp)$ is the LRF energy density obtained from Eq. 2.10, and the minus sign ensures that the angle Φ_n points to the direction where energy density falls fastest. (For fluctuating events, the energy density profile must be re-centered to the origin in the transverse plane before calculating the eccentricities.) However, if the initial conditions feature a non-zero initial hydrodynamic flow profile, as is the case in Eq. (2.10), flow anisotropies cause the Lorentz contraction factor γ between the local and global rest frame to depend on the azimuthal angle ϕ . In the laboratory frame, the initial energy density is thus better characterized by eccentricity coefficients calculated with a modified prescription using the energy density in the laboratory frame:

$$\begin{aligned} \mathcal{E}_n(\tau_s) &= \epsilon_n(\tau_s) e^{in\Phi_n(\tau_s)} \\ &= -\frac{\int_{\tau_s} d^3\sigma_\mu(x) T^{\mu\nu}(x) u_\nu(x) r_\perp^n e^{in\phi}}{\int_{\tau_s} d^3\sigma_\mu(x) T^{\mu\nu}(x) u_\nu(x) r_\perp^n} \\ &= -\frac{\int d^2r_\perp \gamma(\mathbf{r}_\perp) e(\mathbf{r}_\perp) r_\perp^n e^{in\phi}}{\int d^2r_\perp \gamma(\mathbf{r}_\perp) e(\mathbf{r}_\perp) r_\perp^n}, \quad (n > 1) \end{aligned} \quad (2.16)$$

where $d^3\sigma_\mu$ is the normal vector on the switching hypersurface of constant τ_s . Now Φ_n points in the direction of the steepest descent in the lab frame. If need be, the modified eccentricity definition (2.16) can also be used for different switching surfaces.

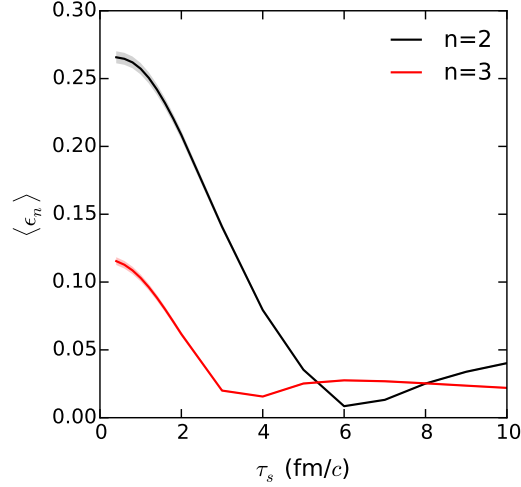


Figure 2.2: Event-averaged spatial eccentricity as a function of switching time for an ensemble of 400 fluctuating Pb+Pb collision events of 10% – 20% centrality at $\sqrt{s} = 2.76$ A TeV.

As shown in Fig. 2.2, the event-averaged ellipticity ϵ_2 and triangularity ϵ_3 at the beginning of the hydrodynamic stage decrease as the length of the free-streaming period increases. However, for $\tau_s > 6$ fm/c, they increase again. Figure 2.1 illustrates why this happens: around 5 fm/c the free-streaming fireball begins to disintegrate and eventually separate into multiple pieces. This disintegration happens due to the absence of interactions between the partons which would otherwise keep the fluid together. So the matter distribution becomes more eccentric for large switching times, and the eccentricity coefficients ϵ_n increase accordingly. Near the minima seen in this figure, each event contributes an eccentricity vector $\mathcal{E}_n$ (16) that changes direction

by π/n in the neighborhood of the minimum. When this happens, the magnitude ϵ_n of that vector vanishes. However, due to event-by-event fluctuations, these zeroes of ϵ_n happen at somewhat different times τ in each event. Since $\epsilon_n \geq 0$ by definition, the mean value $\langle \epsilon_n \rangle$ therefore never reaches zero exactly; however, it still develops a minimum at the average time where these flips of the angles Φ_n by π/n occur.

Free-streaming also drives the system out of equilibrium. For free-streaming (which corresponds to an infinite mean free path $\lambda_{\text{mfp}} = \infty$), the Knudsen number

$$\text{Kn} = \frac{\lambda_{\text{mfp}}}{L_{\text{macro}}}, \quad (2.17)$$

where L_{macro} is the characteristic macroscopic length scale of the system, is infinite. This tells us that, even if the initial momentum distribution were thermal, the system would evolve further and further away from local thermal equilibrium. The inverse Reynolds number uses the hydrodynamic decomposition (3.1) to describe how far away a system is from local thermal equilibrium. For a non-equilibrium pressure caused by shear viscosity, it is defined as the ratio between the scalar $\sqrt{\pi^{\mu\nu}\pi_{\mu\nu}}$ characterizing the magnitude of the shear stress and the thermal pressure $\mathcal{P}$:

$$R_\pi^{-1} = \frac{\sqrt{\pi^{\mu\nu}\pi_{\mu\nu}}}{\mathcal{P}}. \quad (2.18)$$

For an analytic estimate Eq. (2.18) is inconvenient since the thermal pressure $\mathcal{P}$ is related to the energy density e (whose initial profile can be calculated analytically in terms of the distribution function f) only through numerical lattice QCD calculations. This complication can be avoided by using a slightly different definition for the inverse Reynolds number:

$$R^{-1} = \frac{\sqrt{\pi^{\mu\nu}\pi_{\mu\nu}}}{-\Delta^{\mu\nu}T_{\mu\nu}/3} = \frac{\sqrt{\pi^{\mu\nu}\pi_{\mu\nu}}}{\mathcal{P} + \Pi}. \quad (2.19)$$

For a conformal EOS, $\mathcal{P} = \frac{1}{3}e$ and $\Pi = 0$, this definition agrees with Eq. (2.18), but if $\Pi \neq 0$ it allows for the following analytic computation of its initial value.

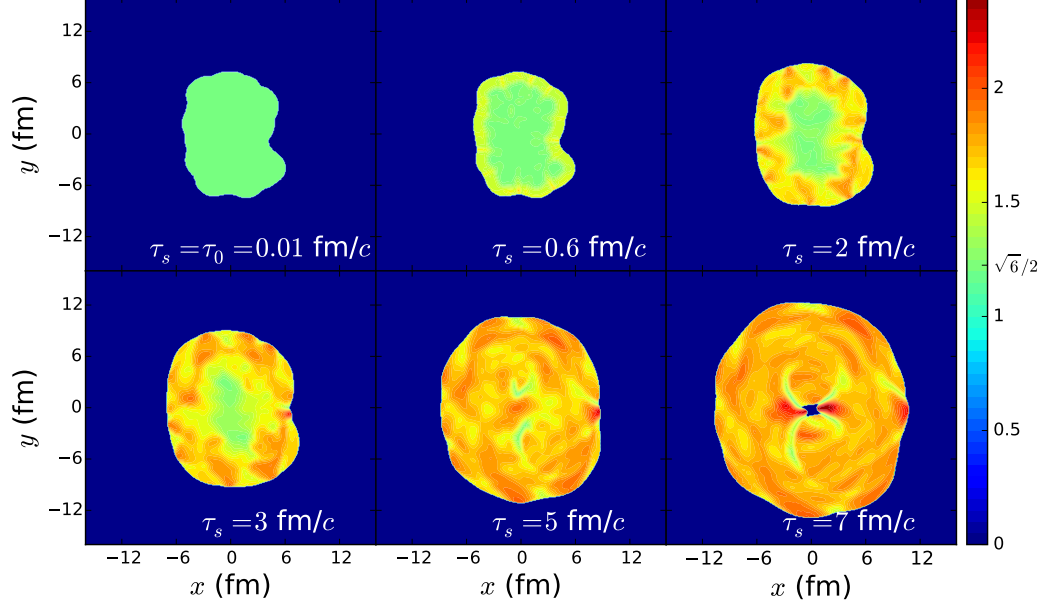


Figure 2.3: Contour plots for the inverse Reynolds number R^{-1} (2.19) in the transverse plane just after the system is switched from free-streaming to hydrodynamics, for several choice of switching time τ_s , for a single fluctuating Pb+Pb collision event of 10% – 20% centrality at $\sqrt{s} = 2.76$ ATeV. See text for discussion.

R^{-1} is a local parameter whose initial value for the case at $\tau_s = \tau_0$ can be calculated analytically, provided the initial momentum distribution is locally isotropic in the transverse plane and the system is boost-invariant. In this case, inserting the definition (2.4) into (2.12) to obtain

$$\begin{aligned}
\pi^{\mu\nu}\pi_{\mu\nu} &= \int \frac{g d^3p}{(2\pi)^3 p^0} \int \frac{g d^3p'}{(2\pi)^3 p'^0} \Delta_{\alpha\beta}^{\rho\sigma} p^\alpha p^\beta p'_\rho p'_\sigma f(p) f(p') \\
&= \int \frac{g d^3p}{(2\pi)^3 p^0} \int \frac{g d^3p'}{(2\pi)^3 p'^0} \left[(\mathbf{p} \cdot \mathbf{p}')^2 - \frac{1}{3} \mathbf{p}^2 \mathbf{p}'^2 \right] f(p) f(p'),
\end{aligned}
\tag{2.20}$$

using local transverse momentum isotropy to recast Eq. (2.2) for massless partons in the transverse plane at $\eta_s = 0$ into

$$f(p)|_{\tau_0, \eta_s=0} = \frac{\delta(y)}{\tau_0 p_\perp} \tilde{f}(p_\perp), \quad (2.21)$$

rewriting $\int \frac{d^3 p}{p^0} = \int dy d^2 p_\perp$, and using the identity $p^0 = p_\perp$ for massless on-shell gluons we find

$$\begin{aligned} \pi^{\mu\nu} \pi_{\mu\nu} |_{\tau_0, \eta_s=0} &= g^2 \int \frac{dy d^2 p_\perp dy' d^2 p'_\perp}{(2\pi)^6 \tau_0^2 p_\perp p'_\perp} \\ &\quad \times \left[(\mathbf{p} \cdot \mathbf{p}')^2 - \frac{1}{3} \mathbf{p}^2 \mathbf{p}'^2 \right] \tilde{f}(p_\perp) \tilde{f}(p'_\perp) \delta(y) \delta(y') \\ &= \frac{g^2}{\tau_0^2} \int \frac{dp_\perp dp'_\perp}{(2\pi)^6} p_\perp^2 p'_\perp{}^2 \tilde{f}(p_\perp) \tilde{f}(p'_\perp) \\ &\quad \times \int \frac{d\phi_p d\phi'_p}{\sin^2 \phi_p \sin^2 \phi'_p} \left[(\sin \theta_p \cos \phi_p \sin \theta'_p \cos \phi'_p \right. \\ &\quad \left. + \sin \theta_p \sin \phi_p \sin \theta'_p \sin \phi'_p + \cos \theta_p \cos \theta'_p)^2 - \frac{1}{3} \right]_{y=y'=0}. \end{aligned} \quad (2.22)$$

In the second line, $\mathbf{p}$ was decomposed as $\mathbf{p} = p(\sin \theta_p \cos \phi_p, \sin \theta_p \sin \phi_p, \cos \theta_p)$ using spherical coordinates, with the polar angle θ_p (θ'_p) being related to the pseudorapidity η (η') (which for massless partons agrees with their rapidity y (y')) through

$$\cos \theta_p = \tanh \eta, \quad \sin \theta_p = 1 / \cosh \eta, \quad (2.23)$$

since $\eta = -\ln [\tan (\theta_p/2)]$. We see that for massless particles the angular integral can be factored from the integration over $p_\perp$. At $y = y' = 0$, $\theta_p = \theta'_p = \frac{\pi}{2}$, and the integration over azimuthal angles ϕ_p and ϕ'_p is easily performed, giving the result $2\pi^2/3$. Thus

$$\pi^{\mu\nu} \pi_{\mu\nu} |_{\tau_0} = \frac{2\pi^2}{3} C^2 \quad (2.24)$$

where $C \equiv \frac{g}{\tau_0} \int \frac{1}{(2\pi)^3} p_\perp^2 dp_\perp \tilde{f}(p_\perp)$.

The value of $\mathcal{P} + \Pi$ (the denominator of R^{-1}) at $\tau = \tau_0$ and $\eta_s = 0$ can be found from Eq. (2.11) (all quantities evaluated at $\tau = \tau_0$ and $\eta_s = 0$):

$$\begin{aligned}
\mathcal{P} + \Pi &= -\frac{1}{3}\Delta^{\mu\nu}T_{\mu\nu} \\
&= -\frac{1}{3}\Delta^{\mu\nu}\int\frac{g\,d^3p}{(2\pi)^3p^0}p_\mu p_\nu\delta(y)\frac{\tilde{f}(p)}{\tau_0 p_\perp} \\
&= \frac{g}{3(2\pi)^3\tau_0}\int\frac{d^2p_\perp}{p_\perp}p_\perp^2\tilde{f}(p_\perp) = \frac{2\pi}{3}C.
\end{aligned} \tag{2.25}$$

Combining Eqs. (2.24) and (2.25), the inverse Reynolds number R^{-1} (2.19) at the matter formation time τ_0 is seen to be independent of position in the transverse plane and equal to

$$R^{-1}|_{\tau_0, \eta_s=0} = \sqrt{\frac{3}{2}} \approx 1.225. \tag{2.26}$$

This non-zero value for the initial inverse Reynolds number is caused by the anisotropy in the initial pressure whose longitudinal component vanishes due to the assumed zero width of the initial rapidity distribution $\sim \delta(y - \eta_s)$. It is consistent with the value obtained in anisotropic hydrodynamics which gives for a conformal system [90]:

$$\frac{(\sqrt{\pi^{\mu\nu}\pi_{\mu\nu}})_{\text{ahydro}}}{\mathcal{P}} = \sqrt{\frac{3}{2}} \frac{1 - \mathcal{P}_L/\mathcal{P}_\perp}{1 + \mathcal{P}_L/(2\mathcal{P}_\perp)}, \tag{2.27}$$

and thus agrees with our results at $\mathcal{P}_L = 0$.

The value of R^{-1} at the beginning of the hydrodynamic stage increases if the matter is allowed to free-stream for a finite time τ_s before switching to hydrodynamics. This is caused by the appearance of additional anisotropies in the transverse plane. As the partons free-stream and the matter expands outward, the transverse momentum distribution becomes locally anisotropic, especially in the regions near the outer edge

of the fireball where the momenta point predominately outward. This breaks the factorization in Eq. (2.23) of the angular integral from the one over the magnitude of $p_\perp$, and the transverse profile of R^{-1} can no longer be calculated analytically. Fig. 2.3 shows how the inverse Reynolds number R^{-1} just after switching varies with τ_s . The constant value of R^{-1} shown in the first panel of this figure (where we switch directly at τ_0) reflects the result (2.26). As τ_s increases in the following panels, R^{-1} first becomes large near the edge, but later also in the core of the profile, indicating that the entire system is moving farther away from local thermal equilibrium if it is allowed to free-stream longer.

One particular feature of the hydrodynamic initial conditions obtained by Landau matching after free-streaming is rather strong initial flow. Its radial part can be quantified by the mean radial velocity

$$\{v_\perp\} = \frac{\int d^2r_\perp \gamma(\mathbf{r}_\perp) v_\perp(\mathbf{r}_\perp) e(\mathbf{r}_\perp)}{\int d^2r_\perp \gamma(\mathbf{r}_\perp) e(\mathbf{r}_\perp)}, \quad (2.28)$$

where the curly bracket stands for the single-event average over the transverse plane. The e and $v_\perp$ profiles are taken from the Landau matching results. For event-by-event hydrodynamical runs, the event-averaged initial radial velocity $\langle v_\perp \rangle$ is obtained by averaging the value (2.28) just after Landau matching over the events:

$$\langle v_\perp \rangle = \frac{1}{N_{events}} \sum_{i=1}^{N_{events}} \{v_\perp\}^{(i)}. \quad (2.29)$$

Fig. 2.4 shows this quantity as a function of switching time. It initially rises very quickly, reaching 25% of the speed of light already after 1 fm/c, and continues to grow at an approximate rate $\langle a_\perp \rangle \approx \frac{d\langle v_\perp \rangle}{d\tau_s} = 0.13 \text{ } c^2/\text{fm}$ over the next 5 fm/c. We reiterate that we expect a free-streaming pre-hydrodynamic stage to yield the largest possible pre-equilibrium effects on the subsequent hydrodynamic evolution. These

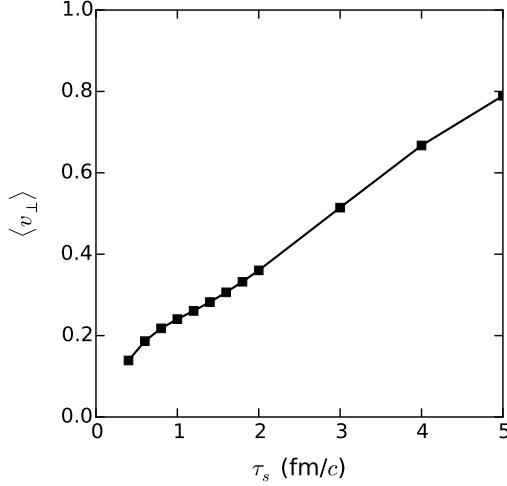


Figure 2.4: Event-averaged initial mean radial velocity as a function of switching time τ_s , for an ensemble of 400 fluctuating Pb+Pb collision events of 10% – 20% centrality at $\sqrt{s} = 2.76$ A TeV.

will be discussed in the following sections; some of the trends we will observe in these sections may manifest themselves in weakened form when free-streaming will be replaced by more realistic pre-equilibrium dynamical models in future studies.

2.4 Effects of free-streaming on hydrodynamical evolution

2.4.1 Radial flow

Pre-equilibrium evolution endows hydrodynamics with significant initial flow but a reduced initial spatial eccentricity. The interplay between these two tendencies controls the radial flow and its anisotropies that are finally observed in the measured hadron momentum distributions. For hydrodynamic simulations starting at different switching times, the initial conditions are rescaled to guarantee constant final total energy per unit space-time rapidity, $dE/d\eta_s$, as calculated from a single-shot hydrodynamic run with an event-averaged initial profile without pre-equilibrium evolution

that has been tuned to reproduce the measured total charged hadron multiplicity density $dN_{\text{ch}}/d\eta$ in central Pb+Pb collisions at $\sqrt{s} = 2.76 \text{ A TeV}$. The final $dE/d\eta_s$ is calculated on the freeze-out surface as

$$\frac{dE}{d\eta_s} = \int_{\Sigma_{\text{fo}}} T^{0\mu}(x) \frac{d^3\sigma_\mu(x)}{d\eta_s}. \quad (2.30)$$

$dE/d\eta_s$ is roughly equal to the total multiplicity density $dN/d\eta$ multiplied by the mean transverse mass for charged hadrons, $\langle m_\perp \rangle^{\text{ch}}$. Note that by varying initial parameters keeping $dE/d\eta_s$ fixed, we allow $dN_{\text{ch}}/d\eta$ to vary: if the parameter change leads to an increase in radial flow, $\langle m_\perp \rangle^{\text{ch}}$ increases and $dN_{\text{ch}}/d\eta$ will decrease accordingly. The reason for using in this work the final energy $dE/d\eta_s$ rather than $dN_{\text{ch}}/d\eta$ for rescaling the initial distribution for each fluctuating event will be explained in Sec. 2.5.

We expect the increase with τ_s of the initial average radial flow shown in Fig. 2.4 to manifest itself in a flow-induced blue shift of the finally measured hadron $p_\perp$ -distributions, caused by the hydrodynamic radial flow on the freeze-out surface. For a single event, the final hydrodynamic radial flow can be characterized by the average radial velocity of the fluid cells on the freeze-out surface

$$v_{\text{fo}} \equiv \frac{\int_{\Sigma_{\text{fo}}} u^\mu d^3\sigma_\mu v_\perp e}{\int_{\Sigma_{\text{fo}}} u^\mu d^3\sigma_\mu e} = \frac{\int_{\Sigma_{\text{fo}}} u^\mu d^3\sigma_\mu v_\perp}{\int_{\Sigma_{\text{fo}}} u^\mu d^3\sigma_\mu}. \quad (2.31)$$

In the second equality we used that our freeze-out surface has constant temperature $T_{\text{dec}} = 120 \text{ MeV}$ and, therefore, constant energy density e_{dec} . The value $\bar{v}_{fo}$ of this quantity obtained from Eq. (2.31) for a single hydrodynamic run with an *ensemble-averaged* MC-KLN initial profile for Pb+Pb collisions at $\sqrt{s} = 2.76 \text{ A TeV}$ and 10% – 20% centrality is shown by the black squares in Fig. 2.5 as a function of switching time τ_s . As expected from Fig. 2.4, it increases with τ_s , contrary to what we observed earlier

in simulations that ignored pre-equilibrium dynamics and started the hydrodynamic evolution with unevolved density profiles and zero transverse flow at the same τ_s (shown as red circles in Fig. 2.5).

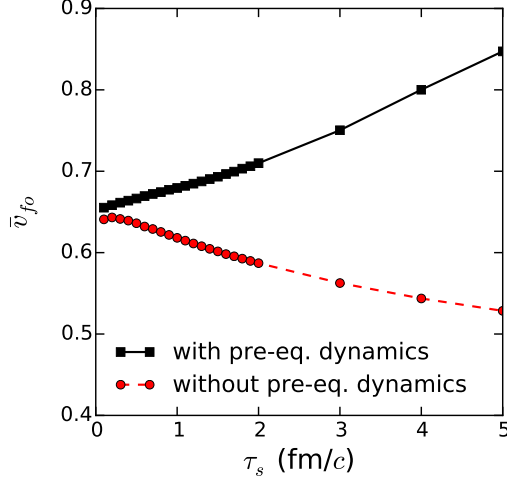


Figure 2.5: $\bar{v}_{fo}$ as a function of switching time τ_s , obtained from a single-shot hydrodynamic event with and without pre-equilibrium evolution, for the same ensemble-averaged MC-KLN initial profile. The solid (dashed) line corresponds to including (excluding) pre-equilibrium flow before beginning of the hydrodynamic evolution stage at τ_s .

2.4.2 Anisotropic flow

The total momentum anisotropy

$$\epsilon'_p = \frac{\int d^2r_\perp (T^{xx} - T^{yy})}{\int d^2r_\perp (T^{xx} + T^{yy})}, \quad (2.32)$$

is directly and monotonously related to the elliptic flow v_2^{ch} of all charged hadron integrated over $p_\perp$ [91, 92]. This quantity includes the collective flow anisotropy generated by pre-equilibrium dynamics as well as a contribution from the anisotropy of the local momentum distribution reflected in $\pi^{\mu\nu}$ [65]. The collective flow part of

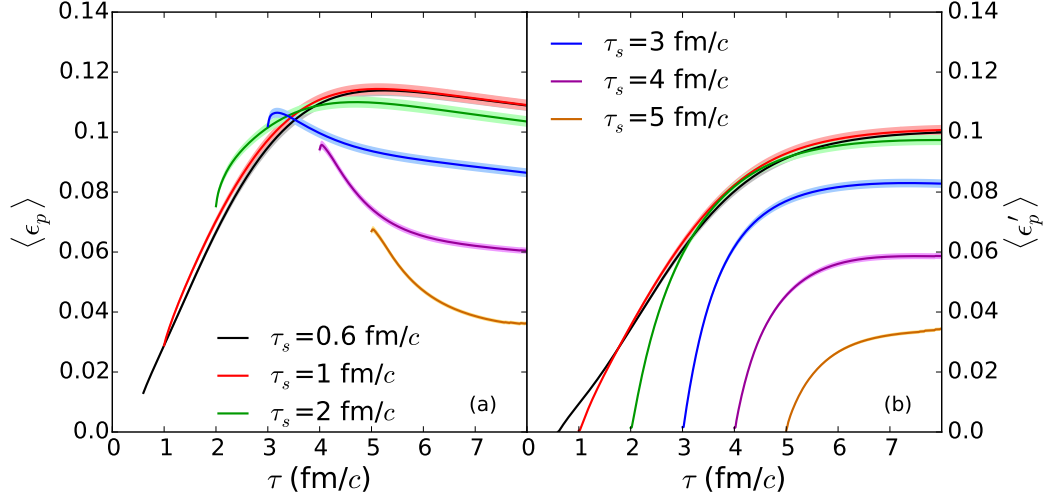


Figure 2.6: Time evolution of the ensemble-averaged total hydrodynamic flow anisotropy $\langle \epsilon_p \rangle$ (a) and total momentum anisotropy $\langle \epsilon'_p \rangle$ (b) (see text for definitions) for different switching times, for an ensemble of 400 fluctuating Pb+Pb collision events of 10% – 20% centrality at $\sqrt{s} = 2.76$ ATeV.

this momentum anisotropy is captured by

$$\epsilon_p = \frac{\int d^2r_\perp (T_{\text{id}}^{xx} - T_{\text{id}}^{yy})}{\int d^2r_\perp (T_{\text{id}}^{xx} + T_{\text{id}}^{yy})}, \quad (2.33)$$

where $T_{\text{id}}^{\mu\nu} = eu^\mu u^\nu - \mathcal{P}\Delta^{\mu\nu}$ is the ideal fluid part of the energy momentum tensor. Starting hydrodynamics at different switching times causes both quantities to saturate at different values. At large times, velocity shear effects die out and Π , $\pi^{\mu\nu}$ become small [65], and hence ϵ_p and ϵ'_p approach each other (see Fig. 2.6). Smaller saturated values of ϵ_p and ϵ'_p indicate weaker final anisotropic flow. Studying how the saturated values of these quantities change with switching time thus may help to constrain that parameter.

In order to calculate the ensemble-averaged total momentum anisotropy $\langle \epsilon'_p \rangle$, we first rotate the transverse components of $T^{\mu\nu}$ in each event to maximize the magnitude

of ϵ'_p and then sum over events. For $\langle\epsilon_p\rangle$ we proceed similarly with the ideal fluid part of $T^{\mu\nu}$. Fig. 2.6 shows how these ensemble-averaged $\langle\epsilon_p\rangle$ and $\langle\epsilon'_p\rangle$ evolve during the hydrodynamic stage, for several choices of the switching time. $\langle\epsilon'_p\rangle$ always starts out with zero magnitude at $\tau = \tau_s$ since the initial parton momentum distribution at τ_0 is isotropic, and this isotropy of the spatially integrated momentum distribution is preserved by free-streaming. In contrast, ϵ_p starts out after Landau matching with non-zero magnitude, as seen in Fig. 2.6a. This is due to anisotropies in the space-momentum correlations that were generated in the pre-equilibrium stage and that, after Landau matching, manifest themselves in anisotropies of the hydrodynamic flow profile $u^\mu(x)$. After the onset of hydrodynamic evolution, $\langle\epsilon'_p\rangle$ initially increases quickly, rapidly approaching ϵ_p , and then saturates. For small switching times $\tau_s < 2$ fm/c, $\langle\epsilon'_p\rangle$ has enough time to fully develop before freeze-out, and the saturated values show little sensitivity to τ_s . However, for larger switching times $\tau_s > 2$ fm/c, $\langle\epsilon'_p\rangle$ saturates at lower values that decrease rapidly with increasing τ_s . If thermalization happens very late, hydrodynamics is no longer able to reach the same degree of final momentum anisotropy as obtained for early thermalization. This agrees with earlier findings in [79, 93].

2.5 Issues of parton-hadron conversion

As shown in Sec. 2.3, free-streaming decreases the local energy density. As the free-streaming time τ_s increases, more cells fall with their energy density below the decoupling value e_{dec} even before the hydrodynamic stage starts. These partons will not be able to thermalize. The sketch shown in Fig. 2.7 illustrates this phenomenon.

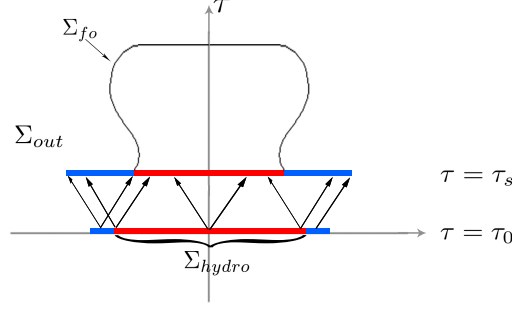


Figure 2.7: Illustration of would-be fluid cells inside (red) and outside (blue) of the freeze-out surface during free-streaming in a (1+1)-dimensional space-time diagram where the horizontal axis represents the transverse plane.

In this figure, the thick colored horizontal lines represent areas occupied by partons. Blue segments stand for regions with energy density below e_{dec} . After Landau matching, these regions would be outside the freeze-out surface Σ_{fo} that separates the thermalized fluid from free-streaming particles. The particles in those regions “decouple” instantaneously on a surface Σ_{out} that is part of the $\tau = \tau_s$ Landau-matching surface. Partons emitted from Σ_{out} neither thermalize nor evolve hydrodynamically. The red segment labeled as Σ_{hydro} indicates the region with $e > e_{\text{dec}}$. After Landau-matching, cells on Σ_{hydro} become part of the thermalized fluid, so Σ_{hydro} forms the initial condition surface from which the hydrodynamic evolution starts. After hydrodynamic evolution, these cells decouple into free-streaming particles once they reach the freeze-out surface Σ_{fo} , i.e. once their local energy density drops below e_{dec} .

At $\tau = \tau_0$, only a small region near the edge of the fireball is on Σ_{out} . When free-streaming starts, the system expands both longitudinally and transversally, leading to a decrease of the local energy density, so Σ_{out} grows and Σ_{hydro} shrinks. At very large

switching times $\tau_s \gtrsim 8 \text{ fm}/c$, Σ_{out} covers the entire $\tau = \tau_s$ surface, and hydrodynamic evolution would never even start.

The non-thermalized partons on Σ_{out} hadronize directly from the free streaming stage. Contrary to the partons at Σ_{hydro} whose hadronization happens only after hydrodynamic evolution on Σ_{fo} and is described by the Cooper-Frye formula [71], partons on Σ_{out} do not have thermal distributions and we cannot use the Cooper-Frye formula to convert them to hadrons. Furthermore, most of the partons generated from the MC-KLN model are soft, with characteristic momenta $< 1\text{--}2 \text{ GeV}$. No reliable models exist to convert such soft partons to hadrons.¹ However, even though we cannot follow their evolution into final hadrons of well-defined mass and flavor, we can still follow their momentum and energy. So in the following sections, we propose to use the system’s total energy flow distribution, instead of the momentum distributions of identified hadrons, to investigate radial and anisotropic flow for late switching times. We will trust our model’s predictions for final identified hadron flows only when the contributions from Σ_{out} can be neglected.

Our inability to hadronize the contribution from Σ_{out} causes a problem for the rescaling of the initial profile. In common practice, the initial entropy profile is rescaled such that the calculated $dN_{\text{ch}}/d\eta$ matches the experimental measurement. This procedure is problematic if there is a significant contribution of final hadrons emitted from Σ_{out} that cannot be included. Our way to work around this problem is to normalize the final *energy* on the transverse plane to a “standard” value. This

¹ One could use parton-hadron duality to calculate the hadron yield from partons on Σ_{out} . Such an approach could be useful for rescaling the initial profile as discussed in the next paragraph. It does not, however, provide the correct chemical composition for the final hadronic state, and it can not be used to compute final hadron spectra and anisotropic flow which are the main interest of this study.

“standard” final energy is obtained from a smooth fireball evolved with single-shot hydrodynamics starting at 0.6 fm/c without pre-equilibrium dynamics, with parameters matched to reproduce the experimental $dN_{\text{ch}}/d\eta$. Using longitudinal boost-invariance, i.e. the fact that the integrand can only depend on the rapidity difference $y-\eta_s$, the total energy per unit rapidity on the freeze-out surface is given by

$$\begin{aligned} \left. \frac{dE}{dy} \right|_{\Sigma_{\text{fo}}} &= \sum_i \frac{g_i}{(2\pi)^3} \int d^2p_{\perp} \int_{\Sigma_{\text{fo}}} p^{\mu} d^3\sigma_{\mu} (n^{\nu} p_{\nu}) f_i \\ &= \sum_i \frac{g_i}{(2\pi)^3} \int dy d^2p_{\perp} \int_{\Sigma_{\text{fo}}} p^{\mu} \frac{d^3\sigma_{\mu}}{d\eta_s} (n^{\nu} p_{\nu}) f_i \\ &= \int_{\Sigma_{\text{fo}}} n_{\nu} T^{\nu\mu} \frac{d^3\sigma_{\mu}}{d\eta_s} = \left. \frac{dE}{d\eta_s} \right|_{\Sigma_{\text{out}}}, \end{aligned} \quad (2.34)$$

where $n^{\nu} = (1, 0, 0, 0)$ is the temporal unit vector in the lab frame and the sum runs over all species. The parton distribution for hadron species i at the freeze-out surface can be written as

$$f_i = f_{0,i} + \delta f_{\text{shear},i} + \delta f_{\text{bulk},i}, \quad (2.35)$$

where $f_{0,i}$ is the local equilibrium distribution for hadron species i while $\delta f_{\text{shear},i}$ and $\delta f_{\text{bulk},i}$ are the shear and bulk viscous corrections to $f_{0,i}$, accounting for the system’s deviation from local thermal equilibrium. For the shear correction we use the ansatz [94, 95]

$$\delta f_{\text{shear},i} = f_{0,i} (1 \pm f_{0,i}) \frac{\pi^{\mu\nu} p_{\mu} p_{\nu}}{2T^2(e + \mathcal{P})}. \quad (2.36)$$

For the bulk correction we use the following expression, derived from the 14-moment approximation for particles with Boltzmann statistics [96]:

$$\delta f_{\text{bulk},i} = -f_{0,i} \Pi \left[B_{0,i} m_i^2 + D_{0,i} u^{\mu} p_{\mu} + E_{0,i} (u^{\mu} p_{\mu})^2 \right], \quad (2.37)$$

For a non-interacting hadron resonance gas the coefficients $B_0(T)$, $D_0(T)$ and $E_0(T)$ were calculated in Ref. [97] in the Boltzmann limit.

Although in our work here the bulk viscous pressure approaches zero on the short bulk relaxation time scale τ_Π , its initial value from the Landau matching is large, and the bulk viscous correction $\delta f_{\text{bulk},i}$ remains significant over the early part of the hydrodynamic freeze-out surface sketched in Fig. 2.7. To match the last two lines of Eq. (2.34) it is therefore important to include $\delta f_{\text{bulk},i}$ in the definition of the distribution function f_i .²

Even if we do not know how to hadronize the partons on Σ_{out} , we can easily add their contribution to dE/dy . At $y = \eta_s = 0$, we find

$$\begin{aligned} \left. \frac{dE}{dy} \right|_{\Sigma_{\text{out}}} &= \frac{g}{(2\pi)^3} \int d^2 p_\perp \int_{\Sigma_{\text{out}}} p^\mu d^3 \sigma_\mu (u^\nu p_\nu) f(x, p) \\ &= \int_{\Sigma_{\text{out}}} n_\nu T^{\nu\mu} \frac{d^3 \sigma_\mu}{d\eta_s} = \tau_s \int_{\Sigma_{\text{out}}} d^2 r_\perp T^{00} = \left. \frac{dE}{d\eta_s} \right|_{\Sigma_{\text{out}}}. \end{aligned} \quad (2.38)$$

Here $f(x, p)$ is the distribution function for the initial free-streaming partons, and we again used the property $f(x, p) \sim \delta(y - \eta_s)$ to convert

$$d^2 p_\perp d^3 \sigma_\mu = (dy d^2 p_\perp) \frac{d^3 \sigma_\mu}{d\eta_s} = n_\mu (dy d^2 p_\perp) (\tau_s d^2 r_\perp). \quad (2.39)$$

The final total energy after free-streaming and hydrodynamical evolution is the sum of the contributions from Σ_{out} and the hydrodynamic freeze-out surface Σ_{fo} . We can now rescale the initial gluon distribution function such that for each switching time τ_s the final total energy reproduces the “standard” value defined above. We

²For a quantitatively accurate matching one actually must correct the ansatz (3.17) and the calculation [97] of its coefficients $B_0(T)$, $D_0(T)$ and $E_0(T)$ for quantum statistical effects. We found a 9% discrepancy between the value of Π obtained by reconstructing it from $\delta f_{\text{bulk},i}$ using its kinetic definition [96] and the value obtained directly by applying the projection (2.11) on the hydrodynamic energy-momentum tensor. Since in our case effects from Π on the hadron spectra and flow coefficients, once integrated over the entire freeze-out surface, are small, we here ignored this 9% discrepancy.

repeat that holding the final energy dE/dy fixed is not equivalent to demanding fixed final multiplicity $dN_{ch}/d\eta$ (see discussion in Sec. 2.4.1). This should be kept in mind when interpreting the results from the following study of the sensitivity of physical observables to the switching time τ_s (i.e. to the time the system needs to thermalize sufficiently for hydrodynamics to become applicable).

Because of our inability to convert the partons on Σ_{out} to hadrons, we do not know how to include their contribution in final hadronic observables such as transverse momentum spectra and flow anisotropies. These observables are computed by only including hadrons emitted from Σ_{fo} :

$$\frac{dN_i}{dyd\phi_p} = \frac{g_i}{(2\pi)^3} \int p_\perp dp_\perp \int_{\Sigma_{fo}} p^\mu d^3\sigma_\mu(x) f_i(x, p), \quad (2.40)$$

$$v_n e^{in\Psi_n} = \frac{\sum_i \int_{-\pi}^{\pi} d\phi_p \frac{dN_i}{dyd\phi_p} e^{in\phi_p}}{\sum_i \int_{-\pi}^{\pi} d\phi_p \frac{dN_i}{dyd\phi_p}}, \quad (2.41)$$

where the sum over i runs over all hadron species. Obviously, theoretical predictions based on this procedure are not trustworthy if the neglected contribution from Σ_{out} presents a significant fraction of the total energy. Fig. 2.8 shows that the associated error increases rapidly with τ_s , but remains below 5% for $\tau_s \lesssim 3 \text{ fm}/c$. If the system takes longer than $3 \text{ fm}/c$ to thermalize, we can no longer ignore the “corona” [98] of particles emerging from Σ_{out} . We will therefore consider comparisons of our predictions for hadronic observables with experimental data “meaningful” only for runs with $\tau_s \lesssim 3 \text{ fm}/c$.

2.6 Energy flow anisotropy

Due to the lack of the contribution from partons on Σ_{out} , for large switching times we are unable to fully reconstruct the hadron azimuthal distribution and its flow

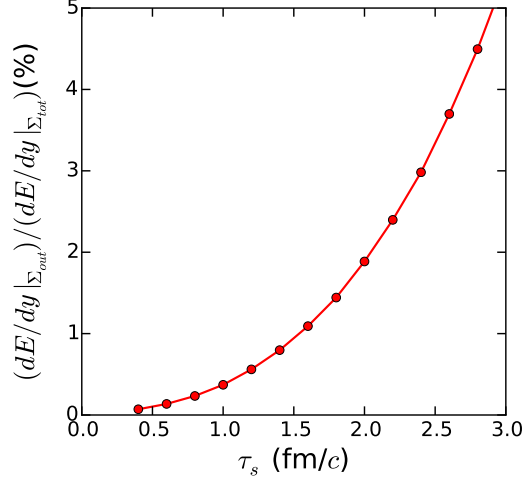


Figure 2.8: The fraction (in percent) of the total final energy $\frac{dE}{dy}$ contributed by non-thermalized particles on Σ_{out} , as a function of the switching time τ_s .

anisotropy. This is a big handicap when trying to explore the effect of large switching times on those physical observables: The largest effects one sees are due to the loss of particles through the Σ_{out} surface.

One way around this problem is to construct the flow anisotropy from the azimuthal distribution of energy instead of that of the hadrons. Since the energy angular distribution closely tracks that of the particles, the energy flow anisotropies should be strongly correlated with the (momentum-integrated) hadron flow anisotropies. In this section, we construct the energy flow anisotropy and calibrate it by comparing it to the hadron flow anisotropy for small switching times, when the contributions from Σ_{out} are negligible.

The azimuthal distributions of energy emitted from Σ_{out} and Σ_{fo} at $y = \eta_s = 0$ are given by

$$\left. \frac{dE}{dyd\phi_p} \right|_{\Sigma_{\text{fo}}} = \sum_i \frac{g_i}{(2\pi)^3} \int_0^\infty n^\nu p_\nu p_\perp dp_\perp \int_{\Sigma_{\text{fo}}} p^\mu d^3\sigma_\mu f_i, \quad (2.42)$$

$$\left. \frac{dE}{dyd\phi_p} \right|_{\Sigma_{\text{out}}} = \frac{g \tau_s}{(2\pi)^3} \int_0^\infty n^\nu p_\nu p_\perp^2 dp_\perp \int_{\Sigma_{\text{out}}} d^2r_\perp f. \quad (2.43)$$

In (2.42) i runs over all hadron species, while (2.43) contains only the gluons generated from the KLN model. In (2.43) we used that on Σ_{out} , $p^\mu d^3\sigma_\mu = p_\perp \tau_s d^2r_\perp$ for massless partons at $y=0$. Note that at $y=0$, $n^\nu p_\nu = p_\perp$ for the massless partons in (2.43) while $n^\nu p_\nu = m_{\perp,i} = \sqrt{m_i^2 + p_\perp^2}$ for the hadron species i in (2.42).

Summing these two contributions to a single distribution $dE/dyd\phi$, the Fourier coefficients of this azimuthal energy distribution can be extracted by the same procedure as used for calculating hadronic anisotropic flow coefficients:

$$w_n e^{in\bar{\Psi}_n} = \frac{\int \frac{dE}{dyd\phi_p} e^{in\phi_p} d\phi_p}{\int \frac{dE}{dyd\phi_p} d\phi_p}. \quad (2.44)$$

w_n is the energy flow anisotropy coefficient, which quantifies the azimuthal distribution of the energy contributed by all the particles – non-thermalized partons as well as frozen-out, hydrodynamically flowing hadrons. $\bar{\Psi}_n$ is the energy flow angle associated with w_n .

We will now show that, for small τ_s whose the contributions from Σ_{out} to energy and particle emission are negligible, w_n from Eq. (2.44) and v_n from Eq. (2.41) are tightly correlated. The advantage of w_n over v_n is that it is easy to include all contributions, including that from Σ_{out} , in our calculation of the energy flow, while v_n only accounts for contributions from Σ_{fo} and thus misses a large fraction of the emitted hadrons when τ_s is large. If w_n and v_n are tightly correlated for small τ_s ,

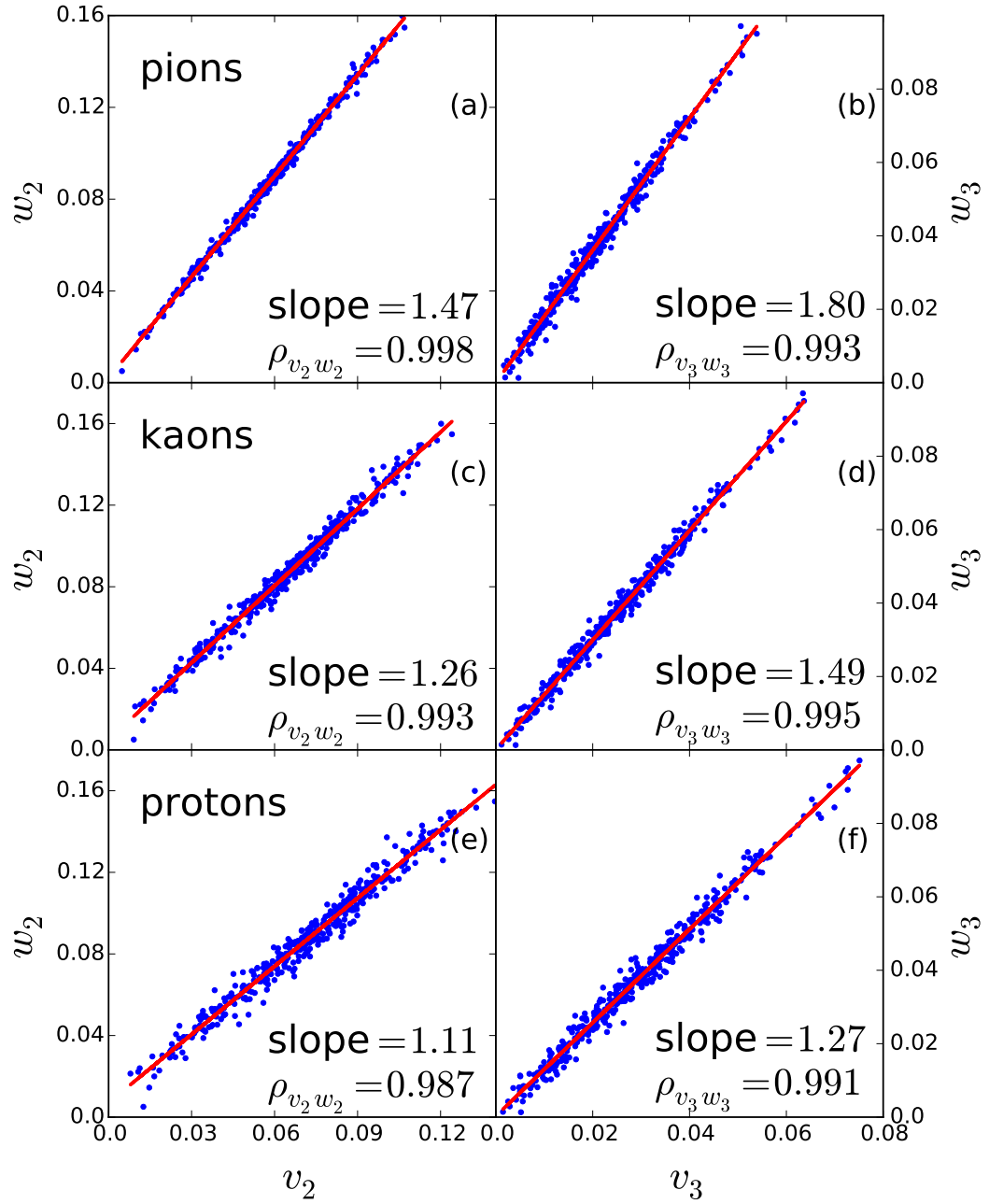


Figure 2.9: Scatter plot of the hadron flow anisotropies $v_{2,3}$ for pions (top panels), kaons (middle panels) and protons (bottom panels), and energy flow anisotropies $w_{2,3}$ from 400 fluctuating hydrodynamic events using $\tau_s = 0.6 \text{ fm}/c$ for the switching time. The left (right) column is for elliptic (triangular) flow. The slope and correlation coefficients from a linear fit to the scatter plots are noted in each panel.

where both v_n and w_n account for essentially all emitted particles, we are allowed to use w_n as a proxy for the true v_n also for large τ_s , where v_n computed from (2.41) no longer faithfully represents the full system.

Fig. 2.9 shows the correlation between the hadron flow anisotropies v_n^i for three selected particle species i and the energy flow anisotropies w_n for harmonic orders $n=2$ and 3. For this comparison we chose $\tau_s=0.6\text{ fm}/c$ to guarantee that the contribution to w_n from Σ_{out} is negligible. We observe almost perfect correlations, with correlation coefficients very close to 1, for both w_2 vs. v_2 and w_3 vs. v_3 . The slopes w_n/v_n^i are larger than 1 for all hadron species i , demonstrating a stronger sensitivity of the energy flow coefficients w_n to the hydrodynamic flow anisotropies than of v_n for individual hadrons. Among the hadrons, heavier species such as protons are more sensitive to hydrodynamic flow than lighter species [79], but even for protons $v_{2,3}$ are still smaller than $w_{2,3}$. We confirmed similarly strong correlations between $v_{2,3}$ and $w_{2,3}$ at other switching times $\tau_s < 2.5\text{ fm}/c$ but saw that the correlation gradually breaks down for large τ_s values $\tau_s > 3\text{ fm}/c$ when too much of the total energy emerges from Σ_{out} .

2.7 Constraining the duration of the pre-equilibrium stage

In this section, we will use the energy flow anisotropies $w_{2,3}$ and the mean transverse momenta for pions, kaons and protons to constrain the duration of the pre-equilibrium stage. It is well known that the average transverse momenta of hadrons with different masses help to separate random thermal motion (i.e. the freeze-out temperature) from the effect of collective radial hydrodynamic flow in the final state. Switching from initial free-streaming to hydrodynamics at later times means more

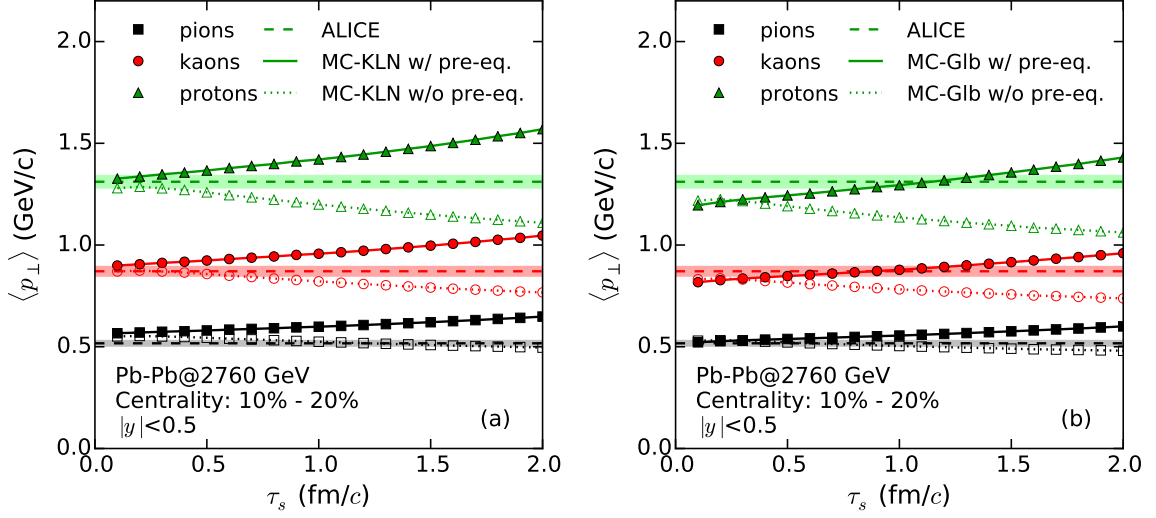


Figure 2.10: Mean transverse momentum for pions, kaons and protons, with and without pre-equilibrium dynamics, compared with data from the ALICE collaboration [99] (horizontal bands), for both MC-KLN (a) and MC-Glauber (b) initial models.

initial flow after Landau matching but less time for developing hydrodynamic flow. Fig. 2.5 has already shown that the net effect is an increased radial flow at freeze-out which will lead to harder momentum spectra and an increase in the average $p_{\perp}$. It is therefore expected that the measured $\langle p_{\perp} \rangle$ values for pions, kaons and protons will put an upper limit on the switching time, by limiting the amount of radial flow at freeze-out.

This is illustrated in Fig. 2.10 where the mean transverse momenta $\langle p_{\perp} \rangle$ for pions, kaons and protons are plotted as a function of switching time τ_s , with MC-KLN initial conditions (propagated with specific shear viscosity $\eta/s = 0.2$) in panel (a) and MC-Glauber initial conditions (propagated with $\eta/s = 0.08$) in panel (b). Shown for comparison are experimental data from the ALICE Collaboration [99] that were obtained by extrapolating the measured spectra to the full $p_{\perp}$ range before calculating

the mean. When pre-equilibrium dynamics is included in the calculations (solid lines with filled symbols), the mean transverse momenta are seen to increase with τ_s , as anticipated. The effect is strongest for protons whose large mass makes them most susceptible to flow. One sees that, with the chosen values for the shear viscosity and freeze-out temperatures, the MC-KLN initializations with free-streaming pre-equilibrium dynamics have difficulties accommodating the data unless one postulates essentially instantaneous thermalization, and even then the pion mean $p_\perp$ is still statistically significantly too large (by about 10%) compared to the measurements. On the other hand, the smaller shear viscosity used for evolving the MC-Glauber initial profiles in panel (b) reduces the transverse shear stress and thus builds less radial flow, giving room for some pre-equilibrium radial flow. With this combination of initial conditions and shear viscosity, a switching time around 1 fm/c appears to be preferred over significantly smaller and larger τ_s values.

In Fig. 2.10 we also show for comparison as dashed lines with open symbols the corresponding results for hydrodynamic evolution without pre-equilibrium dynamics. In this case τ_s has the meaning of the starting time for the hydrodynamic evolution, but with initial conditions that have not evolved in the transverse plane between τ_0 and τ_s . Without pre-equilibrium, delaying the start of the hydrodynamic expansion leads to a reduction of the final radial flow, since less time is available for its generation before the matter reaches the decoupling temperature. As a result, $\langle p_\perp \rangle$ decreases with increasing τ_s , and the effect is again stronger for protons than for pions and kaons, due to their larger mass.

For the purely hydrodynamic runs without pre-equilibrium dynamics, we see in Fig. 2.10 that no choice of τ_s can reproduce all three measured $p_\perp$ values simultaneously, for either of the two initial condition models and associated shear viscosities. The reader may wonder how this can be consistent with successful earlier fits of the measured transverse momentum spectra for these three particle species [100, 101]. Part of the answer is that in [100, 101] the quality of the model description of the data was judged by the overall shape of the $p_\perp$ -distributions whereas here we compare with only a single moment of that distribution which, however, measured with very good precision. We will return to this question in the following section where we look at a somewhat larger set of experimental data that are, in addition to the mean $p_\perp$, also sensitive to the shape of the $p_\perp$ -distributions and try to fit them by simultaneously varying several hydrodynamic parameters.

For anisotropic flow the τ_s dependence is more subtle: as shown in Fig. 2.2, a free-streaming pre-equilibrium stage reduces the source eccentricity at the start of the hydrodynamic evolution, so it reduces the amount of flow anisotropy that can be generated during the hydrodynamic stage in response to this initial eccentricity. However, as shown in Fig. 2.6a, it also creates a non-zero hydrodynamic flow anisotropy at the start of the fluid stage which gives the hydrodynamic evolution of anisotropic flow a boost. Fig. 2.11 shows that, for switching times up to about 2 fm/c, the combined effect are final elliptic and triangular flow anisotropies $w_{2,3}$ that are almost independent of the switching time. In fact, both w_2 and w_3 slightly increase with increasing switching time until τ_s reaches about 1.5 fm/c. Only for larger switching times beyond 2 fm/c does the reduction of $\varepsilon_{2,3}$ before the start of the hydrodynamic

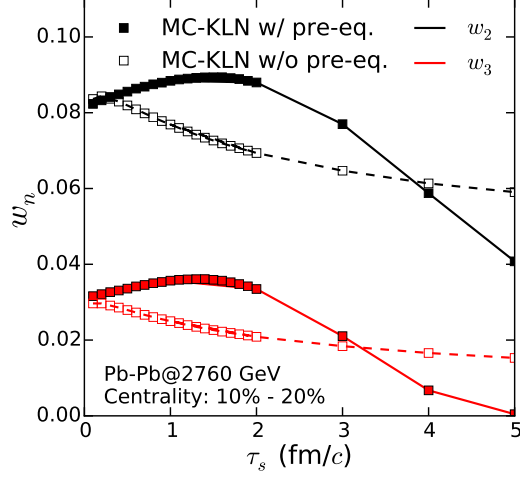


Figure 2.11: Elliptic and triangular energy flow anisotropy coefficients w_2 , w_3 as a function of the switching time from single-shot hydrodynamic simulations with a smooth ensemble-averaged MC-KLN initial profile.

evolution cut into the finally established anisotropic flow coefficients, and for very large switching times both w_2 and w_3 approach zero.

The naive expectation that the pre-equilibrium dilution of the source eccentricity before τ_s should reduce the finally established anisotropic flow [79, 93] is borne out only if one completely ignores the position-momentum correlations created by the pre-equilibrium dynamics and starts the hydrodynamic stage with zero transverse flow. This is illustrated by the dashed lines with open symbols in Fig. 2.11.

Figure 2.11 thus leads, in disagreement with the earlier statements made in Refs. [79, 93], to the (revised) conclusion that elliptic and higher-order anisotropic flow measurements alone cannot put a tight upper limit on the duration of the pre-equilibrium stage. Fig. 2.11 suggests that, as long as pre-equilibrium contributions to the final flow pattern are consistently accounted for, the final anisotropic flows

are insensitive to how strongly the medium is coupled during the first $2\text{ fm}/c$ or so. Whether this stage is described hydrodynamically (very strong coupling) or by free-streaming partons (very weak coupling), one sees the same final flow anisotropy. This finding supports the idea of “universal transverse flow” during the earliest stages of the fireball evolution proposed by Pratt and Vredevoogd [102]. In contrast, radial flow (which affects the slope and mean $p_\perp$ of the transverse momentum spectra) exhibits a strong and monotonic τ_s dependence already for small switching times that can be used much more effectively to put an upper limit on the thermalization time in heavy-ion collisions.

2.8 Chapter summary

In this chapter, we thoroughly investigated the effect of pre-equilibrium flow on heavy-ion collision observables. In order to estimate the maximum difference between simulations where the hydrodynamic stage was initiated with non-zero flow resulting from a preceding stage of pre-equilibrium evolution and others where all dynamical effects before the onset of hydrodynamic expansion were simply ignored (as has been common practice in many earlier studies), we here assumed the pre-equilibrium stage to be non-interacting, i.e. free-streaming. By adjusting the switching time τ_s between the free-streaming and hydrodynamic stages we can thus smoothly switch between a picture where the earliest stage of the collision is coupled infinitely weakly and one where it is coupled infinitely strongly.

The pre-equilibrium and hydrodynamic stages are Landau-matched, conserving energy and momentum and fully accounting for all components of the pre-equilibrium

energy-momentum tensor with non-zero (and possibly large) dissipative pressure components (bulk and shear viscous pressures). The study presented here was done for zero bulk viscosity, i.e. the non-zero bulk viscous pressure generated by the Landau matching procedure was allowed to evolve dynamically to zero with a short microscopic relaxation time. The viscous shear stress at the beginning of the hydrodynamic stage was found to be large, corresponding to an inverse Reynolds number slightly above unity for early switching times and further increasing if one switches from free-streaming to hydrodynamics later. In the hydrodynamic stage, these large starting values for the shear stress decrease quickly on a short microscopic time scale, due to the assumed low shear viscosity η/s of the hydrodynamic fluid.

On the way we had to solve the problem that extended free-streaming leads to a loss of a significant fraction of the energy of the expanding fireball because the volume of the “corona” of dilute matter that never thermalizes and therefore never becomes part of the hydrodynamic fluid increases. While we are not able to convert corona partons into hadrons we can account for their energy, so we can include them in anisotropic flow coefficients w_n that characterize the azimuthal anisotropy of the energy flow even if we cannot account for their contributions to anisotropic particle flow v_n . We demonstrated that for small switching times where corona losses can be neglected, w_n and v_n closely track each other.

Our most important finding is that, contrary to traditional beliefs (see e.g. [15]), the anisotropic flow coefficients are not very sensitive to the thermalization (or switching) time as long as the latter does not significantly exceed about $2 \text{ fm}/c$. The reason is that anisotropic flow is not generated in the hydrodynamic stage, due to a reduced initial fireball eccentricity and shortened hydrodynamic stage when τ_s is allowed to grow

large, is almost precisely compensated for by anisotropies in the space-momentum correlations that develop during the free-streaming phase and manifest themselves as non-zero starting values for the momentum anisotropy of the energy-momentum tensor in the hydrodynamic stage. On the other hand, we found that an extended weakly coupled pre-equilibrium stage leads to stronger radial flow at the end of the hydrodynamic evolution, caused by large initial flow at the beginning of the hydrodynamic stage which is stronger than it would have been if the pre-equilibrium stage had been strongly coupled (i.e. described by hydrodynamics). This is a result of the faster signal propagation speed in the pre-equilibrium stage which, in the free-streaming case, is given by the speed of light and thus exceeds the hydrodynamic speed of sound by almost a factor 2. This kick-start of the radial flow by pre-equilibrium evolution overcompensates the loss of radial flow generated during the hydrodynamic stage which is shortened when the pre-equilibrium stage lasts longer.

It thus turns out that the mean transverse momentum $\langle p_\perp \rangle$ of the finally emitted hadrons, which (especially for the massive baryons) is strongly affected by the final radial flow of the fireball, provides a stronger upper limit on the thermalization time τ_s than the anisotropic flow coefficients. This agrees with recent findings by Romatschke and collaborators [81].

Of course, the switching time τ_s is only one of several model parameters affecting the final observables. In later chapter we perform an extended parameter search where we vary the switching time, decoupling temperature and specific shear viscosity of the fluid simultaneously, for two different initial state models and both runs with and without pre-equilibrium dynamics.

Chapter 3: The effects of bulk viscous and non-linear terms on viscous hydrodynamic evolution

3.1 Introduction

The second order viscous hydrodynamic equations [40,65] previously implemented in the VISH2+1 code were derived from the second law of thermodynamics in the Israel-Stewart formalism [37]. This code gained its success from describing and predicting experimentally observed hadronic spectra and anisotropic flows. However, when this code was written, the implications of the bulk viscous pressure were not well understood. Early studies [87,103] showed effects from bulk viscosity that were much smaller than those caused by the shear stress. Based on these works, most subsequent studies aimed at extracting the shear viscosity from experimental data and ignored the bulk viscosity.

Recently, more detailed studies on the bulk viscous effects have indicated non-negligible contributions from the bulk viscous pressure to the hadron anisotropic flows and mean transverse momenta [97,104–106], indicating that for a precise extraction of QGP transport properties, bulk viscosity can not be ignored. In order to extract the bulk viscosity from a model-to-data comparison, a more complete set of equations is needed which contains the nonlinear terms related to the bulk and shear pressure,

as well as the couplings between these two. This is because, while these nonlinear terms are smaller than the leading shear viscous terms, they still compete with the bulk viscous terms. Therefore, we upgrade the evolution equations in VISHNew to a more complete set derived from the Boltzmann equation [107].

In Section 3.2, we remind the readers of the previously implemented viscous hydrodynamic equations and show their updated versions, specifying the transport coefficients for the new equations. In Section 3.3, we discuss the range of applicability of viscous hydrodynamics with non-zero bulk viscosity and the effect of each of the nonlinear terms on the directly emitted particle spectra and anisotropic flows. In Section 3.5, we explore two different forms of the bulk viscous correction for the distribution function in the Cooper-Frye formula and discuss the effects of their differences on final observables. In Section 3.6, we present a detailed comparison between the updated VISHNew code and the (3+1)D MUSIC code developed at McGill University [69, 70], which evolves the same hydrodynamic equations as our updated VISHNew. We identify and discuss some numerical instabilities we found in VISH2+1 in Section 3.7.

3.2 Non-linear terms in the viscous hydrodynamic equations

In systems with zero net baryon density, hydrodynamics solves the conservation equations $\partial_\mu T^{\mu\nu} = 0$ for the energy momentum tensor

$$T^{\mu\nu} = eu^\mu u^\nu - (\mathcal{P} + \Pi)\Delta^{\mu\nu} + \pi^{\mu\nu}. \quad (3.1)$$

Here e and $\mathcal{P}$ are the energy density and thermal pressure in the local fluid rest frame (LRF), Π is the local bulk viscous pressure, $\pi^{\mu\nu}$ is the shear pressure tensor or “shear stress”, and u^μ is the local fluid velocity. $\Delta^{\mu\nu} \equiv g^{\mu\nu} - u^\mu u^\nu$ is the projection operator which projects onto the spatial coordinates in the LRF. As before, we work in Milne

coordinates (τ, x, y, η_s) , where $\tau = \sqrt{t^2 - z^2}$ and $\eta_s = \frac{1}{2} \ln \frac{t+z}{t-z}$, with spacetime metric $g^{\mu\nu} = \text{diag}(1, -1, -1, -1/\tau^2)$.

The evolution equations for the shear stress tensor and the bulk viscous pressure originally implemented in the VISH2+1 code were:

$$\begin{aligned} \Delta^{\mu\alpha} \Delta^{\nu\beta} u^\lambda d_\lambda \pi_{\alpha\beta} &= -\frac{1}{\tau_\pi} (\pi^{\mu\nu} - 2\eta\sigma^{\mu\nu}) \\ &\quad - \frac{1}{2} \pi^{\mu\nu} \frac{\eta T}{\tau_\pi} d_\lambda \left(\frac{\tau_\pi}{\eta T} u^\lambda \right), \end{aligned} \quad (3.2)$$

$$\begin{aligned} u^\lambda d_\lambda \Pi &= -\frac{1}{\tau_\Pi} (\Pi + \zeta\theta) \\ &\quad - \frac{1}{2} \Pi \frac{\zeta T}{\tau_\Pi} d_\lambda \left(\frac{\tau_\Pi}{\zeta T} u^\lambda \right). \end{aligned} \quad (3.3)$$

In the above equations, d_μ is the covariant derivative given in Eqs. (1.4), $\theta = d_\mu u^\mu$ is the scalar expansion rate, and $\sigma^{\mu\nu} = \frac{1}{2}(\nabla^\mu u^\nu + \nabla^\nu u^\mu - \frac{1}{3}\nabla^{\mu\nu}\theta)$ is the velocity shear tensor, with ∇^ν defined in Eq. (1.8). T is the local temperature, η is the shear viscosity, and ζ is the bulk viscosity. τ_π and τ_Π are the shear and bulk relaxation times; they should be calculated from a microscopic theory of the fluid but will here be treated as phenomenological parameters, with magnitudes estimated from the Boltzmann kinetic theory for a massless parton gas.

Ref. [107] gives the following generalized equations which contain all non-linear and coupling terms for a system with zero net baryon density:

$$\begin{aligned} \Delta_{\alpha\beta}^{\mu\nu} u^\lambda d_\lambda \pi^{\alpha\beta} &= -\frac{1}{\tau_\pi} (\pi^{\mu\nu} - 2\eta\sigma^{\mu\nu}) - \frac{\delta_{\pi\pi} \pi^{\mu\nu} \theta}{\tau_\pi} \\ &\quad + \frac{\varphi_7}{\tau_\pi} \pi_\alpha^{\langle\mu} \pi^{v\rangle\alpha} - \frac{\tau_{\pi\pi}}{\tau_\pi} \pi_\alpha^{\langle\mu} \sigma^{v\rangle\alpha} \\ &\quad + \frac{\lambda_{\pi\Pi}}{\tau_\pi} \Pi \sigma^{\mu\nu}, \end{aligned} \quad (3.4)$$

$$\begin{aligned} u^\lambda d_\lambda \Pi &= -\frac{1}{\tau_\Pi} (\Pi + \zeta\theta) - \frac{\delta_{\Pi\Pi}}{\tau_\Pi} \Pi \theta \\ &\quad + \frac{\lambda_{\Pi\pi}}{\tau_\Pi} \pi^{\mu\nu} \sigma_{\mu\nu}. \end{aligned} \quad (3.5)$$

Here the angular brackets around two indices μ and ν in Eq. (3.4) are a shorthand for the projection with $\Delta_{\alpha\beta}^{\mu\nu}$ given in the following equation:

$$A^{\langle\mu\nu\rangle} \equiv \Delta_{\alpha\beta}^{\mu\nu} A^{\alpha\beta}. \quad (3.6)$$

Comparing Eqs. (3.2) and (3.4), it can be shown [108] that for a massless system, the last term on the right hand side of Eq. (3.2) agrees with the $\delta_{\pi\pi}$ term in Eq. (3.4) for $\delta_{\pi\pi} = \frac{4}{3}\tau_{\pi}$. Eq. (3.4) contains three new terms with transport coefficients φ_7 , $\tau_{\pi\pi}$ and $\lambda_{\pi\Pi}$. φ_7 and $\tau_{\pi\pi}$ multiply higher-order terms that are non-linear in the shear stress tensor, while $\lambda_{\pi\Pi}$ accounts for the coupling of the shear stress tensor to the bulk viscous pressure. In the notation introduced in Chapter 2, the term $\sim \varphi_7$ is of second order in the inverse Reynolds number associated with $\pi^{\mu\nu}$, while the term $\sim \tau_{\pi\pi}$ is of order $\text{Kn} \cdot R_{\pi}^{-1}$. Comparing Eqs. (3.3) and (3.5), the last term on the right hand side of Eq. (3.3) is, for massless systems, equivalent to the $\delta_{\Pi\Pi}$ term in Eq. (3.5) with $\delta_{\Pi\Pi} = \frac{2}{3}\tau_{\Pi}$ [109]³. The only difference between Eq. (3.5) and Eq. (3.3) is the additional term in Eq. (3.5) proportional to $\lambda_{\Pi\pi}$ which takes into account the bulk-shear coupling.

The transport coefficients in the new equations have been calculated in [109] from the Boltzmann equation for a massless Boltzmann gas. For the shear tensor evolution

³For massless (conformally invariant) systems, of course, $\Pi = 0$. What we mean to say here is that, using the scaling relations between τ_{Π} , ζ and T that hold for conformal systems, the last term in Eq. (3.3) can be brought into the form $(\delta_{\Pi\Pi}/\tau_{\Pi})\Pi\theta$ with $\delta_{\Pi\Pi} = (2/3)\tau_{\Pi}$.

equation the authors of [109] give

$$\begin{aligned}
\tau_\pi &= \frac{5\eta}{e + \mathcal{P}}, \\
\delta_{\pi\pi} &= \frac{4}{3}\tau_\pi, \\
\lambda_{\pi\Pi} &= \frac{6}{5}\tau_\pi, \\
\tau_{\pi\pi} &= \frac{10}{7}\tau_\pi, \\
\varphi_7 &= \frac{18}{35(e + \mathcal{P})}.
\end{aligned} \tag{3.7}$$

For the bulk evolution equation, the transport coefficients are [109]

$$\begin{aligned}
\tau_\Pi &= \frac{\zeta}{14.55 \times \left(\frac{1}{3} - c_s^2\right)^2 (e + \mathcal{P})}, \\
\delta_{\Pi\Pi} &= \frac{2}{3}\tau_\Pi, \\
\lambda_{\Pi\pi} &= \frac{8}{5} \left(\frac{1}{3} - c_s^2\right) \tau_\Pi.
\end{aligned} \tag{3.8}$$

where $c_s^2 = \partial\mathcal{P}/\partial e$ is the squared speed of sound. In the absence of baryon flow, $\tau_\pi = \frac{5\eta}{e+\mathcal{P}} = \frac{5\eta/s}{T}$ only depends on the specific shear viscosity η/s and the local temperature T [109]. For simplicity we use a temperature-independent specific shear viscosity η/s in this study, such that $T\tau_\pi = 5\eta/s = \text{const.}$, as expected for an (approximately) conformal system.

For the specific bulk viscosity ζ/s , we adopt the parametrization given in [110] which smoothly matches its behavior in the QGP phase to that in the hadronic phase at a transition temperature $T_{tr} = 180 \text{ MeV}$ ⁴. The left panel of Fig. 3.1 displays this parametrization: the bulk viscosity has a peak at $T_{tr} = 180 \text{ MeV}$, reflecting a

⁴In view of the recent revised value for the pseudo-critical temperature of the quark-hadron phase transition, $T_c \approx 155 \text{ MeV}$ [9], this value for T_{tr} may seem high. We did not adjust it downward, however, since lower values of T_{tr} would maximize the bulk viscosity exactly where we want to match hydrodynamics to the hadron gas afterburner, which leads to uncontrollably large bulk viscous corrections to the distribution function in the Cooper-Frye formula. This issue deserves further study in future work.

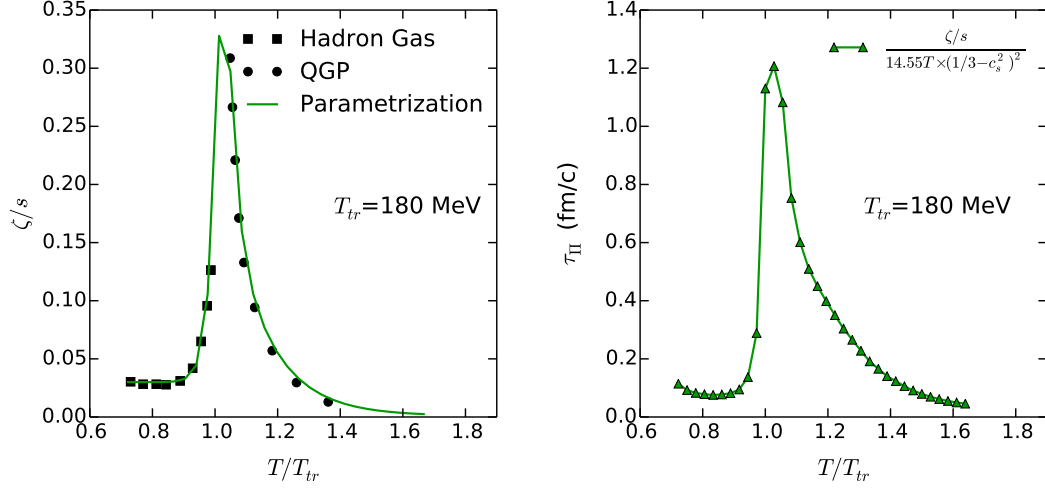


Figure 3.1: Left Panel: the specific bulk viscosity parametrization used here [110]. Right Panel: the bulk relaxation time as a function of T/T_{tr} .

large correlation length due to critical behavior at the quark-hadron phase transition which quickly decreases when the system temperature moves away from T_{tr} . One sees that the effects of bulk viscosity will mostly come from a narrow temperature window near T_{tr} . The right panel of Fig. 3.1 shows the bulk relaxation time from Eq. (3.8)⁵. Although the factor $c_s^2 - 1/3$ in the denominator also peaked near T_{tr} , the shape of τ_{Π} is dominated by the stronger peak of ζ/s at $T \sim T_{tr}$. This causes the bulk pressure to evolve more slowly near T_{tr} . This phenomenon is called “critical slowing down”, and was studied in Ref. [87]. We use the forms shown in Fig. 3.1 for $(\zeta/s)(T)$ and $\tau_{\Pi}(T)$ throughout this chapter.

⁵For this plot, the speed of sound c_s^2 in this plot is taken from lattice QCD results given in [111]. In the hydrodynamic simulation, c_s^2 is calculated on the fly from the energy density and pressure given by the equation of state [112], which is also obtained from lattice QCD results, but somewhat older ones [8].

3.3 Applicability of viscous hydrodynamics with non-zero bulk viscosity

After including bulk viscosity into the hydrodynamic evolution, it is possible that a large bulk viscous pressure may turn the effective pressure $\mathcal{P} + \Pi$ negative. Negative effective pressure makes the liquid mechanically unstable against cavitation [113, 114] and therefore pushes the viscous hydrodynamic formalism beyond its range of validity [115]. So before applying our hydrodynamic code to study the QGP evolution, it is necessary to check its region of validity. In this chapter, we achieve this by monitoring the inverse Reynolds numbers and Knudsen numbers during the hydrodynamic evolution with non-zero bulk viscosity. For simplicity, we use single-shot hydro simulations. The fluctuating initial conditions are averaged over a large number of bumpy events given by the MC-Glb model [49] for Au+Au collision at $\sqrt{s_{NN}} = 200$ GeV and 10% - 20% centrality, resulting in a smooth average initial density profile. We perform this test for top RHIC energy because at this energy the system spends a larger fraction of time in the region where the bulk viscosity is large than at LHC energy, and thus bulk viscous pressure effects will be most prominent. The hydrodynamic evolution is assumed to start at $\tau = 0.6$ fm/ c , and the freeze-out is taken to happen at a constant energy density of $e = 0.18$ GeV/fm³. We fix the specific shear viscosity at $\eta/s = 0.2$. At each time step of the hydrodynamic simulation, we calculate the inverse Reynolds numbers related to the shear stress and bulk pressure, as well as the Knudsen number related to the scalar expansion rate at each spatial

lattice point as

$$R_{\pi}^{-1} = \frac{\sqrt{\pi^{\mu\nu}\pi_{\mu\nu}}}{\mathcal{P}}, \quad (3.9)$$

$$R_{\Pi}^{-1} = \frac{|\Pi|}{\mathcal{P}}, \quad (3.10)$$

$$\text{Kn}_{\theta} = \frac{\lambda_{mfp}}{L_{macro}} = \tau_{\pi}\theta = 5\frac{\eta\theta}{sT}, \quad (3.11)$$

where τ_{π} is taken from Eq. (3.7). When both quantities are much smaller than 1, the hydrodynamic description is applicable. If R_{π}^{-1} or R_{Π}^{-1} do not fulfill this condition, it may indicate that the system is too dissipative and that second-order viscous hydrodynamics is no longer a good approximation. If $\text{Kn}_{\theta} > 1$, collisions are not frequent enough to counter act the expansion rate, driving the system out of thermal equilibrium and stresses the validity of viscous fluid dynamics.

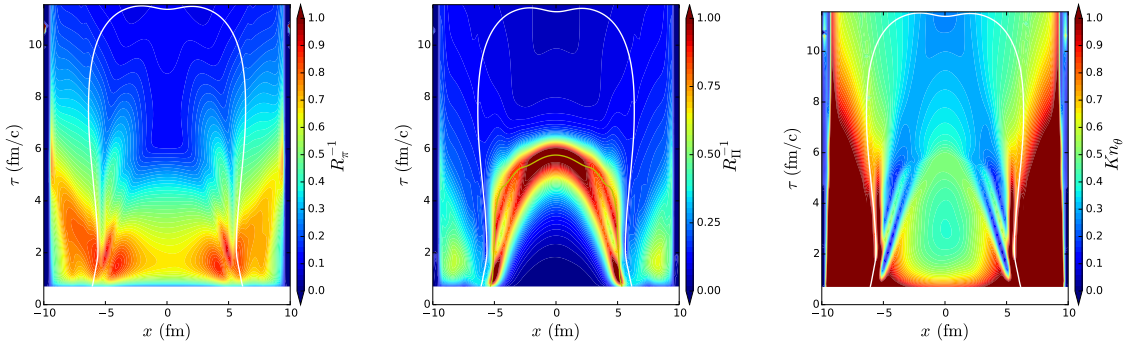


Figure 3.2: Contour plots for the evolution of the inverse shear Reynolds number R_{π}^{-1} (left panel), inverse bulk Reynolds number R_{Π}^{-1} (middle panel), and the Knudsen number Kn_{θ} (right panel) in a viscous hydrodynamic simulation. The white contour line in each plot represents the freeze-out surface at energy density $e = 0.18 \text{ GeV/fm}^3$, and the yellow line in the middle panel denotes $T_{tr} = 180 \text{ MeV}$ where $(\zeta/s)(T)$ reaches its peak value.

Fig. 3.2 shows how the inverse shear Reynolds numbers and the Knudsen number along the x -axis in the transverse plane evolve with time. The white contour denotes

the freeze-out surface. Red regions indicate large R_π^{-1} , R_Π^{-1} or Kn_θ . Large inverse shear Reynolds numbers show up at early times, but as the system evolves, R_π^{-1} decreases. This indicates that the validity of hydrodynamics is problematic only at early times. Large inverse bulk Reynolds numbers occur mostly near the $T_{tr} = 180$ MeV surface where the bulk viscosity peaks. Large Knudsen numbers also show up at early times, but disappear from the inside of the freeze-out surface after the system has evolved for a few fm/c. Noticeably, there are two red ridges just inside the freeze-out surface around $x = \pm 5$ fm/c, which are due to the large expansion rate near the edge of the fireball. Most of the region inside the freeze-out surface, however, has both R_π^{-1} and Kn_θ much smaller than 1. In summary, the regions where viscous hydrodynamics may be operating outside its domain of validity are mostly outside the freeze-out surface and at early times, with a possibility of problems near T_{tr} arising from the large bulk viscous pressure near the quark-gluon phase transition. The problems at early times indicate the need for describing the earliest stages of the collision microscopically with a pre-equilibrium model, while the breakdown of viscous hydrodynamics in the region outside the edge of the fireball has little effect on the calculation of physical observables on the freeze-out surface.

A better strategy inspired by [116] would be to check the magnitude of the second-order terms in the equation of motion for the shear stress $\pi^{\mu\nu}$ against that of the first-order term $\sqrt{4\eta^2\sigma^{\mu\nu}\sigma_{\mu\nu}}$, and similarly for the bulk viscous pressure:

$$\begin{aligned} \left(\tilde{R}_\pi^{(2)}\right)^{-1} &= \frac{\delta_{\pi\pi} |\theta| \sqrt{\pi^{\mu\nu}\pi_{\mu\nu}}}{2\eta\sqrt{\sigma_{\mu\nu}\sigma^{\mu\nu}}}, \\ \left(\tilde{R}_\Pi^{(2)}\right)^{-1} &= \frac{\delta_{\Pi\Pi} |\theta\Pi|}{\zeta |\theta|} = \frac{\delta_{\Pi\Pi} |\Pi|}{\zeta}. \end{aligned} \quad (3.12)$$

Additionally, we can also check the magnitude of the second-order correction to the leading order:

$$\begin{aligned}\left(R_{\pi}^{(2)}\right)^{-1} &= \frac{\delta_{\pi\pi} |\theta| \sqrt{\pi^{\mu\nu} \pi_{\mu\nu}}}{\mathcal{P}}, \\ \left(R_{\Pi}^{(2)}\right)^{-1} &= \frac{\delta_{\Pi\Pi} |\theta\Pi|}{\mathcal{P}}.\end{aligned}\tag{3.13}$$

Fig. 3.3 displays the time evolution of these quantities measured along the x -axis. For the bulk viscous part, the second-order correction is much smaller than both the first-order and leading-order terms. Large second-order corrections only exist near T_{tr} where the bulk viscosity peaks. In the shear viscous part, however, the second-order correction is generally smaller than the leading-order term except for at very early times. It is surprising the second-order correction is no smaller than the first-order correction. This is shown in Fig. 3.3 with a large yellow - red region inside the freeze-out surface in the $\left(\tilde{R}_{\pi}^{(2)}\right)^{-1}$ evolution plot. This is surprising because in Section 3.4 below we found that the second-order corrections $\sim \varphi_7$, $\tau_{\pi\pi}$ and $\lambda_{\pi\Pi}$ show only very weak effects on the hadron spectra and anisotropic flows. In contrast to that, the left upper panel in Fig. 3.3 shows that the second-order term $\sim \delta_{\pi\pi}$ has a size that is comparable with the Navier-Stokes terms. While the importance of the $\delta_{\pi\pi}$ term has been noticed before [41], it is not clear to us why the remaining second-order terms are so much smaller.

In Fig. 3.3, the yellow - red region has some similarity in shape with $T_{tr} = 180$ MeV. We therefore suspected that this large second-order correction maybe caused by feed back from the bulk viscous pressure evolution into the shear stress through the shear - bulk coupling term $\sim \lambda_{\pi\Pi}$ in Eq. (3.4). To test this hypothesis we set this coupling term to zero, and plot the results in Fig. 3.4. Clearly, the ratio $\left(\tilde{R}_{\pi}^{(2)}\right)^{-1}$ hardly changes from Fig. 3.3 to Fig. 3.4 when we turn off the shear - bulk coupling

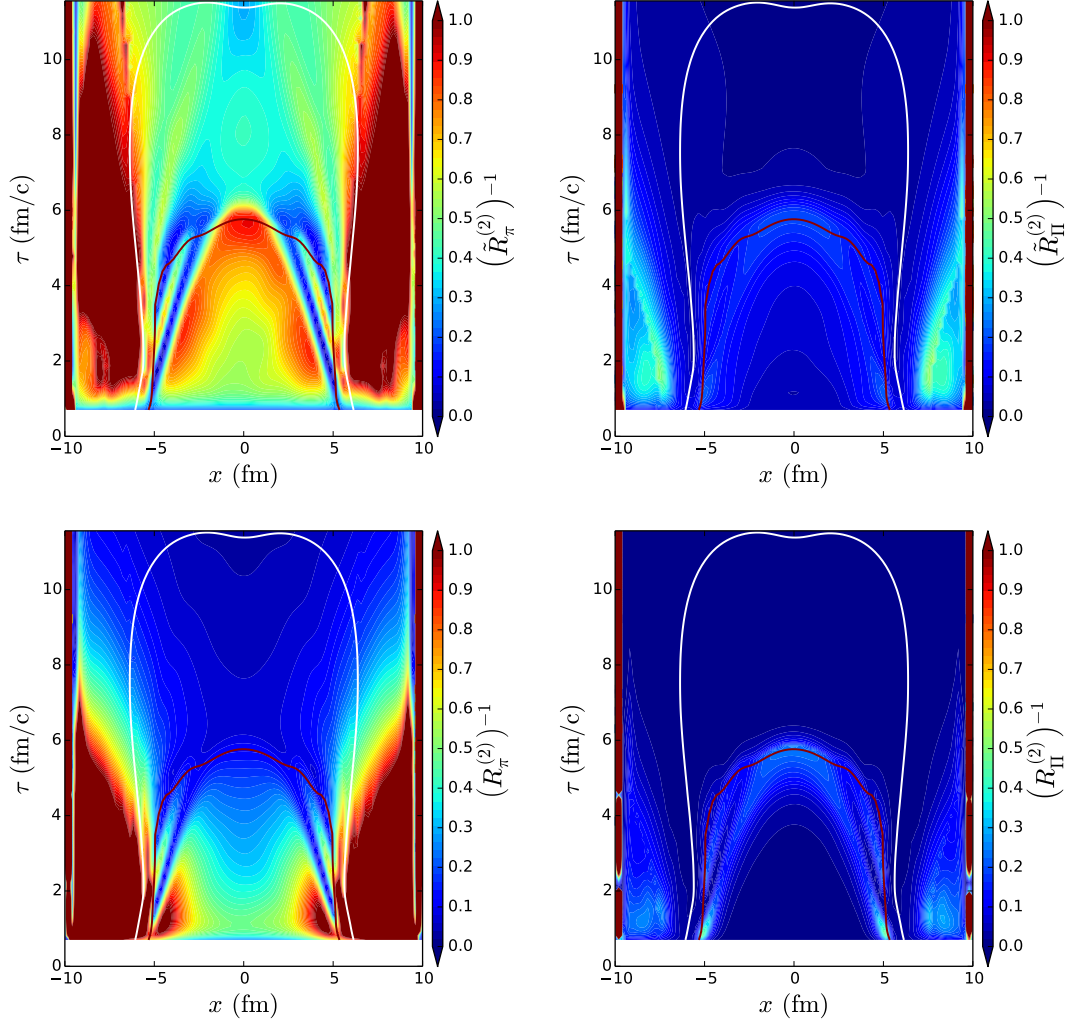


Figure 3.3: Contour plots for the evolution of the higher-order inverse Reynolds numbers in a viscous hydrodynamic simulation. The two upper panels show the ratio of the second-order to the first-order corrections for both shear and bulk viscous pressure, as defined in (3.12). The two lower panels show the ratio of the second-order to the leading-order corrections defined in (3.13). The white line in each panel represents for the freeze-out surface at $e = 0.18$ GeV/fm³ and the dark red lines denote $T_{tr} = 180$ MeV where $(\zeta/s)(T)$ (both ζ and s depend on T , but here we are focusing on the T -dependence of the ratio ζ/s : $(\zeta/s)(T)$) reaches its peak value.

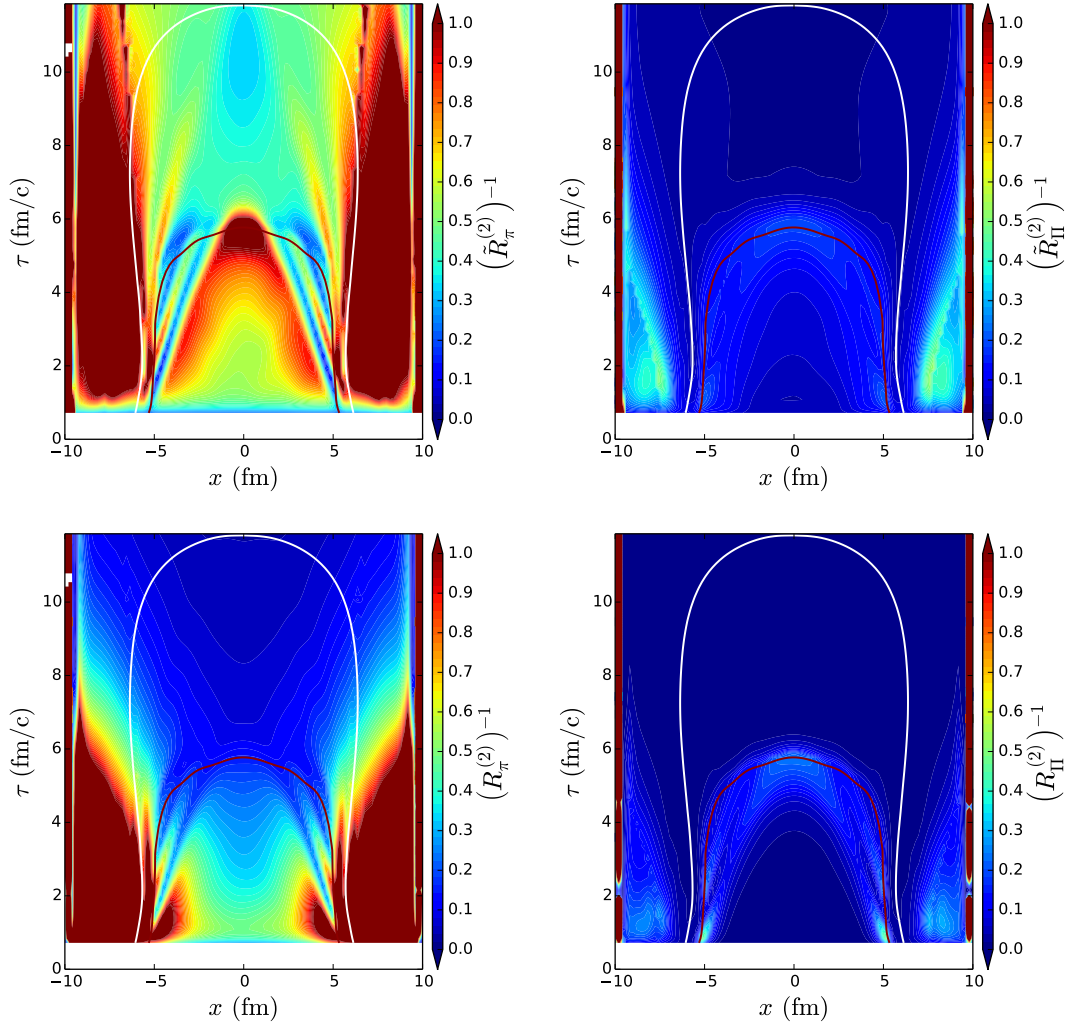


Figure 3.4: Same as Fig. 3.3 but for zero shear - bulk coupling $\sim \lambda_{\pi\Pi}$ in Eq. (3.4).

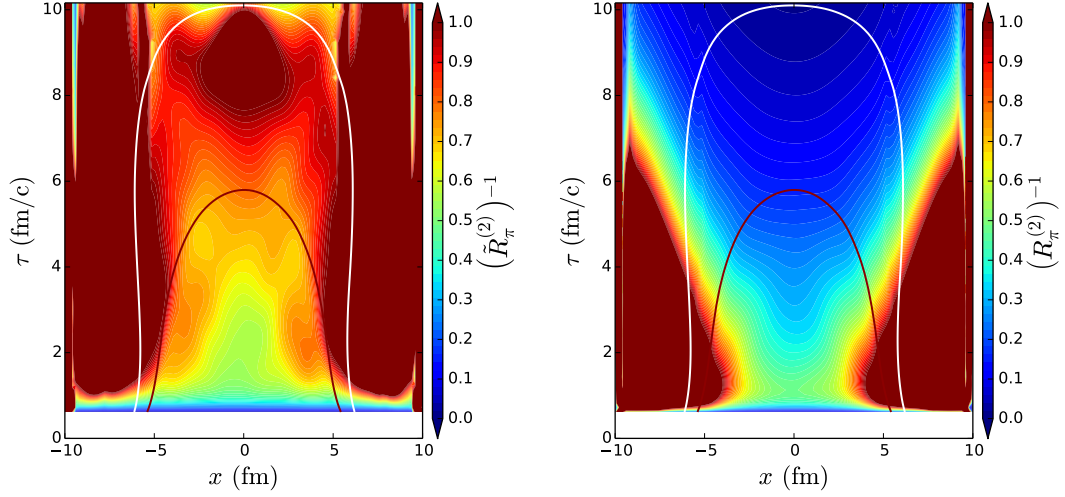


Figure 3.5: Same as Fig. 3.3, for zero bulk viscosity, $\zeta/s = 0$.

term. Therefore the relatively large second-order corrections seen in Fig. 3.3 are not due to the bulk viscous pressure. If we check the shape of the red triangular region inside the freeze-out surface in the top left panel, it suggests a signal propagating from the edge of the fireball to the center of the fireball with a speed $\sim 0.76c$, which is larger than the speed of sound. We suspect that this could be a numerical effect or a deflagration shock. Its origin requires further studies.

Fig. 3.5 shows additionally that $\left(\tilde{R}_\pi^{(2)}\right)^{-1}$ becomes large inside the entire fireball if we set the bulk viscosity to zero. We do not have a thorough understanding of this phenomenon either. We expect the bulk viscous pressure to reduce the scalar expansion rate, which should make the first ratio in Eq. (3.12) smaller. Again, we have to leave the resolution of this puzzle to future studies.

3.4 The effects of the non-linear terms

In this section, we discuss the effects of the newly added non-linear and coupling terms in Eqs. (3.4) and (3.5) on the spectra and elliptic flow of directly emitted (“thermal”) pions escaping from the freeze-out surface. To illustrate the effect of each term, we begin this investigation by setting ζ/s and the transport coefficients (i.e. φ_7 , $\tau_{\pi\pi}$ and $\lambda_{\pi\Pi}$) for the non-linear terms in Eq. (3.4) to zero. We will then turn on these coefficients one by one while keeping $\zeta/s = 0$. In each run, thermal pion spectra and elliptic flow are calculated with the Cooper-Frye formula [71]

$$\frac{dN_i}{dy p_\perp dp_\perp d\varphi_p} = \frac{g_i}{(2\pi)^3} \int_{\Sigma_{fo}} p \cdot d^3\sigma(x) f_i(x, p). \quad (3.14)$$

Then we repeat the above process with the nonzero ζ/s shown in Fig. 3.1, eventually also turning on the non-linear term $\sim \lambda_{\Pi\pi}$ in Eq. (3.5). The distribution for hadron species i after freeze-out is given by

$$f_i = f_{0,i} + \delta f_{\text{shear},i} + \delta f_{\text{bulk},i}, \quad (3.15)$$

where $f_{0,i}$ is the equilibrium distribution, and $\delta f_{\text{shear},i}$ and $\delta f_{\text{bulk},i}$ account for the shear and bulk viscous corrections, respectively. The shear viscous correction is given by [94, 95]

$$\delta f_{\text{shear},i} = f_{0,i}(1 \pm f_{0,i}) \frac{\pi^{\mu\nu} p_\mu p_\nu}{2T^2(e + \mathcal{P})}. \quad (3.16)$$

For the bulk correction, we use the formula given in [105], derived from the Boltzmann equation in the relaxation time approximation :

$$\delta f_{\text{bulk},i} = -f_{0,i}(1 \pm f_{0,i}) \frac{\Pi}{C_\Pi} \left[\frac{1}{u \cdot p} \frac{m_i^2}{3} - \left(\frac{1}{3} - c_s^2 \right) (u \cdot p) \right], \quad (3.17)$$

where C_{Π} is a temperature-dependent coefficient. The v_2 and hadron $p_{\perp}$ -distributions resulting from the use of (3.17) differ from those resulting from the results of the analysis given in [96], especially at high $p_{\perp}$. We will explore these differences in Section 3.5.

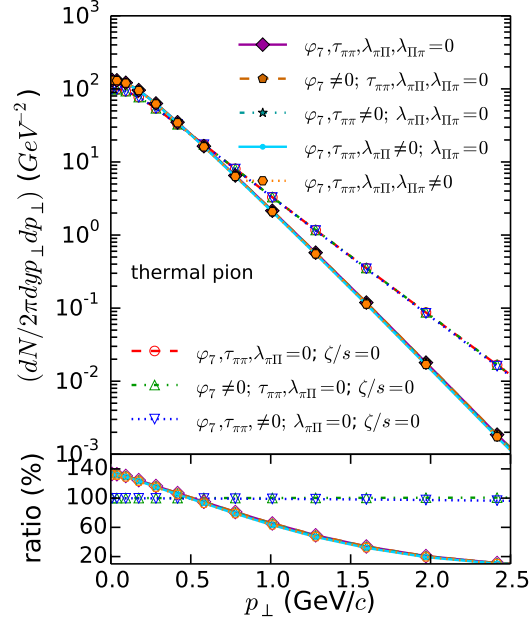


Figure 3.6: Thermal pion spectra (upper panel) and ratio (lower panel) with non-linear terms turned on one by one. Lines with unfilled markers stand for the runs with zero bulk viscosity, while the lines with filled marker are for those with temperature dependent bulk viscosity. In the lower panel, the spectra of each run is contrasted with the run in which the transport coefficients for non-linear terms are zero and $\zeta/s = 0$.

Figures 3.6 and 3.7 show the spectra and $p_{\perp}$ -differential elliptic flow of thermal pions, with non-linear terms turned on one by one. In Fig. 3.6 we observe that the lines fall into two groups, one corresponding to zero bulk viscosity and the other corresponding to non-zero bulk viscosity. This shows that the presence or not of

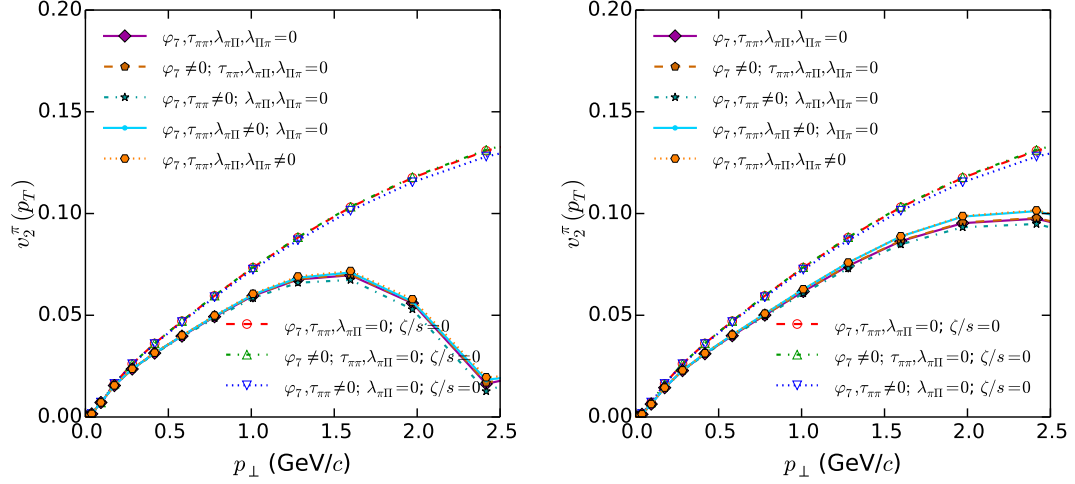


Figure 3.7: Left: $p_{\perp}$ -differential thermal pion elliptic flow with non-linear terms turned on one by one. Line styles are the same as in Fig. 3.6. The upper (lower) set of curves correspond to $\zeta/s = 0$ ($\zeta/s \neq 0$). Right: the same as the left panel but without the bulk viscous correction to the hadron distribution, i.e. for $\delta f_{\text{bulk}} = 0$.

bulk viscosity is more important than all the non-linear terms, individually or taken together. As we see in Fig. 3.6, the spectra become steeper when $\zeta/s > 0$ is accounted for. This is easily understood: bulk viscosity resists the expansion of the system and the generation of radial flow. Decreasing radial flow reduces the flow - induced blue-shift of the emitted particle momenta, leading to steeper $p_{\perp}$ -spectra. As a result of the action of the bulk viscous pressure, the pion spectra can be increased by 40% at low $p_{\perp}$ while decreasing by up to a factor 5 at $p_{\perp} \sim 2$ GeV/c. This obviously reduces the mean transverse momentum but also affects the $p_{\perp}$ -distributions of the anisotropic flows. In each cluster of curves in Fig. 3.6, however, the inclusion of non-linear terms or shear bulk coupling terms does not lead to any visible difference in the $p_{\perp}$ -spectra.

The effect on the $p_{\perp}$ -distribution of the elliptic flow is studied in Fig. 3.7. The bulk pressure is still the dominant factor while non-linear terms have only a minor

influence on $v_2^\pi(p_\perp)$. Bulk pressure strongly suppresses the elliptic flow above $p_\perp \sim 0.3$ GeV/ c . The large suppression at high $p_\perp$ seen in the left panel is mostly caused by the large bulk viscous correction to the pion distribution function on the decoupling surface. To show this, we present the same quantities shown in the left panel of Fig. 3.7 again in the right panel, but this time setting $\delta f_{\text{bulk}} = 0$ in Eq. (3.14). We see that with δf_{bulk} this suppression of $v_2^\pi(p_\perp)$ by bulk viscous effect is much smaller. We will discuss this more in the following section. Shear-bulk coupling terms do not exhibit a strong effect on the observables. This appears to be different from (0+1)D systems where shear-bulk coupling terms were found to be important in [104].

3.5 Comparison of two types of bulk viscous corrections

Significant theoretical uncertainties are associated with the form of the bulk viscous correction δf_{bulk} . Several ansätze were discussed in [97]. Here we compare the thermal particle spectra and elliptic flow calculated with two different versions of the bulk viscous corrections δf_{bulk} - the 14-moment approximation [96] and the relaxation time approximation [105] - to illustrate the theoretical uncertainty in several physical observables induced by the bulk viscous correction. Unfortunately, we cannot offer a resolution of this ambiguity.

In [78], we used the bulk viscous correction formula derived from the 14-moment approximation for particles with Boltzmann statistics [96]:

$$\delta f_{\text{bulk},i} = -f_{0,i} \Pi \left[B_{0,i} m_i^2 + D_{0,i} u^\mu p_\mu + E_{0,i} (u^\mu p_\mu)^2 \right], \quad (3.18)$$

where the coefficients $B_0(T)$, $D_0(T)$ and $E_0(T)$ were calculated in [97] from a non-interacting hadron resonance gas in the Boltzmann limit.

Comparing with (3.17), which was derived from the relaxation time approximation for the collision term in [109, 117], the 14-moment formula is a quadratic function of the hadron mass m_i at low momentum and a quadratic function of $p_\perp$ at high momentum, while the relaxation time form for $\delta f_{\text{bulk},i}$ has a more moderate linear mass dependence at low momentum and linear $p_\perp$ -dependence at high momentum. Therefore at high momentum the 14-moment $\delta f_{\text{bulk},i}$ modifies f_i more aggressively. We also notice that in the high-momentum region the 14-moment $\delta f_{\text{bulk},i}$ sometimes overwhelms the thermal distribution and turns f_i negative, which means that particles move into the freeze-out surface instead of leaving it. We avoid this unphysical picture by manually setting f_i to zero in such a situation.

Fig. 3.8 shows a comparison of the thermal particle spectra calculated with different assumptions for δf_{bulk} . Dash-dotted lines stand for $\delta f_{\text{bulk}} = 0$ in Eq. (3.15). Dashed lines are the spectra calculated after including in (3.15) the 14-moment bulk viscous correction (3.18), and the solid lines correspond to using the relaxation time formula (3.17) instead of (3.18). We notice that including a non-zero δf_{bulk} affects the spectra over the entire $p_\perp$ range. Both the 14-moment and the relaxation time formulae lead to a suppression on of the spectra at high $p_\perp$ and an enhancement at low $p_\perp$. We also note that the 14-moment f_{bulk} decreases the spectra almost by a factor of 5 near $p_\perp = 2.5 \text{ GeV}/c$.

Fig. 3.9 shows a similar comparison for $v_2(p_\perp)$. The results using these three δf_{bulk} are similar at low $p_\perp$, but diverge above $p_\perp = 0.6 \text{ GeV}/c$. We notice that the relaxation time bulk viscous correction suppresses the elliptic flow most strongly at high momentum. This suppression is more prominent than the one seen in the results

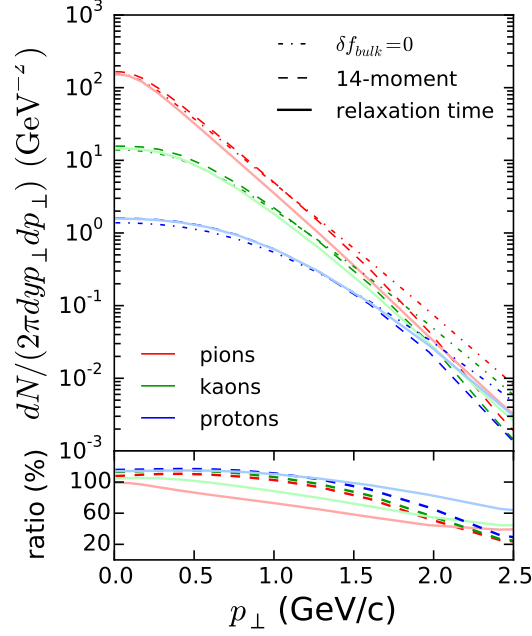


Figure 3.8: Upper panel: a comparison of the $p_{\perp}$ -spectra for thermal pions, kaons and protons calculated with different assumptions for δf_{bulk} as described in the text. Different colors represent different particle species, and different line types represent different choices of δf_{bulk} . Lower panel: the ratio of the spectra calculated with the 14-moment (dashed line) and the relaxation time (solid line) δf_{bulk} to the spectra calculated with $\delta f_{\text{bulk}} = 0$.

of Ref. [97], where ζ/s was taken to be smaller than ours by almost a factor of 20 (but with a similar temperature dependence).

In Table 3.1, we compare the $p_{\perp}$ -integrated elliptic flow and the mean hadron transverse momentum resulting from the three different choices for δf_{bulk} . Both elliptic flow and mean transverse momentum are calculated for particles with $p_{\perp} > 0$ and within the rapidity range $-0.5 < y < 0.5$. The differences in the integrated elliptic flow and the mean $p_{\perp}$ reflect the fact that the different forms of the bulk viscous correction give different shapes for the $p_{\perp}$ -spectra. The integrated elliptic flow exhibits sensitivity to the choice of δf_{bulk} at the level of about 5%. The sensitivity of the mean

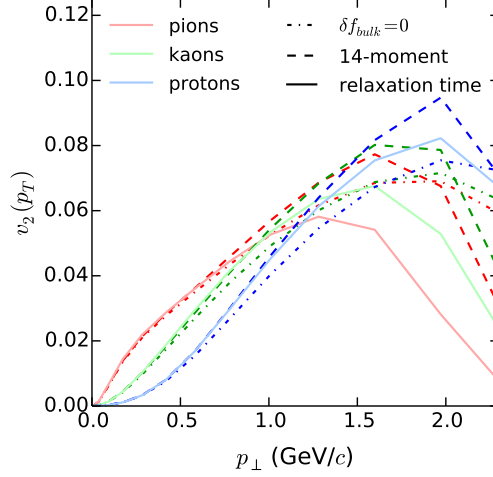


Figure 3.9: A comparison of $p_{\perp}$ -differential elliptic flow for thermal particles between calculations where δf_{bulk} is set to zero in Eq. (3.15) (dash-dotted lines) and others where δf_{bulk} is included in the 14-moment (dashed line) and relaxation time (solid line) approximation. Legends are the same as Fig. 3.8.

transverse momentum to δf_{bulk} is larger and can reach 10%. Clearly, this will result in theoretical uncertainties when trying to extract η/s and ζ/s from a model-data comparison.

Mode	$\delta f_{\text{bulk}} = 0$	14-moment	relaxation time
$\bar{v}_2^{\pi^+}$	0.030	0.031	0.029
$\bar{v}_2^{K^+}$	0.031	0.032	0.031
$\bar{v}_2^p$	0.033	0.035	0.033
$\langle p_{\perp} \rangle_{\pi^+}$ (GeV/c)	0.507	0.491	0.469
$\langle p_{\perp} \rangle_{K^+}$ (GeV/c)	0.686	0.654	0.644
$\langle p_{\perp} \rangle_p$ (GeV/c)	0.903	0.848	0.867

Table 3.1: A summary of $p_{\perp}$ -integrated elliptic flow and mean transverse momentum values for thermal pions, kaons, and protons with $p_{\perp} > 0$ and rapidity $-0.5 < y < 0.5$, calculated with choices for δf_{bulk} discussed in the text.

3.6 Code comparison between VISH2+1 and MUSIC

In this section, we present a code comparison between two numerical codes for viscous hydrodynamics: VISH2+1 (in its more robust VISHNew version [18]) and MUSIC [69,70]. The hydrodynamic equations solved by both programs are the same. The differences are the dimensionality of the system and the numerical algorithm used for propagating the solution in time. VISH2+1 assumes longitudinal boost-invariance and solves the hydrodynamic equations in two spatial dimensions, while MUSIC solves the equations in three spatial dimensions, without assuming boost invariance in the longitudinal direction. This code comparison aims to test their convergence, in addition to identifying and eliminate possible coding errors. In this test, MUSIC is run with boost-invariant initial conditions such that the same physical situations are implemented in both codes. The initial conditions in the transverse plane, the hydrodynamic starting time and the decoupling energy density are the same as discussed above in this chapter. We use the chemical equilibrium equation of state from [112]. Our comparison includes the evolution of a number of hydrodynamic quantities throughout the evolution and thermal particle observables after freeze-out.

The left panel of Fig. 3.10 shows a comparison of temperature evolution between these two codes. Each curve represents a temperature profile in the transverse plane along the axis $y = 0$ for a constant proper time, with solid lines for VISH2+1 and markers for MUSIC. The two codes generally agree with each other very well. However, we observe some discrepancies at the edge of the fireball at late times, where the temperature of VISH2+1 drops faster than in MUSIC. This is due to the edge regularization used in VISH2+1, which suppresses the energy momentum tensor at the edge to stabilize the code. This regularized region is far outside the freeze-out

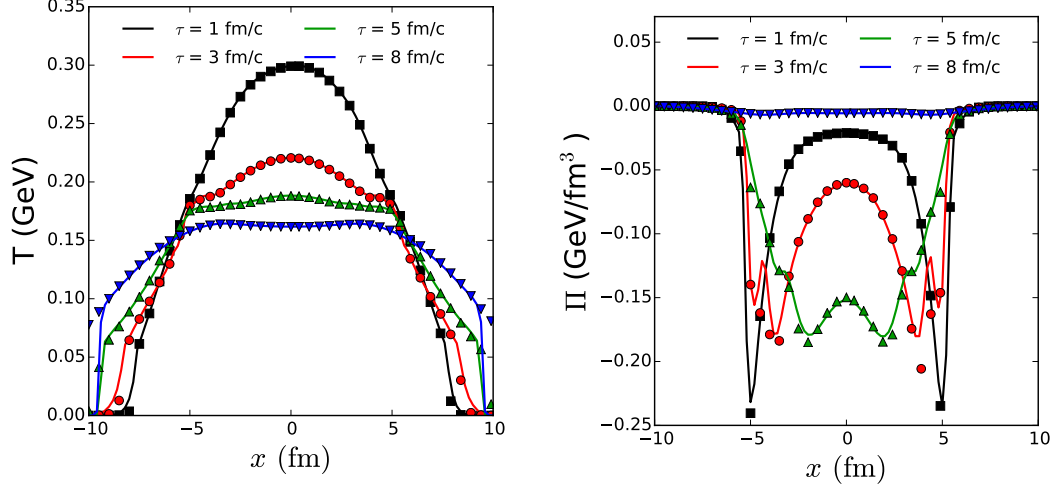


Figure 3.10: Time evolution of the temperature (left panel) and bulk viscous pressure (right panel) along the x axis in the transverse plane. Solid lines are the results from VISH2+1, while filled markers are from MUSIC.

surface, so it does not affect the physical observables. The right panel of Fig. 3.10 displays the bulk viscous pressure evolution, and again the two codes give generally very similar results. We note, however, that at $\tau = 3$ fm/ c VISH2+1 shows for Π two pairs of spikes near $x = \pm 5$ fm where MUSIC has single spikes. The temperatures of these two regions are close to $T_{tr} = 180$ MeV where the bulk viscosity ζ/s peaks. These spikes indicate a possible instability in VISH2+1. We will explore this in more detail in Section 3.7. In Fig. 3.11 we compare several components of the shear stress tensor. The two codes are seen to give almost identical shear viscous pressure components along the x -axis throughout the evolution, except for some minor discrepancies around $x = \pm 5$ fm. The latter are likely caused by feedback of the above instability in the bulk viscous pressure Π into the shear stress $\pi^{\mu\nu}$ via bulk-shear coupling.

Having confirmed that the two codes give very similar results throughout the hydrodynamic evolution stage, we compare the thermal particle spectra and flow

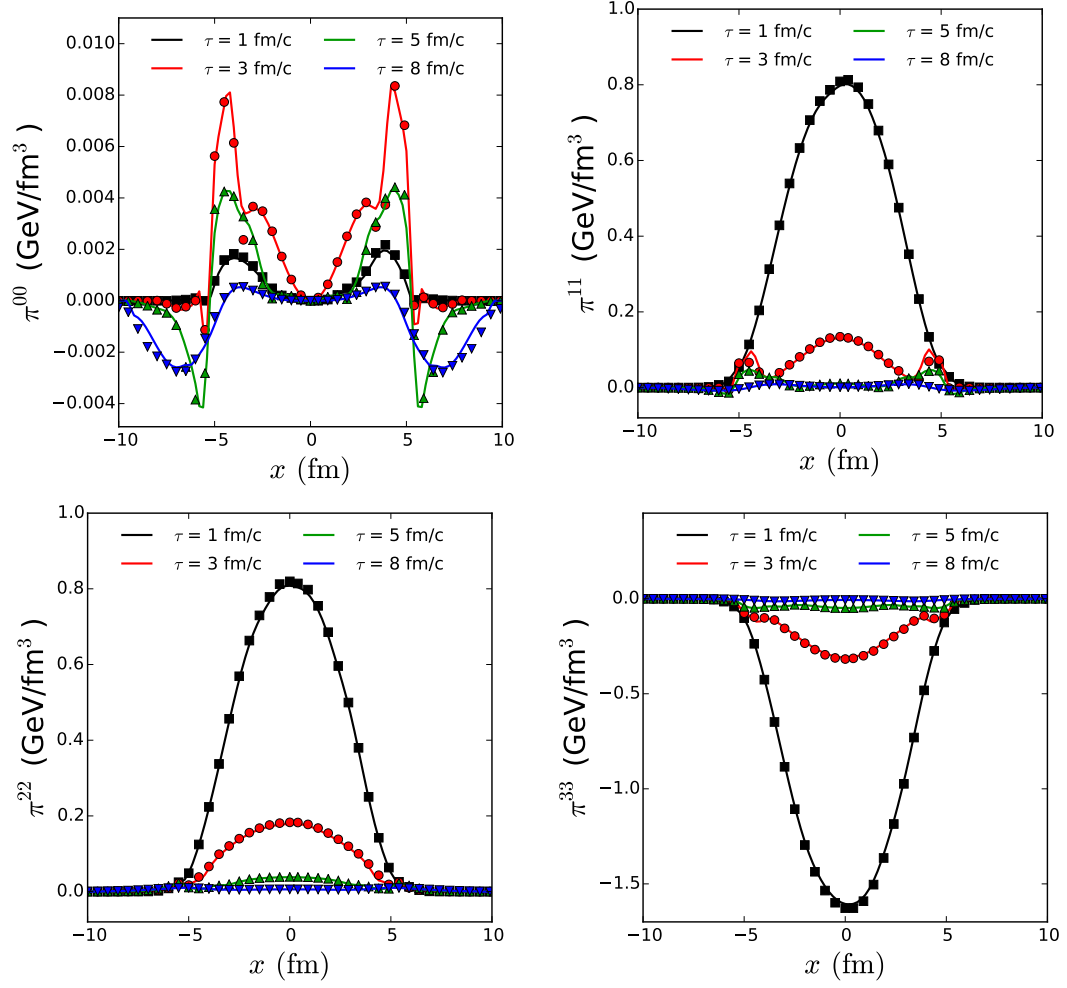


Figure 3.11: A comparison of the diagonal components of the shear stress tensor between VISH2+1 and MUSIC. Legend is the same as in Fig. 3.10.

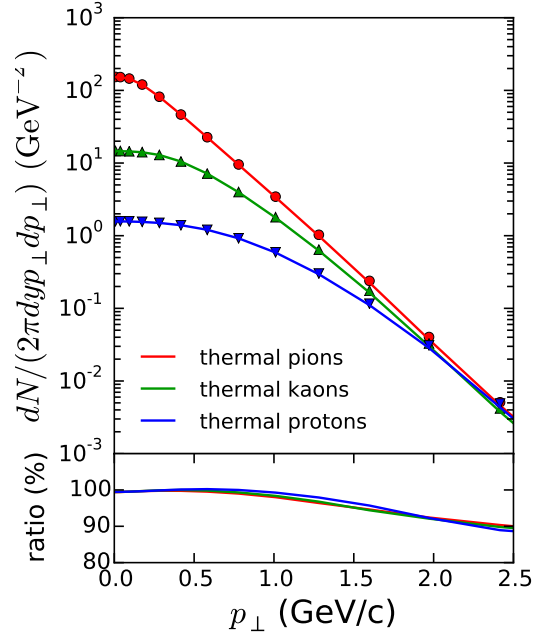


Figure 3.12: Upper panel: a comparison of thermal pion, kaon and proton spectra between VISH2+1 and MUSIC. The legend is the same as in Fig. 3.10. Lower panel: the ratio of VISH2+1 over MUSIC spectra.

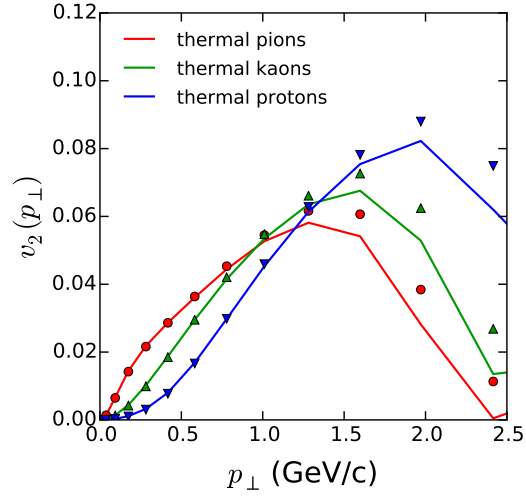


Figure 3.13: A comparison of $p_{\perp}$ -differential flow for thermal particles between VISH2+1 and MUSIC. The legend is the same as Fig. 3.10.

after converting the hydrodynamic quantities to hadrons on the freeze-out surface, using the same numerical Cooper-Frye code. For bulk viscous correction we use the relaxation time formula (3.17) in both cases. Fig. 3.12 compares the $p_\perp$ -spectra. We see that the spectra agree with each other at the level of a few percent for $p_\perp < 1$ GeV/ c but disagree by up to 10% at $p_\perp \approx 2.5$ GeV/ c . This is consistent with an earlier comparison which was conducted with zero bulk viscosity and showed a 10% difference between the two codes [118]. The $p_\perp$ -differential elliptic flow agrees for $p_\perp < 1.3$ GeV/ c , but diverges at large $p_\perp$, with VISH2+1 producing much smaller elliptic flow than MUSIC. We also compared the $v_2(p_\perp)$ for ideal hydrodynamics and we observed no differences between the codes; the differences appear only for non-zero viscosities. They point to differences in the numerical precision with which the two codes propagate the viscous pressure components. Unfortunately, we were not able to assess which of the two codes has higher precision. Comparison of the “Gubser test” of VISH2+1 in [18] with that of MUSIC presented in [119] suggests that VISH2+1 may be slightly more accurate, due to the exact implementation of boost-invariance. The ability of MUSIC to handle 3-dimensional initial conditions may have been bought by sacrificing some precision in the 2-dimensional case with boost-invariance.

3.7 Instability in bulk viscous pressure evolution

In the right panel of Fig. 3.10, we saw an instability of VISH2+1 in its propagation of the bulk viscous pressure. Here we explain what causes the spikes in Fig. 3.10 and how these spikes affect the final observables. The spikes indicate discontinuities along the x -direction. As shown in Fig. 3.14, spikes appear in the scalar local expansion rate at the same locations as those in the right panel of Fig. 3.10. MUSIC suffers

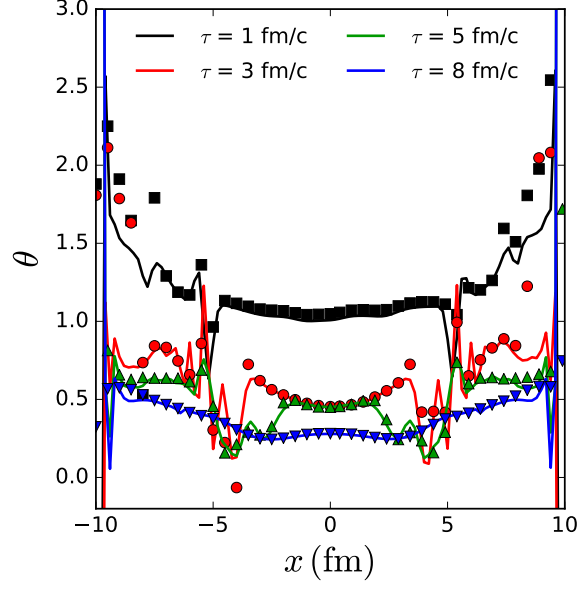


Figure 3.14: Time evolution of the local scalar expansion rate along the x axis in the transverse plane. The solid lines are given by VISH2+1 while the solid markers denote the results from MUSIC.

from the same problem, but with less severity. To check whether the discontinuities might be due to a spatial grid spacing which is too large and can cause the spatial derivatives to be unreliable, we decreased the spatial grid spacing from the default value $\Delta x = \Delta y = 0.1$ fm to $\Delta x = \Delta y = 0.05$ fm, keeping the proper time spacing $\Delta t = 0.02$ fm/c fixed. However, this change introduces lots of regulations on the bulk viscous pressure in fireball domains with temperatures near $T_{tr} = 180$ MeV (whenever $|\Pi|$ becomes larger than $\mathcal{P}$, the code regulates Π to smaller values [18]). These regulations were found to worsen the agreement with MUSIC. To find the reason for the increase of the number of Π -regulations, we compared the corresponding Navier-Stokes limits of the bulk pressure, $\Pi_{NS} = -\zeta\theta$, for these two grid settings with each other and with MUSIC, as shown in Fig. 3.15. In this figure, we use unfilled markers

to denote instances where bulk viscous pressure regulation happens. MUSIC and VISH2+1 with the larger grid spacing do not show any instances of Π regulation. VISH2+1 with the smaller grid spacing experiences Π regulations at both high and low temperatures. It turns out that these regulations are all triggered by fluid cells near the edge of the fireball, where the thermal pressure is much smaller than the bulk viscous pressure and the system is mechanically unstable. These regulations are therefore triggered automatically in order to suppress the bulk viscous pressure and prevent this instability. As a result of this, however, the regulation equation severely modifies the hydrodynamic evolution equation, leading to a different evolution. Additionally, all three curves feature oscillations in the temporal direction, which points to numerical issues which we have not yet fully understood. Choosing $\Pi_{NS} = -\zeta\theta$ with smaller grid spacing leads to more such oscillations. We were able to trace these oscillations to an instability in the time evolution of the fluid velocity: Fig. 3.16 shows that this instability originates from oscillations of the various components of the fluid velocity and the corresponding derivatives $\partial_\tau u^\tau$ and $\partial_x u^x$.

The same instability appears when we vary the time step of the VISH2+1 code. Fig. 3.17 shows a comparison of the bulk viscous pressure evolution between VISH2+1 and MUSIC at a fixed point on the transverse plane for different time steps in VISH2+1. Decreasing the time step in VISH2+1 shrinks the “amplitude” of $-\zeta\theta$, causing it to diverge from the MUSIC result. However, decreasing Δt does not introduce additional oscillations as decreasing Δx did in Fig. 3.15.

The spikes in the bulk viscous pressure and the oscillations in the fluid velocity only appear around $T = T_{tr}$ where the bulk viscosity is large. VISH2+1 results agree again with MUSIC results once the system approaches the decoupling temperature.

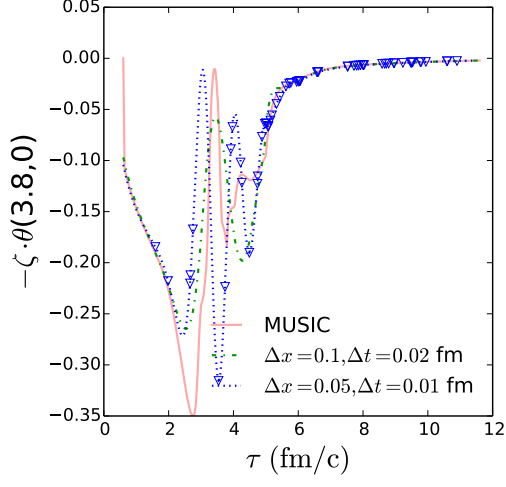


Figure 3.15: A comparison of the time evolution of the Navier-Stokes limit of the bulk viscous pressure $\Pi_{NS} = -\zeta\theta$, from MUSIC (solid line) and VISH2+1 (dash-dotted and dashed lines) at the point $(x = 3.8 \text{ fm}, y = 0)$ in the transverse plane. The dash-dotted line represents the results from $\Delta x = \Delta y = 0.1 \text{ fm}$ and $\Delta t = 0.02 \text{ fm}/c$, while the blue line shows results from $\Delta x = \Delta y = 0.05 \text{ fm}$ with $\Delta t = 0.01 \text{ fm}/c$.

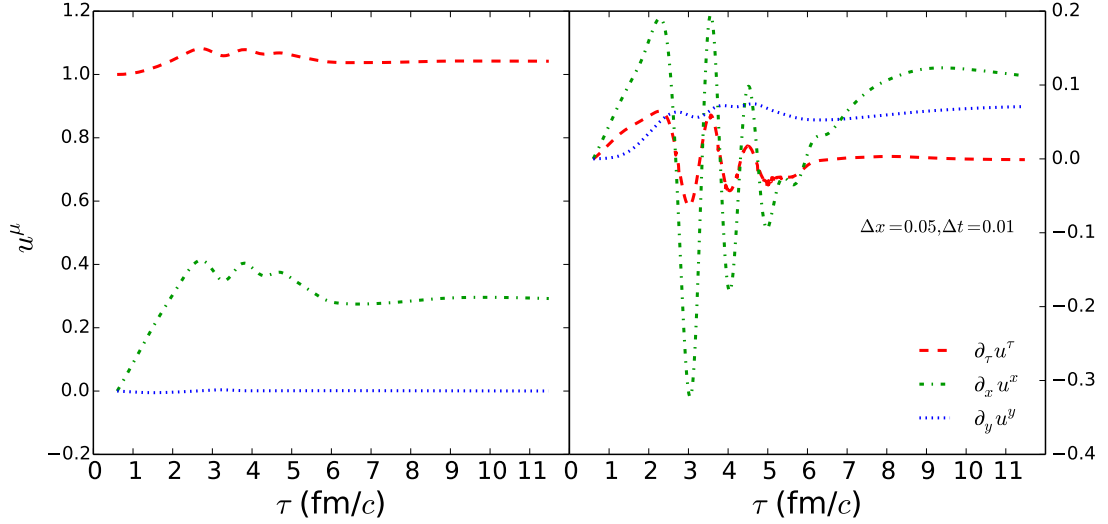


Figure 3.16: Left panel: the time evolution of the fluid velocity components u^τ (red), u^x (green) and u^y (blue) at the point $(x = 3.8 \text{ fm}, y = 0)$ in the transverse plane. Right: the time evolution of derivatives of the fluid velocity components.

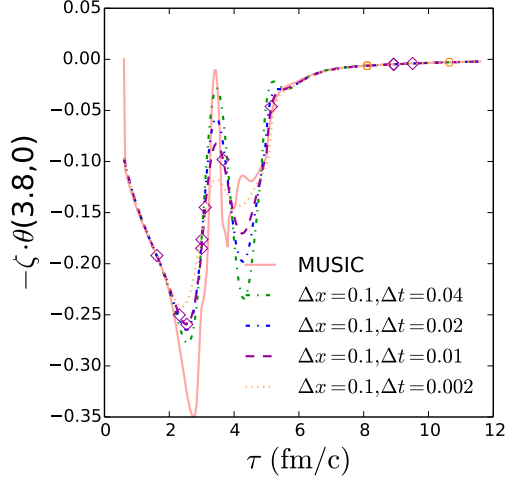


Figure 3.17: A comparison of the time evolution of the Navier-Stokes limit of bulk pressure from MUSIC (solid line) and VISH2+1 (dash-dot and dashed lines) for the point $(x = 3.8 \text{ fm}, y = 0)$ at the transverse plane.

We should therefore expect that changing the grid spacing will only bring a very small change to the final observables. Fig. 3.18 supports this expectation: changing the spatial grid spacing alters the spectra by only a few percent at high $p_{\perp}$. Fig. 3.19 shows a more visible difference in the $p_{\perp}$ -differential elliptic flow. We also observe that continuously decreasing Δt but holding Δx fixed leads to a monotonic decrease of the elliptic flow at high $p_{\perp}$. However, the $p_{\perp}$ -integrated observables are not sensitive to changes in the grid spacing, because the largest changes occur in the high- $p_{\perp}$ region where the contributions are negligibly small. Tables 3.2 and 3.3 show the mean transverse momenta and the integrated elliptic flow, respectively, for different grid spacings in VISH2+1. We see that varying the grid spacing only weakly affects these quantities.

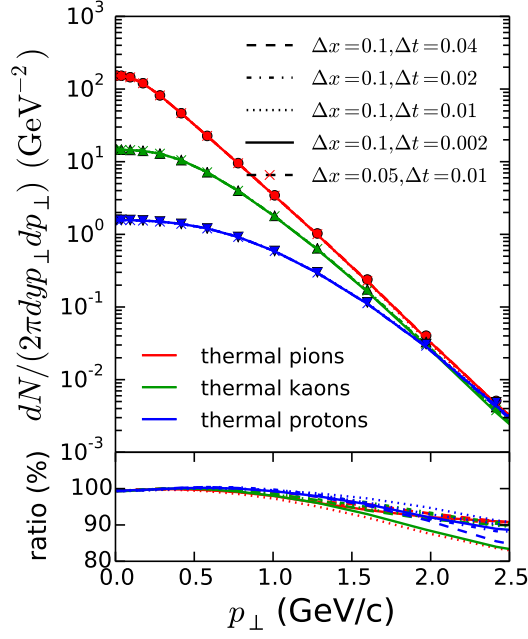


Figure 3.18: Comparison the thermal particle spectra generated by MUSIC with those generated by VISH2+1. Upper panel: the spectra of thermal pions, kaons and protons. Lines correspond to VISH2+1 results, while the points represent the MUSIC results. Different colors represent different hadron species, while different line types represent different grid spacings. Lower panel: the ratio of of VISH2+1 results to MUSIC results.

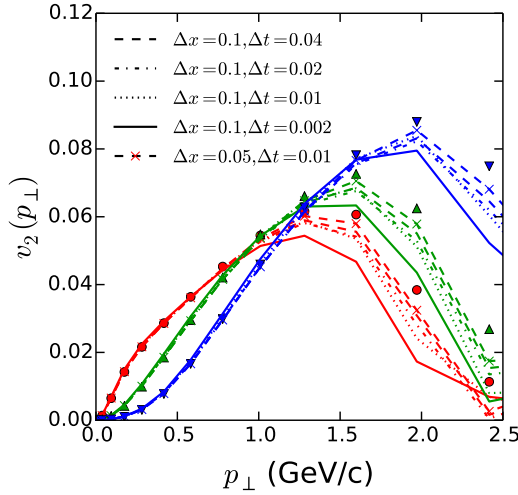


Figure 3.19: Comparison of the $p_{\perp}$ -differential elliptic flow between MUSIC and VISH2+1 with different grid spacings. The legend is the same as in Fig. 3.18.

model	$\langle p_{\perp} \rangle_{\pi^+}$ (GeV/c)	$\langle p_{\perp} \rangle_{K^+}$	$\langle p_{\perp} \rangle_p$ (GeV/c)
MUSIC	0.472	0.648	0.875
$\Delta x=0.1, \Delta t=0.04$	0.469	0.644	0.868
$\Delta x=0.1, \Delta t=0.02$	0.469	0.644	0.867
$\Delta x=0.1, \Delta t=0.01$	0.468	0.642	0.866
$\Delta x=0.1, \Delta t=0.002$	0.469	0.644	0.867
$\Delta x=0.05, \Delta t=0.01$	0.470	0.645	0.870

Table 3.2: Mean transverse momenta of thermal hadrons calculated from different VISH2+1 grid spacing settings. The MUSIC results are also listed for comparison. In this calculation, we integrate over all $p_{\perp} > 0$ and rapidity $-0.5 < y < 0.5$.

model	$v_2^{\pi^+}$	$v_2^{K^+}$	v_2^p
MUSIC	0.029	0.032	0.036
$\Delta x=0.1, \Delta t=0.04$	0.029	0.031	0.035
$\Delta x=0.1, \Delta t=0.02$	0.029	0.031	0.035
$\Delta x=0.1, \Delta t=0.01$	0.029	0.031	0.035
$\Delta x=0.1, \Delta t=0.002$	0.029	0.032	0.036
$\Delta x=0.05, \Delta t=0.01$	0.029	0.031	0.035

Table 3.3: Same as in Table 3.2, but for the $p_{\perp}$ -integrated elliptic flows.

3.8 Chapter summary

In this chapter, we investigated the effects of non-zero bulk viscosity and of the non-linear and shear-bulk coupling terms on the hydrodynamic evolution. For $\zeta/s \neq 0$, the bulk viscous pressure causes a significant suppression of particle spectra at higher momenta, resulting in a decrease of the mean transverse momenta of the emitted hadrons. It also changes the $p_{\perp}$ -differential elliptic flow. These changes need to be taken into consideration when extracting the shear viscosity from model-data

comparisons. However, the non-linear second-order terms do not show noticeable effects on either particle spectra or flow. This indicates that the gradient expansion converges well, and second-order viscous hydrodynamics is a robust tool for describing relativistic heavy-ion collision dynamics. The only limitations to this statement we observed when studying the evolution of the bulk viscous pressure. For a temperature-dependent specific bulk viscosity $(\zeta/s)(T)$ as given in Fig. 3.1, which exhibits a large peak near T_{tr} , Israel-Stewart theory gives such large values for the bulk viscous pressure near T_{tr} that the numerical code begins to become unstable. While these instabilities are under control in the work shown here, in the sense that their effects on observables are small, we note that anisotropic hydrodynamics, which handles large first-order corrections to ideal hydrodynamics non-perturbatively [120], may be able to alleviate this problem.

We also compared two ansätze for the bulk viscous correction to the particle distribution function at freeze-out. We showed that the uncertainties brought by this correction affect the calculated integrated elliptic flow and mean transverse momenta at the 5% and 10% level, respectively, which will have consequences for shear viscosity and bulk viscosity extraction from experimental data. A comparison between VISH2+1 and MUSIC was also presented. The results from these two codes generally agree with each other very well, but exhibit some noticeable differences at higher transverse momenta.

Chapter 4: Parameter Optimization: Introduction and application to pure hydrodynamic simulations

4.1 Chapter introduction

In order to gain generic insights into which of the different observables at our disposal provide the strongest constraints on the pre-equilibrium to hydrodynamic switching time τ_s , we varied τ_s in Chapter 2 while leaving all other model parameters unchanged. However, in addition to the switching (or hydrodynamic starting) time τ_s , our hydrodynamical model has several other input parameters whose choice influences the final physical observables. It is immediately obvious that there should be some sort of tradeoff between effectively weakening the interactions in the pre-equilibrium stage, say, by lengthening the free-streaming period, and weakening the interactions during the later hydrodynamic stage, say, by shortening the free-streaming stage and increasing the shear viscosity during the subsequent hydrodynamic evolution. The effects of changing the transition time between free-streaming and hydrodynamic evolution and of changing the shear viscosity during the hydrodynamic evolution are therefore entangled, and we should optimize both parameters simultaneously. Furthermore, since the slopes of the final spectra are controlled by a combination of the temperature and radial flow on the freeze-out hypersurface, and a change in

viscosity affects the transverse pressure gradients and thus the radial flow, we should allow T_{dec} to vary together with η/s .

In this chapter, we perform a 3-parameter fit of the measured values for the average transverse momenta $\langle p_{\perp} \rangle$ for pions, kaons and protons, as well as the elliptic and triangular flows of charged hadrons $v_{2,3}^{\text{ch}}$, by taking the switching time τ_s , the specific shear viscosity η/s during the hydrodynamic stage, and the kinetic decoupling temperature T_{dec} as free parameters, thus find the preferred “thermalization” times τ_s , the specific shear viscosity η/s and the kinetic freeze-out temperature T_{dec} for pure hydrodynamics evolution.

4.2 Latin hypercube sampling

In order to find the optimized τ_s , η/s and T_{dec} , we need to explore the 3-dimensional parameter space constructed from these three parameters. This means we need to run our model on a huge number of possible parameter triplets. One such run generally requires 1 CPU hour. If we need n distinct values for k parameters, the regular grid method gives n^k triplets. If $n \sim \mathcal{O}(10^3)$, this implies a computation time $\sim \mathcal{O}(10^9)$ CPU hours when we have 3 parameters to tune; this is intractable. Therefore we prefer a smaller subset of parameter combinations which can equally effectively represent all possible parameter combinations in the entire parameter space.

Latin hypercube sampling [121, 122] is a method for optimizing the selection of parameter combinations from a high dimensional parameter space. Parameter combinations sampled from this method efficiently span the parameter space because no two parameter triplets share the same value for any of the three components. After

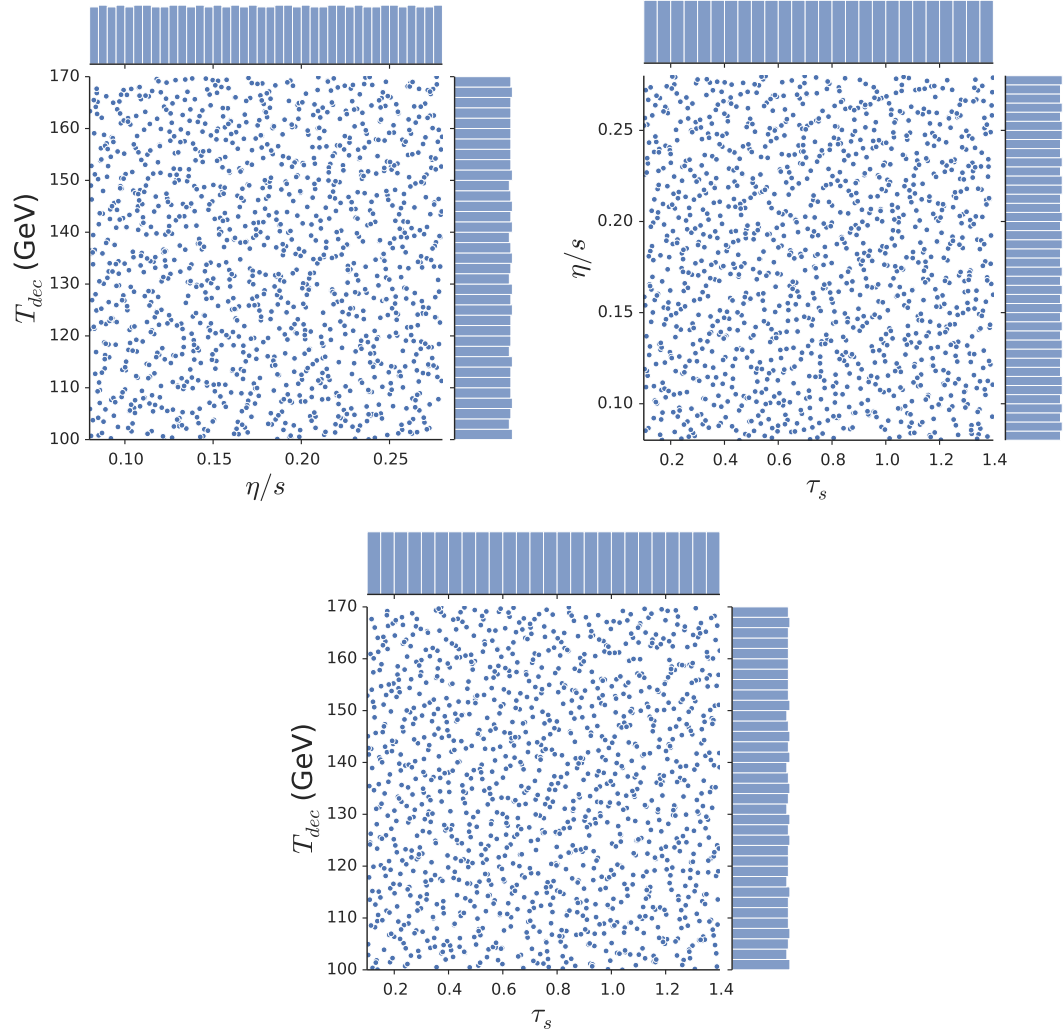


Figure 4.1: Projection of the Latin hypercube sampled 1,300 parameter triplets for the MC-KLN initial-state model onto the 2-dimensional 2-parameter subspace. The histograms at the edges of each panel show the distributions of each single parameter. The ranges for each of the three parameters is specified in Section 4.3.

projecting the sampled triplets onto any of three components, the marginal distribution is uniform, which reflects the fact that we do not have prior information about the distribution of these parameters. In Fig. 4.1, we project the parameter triplets sampled for optimizing our hydrodynamic model with MC-KLN initial-state in three

directions. The margins of each panel show the distribution of the parameters labeled along the corresponding axes. These distributions are uniform, with only small fluctuations due to the finite statistics in each bin.

4.3 Parameter optimization for pure hydrodynamic simulation with pre-equilibrium dynamics

Here we report on a study where we allow τ_s , η/s and T_{dec} to vary simultaneously, trying to find the best combination by comparing the model predictions for v_2^{ch} , v_3^{ch} , $\langle p_{\perp} \rangle_{\pi^+}$, $\langle p_{\perp} \rangle_{K^+}$, and $\langle p_{\perp} \rangle_p$ for 2.76 A TeV Pb+Pb collisions of 10–20% centrality with experimental data from the ALICE [99] and ATLAS [123] collaborations and minimizing the value of χ^2 . The values of the experimental measurements for these observables are summarized in Table 4.1.

$\langle v_2^{\text{ch}} \rangle$	0.0782 ± 0.0019
$\langle v_3^{\text{ch}} \rangle$	0.0316 ± 0.0008
$\langle p_{\perp} \rangle_{\pi^+} \text{ (GeV}/c\text{)}$	0.517 ± 0.017
$\langle p_{\perp} \rangle_{K^+} \text{ (GeV}/c\text{)}$	0.871 ± 0.027
$\langle p_{\perp} \rangle_p \text{ (GeV}/c\text{)}$	1.311 ± 0.034

Table 4.1: Experimental data for the five hadronic observables from 2.76 A TeV Pb+Pb collisions of 10–20% centrality that were considered in our fit. The mean $p_{\perp}$ -integrated elliptic and triangular flow values for charged hadrons were measured by ATLAS [123], the mean transverse momenta for positively charged pions, kaons and protons (extrapolated to the full $p_{\perp}$ range) by the ALICE Collaboration [99].

A somewhat more ambitious fit with five hydrodynamic model parameters and three experimental observables (charged multiplicity, $\langle v_2^{\text{ch}} \rangle$ and $\langle v_3^{\text{ch}} \rangle$) at six collision centralities each (i.e. altogether 18 observables), including a hadronic afterburner but no pre-equilibrium dynamics, was recently reported in [124], and a 8-parameter

fit including bulk viscosity, but without pre-equilibrium flow was reported the same group at the Quark Matter 2015 conference. We perform simulations both with and without pre-equilibrium dynamics, in order to assess its impact on the best-fit values for the other model parameters. Our simulations are done in single-shot mode with smooth ensemble-averaged initial density profiles, not in event-by-event mode with fluctuating initial profiles as the work reported in [124]. Since we used data on the mean elliptic and triangular flows of charged hadrons, obtained by ATLAS [123] from their full reconstructed event-by-event probability distributions, instead of their rms values that were used in [124] and which are affected by the variance of their event-by-event fluctuations, the added numerical cost of event-by-event hydrodynamic simulations could be avoided in our analysis.

After running the hydrodynamic simulation for a given triplet of parameters from the Latin hypercube sample, the quality of the description obtained with this parameter set is estimated by computing the χ^2 of the resulting fit of the selected experimental data:

$$\chi^2 = \sum_i \frac{(O_i - E_i)^2}{\sigma_i^2}. \quad (4.1)$$

Here the sum runs over the five observables, E_i is the value and σ_i the combined statistical and systematic error of the experimental measurement of the observable, and $O_i(\tau_s, \eta/s, T_{\text{dec}})$ is the value of the observable from the simulation with parameter set $(\tau_s, \eta/s, T_{\text{dec}})$. Since we are using single-shot hydrodynamics with an ensemble-averaged initial profile, O_i has no statistical error. Assuming that the five chosen observables are uncorrelated, with three fit parameters we have two statistical degrees of freedom, and a good fit of the data should thus have $\chi^2/2 \simeq 1$. The best fits we have been able to achieve with the three selected model parameters have $\chi^2/2 \sim 9 - 15$

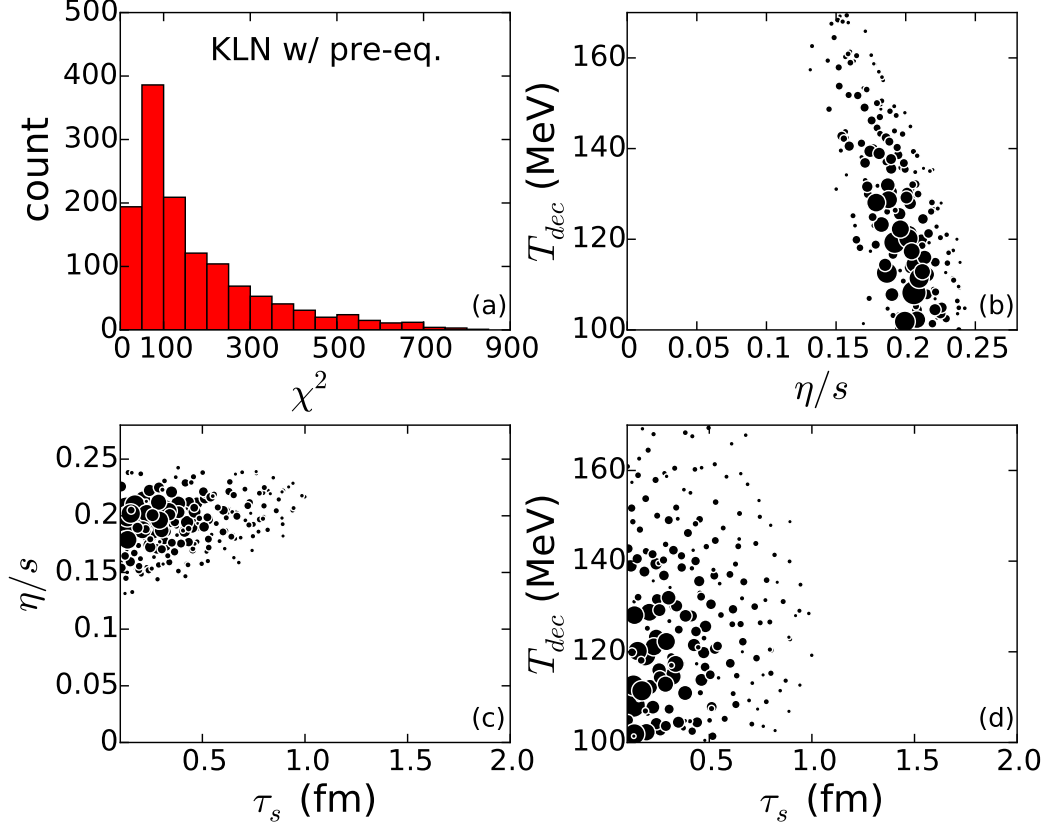


Figure 4.2: Parameter search result for the KLN initial-state model, evolved in single-shot hydrodynamic mode following a free-streaming stage of duration $\tau_s - \tau_0$. (a) Histogram of the χ^2 distribution. (b-d) 2-dimensional projections of those parameter triplets $(\tau_s, \eta/s, T_{dec})$ corresponding to $\chi^2 < 50$. The size of the rings around their positions increases with decreasing χ^2 , i.e. with increasing fit quality.

(see Table 4.3). This suggests that at least one additional physical mechanism not captured by these three model parameters may play an important role in describing the chosen observables. This could be, for example, that hydrodynamics breaks down during the final hadronic stage of the fireball expansion and needs to be replaced there by a microscopic model for hadronic rescattering [72, 124]. We have not tested this hypothesis.

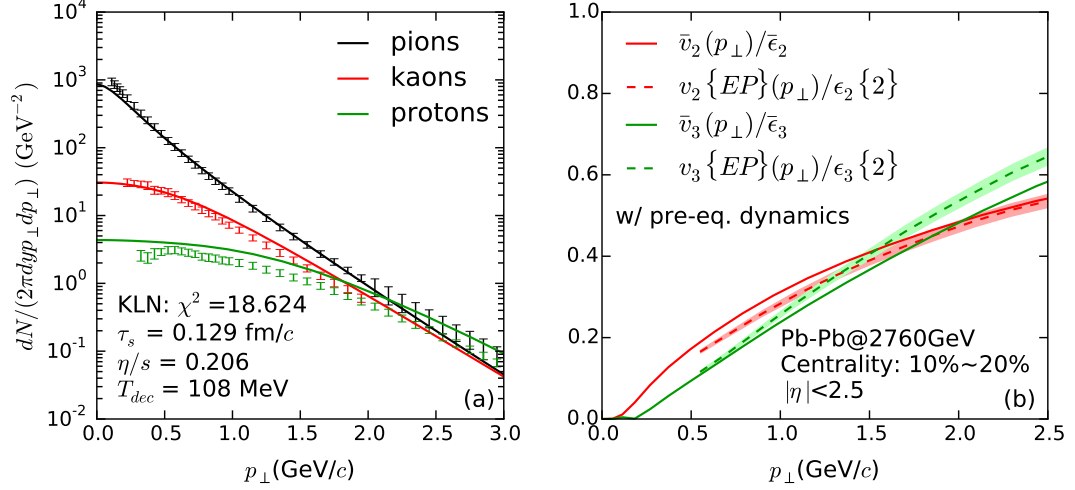


Figure 4.3: Comparison with experimental data of single-shot hydrodynamic model predictions with the best fit parameter combination (smallest χ^2 value) for KLN-initialized simulations with pre-equilibrium free-streaming dynamics, for 2.76 A TeV Pb+Pb collisions at 10%–20% centrality. The best-fit parameter values are listed in panel (a). (a) Transverse momentum spectra for π^+ , K^+ and protons, compared with ALICE data [125]. (b) Eccentricity-scaled $p_\perp$ -differential elliptic and triangular flow anisotropies for charged hadrons, compared with ATLAS data [126]. Single-shot hydrodynamic simulations predict the ensemble averaged flow $\bar{v}_n$ which was scaled by the corresponding ensemble-averaged eccentricity $\bar{\epsilon}_n$ (solid lines). The ATLAS anisotropic flow data are measured with the event-plane method and are thus affected by the variance of the event-by-event v_n distribution. They were fitted with a smooth curve and scaled by the rms eccentricity $\epsilon_n\{2\}$ (dashed lines). The shaded area around the dashed lines represents the experimental error of the ATLAS $v_n\{EP\}$ measurements [126].

For the KLN initial-state model we drew a Latin hypercube sample of 1300 points covering the following parameter ranges: $0.1 \text{ fm}/c < \tau_s < 1.4 \text{ fm}/c$, $0.08 < \eta/s < 0.28$, and $100 \text{ MeV} < T_{dec} < 170 \text{ MeV}$. For the Glauber initial-state model we sampled 950 points in the range $0.1 \text{ fm}/c < \tau_s < 2 \text{ fm}/c$, $0 < \eta/s < 0.16$, and $100 \text{ MeV} < T_{dec} < 170 \text{ MeV}$.⁶

Figs. 4.2, 4.4, 4.6 and 4.8 show the corresponding χ^2 distributions for simulations with

⁶In both cases the upper end of the explored range for τ_s is small enough that the particle and energy losses through the corona studied in Sec. 2.5 can be ignored.

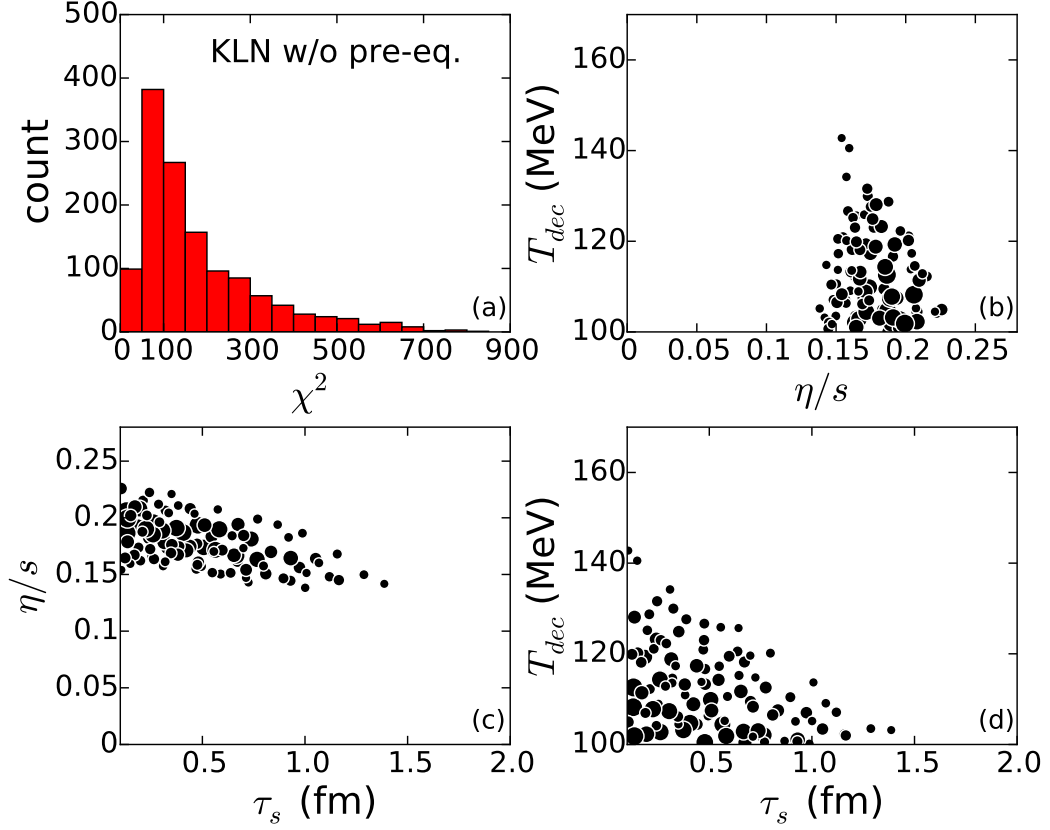


Figure 4.4: Same as Fig. 4.2, but for single-shot hydrodynamic simulations starting at τ_s without preceding pre-equilibrium stage.

KLN and Glauber initial conditions with and without a free-streaming pre-equilibrium stage, respectively (see captions). The best-fit values for the three model parameters in each of the four cases, and the predictions the model makes for these best-fit parameter values for the observables listed in Table 4.1, are summarized in Tables 4.2 and 4.3.

Panels (b-c) in Figs. 4.2, 4.4, 4.6 and 4.8 show scatter plots of all simulations with a total $\chi^2 < 50$ in each of the three 2-dimensional projections of the 3-dimensional parameter space. The size of each blob indicates the quality of the description of the

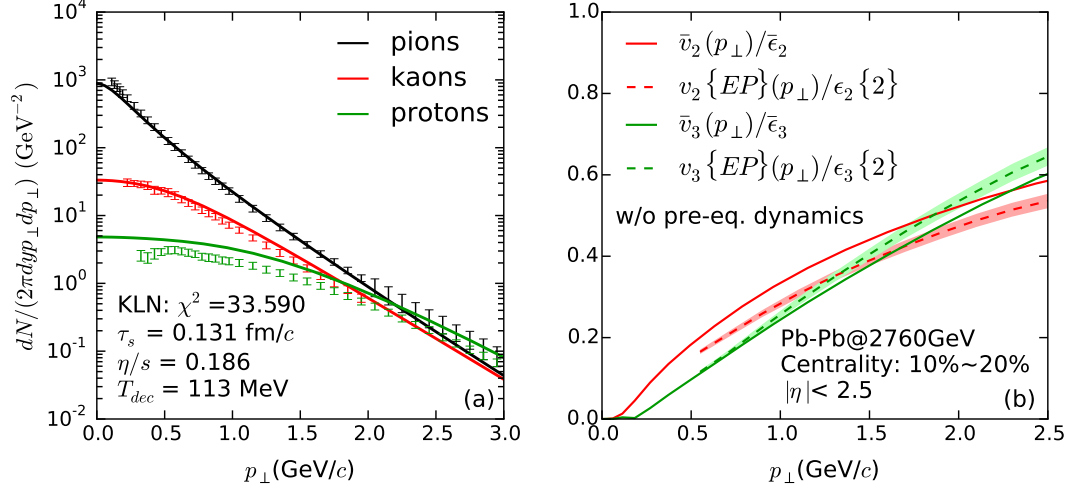


Figure 4.5: Same as Fig. 4.3, but for single-shot hydrodynamic simulations starting at τ_s without preceding pre-equilibrium stage.

data achieved with the corresponding parameter set: The larger the blob, the smaller the total χ^2 and the better the fit.

Figures 4.3, 4.5, 4.7 and 4.9 show the $p_\perp$ distributions of pions, kaons and protons (a) and of the charged hadron elliptic and triangular flows predicted by the simulations with the best-fit parameter sets, for each of the four simulation modes listed in Tables 4.2, 4.3. We use the equation of state s95p-PCE [112, 127] which assumes chemical freeze-out of hadron abundances at $T_{\text{chem}} = 165$ MeV and therefore overpredicts the measured proton yields by about 50% (without the hadronic afterburner, our hydrodynamic approach cannot account for baryon-anti-baryon annihilation during the final hadronic rescattering stage, which is required to reproduce the experimental yields [128]). For the protons one should therefore ignore the normalization of the $p_\perp$ spectra and focus instead on their shape. Clearly, the description of the experimental data in Figs. 4.3, 4.5, 4.7 and 4.9 (of which only the lowest non-trivial moments were

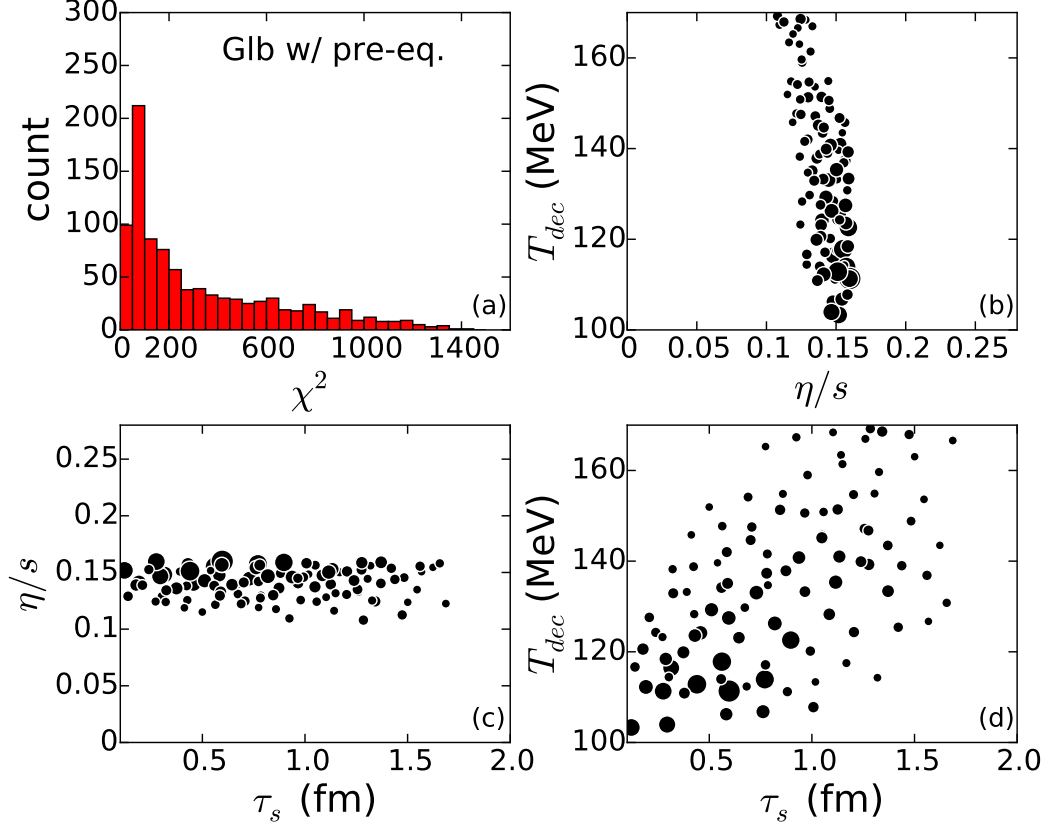


Figure 4.6: Same as Fig. 4.2, but for MC-Glauber initial conditions, free-streamed to τ_s and then evolved hydrodynamically.

used in the fit) is not perfect, but of similar quality as most other, less systematic parameter fits published in the literature.

At first sight, though, there appears to be one exception: As seen in Fig. 4.9b, the MC-Glauber model *without* pre-equilibrium dynamics appears to provide a qualitatively better simultaneous description of the differential charged hadron elliptic and triangular flows than the other approaches. (In particular, the KLN model has troubles to describe these two observables simultaneously, as has been noted before [129].) However, the overall χ^2 of this “Glauber without pre-equilibrium” fit is

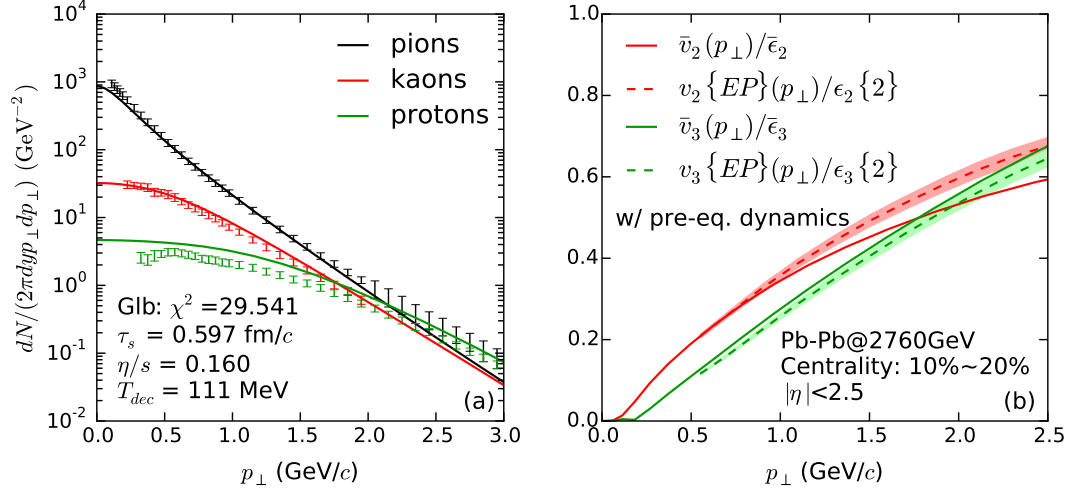


Figure 4.7: Same as Fig. 4.3, but for MC-Glauber initial conditions, free-streamed to τ_s and then evolved hydrodynamically.

worse than that for the “KLN with pre-equilibrium” fit, due to a larger discrepancy with the data of the predicted mean $p_\perp$ for kaons and pions. Fig. 4.9a also shows that the best “Glauber without pre-equilibrium” simulation does not describe the slope of the pion spectrum quite as well as the best “KLN with pre-equilibrium” fit in Fig. 4.3a. This clearly detracts from the apparently much better description of the $p_\perp$ -differential $v_{2,3}^{\text{ch}}(p_\perp)$ in Fig. 4.9b compared to Fig. 4.3b which may simply reflect an incorrect weighting of regions of high and low $p_\perp$ in the best-fit “Glauber without pre-equilibrium” simulation.

Let us discuss a few other trends that are visible in Figs 4.2-4.9. First, panels b and c in Figs. 4.2, 4.4, 4.6 and 4.8, as well as Table 4.2, show that the inclusion of pre-equilibrium dynamics puts some upward pressure on the best-fit value of η/s , for both types of initial conditions. The effect is not large (of order 10%) but appears to be significant. (We will not be absolutely certain of the significance of this observation

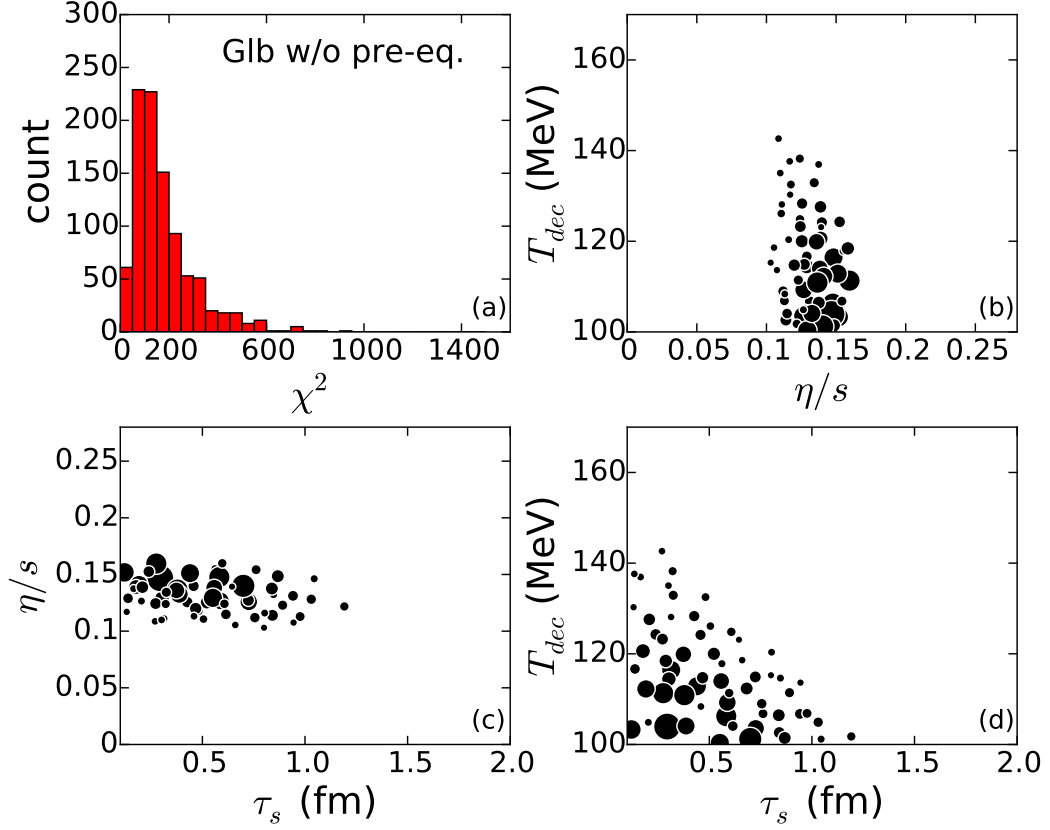


Figure 4.8: Same as Fig. 4.6, but for single-shot hydrodynamic simulations starting at τ_s without preceding pre-equilibrium stage.

until we have completed a full Markov Chain Monte Carlo (MCMC) simulation of the posterior model parameter distributions [124, 130] which is beyond the scope of this

Model	Pre-eq.	τ_s (fm/c)	η/s	T_{dec} (MeV)
MC-KLN	Yes	0.129	0.206	108
MC-KLN	No	0.131	0.186	113
MC-Glb	Yes	0.597	0.160	111
MC-Glb	No	0.295	0.147	104

Table 4.2: Best-fit parameters from a parameter search for four different types of simulations.

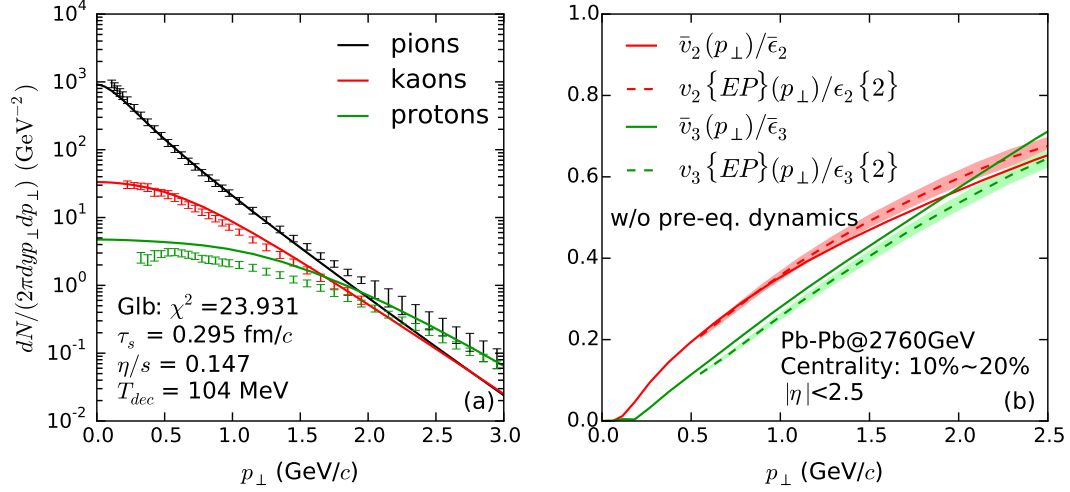


Figure 4.9: Same as Fig. 4.7, but for single-shot hydrodynamic simulations starting at τ_s without preceding pre-equilibrium stage.

paper.) Second, by looking at the spread of the blobs shown in panel b of Figs. 4.2, 4.4, 4.6 and 4.8, we see a reduced sensitivity of the fit quality to the decoupling temperature when pre-equilibrium dynamics is accounted for in the simulations: the same upper limit of 50 for the total χ^2 allows for larger deviations of T_{dec} from the best-fit value if the simulations include a pre-equilibrium stage. Third, it can

Model	MC-KLN	MC-KLN	MC-Glb	MC-Glb
Pre-eq.	Yes	No	Yes	No
$\bar{v}_2^{\text{ch}}$	0.083	0.088	0.070	0.071
$\bar{v}_3^{\text{ch}}$	0.030	0.030	0.034	0.034
$\langle p_{\perp} \rangle_{\pi^+}$ (GeV/c)	0.550	0.545	0.539	0.518
$\langle p_{\perp} \rangle_{K^+}$ (GeV/c)	0.900	0.877	0.869	0.852
$\langle p_{\perp} \rangle_p$ (GeV/c)	1.349	1.302	1.293	1.279
χ^2	18.624	33.590	29.541	23.931

Table 4.3: Model predictions for the five observables listed in Table 4.1 with the best-fit parameters listed in Table 4.2.

be seen from panel c in the same figures that allowing for pre-equilibrium build-up of flow reduces the probability of a good fit for switching times that significantly exceed the best-fit value in the KLN model but not in the Glauber model. This is consistent with Fig. 2.10 where we observed that allowing for any appreciable delay τ_s of the hydrodynamic stage due to pre-equilibrium dynamics tends to cause the model to overpredict the mean $p_\perp$ of the hadrons (especially the protons) for KLN initial profiles (panel a) but not for the Glauber model profiles (panel b). Indeed, for the Glauber model the neglect of pre-equilibrium flow puts downward pressure in τ_s , because of the effect of missing radial flow on the mean hadron $p_\perp$. One sees this in both Fig. 2.10b and when comparing panels c in Figs. 4.6 and 4.8.

4.4 Chapter summary

In this chapter, we implement a 3-dimensional parameter search to optimize the switching time, the specific shear viscosity and the kinetic freeze-out temperature simultaneously for MC-KLN and MC-Glb initial model, with and without pre-equilibrium dynamics. We find that the switching time τ_s depends strongly on the model of the initial conditions. MC-KLN initial conditions require an earlier transition to hydrodynamic behavior (at $\tau_s \approx 0.13$ fm/c), followed by hydrodynamic evolution with a larger specific shear viscosity $\eta/s \approx 0.2$, than MC-Glb initial conditions which prefer switching at a later time ($\tau_s \approx 0.6$ fm/c) followed by a less viscous hydrodynamic evolution with $\eta/s \approx 0.16$. These new results including pre-equilibrium evolution are compared to fits without a pre-equilibrium stage where all dynamic evolution before the onset of hydrodynamic behavior is ignored. In each case, the quality of the dynamical descriptions for the optimized parameter sets, as well as the

observables which show the strongest constraining power for the thermalization time, are discussed. While this parameter optimization does not exhaust the list of parameters and possibilities, this exercise provides a more holistic picture of the effects of pre-equilibrium dynamics on final observables and on the values of medium parameters extracted from a comparison of the model predictions with experimental data. We found for both initial state models that accounting for pre-equilibrium dynamics slightly increases the optimal values for the specific shear viscosity η/s extracted from mean $p_\perp$ and anisotropic flow measurements and reduces the sensitivity of the observables to the decoupling temperature. However, the extracted limits for the thermalization time τ_s turned out to depend sensitively on the model for the initial density profiles.

Chapter 5: Parameter Optimization: Application to hybrid simulations

5.1 Chapter introduction

The VISHNU hybrid model [72], which incorporates the hadronic afterburner UrQMD to simulate the hadronic rescattering after the hydrodynamic evolution, has successfully reproduced and predicted the experimentally observed non-strange hadron spectra and anisotropic flows [72, 131–133]. Recently this model has been implemented to study the strange and multi-strange hadronic elliptic flow mass-ordering observed at the Large Hadron Collider (LHC) [134, 135]. The anisotropic flows of strange and multi-strange particles, Λ , Ξ , and Ω , are of particular interest due to the smaller scattering cross-sections associated with strange quarks and a correspondingly reduced probability for participating in the hadronic interactions [136]. Therefore they are widely considered as “cleaner” probes for the prehadronic hydrodynamic stage than other hadronic species that suffer more hadronic rescattering. However, the VISHNU hybrid model without pre-equilibrium flow fails to explain the experimentally measured mass-ordering of the elliptic flows for protons and Λ [135]. Standard elliptic flow mass-ordering was observed in the experiments for proton, Λ , Ξ , and

Ω [137, 138], while the VISHNU hybrid model predicted an inverted mass-ordering for the proton and Λ elliptic flows [135].

This failure may be due to an incomplete physical picture and poorly optimized model parameters. From a physical point of view, the implementation of the hybrid model used in [135] ignores the pre-equilibrium stage and starts the hydrodynamic evolution with some delay after the initial gluon production, but without taking into account the necessary dynamical evolution of the fireball in size and shape during this delay. We have shown in Chapter 2 that pre-equilibrium generated flow has non-negligible effects on the final observed flows, meaning that it is necessary to include a pre-equilibrium evolution stage in the hybrid model. Moreover, the VISHNU version used up to now evolves the QGP with zero bulk viscous pressure, even though recent studies have shown that the bulk viscous pressure has visible effects on the final observed hadronic spectra and flows (see [97, 104–106] and Chapter 3 above). Finally, the free parameters used in this model are not necessarily optimized. The free parameters in the hybrid model are only constrained experimentally by the observed charged multiplicity, thus leaving some room for improving the model by choosing a better set of values for the remaining free parameters.

In this chapter, we upgrade the VISHNU model mentioned above and use it to try to resolve the elliptic flow mass-ordering problem. We include the pre-equilibrium evolution described in Chapter 2 to complete the evolution process. We adopt the more complete hydrodynamic evolution equations discussed in Chapter 3, which also evolve the system with non-zero bulk viscosity. We implement the parameter optimization technique developed in Chapter 4 to optimize the free parameters in our updated VISHNU hybrid model. Finally, instead of using the single-shot hybrid approach

used in Ref. [135] throughout, we only use it in the parameter optimization stage but resort to full event-by-event hybrid simulations with optimized model parameters at the end, to properly include the initial states fluctuations in the calculation of the elliptic flow measured with the scalar product method [134].

In our study, we simulate Pb-Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV. In order to limit the necessary computation time we focus only on the 10% – 20% centrality class. We employ the Monte Carlo Kharzeev-Levin-Nardi (MC-KLN) [46, 47] and Monte Carlo Glauber (MC-Glb) [49] models to generate the initial parton density distributions. To determine which events belong to the 10% - 20% centrality class, we then cut the total initial entropy distribution in centrality bins which was shown in [139] to closely match the experimental centrality cut. We perform a single-shot hydrodynamic simulation when optimizing parameters in Section 5.3. In order to get good statistics, we oversample directly emitted hadrons from the Cooper-Frye spectra 1,000 times and run each of these 1,000 samplings through UrQMD. The number oversampling of each hydrodynamic event is dictated by the event statistics needed to reduce the statistical uncertainties of the model calculations to values comparable with the experimental uncertainties. We resume event-by-event hybrid simulations in Section 5.5 where we compare best fit results with additional observables, especially the spectra and the differential elliptic flow of hyperons.

The sections in this chapter are arranged as follows: Section 5.2 shows how we upgraded the VISHNU hybrid model. Section 5.3 presents the results of the parameter optimization. In Section 5.4, we investigate the posterior probability distribution of the fitted free parameters using the Markov Chain Monte Carlo (MCMC) technique.

In Section 5.5, we report our results for the elliptic flow mass-ordering after implementing an event-by-event hybrid run with the best parameter combination found in Section 5.3. We also show results from the best-fit parameters from an additional 4-parameter optimization campaign. Finally, we summarize our findings in Section 5.6.

5.2 Updates to the VISHNU hybrid model

In this section, we give a brief review of our updated VISHNU hybrid model. First of all, we supplement the evolution process by including a pre-equilibrium phase, which is modeled by free-streaming, introduced in Chapter 2. The pre-equilibrium phase generates an energy momentum tensor that is matched to hydrodynamic initial conditions at the switching time τ_s . This set of initial conditions includes a non-zero value for the shear stress tensor and bulk viscous pressure, and a significant pre-equilibrium flow as mentioned in Chapter 2.

The work described in Chapter 2 set the bulk viscosity ζ to zero, since during that part of the project we had not yet properly implemented bulk viscous pressure evolution in our model. In order to address the bulk viscous pressure evolution and the shear - bulk coupling in the hydrodynamic stage, we now replace the evolution equations used in the original version of the hydrodynamic simulation code VISH2+1 [40,65] by the more complete set discussed in Chapter 3. The parametrization for the temperature-dependent specific bulk viscosity ζ/s is taken from Ref. [110] and was shown in Fig. 3.1.

Additionally, we update the UrQMD module of the hybrid model to its latest version UrQMD v3.4, because this version improves the description of strange hadron

interactions by including additional reactions of strange and multi-strange particles at low relative momentum [140]. When making that update we realized that different versions of UrQMD lead to somewhat different values for the model parameters extracted from a model-data comparison.

We also update the hydro - hadron cascade switching temperature and the equation of state. The system is switched to the hadronic stage at $T_{sw} = 155$ MeV, since recent lattice QCD studies have converged to the new, lower value $T_c = 154 \pm 9$ MeV [9]. This parameter can also be treated as a free parameter and be tuned to match the experimentally measured hadron yield ratios. We fix it in most of the studies reported in this chapter, but allow it to vary in Section 5.5. We also used a new equation of state (EOS) that smoothly connects the latest lattice QCD results to a hadron resonance gas EOS at $T < 110$ MeV [111]. Because UrQMD includes most but not all known resonances, the EOS of the hadron resonance gas is calculated including only those particle species that exist in UrQMD.

We understand that there is theoretical uncertainty associated with the form of the bulk viscous correction δf_{bulk} , as discussed in some detail in Chapter 3. However, the effects of bulk viscosity should be smaller at LHC energies than at the RHIC energies studied earlier in Chapter 3, because the initial temperature is higher than at RHIC and thus the system spends a smaller fraction of its life time in the region where the specific bulk viscosity ζ/s is large. At freeze-out, the bulk viscosity is small. In this study, we adopt the relaxation time bulk viscous correction (3.17) [105], but keep in mind that other forms for δf_{bulk} may affect our results. We leave additional studies of δf_{bulk} to the future.

5.3 Parameter optimization

There are a few free parameters in our hybrid model that have decisive effects on the final observables. The switching time τ_s controls the equilibration time of the system, the size of initial flow, and the initial shear and bulk viscous pressures for the hydrodynamic evolution. We have shown the influence of the initial flow on the hydrodynamic flow and the hadrons' mean transverse momenta in Chapter 4. At the same time, the specific shear viscosity η/s changes the shear stress tensor, which modifies the gradients of the transverse pressure and eventually the radial flow. The bulk viscous pressure counteracts the radial expansion and suppresses the development of radial flow. It turns out that the inclusion of bulk viscosity into the hydrodynamic evolution significantly decreases the value of the shear viscosity in order to fit the data. A study using IP-Glasma initial conditions in the (3+1)D hydrodynamic code MUSIC has shown that in order to fit the experimental flow and mean transverse momentum simultaneously, the shear viscosity is almost halved when the bulk viscosity is included in the hydrodynamic evolution [106]. Therefore the switching time and the shear and bulk viscosities should be optimized together.

In our study, we adopt the temperature-dependent specific bulk viscosity parametrization given in Ref. [110], with ζ/s exhibiting a peak value of approximately 0.33 at $T_{tr} = 180$ MeV. In order to study the sensitivity of the model predictions to the bulk viscosity, we vary the normalization of the curve $(\zeta/s)(T)$ shown in Fig. 3.1 by multiplying this parametrization by an overall “normalization” factor, or scale factor, ranging from 0 to 3. This keeps the peak value of ζ/s between 0 and 1. In this section, we optimize three parameters: τ_s , η/s and the bulk normalization factor simultaneously, and find the preferred regions for each of them.

We utilize the parameter optimization framework developed in Chapter 4 to find the preferred region of these three parameters. Namely, we sample the parameter triplets using the Latin hypercube method [121, 122], then run the hybrid model and assess the “goodness of fit” through χ^2 defined as

$$\chi^2 = \sum_i \frac{(O_i - E_i)^2}{\sigma_i^2}. \quad (5.1)$$

The summation runs over all five observables listed in Table 4.1. E_i is the value of the observable from the experimental measurement, while $O_i(\tau_s, \eta/s, b_{norm})$ is the value from the hybrid simulation. σ_i consists of both experimental error, which includes systematic and statistical uncertainties, and simulation error due to the finite statistics. Because single-shot hydro does not have fluctuations in the initial state, we compare our flows to the ATLAS measurements of the mean elliptic and triangular flows [123], reconstructed from event-by-event probability distributions for v_2 and v_3 .

We sampled 1,024 points with the Latin hypercube method to cover the parameter space presented in Table 5.1. Note that we choose a larger range for τ_s for MC-Glb initial conditions, because runs with the MC-Glb model prefer larger switching times as we found in Ref. [78]. For any parameter triplet, we match the charged multiplicity $dN_{ch}/d\eta$ to the experimental measurement (966 ± 37) [141]. As we pointed out in Chapter 2, late switching causes a large fraction of particles to be pushed outside of the freeze-out surface before the hydrodynamic evolution even starts losing them from the Cooper-Frye freeze-out integral. Our inability to convert these partons to hadrons makes the contribution from these partons unrecoverable. This brings an uncertainty into our model. However, we also showed that for switching times $\tau_s \leq 3 \text{ fm}/c$, this loss amounts to less than 5% percent of the total energy dE/dy . We therefore expect the parameter uncertainties resulting from this effect to be small.

Model	τ_s (fm/c)	η/s	bulk norm.
MC-KLN	0.1 - 2.0	0.08 - 0.28	0 - 3
MC-Glb	0.1 - 3.5	0 - 0.21	0 - 3.5

Table 5.1: The ranges of each parameter in parameter search.

We now present the results of our parameter search. Figs. 5.1, 5.2 show scatter plots for MC-KLN and MC-Glb initial conditions including pre-equilibrium dynamics. We project the 3-dimensional parameter space into various 2-dimensional planes, and plot those parameter combinations that give $\chi^2 < 50$. Table 5.2 summarizes the best-fit parameters for each of these two run modes and Table 5.3 lists the model output corresponding to each best parameter triplet.

From Fig. 5.1, we see that the shear viscosity is tightly constrained to be around 0.17. MC-KLN initial conditions prefer early switching at $\tau_s \lesssim 1.5$ fm/c when a pre-equilibrium stage is included. The bulk normalization factor is generally larger than 0.7 for the MC-KLN initial state. The switching time and bulk norm factor are positively correlated (cf. the last panel of Fig. 5.1), reflecting the fact that a larger bulk viscosity is required to suppress the excessive initial radial flow caused by a longer initial free-streaming stage. It is a bit surprising that the shear viscosity does not correlate with the switching time. In Chapter 4, we saw these two parameters are slightly positively correlated because shear viscosity is required to suppress the initial flow for late switching times, but here η/s is seen to not depend on the choice of τ_s . This may be due to the presence of the bulk viscosity. Fig. 5.2 shows that MC-Glb model prefers a larger switching ~ 2.5 fm/c, a larger bulk normalization factor, and a slightly smaller η/s than MC-KLN initial conditions. We also see stronger correlations

between any two of these free parameters, especially a negative correlation between τ_s and η/s , which was not observed in the pure hydro parameter search of Chapter 4 (Fig. 4.6). We will assess these correlations in the next section.

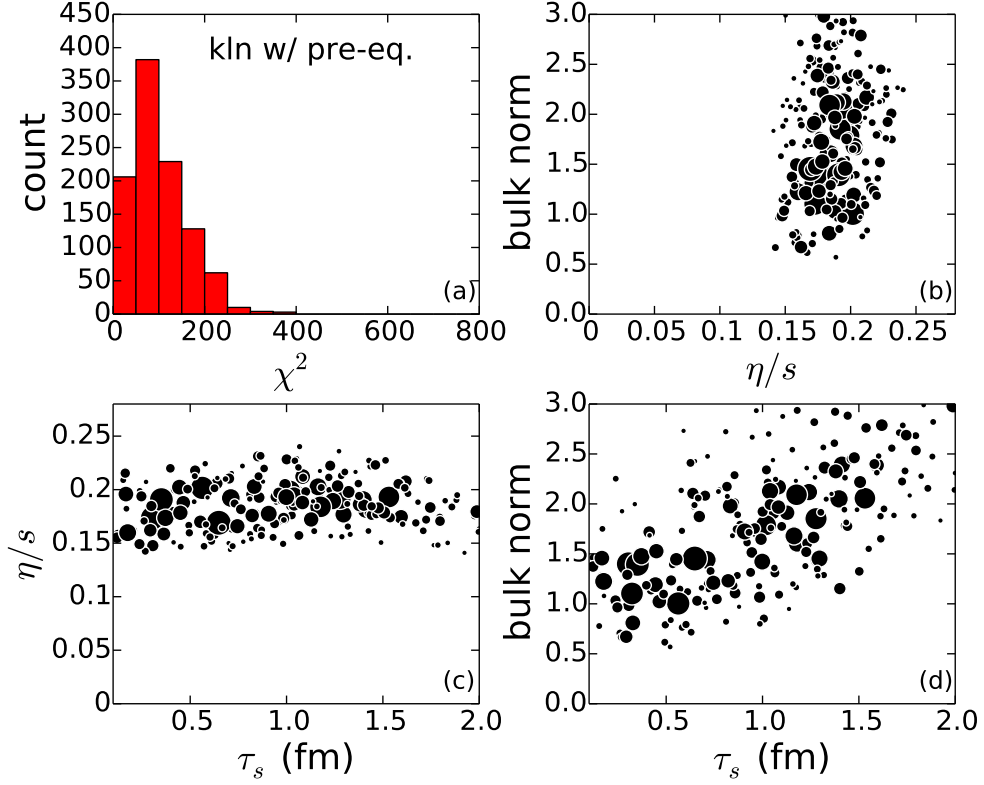


Figure 5.1: Parameter search result for the KLN initial-state model, evolved in hydrodynamic + hadronic afterburner following a free-streaming stage of duration $\tau_s - \tau_0$. (a) Histogram of the χ^2 distribution. (b-d) 2-dimensional projections of those parameter triplets ($\tau_s, \eta/s$, bulk norm.) corresponding to $\chi^2 < 50$. The size of the rings around their positions increases with decreasing χ^2 , i.e. with increasing fit quality.

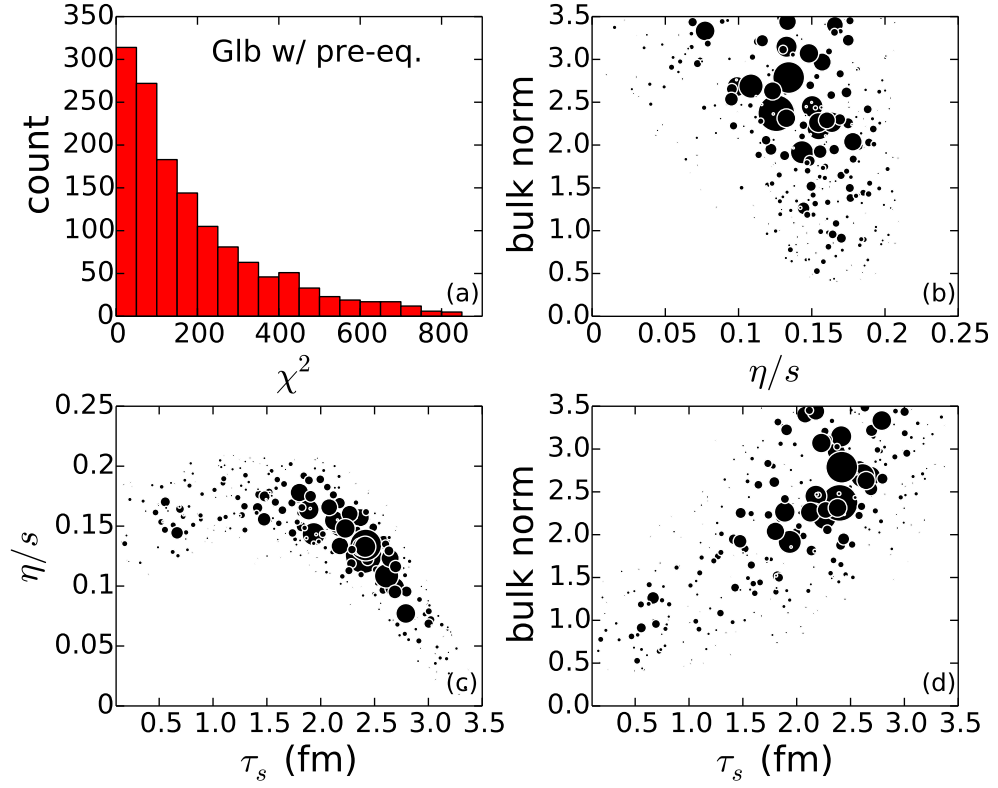


Figure 5.2: Same as Fig. 5.1, but for MC-Glb initial states with pre-equilibrium evolution.

Model	Pre-eq.	τ_s (fm/c)	η/s	bulk norm.	χ^2
MC-KLN	Yes	0.648	0.169	1.453	21.812
MC-Glb	Yes	2.398	0.126	2.371	8.534

Table 5.2: Best-fit parameters from a parameter search for two different types of simulations.

Model	MC-KLN	MC-Glb
Pre-eq.	Yes	Yes
$\bar{v}_2^{\text{ch}}$	$0.087 \pm 6.1\text{e-}4$	$0.075 \pm 6.2\text{e-}4$
$\bar{v}_3^{\text{ch}}$	$0.0306 \pm 6.2\text{e-}4$	$0.0328 \pm 6.2\text{e-}4$
$\langle p_\perp \rangle_{\pi^+}$ (GeV/c)	$0.520 \pm 1.3\text{e-}2$	$0.531 \pm 1.3\text{e-}2$
$\langle p_\perp \rangle_{K^+}$ (GeV/c)	$0.848 \pm 1.6\text{e-}2$	$0.884 \pm 1.7\text{e-}2$
$\langle p_\perp \rangle_p$ (GeV/c)	$1.323 \pm 2.2\text{e-}2$	$1.397 \pm 2.3\text{e-}2$
χ^2	21.812	8.534

Table 5.3: Model predictions for the five observables listed in Table 4.1 with the best-fit parameters listed in Table 5.2.

5.4 Bayesian analysis of the distributions of model parameters

In the preceding section we explored a subset of parameter triplets sampled by the Latin hypercube method and identified the preferred region of each parameter by identifying the region where the fit is best. However, even though we carefully selected parameter triplets to effectively represent the whole parameter space, there is plenty of parameter space left unexplored. Moreover, we are interested in knowing how the likelihoods for the parameters are distributed over the entire parameter space. Additionally, different run modes show different preferred regions for the same parameter, and it is worth knowing if this observation is significant. For this we need a

quantitative way to measure the uncertainties associated with each parameter. In this section, we use “Distribution Sampling” tools developed by the MADAI collaboration [142] to achieve these goals.

“Distribution Sampling” tools contain the Gaussian Process (GP) emulator and a Markov Chain Monte Carlo (MCMC) sampling routine. MCMC presents itself as an efficient way of exploring high dimensional parameter spaces. This method has been used to generate the posterior distributions of free parameters in heavy-ion collisions and in other physical models. Readers can refer to Refs. [75, 124, 143] for more details. MCMC samples points from a parameter space by conducting a weighted random walk. The weight is the posterior distribution of parameters calculated by Bayes’ theorem once the parameters, their corresponding model results and the experimental observations are all given. One can show that this posterior distribution is equal to the likelihood $P(\mathcal{D}^{(exp)} \mid \mathbf{x})$, which is the conditional probability of observing experimental data $\mathcal{D}^{(exp)}$ when a parameter combination $\mathbf{x}$ is given. This likelihood is assumed to have a Gaussian form

$$P(\mathcal{D}^{(exp)} \mid \mathbf{x}) \sim \exp\left(-\sum_i \frac{(\mathcal{D}_i^{(exp)} - \mathcal{D}_i^{(mod)}(\mathbf{x}))^2}{2\sigma_i^2}\right), \quad (5.2)$$

where i runs over the five observables we mentioned in the preceding section. σ_i is the uncertainty which includes both experimental and model uncertainties. MCMC applies the Metropolis algorithm to sample from the posterior distribution. This algorithm records the likelihood of every step in the random walk process, such that the acceptance of a new step depends only on the likelihood of the immediately preceeding step. If the likelihood of the new step is higher, then this new step is accepted; if not, the new step is accepted with a probability proportional to the relative likelihood between these two steps.

However, using the hybrid model to obtain model results for MCMC sampling is impractical. Typically, MCMC takes ~ 10 million steps in a random walk to get a good representation of the posterior distribution. Therefore the hybrid model has to be executed ~ 10 million times, which takes an excessively long computation time. Therefore we train a GP emulator [144] to act as a proxy of the hybrid model. After training (conditioning) the emulator on the results of thousands of hybrid model runs, the GP emulator is able to make predictions for new input parameter combinations by interpolating between the parameter set on which it was trained. In addition to the predicted values, it also reports the associated uncertainties, which is desirable for calculating likelihoods.

In this section, we train the GP emulator with full model runs for each of the two initial states model with 1,024 parameter triplets in the latin hypercube, using 5 observables computed from the hybrid simulation. After training is complete, MCMC sampling uses this emulator to calculate the final observables for a large number of newly sampled parameter triplets. The random walk in the parameter space takes 10 million steps in order to guarantee that the sampled points reflect the posterior distribution. We analyze the MCMC sampled parameter triplets and report the results in Tables 5.4, 5.6 and Figs. 5.3, 5.4. Table 5.4 summarizes the optimal values and the mean of each parameter with 95% confidence interval estimated from MCMC sampled points.

In Figs. 5.3 and 5.4, the diagonal panels show the histogram and estimated probability distribution for each of the three parameters. The probability curve is calculated from the Gaussian Kernel Density Estimate (KDE) [145, 146]. This is a non-parametric method, therefore we cannot write down functional forms for these

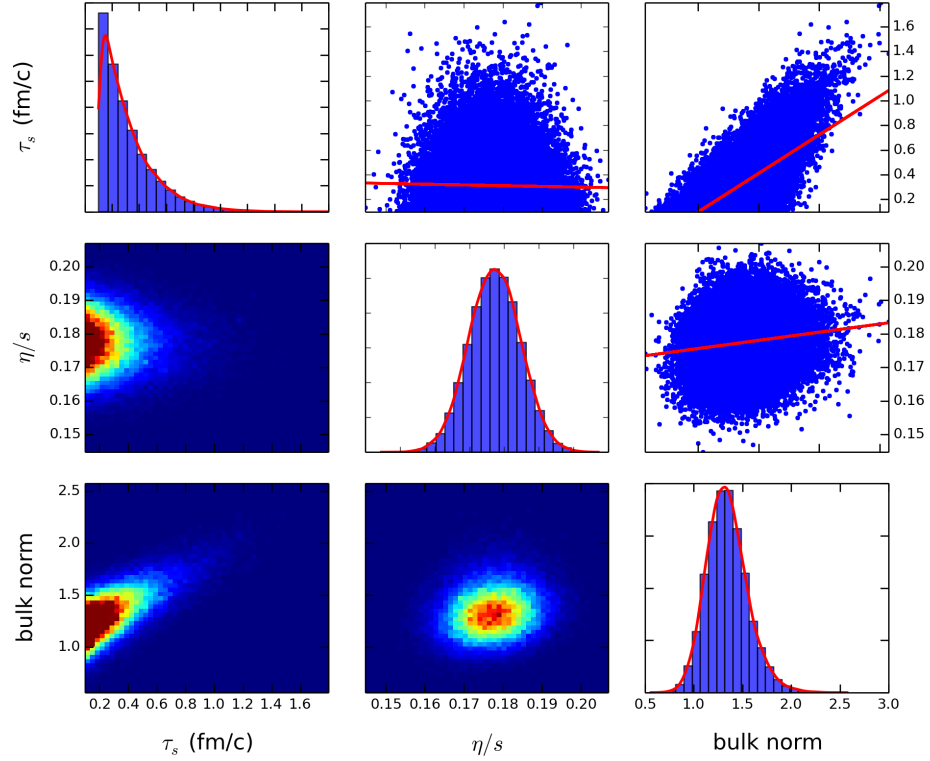


Figure 5.3: MCMC results for MC-KLN initial states with pre-equilibrium dynamics. The data used for this plot is a randomly chosen subset of 50,000 parameter triplets from 10 million MCMC sampled points.

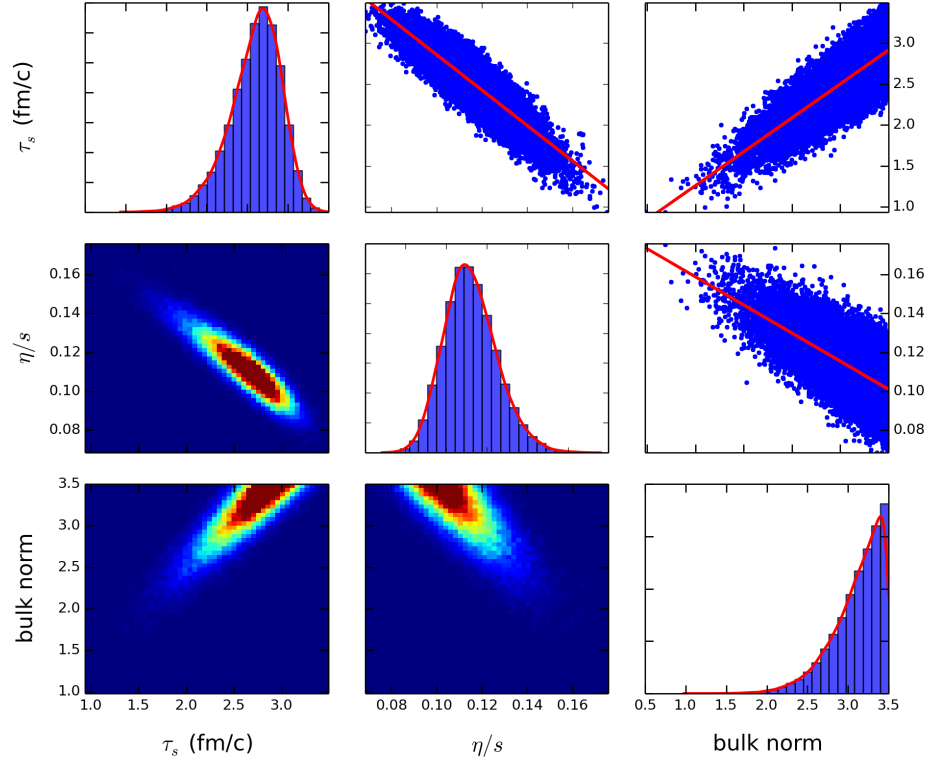


Figure 5.4: MCMC results for MC-Glb initial states with pre-equilibrium dynamics. The procedure is the same as that used for Fig. 5.3.

curves. The panels on the upper triangle are scatter plots for combinations of two parameters, with the red solid line showing any linear relationship between the two parameters. The panels on the lower triangle are the density plots of the various projections of the 3-dimensional parameter space into lower dimensions, color-coded by the relative number of runs (i.e. the probability) for these parameter combinations. Red areas indicate the most likely parameter regions. We again observe that, for both kinds of initial conditions, a larger switching time demands a larger bulk viscosity to counteract the excessive radial flow developed in the pre-hydrodynamic stage. However, these two sets of initial conditions reveal different correlations between parameters. For MC-KLN initial conditions in Fig. 5.3, the switching time and bulk viscosity, as well as shear viscosity and the bulk normalization factor, have nearly zero correlation. This indicates that the parameters in each pair are independent, which is very different from what we saw for MC-Glb initial conditions in Fig. 5.4, where strong linear correlations are exhibited between τ_s and η/s as well as between η/s and the bulk normalization factor. This difference may be due to the fact that pre-equilibrium evolution with MC-Glb initial conditions cannot generate enough anisotropic pre-equilibrium flow as the switching time increases. Therefore a smaller η/s is required for a larger τ_s in order to reduce viscous suppression of v_2 during the hydrodynamic stage. However, the pre-equilibrium radial flow generated at a late switching time is large, which calls for a large bulk viscosity in order to avoid too much radial flow at freeze-out.

Table 5.4 summarizes the posterior distribution of each parameter given by the MADAI tools including best parameter, mean parameter and confidence interval. We should be aware that these confidence intervals are calculated assuming each

Model	Pre-eq.	Parameters	Best	Mean	95% C.I.
MC-KLN	Yes	τ_s (fm/c)	0.650	0.313	0.1-0.702
		η/s	0.169	0.177	0.163-0.193
		bulk norm.	1.454	1.343	0.927-1.759
MC-Glb	Yes	τ_s (fm/c)	2.915	2.596	1.975 - 3.217
		η/s	0.101	0.112	0.086 - 0.138
		bulk norm.	3.450	3.115	2.504 - 3.5

Table 5.4: Best-fit parameters and 95% confidence intervals (C.I.) given by MCMC sampling after assuming all parameters follow normal distribution.

posterior distribution is a Gaussian. For highly skewed distributions, such as the τ_s distribution from MC-KLN initial conditions and the bulk normalization factor from MC-Glb initial conditions, this kind of estimation is problematic.

In the hope of finding the location of the peak in the probability distribution for the bulk normalization factor, we extended the upper bound of this parameter from 3.5 to 4.5 and repeated the parameter optimization. The results are shown in Figs. 5.5 and 5.6. Fig. 5.6 shows that the peak of the bulk normalization factor remains elusive. However, panel (b) and (d) of Fig. 5.5 appear to show two minima for χ^2 when we vary the bulk normalization factor: one around 2.5 and the other around 4.2. The second χ^2 minimum at large bulk viscosity is problematic because for such large ζ/s the viscous hydrodynamic code may operate outside its region of validity for a significant fraction of the evolution history. We can check this by plotting the time evolution of the inverse bulk Reynolds numbers mentioned in Chapter. 3.

The result is shown in Fig. 5.7 where we plot the inverse bulk Reynolds number R_{Π}^{-1} (3.11) in the hydrodynamic simulation for the best-fit parameter triplet, which is $\tau_s = 2.542$, $\eta/s=0.106$ and (bulk norm.)=4.053. We note that the red region, where

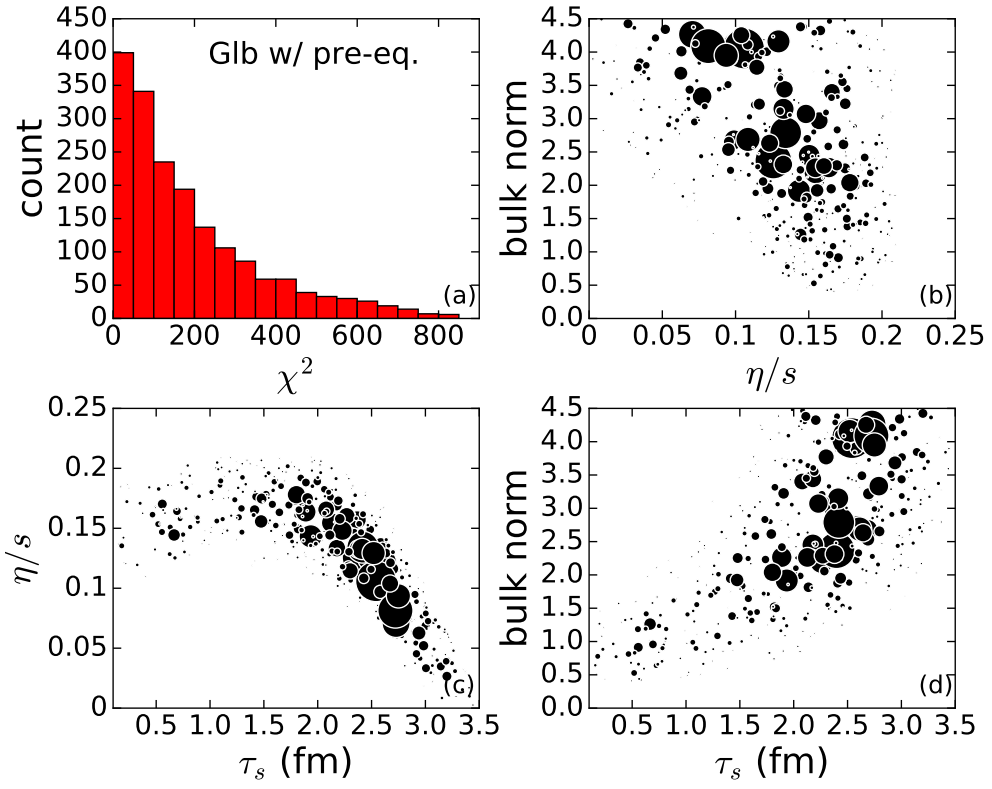


Figure 5.5: Same as Fig. 5.2, but for a larger range of the bulk normalization factor.

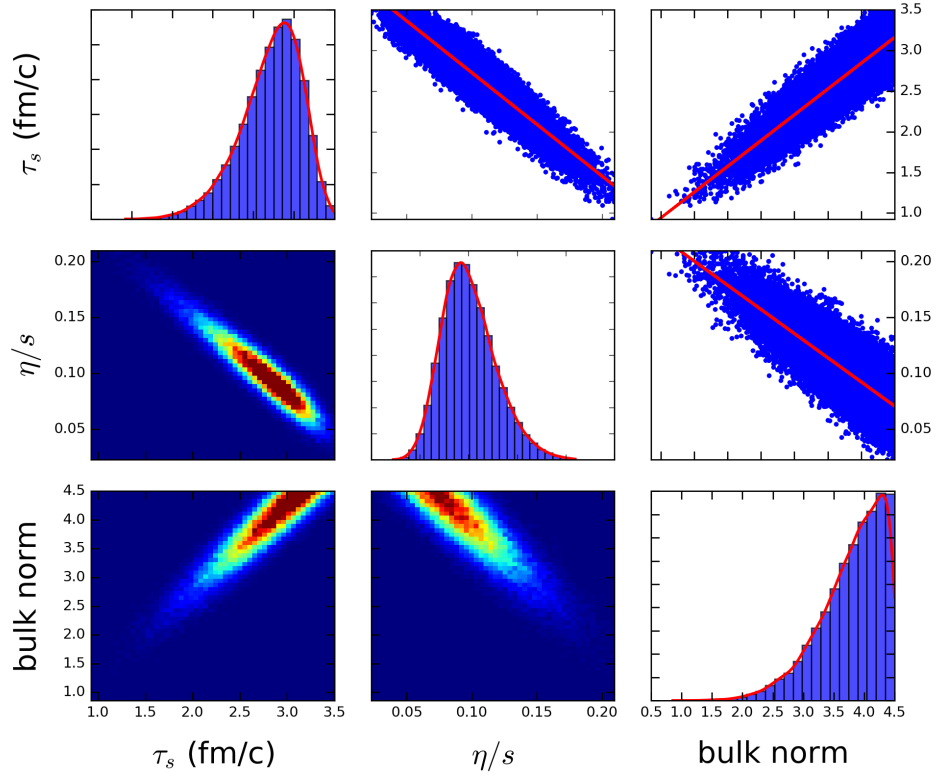


Figure 5.6: Similar as Fig. 5.4, but for a range of 0 - 4.5 for the bulk normalization factor.

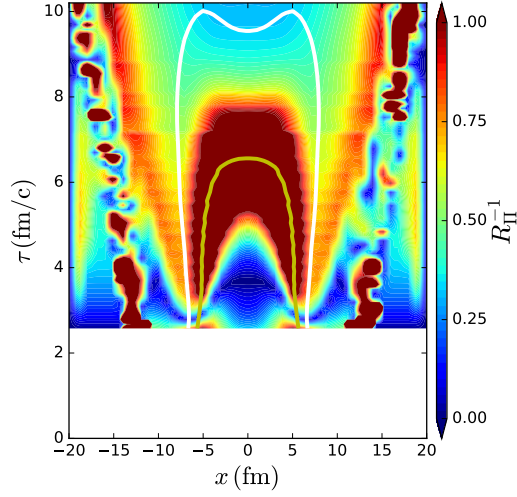


Figure 5.7: False color plots for the evolution of the inverse bulk Reynolds number R_{Π}^{-1} in the viscous hydrodynamic simulation. The white contour line represents the freeze-out surface, while the yellow line denotes the surface $T_{tr} = 180$ MeV where $(\zeta/s)(T)$ reaches its peak value.

R_{Π}^{-1} is of the order of 1 or larger, covers almost half of the space-time volume inside the freeze-out surface. While the regulation routine in VISH2+1 regulates exceedingly large values for the bulk viscous pressure, the system is numerically unstable, as shown by the yellow-red alternating pattern near the freeze-out surface. This numerical instability, likely caused by a mechanical instability due to the negative total pressure, combined with the large inverse bulk Reynolds number inside the freeze-out surface, indicates that applying viscous hydrodynamics with such a large bulk viscosity normalization factor is problematic.

Fig. 5.8 shows the hadron spectra from the best-fit parameter triplet from this campaign. As seen in the left panel, our simulation overpredicts the proton spectra at both low and high $p_{\perp}$ and therefore the total proton yield. Because the parameter optimization did not use hadron yields as experimental constraints, this parameter

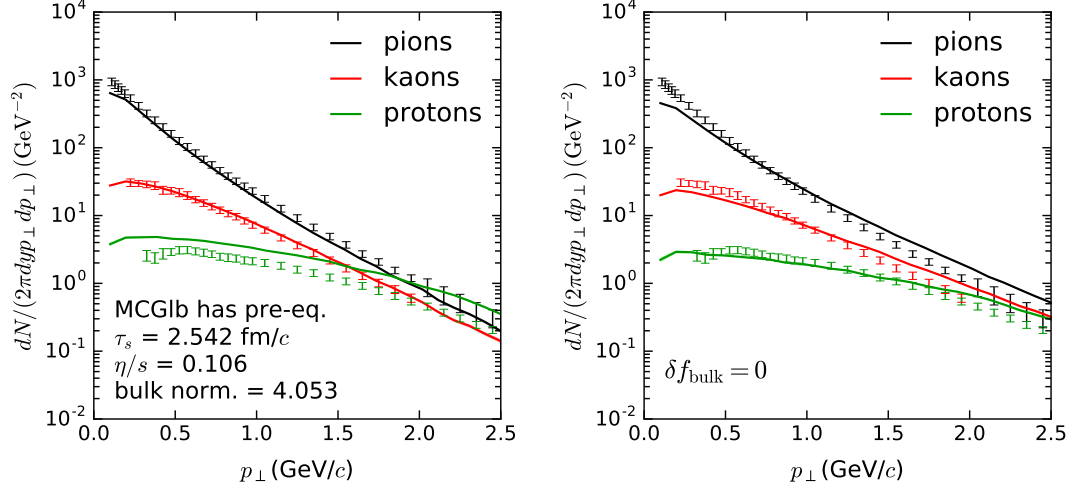


Figure 5.8: Comparison of transverse momentum spectra for π^+ , K^+ and protons between the VISHNU results and ALICE data [125]. Solid lines represent the results from the VISHNU simulation with best-fit parameter triplet, and the error bar stands for the experimental data with uncertainties. In the left panel we include the bulk viscous correction (3.17) to the hadron distribution (3.15) at freeze-out, while in the right panel we ignore the bulk viscous correction in the hadron distribution function.

triplet is still regarded as the best one even though it does not reproduce the correct proton number. The overprediction of the proton spectra at low $p_\perp$ is probably due to the bulk viscous correction (3.17), which increases particle spectra significantly in this $p_\perp$ range (see Fig. 3.8 in Chapter 3). The large values of the calculated proton spectrum at high $p_\perp$ reflects the large radial flow generated in the rather long pre-equilibrium stage in this simulation. In order to investigate the role of the bulk viscous correction at freeze-out, we show in the right panel of Fig. 5.8 the spectra obtained when setting to zero. Comparing the two plots in Fig. 5.8, we find that, the effect of δf_{bulk} is very strong at low $p_\perp$. Both the mechanical instability during the hydrodynamic stage and the large bulk viscous correction on the proton $p_\perp$ -spectra cast doubts on the reliability of our model when used for such large bulk

viscosity normalization factor. Therefore the minimum of χ^2 at large values for the bulk normalization factor is probably non-physical. It is likely that the secondary χ^2 minimum near (be the norm) 2.5 is a better candidate for the preferred parameter triplet, but we cannot be sure because our code becomes increasingly unreliable at large values for this parameter.

We are most interested in constraining the switching time τ_s . We know that hydrodynamics does not apply at very small switching times because for very small switching times the initial pressure anisotropies are too large. We therefore set a lower limit on τ_s when we performed the parameter search. This causes the distribution of the MCMC-sampled τ_s to be asymmetric, and when the τ_s likelihood distribution peaks at too small values, we can only extract an upper limit, but not a preferred range for τ_s . In the top left panel of Fig. 5.3, we observe that the distribution of τ_s is not a Gaussian: it is highly skewed to the right since τ_s cannot take negative values. So it is problematic to calculate the confidence interval of τ_s assuming it follows a normal distribution. Instead, we find that the log-normal distribution fits the MCMC-sampled τ_s data well (cf. see Fig. 5.9 for such a fit). The log-normal distribution for a variable x has the form

$$f(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi}x\sigma} \exp\left(-\frac{(\ln x - \mu)^2}{2\sigma^2}\right), \quad (5.3)$$

where μ is the mean and σ is the standard deviation for the log-transformed data $\ln x$. We estimate these two parameters by the maximum likelihood method [147] and obtain $\hat{\mu} = -1.333$ and $\hat{\sigma} = 0.575$, where the “hat” denotes the estimated value. The mean and its confidence interval of un-transformed data are shown in Table 5.5. The mean of the original data (not log-transformed) is $\exp(\hat{\mu} + \hat{\sigma}^2/2)$. The 95% confidence intervals for the estimated mean is calculated by using Cox’s

formula [148]. This estimated mean is the same as the arithmetic mean we saw in Table 5.4. However, because the sample size is too large, the 95% confidence interval is tightly constrained around the mean. This overly constrained C.I. rules out most τ_s , in contradiction with what we observe in Fig. 5.9. Therefore, in order to give a more meaningful estimate of the upper limit of τ_s , we also report the 95% quantile of MCMC sampled data in this table, which tells us that 95% of MCMC-sampled τ_s are below $\tau_s = 0.714 \text{ fm}/c$.

Model	Pre-eq.	Parameters	Mean	95% C.I.	99.7% C.I.	95% quantile
MC-KLN	Yes	$\tau_s \text{ (fm}/c)$	0.311	0.309 - 0.313	0.308 - 0.314	0.714

Table 5.5: Estimate the mean and its confidence interval of τ_s from MCMC resampled parameter triplets after assuming τ_s follows log-normal distribution.

Model	MC-KLN	MC-Glb
Pre-eq.	Yes	Yes
$\bar{v}_2^{\text{ch}}$	0.087	0.075
$\bar{v}_3^{\text{ch}}$	0.0305	0.032
$\langle p_\perp \rangle_{\pi^+} \text{ (GeV}/c)$	0.520	0.507
$\langle p_\perp \rangle_{K^+} \text{ (GeV}/c)$	0.847	0.853
$\langle p_\perp \rangle_p \text{ (GeV}/c)$	1.325	1.372
LogLikelihood	-12.710	-4.356

Table 5.6: MCMC predictions for the five observables listed in Table 4.1 with the best-fit parameters listed in Table 5.4.

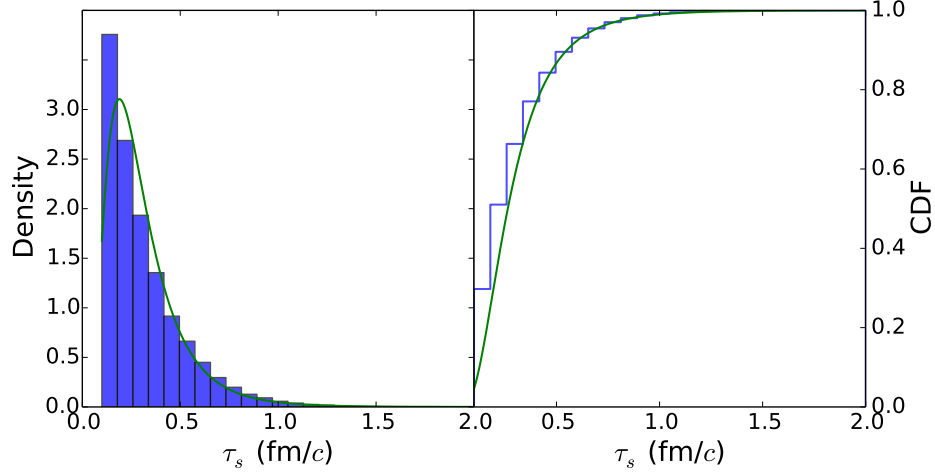


Figure 5.9: Log-normal fit to the τ_s distribution generated from MCMC with MC-KLN initial states with pre-equilibrium stage. The parameters for the inverse Gaussian curves are estimated by the maximum likelihood method. Left panel: a comparison of the histogram (blue) of MCMC τ_s with the fitted curve (green); right panel: a comparison of the cumulative distribution with the same color code as the left panel.

5.5 Trying to resolve the mass ordering problem

With the best-fit parameters shown in Table 5.2, we now run the hybrid model in event-by-event mode with MC-KLN initial conditions in order to calculate the $p_\perp$ -differential anisotropic flows using the scalar product method (which is sensitive to the variance of flow fluctuations). We simulated a total of 160,000 events, with 400 separate hydro events while each hydro event was oversampled 400 times. The results are displayed in Fig. 5.10. We include the electromagnetic decay $\Sigma^0 \rightarrow \Lambda + \gamma$ by hand (it is not contained in UrQMD) to account for the feed-down from non-weak decays in the ALICE measurement [137]. The transverse momentum spectra given by the hybrid model shown in the left and middle panels generally reproduce the shape of experimentally measured spectra. We see, however, a deviation at large $p_\perp$ for the

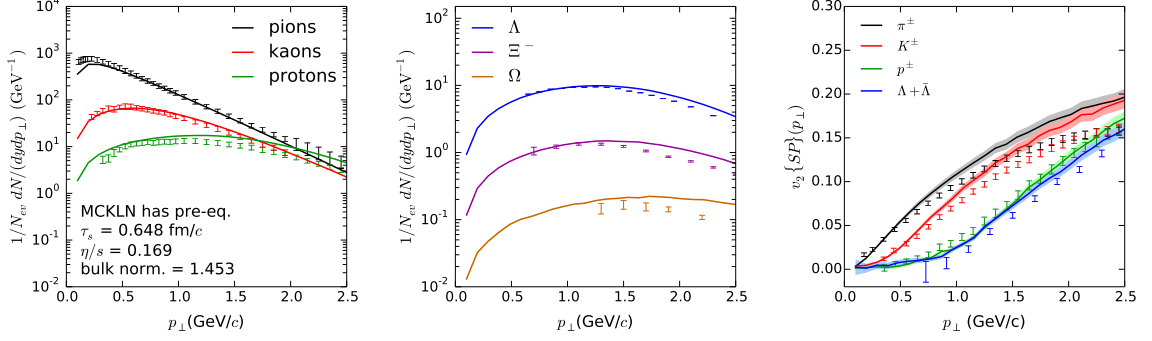


Figure 5.10: Comparison with experimental data of event-by-event hybrid model predictions with the best fit parameter combination (the one with the smallest χ^2 value in Table 5.2) for KLN-initialized simulations with pre-equilibrium free-streaming dynamics, for 2.76 A TeV Pb+Pb collisions at 10%–20% centrality. The event-by-event hybrid simulation used 400 fluctuating MC-KLN initial density profiles. The spectra calculated from the Cooper-Frye formula are oversampled for 400 times and fed into UrQMD. The left panel shows a comparison of the transverse momentum spectra of positively charged pions, kaons and protons from the hybrid model output with ALICE data [125]; the middle panel shows a similar comparison for Λ , Ξ and Ω using ALICE data from [137, 138]. The right panel compares the scalar product $p_{\perp}$ -differential elliptic flow to measurements presented in Ref. [134]. The experimental data are plotted as points with error bands while the simulation results are plotted as color-coded solid lines with a shaded band indicating the statistical uncertainties of the simulated results.

heavier particles (protons, Λ , Ξ and Ω), which indicates that our simulations with best-fit parameters produce too much radial flow in the simulation. Constraining our model with data for the mean $p_{\perp}$ of protons is unable to prevent this from happening, therefore a parameter search with additional input from higher $p_{\perp}$ moments (e.g. $\langle p_{\perp}^2 \rangle$) of the proton spectrum is necessary to eliminate this problem. We will implement this at the end of this section.

Fig. 5.10 compares the $p_{\perp}$ -differential scalar product elliptic flow with experimental data. The theoretical results correctly predicts the trends of $p_{\perp}$ differential flow. However, the elliptic flow spectra for proton and Λ are not as well separated as in the

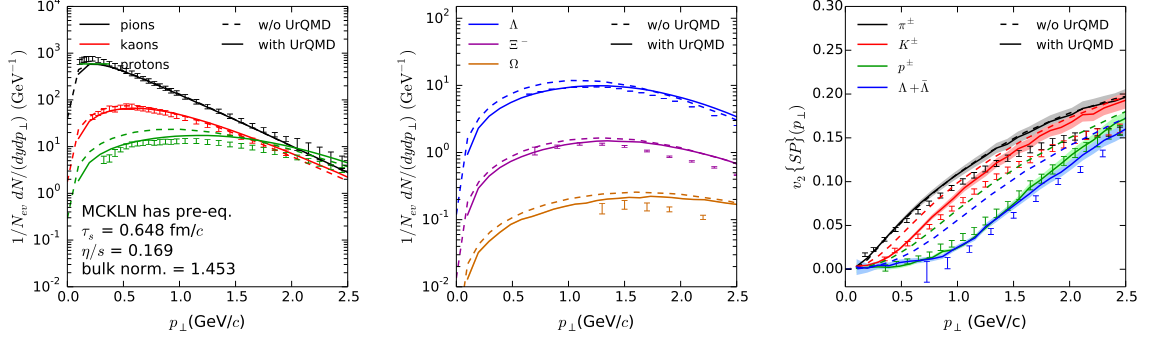


Figure 5.11: Same as Fig. 5.10 (solid lines), but including the results from a pure hydrodynamic run with the same parameters, without any hadronic rescatterings (dashed lines).

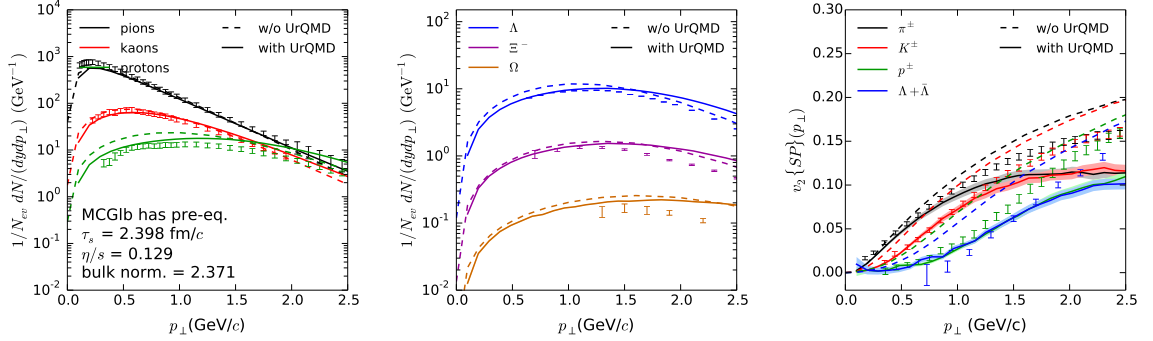


Figure 5.12: Same as Fig. 5.11, but with MC-Glb initial conditions and the corresponding best-fit parameters shown in Table. 5.2.

experimental data. In order to assess the role of the hadronic afterburner in this observation, we performed a set of event-by-event simulations with the best-fit parameters, without the UrQMD afterburner, decoupling directly at $T_{sw} = 155$ MeV. The results are shown in Fig. 5.11 (for MC-KLN initial conditions) and 5.12 (for MC-Glb initial conditions). In both plots, the solid lines stand for the full VISHNU runs while the dashed lines represent the same runs without the hadronic afterburner. Comparing

the shapes of the curves for the $p_\perp$ -spectra, we see that UrQMD generates additional radial flow for protons and Λ , but not so much for Ξ and Ω . On the other hand, the radial flow effects generated by both the full VISHNU and the pure hydrodynamic runs for Ξ and Ω are stronger than in the measured spectra. Standard elliptic flow mass-ordering for protons and Λ is observed before hadronic rescattering, but the hadronic afterburner pushes the elliptic flow of protons to larger $p_\perp$ more strongly than for Λ 's, due to the larger scattering cross-section for protons. This leads to an almost complete disappearance of the p - Λ mass splitting in $v_2(p_\perp)$ at the end of the hadronic stage. The experimental data, on the other hand, show that the p - Λ mass splitting of $v_2(p_\perp)$ survives the hadronic stage. The hadronic afterburner effects on both $v_2^p(p_\perp)$ and $v_2^\Lambda(p_\perp)$ are large, and the effect that leads to the approximate disappearance of the p - Λ mass splitting in the theoretical simulations is subtle. It would be easier to understand the experimental data if the dynamic model spent less time in the hadronic phase, establishing more of the radial flow earlier.

We conclude this section by showing results from one final campaign in which included the switching temperature T_{sw} at which we switch from hydrodynamics to UrQMD as a forth parameter in the parameter optimization. We allow it to vary between 130 MeV and 170 MeV. This parameter is sensitive to the final hadronic particle ratios, so we included the π^+/K^+ , π^+/p and π^+/Λ ratios measured by ALICE [99, 137] into the list of our final observables used to constrain the model parameters. Furthermore, instead of using the mean transverse momenta calculated from the experimental data by first extrapolating them to $p_\perp = 0$ [99], we constrain our parameter search with truncated $\langle p_\perp \rangle$ values calculated directly from the measured data for the hadron spectra reported in Ref. [99]. We also include the second $p_\perp$ -moment

of proton spectra, $\langle p_{\perp}^2 \rangle$, in order to avoid the problem of generating too much radial flow as seen in Figs. 5.10 - 5.12 and to obtain a better description of $p_{\perp}$ -spectra at high $p_{\perp}$. The updated final observables are listed in Table. 5.7.

The 1,024 parameter combinations sampled by the Latin hypercube method cover the following ranges: $0.1 \text{ fm}/c < \tau_s < 3.5 \text{ fm}/c$, $0 < \eta/s < 0.21$, $0 < (\text{bulknorm.}) < 4$ and $130 \text{ MeV} < T_{sw} < 170 \text{ MeV}$. For this campaign, we only optimized these parameters for MC-Glb initial conditions.

$\langle v_2^{\text{ch}} \rangle$	0.0782 ± 0.0019
$\langle v_3^{\text{ch}} \rangle$	0.0316 ± 0.0008
$\langle p_{\perp} \rangle_{\pi^+} \text{ (GeV}/c\text{)}$	0.542 ± 0.018
$\langle p_{\perp} \rangle_{K^+} \text{ (GeV}/c\text{)}$	0.825 ± 0.028
$\langle p_{\perp} \rangle_p \text{ (GeV}/c\text{)}$	1.311 ± 0.043
$\langle p_{\perp}^2 \rangle_p \text{ (GeV}^2/c^2\text{)}$	2.085 ± 0.070
$(dN_{\pi^+}/dy)/(dN_{K^+}/dy)$	6.691 ± 0.670
$(dN_{\pi^+}/dy)/(dN_p/dy)$	21.667 ± 2.292
$(dN_{\pi^+}/dy)/(dN_{\Lambda}/dy)$	26.765 ± 3.639

Table 5.7: Experimental data for the nine hadronic observables from 2.76 A TeV Pb+Pb collisions of 10–20% centrality that were used as constraints for our 4-parameter fit. The mean $p_{\perp}$ -integrated elliptic and triangular flow values for charged hadrons were measured by ATLAS [123], the mean transverse momenta for positively charged pions, kaons and protons, and the second moment of protons are calculated from the corresponding spectra reported by the ALICE Collaboration [99]. The hadron ratios are calculated from the identified hadronic yields given by the ALICE Collaboration [99, 137].

Fig. 5.13 shows the results of the 4-parameter optimization for MC-Glb initial conditions. We notice that the system actually prefers a lower switching temperature around 135 - 140 MeV, instead of the higher value of 155 MeV assumed in our earlier fits. Compared with the earlier 3-parameter optimization, the 4-parameter fit

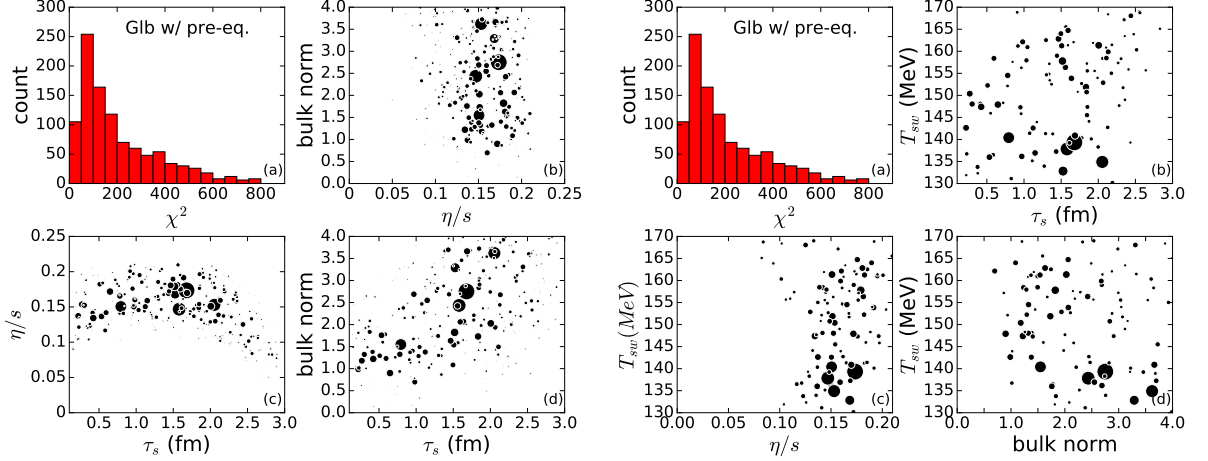


Figure 5.13: Same as Fig. 5.2, but with 4 parameters used in the optimization process. The left plot shows the projection of the 4-dimensional parameter space onto 2-dimensional subspaces consisting of any two of τ_s , η/s and bulk normalization factor, while the right plot shows such projections on the three 2-dimensional subspaces containing T_{sw} .

prefers smaller values for the switching time τ_s around $\tau_s \approx 1.7$ fm/c. In order to check the posterior parameter distributions, we again employ the MCMC technique described in Section 5.4. The results are shown in Fig. 5.14. In this plot the probability distribution for T_{sw} peaks around 140 MeV, which is well below the switching temperature we used before. This figure also reveals that T_{sw} is weakly correlated with the switching time, which means it is not very sensitive to the length of the pre-equilibrium stage; it is positively correlated with the shear viscosity but negatively correlated with the bulk viscosity. The best-fit parameter combination given by this optimization is: $\tau_s=1.678$ fm/c, $\eta/s=0.174$, $T_{sw}=139.3$ MeV and (bulk norm.)=2.752.

Finally, we simulated 160,000 events in VISHNU (400 hydrodynamic events, each of them is oversampled 400 times for the hadronic afterburner) using this best-fit parameter combination. The resulting hadron spectra and elliptic flows are shown in

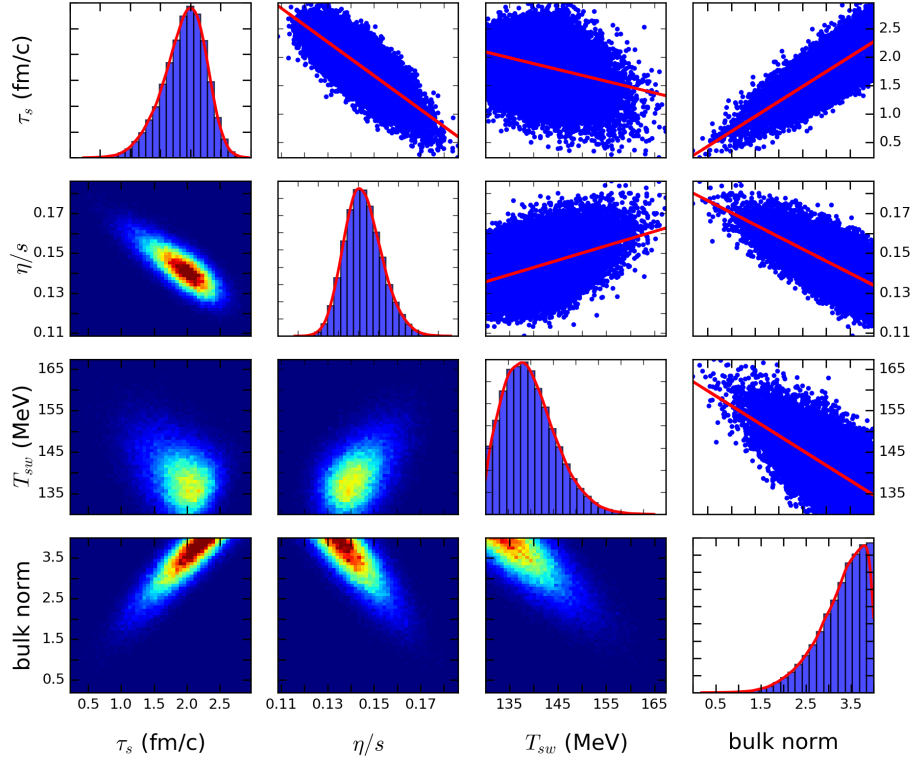


Figure 5.14: MCMC simulation results for MC-Glb initial conditions with pre-equilibrium dynamics for the runs shown in Fig. 5.13. The procedure is the same as that used in Fig. 5.3.

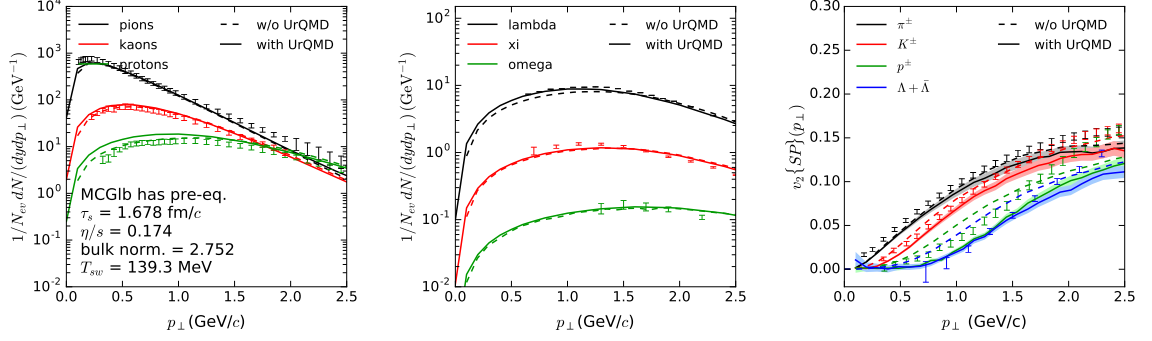


Figure 5.15: Same as Fig. 5.12, but with the best-fit 4 parameters.

Fig. 5.15. In this figure, we also compare the results from the full VISHNU run (solid lines) with those from a simulation without the hadronic afterburner. Comparing with the full VISHNU results shown in Fig. 5.12, the hadron spectra and elliptic flows in Fig. 5.15 describe the experimental data much better, especially at higher $p_{\perp}$ values. This is undoubtedly due to the additional $\langle p_{\perp}^2 \rangle$ constraint for the protons. However, this run with the optimized 4 parameters still does not resolve the mass ordering issue of the proton and Λ elliptic flows. We observe that the effect of UrQMD is still large, even though we now switch to the hadronic stage at a lower temperature. A more thorough understanding of the hadron rescattering processes may be required to resolve this problem.

5.6 Chapter summary

In this chapter, we improved the VISHNU hybrid model by including a pre-equilibrium evolution stage and switching to a more complete set of viscous hydrodynamic equations. We optimized the free parameters in the updated hybrid model by implementing a parameter search, which is then supplemented by a more thorough

parameter space exploration using MCMC sampling. The results show that the MC-KLN initial states model prefers an earlier switching time and a smaller bulk viscosity than the MC-Glb model.

We thank Jonah Bernhard for kindly providing the EOS for the hybrid model and helping with the UrQMD code.

Chapter 6: Conclusions and Outlook

Viscous hydrodynamics, together with the initial condition models, a pre-equilibrium stage, and a hadronic after-burner, constitutes a powerful framework for the phenomenological study of relativistic heavy-ion collisions. This framework successfully describes the soft part of hadronic observables, which covers approximately 99% of all particles produced in heavy-ion collisions. One of the most notable aspects of this model is its power in constraining transport coefficients of the QGP, such as its shear and bulk viscosities.

As we showed in Chapter 2, the pre-equilibrium stage has non-negligible effects on heavy-ion collision observables. We studied this by comparing hydrodynamic simulations with no pre-equilibrium evolution, assuming thermalization after a certain time delay to where this time interval was filled with a free-streaming pre-equilibrium stage. The pre-equilibrium stage is matched to the hydrodynamic stage by applying Landau matching conditions, which translate the pre-equilibrium energy momentum tensor to a complete set of hydrodynamical initial conditions, including pre-equilibrium flow, and non-zero starting values for the shear stress tensor and bulk viscous pressure. Our investigation showed that with pre-equilibrium evolution, the anisotropic flow coefficients are only weakly sensitive to the switching time all the way up to about $2 \text{ fm}/c$, due to significant anisotropic flow generated in the pre-equilibrium stage,

which compensates for the reduced anisotropic flow created by hydrodynamics if the hydrodynamic stage starts only after this delay. We also found that the hadron mean transverse momenta are highly sensitive to the length of the pre-equilibrium stage. A free-streaming pre-equilibrium stage generates more radial flow than if the system had thermalized earlier. Compared with anisotropic flows, the mean transverse momentum puts a tighter constraint on the thermalization time.

In order to study the effects of non-zero bulk viscosity, we updated the hydrodynamic equations in VISH2+1 to include the evolution of the bulk viscous pressure, including all non-linear second-order terms. We analyzed the effect of each non-linear term individually and found that they only weakly alter the spectra and anisotropic flow coefficients. The presence of non-zero bulk viscosity leads to steeper spectra and suppresses the elliptic flow at large $p_{\perp}$. In spite of presently unavoidable uncertainties arising from specific parameterization of the temperature dependent bulk viscosity and the form of the bulk viscous correction of the distribution function at freeze-out, a credible extraction of the shear viscosity from experimental data requires accounting for the effects of bulk viscosity and the two transport coefficients should therefore be extracted simultaneously.

Chapters 4 and 5 show our effort in optimizing the free model parameters simultaneously by comparing the model predictions to experimental data. Chapter 4 focuses on pure hydrodynamic simulations with the switching time, shear viscosity and kinetic decoupling temperature as free parameters. We optimized them simultaneously using a 3-dimensional parameter search. This study showed that the thermalization time as well as the shear viscosity are model dependent: MC-KLN initial conditions prefer earlier thermalization ($\tau_s \approx 0.13$ fm/c) and larger shear viscosity $\eta/s \approx 0.2$

than MC-Glb initial conditions ($\tau_s \approx 0.6$ fm/c, $\eta/s \approx 0.16$), if pre-equilibrium evolution is included. In Chapter 5 we optimized the switching time, shear viscosity and bulk viscosity normalization factor using the VISHNU hybrid model with MC-KLN and MC-Glb initial conditions, respectively. We also studied the posterior parameter distribution calculated from a Bayesian analysis with MCMC sampling. We showed that this optimization gives qualitatively similar results as the one using pure hydrodynamic simulations - namely, that MC-KLN initial conditions prefer an earlier switching time and a larger shear viscosity than the MC-Glb initial conditions. Because MC-Glb prefers later switching, it requires a larger bulk viscosity than MC-KLN to suppress the excessive radial flow from the pre-equilibrium stage. In this chapter, we also showed that the proton and Λ elliptic flow distributions are very close to each other, showing nearly no separation at $p_\perp \lesssim 1.5$ GeV. We also conducted a more comprehensive parameter optimization, which included the switching temperature from the partonic phase to the hadronic phase as a fourth parameter, as a last attempt to solve this problem. The resulting best-fit spectra and elliptic flows describe the data much better but the elliptic flow mass-ordering problem for p and Λ persists. It is possible that an update to the strange particles' cross-sections in UrQMD is required to resolve the elliptic flow mass-ordering problem. We keep this for future work.

With more abundant and precise experimental measurements on the heavy-ion collision observables, our iEBE-VISHNU package will need to be upgraded for more detailed phenomenological study, such as a realistic pre-equilibrium evolution in which the matter can thermalize and a 3+1D viscous hydrodynamic model which is capable of handling the breakdown of boost-invariance. These will pave the way for the

investigation of heavy-ion collisions in smaller collision systems and at lower collision energies at RHIC. The author thanks The Ohio Supercomputer Center [149] for providing the computation resources.

Appendix A: Building a predictive model for the hydrodynamic scaling factor

A.1 Introduction

In hydrodynamic simulations, it is common practice to rescale the initial entropy profile by multiplying with a scaling factor so that the simulated charged particle multiplicity $dN_{ch}/d\eta$ matches the experimental measurement. This scaling factor, although roughly centrality independent, depends on several other model parameters: the initial-state model, the switching time between pre-equilibrium and hydrodynamics, the freeze-out temperature, etc. In the default mode of the iEBE-VISHNU package, these model parameters are carefully tuned to reproduce the multiplicity in the most central collisions at midrapidity, see Table A.2 in Ref. [150] for details. However, if one needs to vary any model parameter, a refit of the initial profile scaling factor to the experimental multiplicity needs to be done.

Our program **smoothHydropackage**, originally written by Chun Shen and significantly customized by the author ⁷, is designed to find the scaling factor for a new set of model parameters in an iterative manner. Starting with an initial guessed scaling factor, this program runs **VISH2+1**, **iS** and resonance decays sequentially to get

⁷see <https://github.com/JiaLiu11/smoothHydropackage>

the charged particle multiplicity $dN_{ch}/d\eta$ within $|\eta| < 0.5$ and compares it with the experimental data. It decreases (increases) the scaling factor in the next run if the current run gives a simulated $dN_{ch}/d\eta$ above (below) the experimental value. Typically this takes about 3 iterations, which is approximately 3 CPU hours, and could be longer if the initial guessed scaling factor is very far from the correct scaling factor. When we need to run a large batch of different parameter combinations, finding the scaling factors in this way takes too much time. It is imperative to find a way to accelerate this process. One approach to this is to predict the scaling factor instead of randomly assigning one.

Through the parameter optimization conducted in Chapter 4, we have already found a decent number of scaling factors corresponding to different parameter combinations. For example, we found 1,300 scaling factors corresponding to 1,300 different parameter triplets using MC-KLN initial profiles with pre-equilibrium evolution. With this data set, we can build a statistical model to predict the scaling factor for a new $\tau_s, \eta/s, T_{dec}$ combination. In this appendix, we build a linear regression model from this data set, evaluate our model performance and improve our model by systematically selecting and including new predictors.

A.2 Introduction to linear regression

Linear regression is a simple yet powerful parametric model to make numerical predictions from known data. The basic assumption of linear regression is that the true outcome y (e.g. the hydrodynamic scaling factor) is linearly related to all its predictors x_i (e.g. $\tau_s, \eta/s, T_{dec}$ and etc.) [151]

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p + \epsilon, \quad (\text{A.1})$$

where $\beta_0, \beta_1, \dots, \beta_p$ are unknown coefficients. ϵ is the error term, which captures the variation in y that cannot be explained by the predictors.

If we have n observations $(x_{11}, x_{12}, \dots, x_{1p}, y_1), (x_{21}, x_{22}, \dots, x_{2p}, y_2), \dots, (x_{n1}, x_{n2}, \dots, x_{np}, y_n)$, we can estimate the coefficients β_i by minimizing the “Residual Sum of Squares” (RSS)

$$\text{RSS} = \sum_{i=1}^n \left[(y_i - \hat{\beta}_0 - \sum_{j=1}^p \hat{\beta}_j x_{ij})^2 \right], \quad (\text{A.2})$$

where $\hat{\beta}_0$ and $\hat{\beta}_i$ are the estimated coefficients, and the “hat” symbol indicates they are estimated values from the data.

Once we have all the estimated coefficients, we can use Eq. (A.1) to predict y , i.e. $\hat{y}$ as $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \dots + \hat{\beta}_p x_p$. We call the predicted outcome as $\hat{y}$ to distinguish it from the true outcome y . Generally the predicted $\hat{y}$ does not equal the true outcome y , but a good linear model should result in a very small difference between them.

If one wants to improve the fit, the usual way is to include predictors with more complex forms, such as $x_{p+1} = x_2^2$, $x_{p+2} = x_1 x_2$. Because the assumption that y is linearly depends on x_{p+1} and x_{p+2} still holds, this is of course a linear model.

In our case, we have $n = 1300$ observations from MC-KLN initial-state runs with pre-equilibrium evolution. We have $p = 3$ predictors: τ_s , η/s and T_{dec} . We use these to train a linear regression model. The trained linear regression model serves as a surrogate for the true simulation model, which takes new parameter triplets and outputs the scaling factor, but it is much faster than the true model.

A.3 Implementing the linear regression model

Linear regression is implemented in most numerical analysis softwares. In this study, we use **R** [152], because of its vast collection of packages for the predictive model building and diagnosing. We fit a linear regression model using τ_s , η/s and T_{dec} as predictors to predict scaling factor s

$$s = \beta_0 + \beta_1\tau_s + \beta_2\eta/s + \beta_3T_{dec} + \epsilon, \quad (\text{A.3})$$

	Estimate	Std. Error	t value	Pr(> t)
β_0	12.46	0.08	164.84	0.00
β_1	-0.18	0.03	-6.82	0.00
β_2	-12.84	0.17	-75.21	0.00
β_3	-4×10^{-4}	0.00	-7.92	0.00

Table A.1: The linear regression estimated coefficients for predicting scaling factor s using τ_s , η/s , T_{dec} as predictors. The 2nd column is the standard error for the estimated coefficients. While the 3rd and 4th columns are the results from Wald's t-test. The training data for this run is from MC-KLN initial-state with pre-equilibrium in pure hydrodynamic simulation.

Table A.1 shows the estimated constant term $\hat{\beta}_0$ and coefficients for predictors τ_s , η/s and T_{dec} . We notice that the coefficients for these three parameters are all negative. This agrees with our expectation. For example, after we find the correct scaling factor for a particular parameter combination, if we hold η/s and T_{dec} constant and delay the equilibration, the system would spend more time free-streaming and less in the hydro stage. Because energy is conserved in free-streaming, a shorter hydro stage means less dissipated energy. So we decrease the scaling factor to reduce the initial total energy to keep the final total energy unchanged. The standard error is

calculated by assuming that the error term ϵ in (A.3) follows a normal distribution. Wald’s t-test intends to point out which predictors cannot be excluded from the linear regression model. However, when the number of observations is much larger than the number of predictors, Wald’s t-test easily fails to exclude any predictor. Therefore we will not discuss the last two columns in Table A.1, but instead turn to use the mean squared error (MSE) to assess the model’s performance.

A.4 Model diagnostics

MSE measures the overall difference between model prediction and true outcome

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (\text{A.4})$$

However, the MSE we calculated from the training data set is not necessarily generalized to the new data set because estimated parameters are only optimized to reduce the MSE for the training data set. So a small MSE calculated from the data we used to train the model does not necessarily mean that the MSE would be equally small for the new parameter triplets. One way out is to discard the first portion of our training data and use the rest to train our model. After the training, the discarded data is used as “new” data to calculate MSE and measure the model performance. This is called the “cross-validation” method [153]. We can do cross-validation several times, each time randomly separating the original data set into the training data and the held-off data, train the model with the training data, then use held-off data to make prediction and calculate MSE. After that, we use the mean MSE from this cross-validation result to measure the model performance. In our test, we do this cross-validation 10 times, each time we reserve 10% of the data and train the model using the remaining 90% of the data. Then we calculate the mean MSE to be 0.26.

This means on average, the difference between predicted and the true scaling factor is 0.5. While most of scaling factor is around 6 to 9, a 0.5 difference is too large. Additionally, a careful check on the data reveals that this model does not give good prediction around the lower limit of τ_s . This suggests that we should improve our linear regression model.

A.5 Improving the model's performance

As mentioned above, we can add polynomials of τ_s , η/s , or T_{dec} into the predictors. Now we include the polynomials of only a single predictor into our model individually, up to its 5th order. For example, when the order of polynomial for τ_s is 3, our model becomes

$$s = \beta_0 + \beta_1\tau_s + \beta_2\eta/s + \beta_3T_{dec} + \beta_4\tau_s^2 + \beta_5\tau_s^3 + \epsilon. \quad (\text{A.5})$$

At each order of the polynomial for each predictor, we do the cross-validation test for 10 times and calculate $\langle \text{MSE} \rangle$. The results are shown in Fig. A.1. We observe that including higher orders of polynomials of τ_s or η/s decreases $\langle \text{MSE} \rangle$, but adding higher order of T_{dec} does not reduce $\langle \text{MSE} \rangle$. Moreover, $\langle \text{MSE} \rangle$ decreases slowly when the order of polynomials goes beyond 3 for τ_s and 2 for η/s . Therefore we will only include τ_s^2 , τ_s^3 and $(\eta/s)^2$ into our model (A.3).

In addition to integer polynomials, fractional polynomials are also possible. But after checking the cross-validation results, they do not improve the model significantly. There is one more possibility to consider, which is the coupling terms between any two predictors. We add either $\tau_s \cdot \eta/s$, $\tau_s \cdot T_{dec}$ or $\eta/s \cdot T_{dec}$ into the simplest model (A.3) one at a time, and check how each of them changes the mean MSE individually.

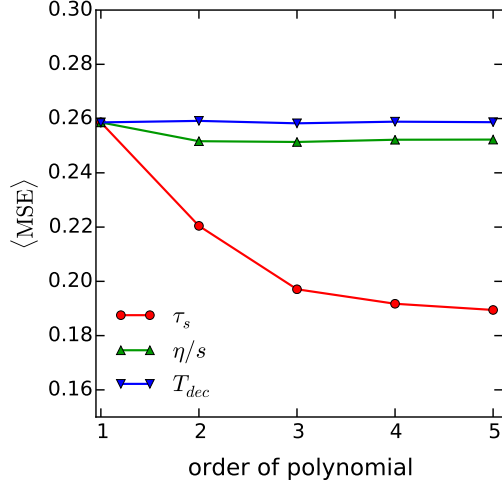


Figure A.1: Results of the cross-validation test for the linear regression model including higher powers of the predictors.

Table A.2 shows the $\langle \text{MSE} \rangle$ calculated from 10 cross-validation tests after adding a specific corresponding coupling term to the model.

coupling	$\langle \text{MSE} \rangle$
none	0.26
$\tau_s \cdot \eta/s$	0.11
$\tau_s \cdot T_{dec}$	0.26
$\eta \cdot T_{dec}$	0.26

Table A.2: Averaged mean squared error after including a coupling term to the linear regression model (A.3).

Including the coupling between the switching time and the specific shear viscosity greatly reduces the MSE, while other two coupling terms have no effect. Therefore we add $\tau_s \cdot \eta/s$ to our linear regression model. After refitting the data and recalculating

the coefficients, our model becomes

$$\begin{aligned}\hat{s} = & 14.163 + 3.908 \tau_s - 36.135 \frac{\eta}{s} - 0.00382 T_{dec} \\ & - 9.335 \tau_s^2 + 3.464 \tau_s^3 + 28.078 \left(\frac{\eta}{s}\right)^2 + 17.865 \tau_s \cdot \frac{\eta}{s}.\end{aligned}\quad (\text{A.6})$$

The $\langle \text{MSE} \rangle$ for this model is 0.04, which is about 5 times smaller than the model A.3.

We apply the above method to construct linear regression models for . These linear regression models are now incorporated in our iEBE package. They provide a fairly good initial estimate of the scaling factor for new parameter combinations. With the help of this linear regression model, our simulation model only takes about two runs (~ 2 CPU hours) to find the correct scaling factor, compared to 3 or 4 runs if the initial guess is chosen randomly.

A.6 Summary and outlook

Now we are able to predict the scaling factor in the pure hydro run mode and use it as a reasonable initial value. In fact, there are many other models for that can make more precise numerical prediction than linear regression [153]. The predictive model building, diagnosing and improvements we presented in this appendix for the linear regression model can be applied to other models. Moreover, we should not confine ourselves in only predicting the scaling factor. By including more parameters which properly specify the properties of initial state and evolution stage, we can build a predictive model, or emulator, to produce observables, such as the hadron spectra and anisotropic flow. Such a predictive model can help explore the parameter space much faster than the true simulation model.

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