OSG Final Assignment: HTC for Relativistic Heavy-Ion Collisions

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1. Introduction

It is widely agreed that shortly (10^{-6} sec) after the big bang, the universe was in a hot and dense state: quark-gluon plasma (QGP). This is a new state of matter other than solid, liquid or gas familiar to us. In this state, nuclear matters interact with each other through strong force, which is described by Quantum chromodynamics (QCD). One way to produce QGP in laboratory is through collisions of heavy-ions with relativistic speed, such as the ones at the RHIC PHENIX Experiment. Our job is to examine the properties of QGP and calculate out the physical measurables that can be compared to the data recorded by detectors.

My current project is on "anomalous viscosity", one of the possible reasons for high v_2 coefficient (elliptic flow) measured for D-mesons. One would expect from kinetic theory that v_2 of mesons containing charmed quarks is much lower than that for lighter mesons. "Anomalous viscosity" is a concept contrary to "collisional viscosity", where drag force in the medium is due to collisions between particles. Anomalous viscosity can be originated from various sources, among which I concentrate on turbulent color field. I will attempt to develop a new algorithm to calculate the diffusion of heavy quark in the framework of Langevin equation. The core of this project is to modify the original diffusion code, trying to incorporate memory effect due to the turbulent color field. With this modified code, physical measurables like v_2 will be recalculated and compared to experimental data.

In Section 2, the workflow of the above computation job will be analyzed in detail. However, honestly speaking, I do not expect an urgent need of OSG for this project right now. Therefore, in Section 3, I would like to present some other potential projects in our research group, where HTP is indeed necessary.

2. Computation of Anomalous Viscosity

Fig.1 shows the workflow of the computation. As indicated by the figure, the workflow can be divided into five parallel flows, each of which corresponds to a

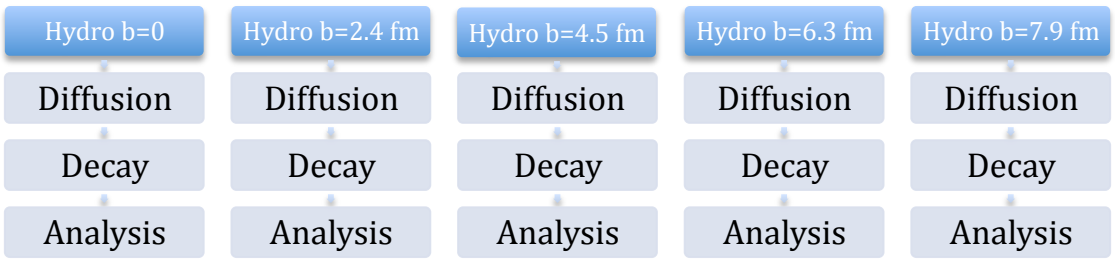

Figure 1 Flow of Calculation

specific impact parameter of the collisions. Firstly, the QGP medium is generated by the hydro code. This step consumes the most CPU time among the whole flow: about 10 hours on our local server. And the result of this step takes up approximately 40G space for each impact parameter. After the medium is prepared, we run the diffusion code, i.e. let the heavy quark diffuse in the QGP medium. This step reads in the 40G hydro result and generates an output file around 200M. Next, the decay code simulates the decay process of a heavy quark into light particles that can be detected by experiments. Finally, analysis program is applied to obtain the distribution plot of various physical quantities. Each step uses the output of the previous step as its input. And the CPU time need for an individual step after the hydro code is no more than 10 minutes on our server, and the storage space no more than 200M.

To use OSG, we should prepare the code and submission file and submit them to RENCI at UNC-Chapel hill. They will help us submit the job to OSG and return the final results to our server at Duke.

3. Potential Application of OSG on RHIC Projects

My current job concentrates on the modification of the diffusion code: to introduce memory effect originated from turbulent color field. Since the running of this part of the workflow does not take up a huge amount of CPU time, the benefit from OSG may not be obvious. However, some of the other parts of the workflow may require the help of OSG urgently. For instance, Dr. Hannah Peterson, a post-doc in our group is currently working on the modification of hydro code. Since she needs the statistic average after running the code "event by event", thousands of hydro runs are supposed to be carried out. Since each hydro code takes 10 hours CPU time on our local server and 40G storage space, this requires huge computation resources. Hopefully, since these hydro runs are parallel to each other, they can be submitted to different servers, and therefore, OSG becomes an ideal choice.

Below, I would like to cite the computational challenges of the three priority research directions in QGP with large-scale computing summarized in the 2009 NPReport -- *Scientific Grand Challenges: Forefront Questions in Nuclear Science and the Role of Computing at the Extreme Scale* (91-116). These projects are supposed to be carried out through a combination of HTC and HPC.

(a) Precision Calculation of Bulk Thermodynamics

Calculations with domain wall fermions or overlap fermions require approximately two orders of magnitude more computational resources than calculations performed with staggered fermions. Prospects for the next generation of studies of bulk thermodynamics based on the staggered fermion discretization scheme have been examined in a white paper written in 2007 by the USQCD collaboration (USQCD 2007). This led to the conclusion that a thorough analysis of the equation of state at temperatures below twice the transition temperature will require approximately 100 sustained teraflop-years. Extending such a study to temperatures twice as high will increase the numerical effort by almost an order of magnitude. A thorough study of the QCD equation of state in the transition from low to high temperature needs to be performed with domain wall or overlap fermions.

(b) Quantum Chromodynamics Phase Structure at Nonzero Net Baryon Number Density

At present, calculations of Taylor expansions up to the third order in the squared baryon chemical potential require about 100 teraflop-years. Extending these expansions to the fifth order will require resources of 1 exaflop-year. To pursue calculations at these high orders, it is necessary to improve the numerical techniques used to calculate Taylor expansion coefficients. Improved techniques for the inversion of large, sparse matrices (deflation) and the optimization of random source vectors (dilution) are currently being tested and are expected to significantly expedite these calculations. The computational challenges that must be addressed in calculations with imaginary chemical potentials are similar. Quantitative studies of finite density QCD, and a decisive calculation that verifies or excludes the existence of a critical point in the QCD phase diagram, require extreme scale computing.

(c) Transport Coefficients of Quantum Chromodynamics and Spectral Functions of Hadrons in Medium

The major computational challenge in studies of the excitation spectrum of hot and dense matter is the quest for statistically accurate data on correlation functions on large lattices. These lattices are typically a factor of 50 larger than those used in calculations of static, bulk thermodynamics. The size of data samples needed to reach sufficiently small uncertainties in the correlation functions is approximately an order of magnitude larger. Fortunately, such calculations would only be performed at a few selected values of the temperature rather than at the large set of temperature values needed to control properties of the equation of state. Still, this presents a computational challenge, and requires a few petaflop-years to perform calculations within the quenched approximation to QCD.