Nuclear Thermodynamics and Equations of State in Relativistic Astrophysics

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This proposed dissertation divides into two parts. The first part is on understanding the nuclear energy distribution during big bang nucleosynthesis (BBN). To do this I have developed a new simulation tool that exactly replicate the thermalization process, and I have worked on a new solution of the multi-component relativistic-Boltzmann equation. Each of these approaches give us the actual energy distribution of nuclei in BBN plasma. In the second part of this thesis I will explore the explosive collisions of two neutron stars. In particular, I will examine effects of various equations of state on binary neutron star merger simulations by analyzing the resultant gravitational wave emission. I will also be examining effects of extended theories of gravity, i.e $f(R)$ gravity on neutron stars.

I. INTRODUCTION

Relativistic astrophysics is at the frontier of physics research. It is one of the most theoretically and computationally interesting as well as demanding fields in physics. Relativity plays a key role in governing the dynamics from the smallest mass scales (e.g. particle scatterings) to the largest mass scales (e.g. in interactions between compact stars and even the big bang itself). This dissertation proposal pertains to research in different regimes of relativistic astrophysics and is thus divided into three parts.

The first is concerned with the relativistic thermodynamics during big bang nucleosyntheis (BBN). I am studying thermalization of nuclei in the background cosmic plasma of relativistic particles. My work on this is nearly completed. I have submitted a co-authored paper, will be submitting a first author paper within a month and have a published conference proceedings [1–3].

The second study concerns gravitational waves emitted during binary neutron star mergers (BNSM). I will perform exact numerical relativity simulations for different nuclear equations of state.

The goal of these studies will be done to gain understanding about the behaviour of nuclear matter in extreme environments such as the dense condensate state of a neutron star, via studies of equations of state, and the ionized plasma state during BBN.

II. BIG BANG NUCLEOSYNTHESIS

Big bang nucleosynthesis (BBN) is a pillar of the modern precision cosmology [4, 5]. It refers to the epoch of the early universe which the synthesis of light elements nuclei such as H, ^{2}H (Deuterium), ^{3}He, ^{4}He, and ^{7}Li. As the universe expands during BBN it cools down from ~ 10 GK to ~ 0.1 GK. Within this temperature range the energies of nuclei are sufficient to overcome the Coulomb barrier to permit the synthesis of other nuclei.

The resultant abundance of light nuclei during the BBN era are calculated by running a network of nuclear reactions that starts with a neutron and proton mixture and uses cosmologically-evaluated temperatures and densities as the conditions for the reactions along with scattering cross sections measured empirically in nuclear physics experiments [6–8].

Decades ago the cosmology community calculated the light nuclear abundance resulting from BBN and found them to be in agreement with various primordial astrophysical sources. However, ^{7}Li had always been calculated to be three times higher than the observed abundance. This discrepancy was called the Cosmic Lithium problem and still is an area of active research. Various solutions to the problem have been suggested based on convection in stars, nuclear reaction uncertainties, and many others. Hou *et al.* recently suggested that this problem is solvable by imposing a Tsallis statistics based distribution on nuclei such that their distribution is deviated to higher energies compared to the standard Maxwell-Boltzmann (MB) distribution [9, 10]. However, the origin of the Tsallis distribution was seemingly unphysical and unmotivated. My research began with the motivation of finding a physical reasoning behind the Tsallis statistics.

The reaction rate between two nuclei 1 and 2 is written as [6, 8]

$$R = n_1 n_2 \langle \sigma(v) v \rangle = n_1 n_2 \int v\sigma(v) f(v) dv \quad , \qquad (1)$$

where n_1 and n_2 are the number densities of the two species, $\sigma(v)$ is the reaction cross section, v is the relative center-of-mass velocity of the two species and $f(v)$ is the relative velocity distribution function. In my research I obtain the distribution function $f(v)$ starting from first principles of statistical physics and collision mechanics.

Due to the high temperatures during the early universe the BBN plasma initially consists primarily of relativistic $e^+ - e^-$ pairs, photons, and neutrinos. Table (I) shows that of the constituents of the BBN plasma, only $e^+ - e^-$ pairs are highly interactive with the charged nuclei present. Hence, the nuclear energy distribution

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TABLE I: Temperature dependence of various ratios relevant to proton elastic-scattering reaction rates with $e^- - e^+$ plasma, photons and other protons (From [1]). I use the minimum among the two cross section ratios (4^{th} or 5^{th} column) to obtain the reaction rates for $e^- - e^+$ plasma.

T		$n_\pm/n_\gamma$	$\sigma_\pm/\sigma_\gamma$		$\Gamma_\pm/\Gamma_\gamma$	$\Gamma_\pm/\Gamma_p$
T_9	MeV		$\sigma_\pm = \pi r_D^2$	$\sigma_\pm = \sigma_{Mott}$		
11.6	1	1.43	5×10^4	10^5	10^5	10^9
1.16	0.1	0.102	10^7	10^5	10^3	10^{10}
0.116	0.01	10^{-13}	2×10^{28}	10^{29}	10^{14}	10

must be derived from its interactions with this background relativistic $e^+ - e^-$ plasma. We approximately solved the relativistic multi-component Boltzmann equation [1]. Moreover, I built an exact 3-dimensional relativistic Brownian motion simulation [2]. Each of these independently leads to the distribution the nuclei present during BBN.

A. 3-D multi-component Relativistic Boltzmann Equation

To obtain the distribution of nuclei present in the expanding universe during the BBN phase, one needs to solve the 3D relativistic multi-component Boltzmann equation [11, 12], i.e.

$$p_a^\alpha \partial_\alpha f_a = \sum_{b=1}^{r} \int (f_a' f_b' - f_a f_b) F_{ba} \sigma_{ab} d\Omega \frac{d^3 p_b}{p_{b0}} \quad , \qquad (2)$$

here subscripts a and b stand for the two different species. In our case they are nuclei and e^- or e^+ respectively. p is four-momentum, f is the distribution, F is the flux between the two species, σ is the cross-section between the two species, Ω is the angle and the primed indicates quantities after undergoing a scattering event. This differential equation describes how the phase space distribution of the species a evolves upon undergoing stochastic scatterings by the constituents of species b, i.e. the plasma.

As part of my thesis I contributed in finding the approximate solution to this equation in the dilute plasma case relevant for BBN [1].

B. Monte-Carlo Scattering thermalization simulation

To replicate the thermalization process exactly as Nature does one would have to develop a thermalization simulation. I built such an an unprecedented 3-D multi-component relativistic thermalization simulation

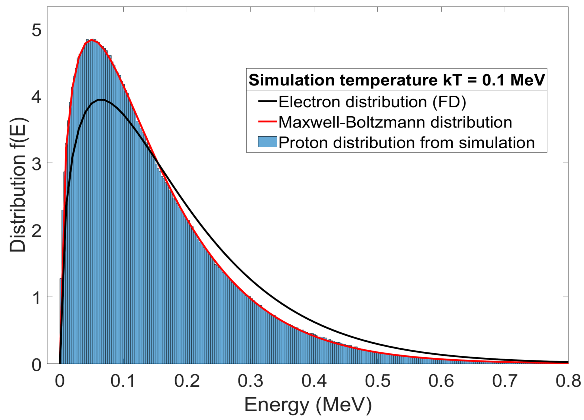


FIG. 1: Monte-Carlo histogram (blue bars) of the kinetic energy distribution of nucleus scattering in a bath of relativistic $e^+ - -e^-$ plasma (black curve) (at $kT = 0.1$ MeV) compared to the kinetic energy distribution of a classical Maxwell-Boltzmann distribution (red curve). From Refs. [1, 2]

[2]. This simulation allows for a nucleus to be thermalized in a bath of relativistic electrons, photons, etc. The resultant equilibrium nuclear distribution of such a simulation would be as it was during the standard BBN.

Fig. 1 shows a result from our simulation. The figure shows the resultant distribution (blue histogram) obtained for the nuclei for one simulation run after scattering off background relativistic electron distribution (red) and the MB distribution for the same temperature as that of the electrons. The figure shows that resultant distribution of the nuclei fit closely with the traditional MB distribution implying the nuclei (and indeed any other specie) follow their independent distribution in a mixture of gases. This distribution is the relativistic Fermi-Dirac (RFD) distribution, although in special cases it approximates to other distributions. For the BBN era where temperatures are much lower than masses of nuclei, this RFD distribution reduces to the MB distribution. This confirms our result from the approximate theoretical approach of solving the Boltzmann equation.

1. *Importance of instantaneous viscosity*

In our earlier report we noted that the distribution of a nucleus after undergoing thermalization in an environment of relativistic electrons deviated away from the traditional Maxwellian distributions [13]. These were being quantified in the form of an increase in effective temperature of the nucleus. This effect was pushing nuclear distributions to higher temperatures and therefore lead to an overproduction of Lithium along with introducing a discrepancy in the Deuterium abundance.

After carefully studying this result by simulating thermalization in different 1, 2, and 3 dimensions I determined that this discrepancy could be attributed to an absence of instantaneous viscosity in our previous simulations. Even though the nucleus is present in an isotropic environment where electron velocity directions are uniformly distributed in all directions, in the nuclear frame the flux of relativistic electrons from different directions is non isotropic. This angular distortion is observed only in a moving frame, such as that of a nucleus, and hence needed to be accounted for. The distorted distribution is critical in deciding the reaction rate of the test nucleus with electrons travelling in different directions. Once I accounted for this in our simulations the nuclear distribution got pushed to lower energies by the exact amount that would bring it down to classically understood results, i.e. an MB distribution.

C. Conclusion of thermalization of nuclei in BBN

The result we found through our independent theoretical and computational approaches is that the nuclei and $e^- - e^+$ plasma attain the same pressure per particle which is equivalent to being in thermal equilibrium. In terms of the species distributions, we found that the different components of the plasma attain their independent RFD distribution.

I have discussed this research in a submitted paper specifically on thermalization of nuclei during BBN and am writing another which has summarizes the simulation technique. The implication of these papers is that the nuclear distribution taken for decades were indeed correct and thus does not provide a solution for the Cosmic lithium problem. However, both the theoretical solution and the simulation technique are the first of their kinds and are thus of importance to the statistical physics and fluid dynamics communities.

III. BINARY NEUTRON STAR MERGER SIMULATIONS

Another aspect of this Ph.D. proposal is on simulating gravitational waves emitted during binary neutron star mergers as a means to better constrain the nuclear equation of state (EoS). These simulations involve solving the Einstein equations and relativistic hydrodynamics in the ADM or BSSN formalisms (as explained below). I will model effect different stiff vs. soft EoS have on the merger process and its outcome, and the associated gravitational wave chirp.

On 17th August 2017, LIGO international collaboration observed the gravitational wave (GW) signal from the merger of two neutron stars [14]. The event was the first observation of a binary neutron star merger (BNSM) system and was followed up by observations in the electromagnetic spectra. Given these, the evolution history of mergers and the structure of nuclear matter in neutron stars (in the form of EoS) can now be study with great precision by simulating the merger event and constraining the emitted GW with the LIGO observed GW.

A. Numerical Relativity (ADM, 3+1 split)

Einstein's theory of gravity postulates that space and time are inseparable and treats them indistinguishably. The Einstein equations that govern the evolution of matter are dependent on both space and time. However, solving them for an astrophysical system (like the merger of two neutron stars) traditionally would imply getting a solution for the entire space-time evolution at once, i.e. obtaining the solution for all spatial and temporal coordinates simultaneously. This is impossible both analytically and numerically given the complexity of the physical system and the system of evolution equations.

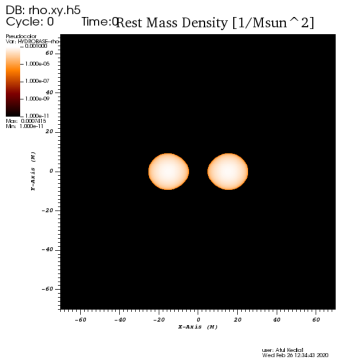
ADM formalism is a Hamiltonian formalism of GR that provides a framework of separating time evolution from spatial evolution in the Einstein equations in the form of a 3+1 split. The split creates "slices" of three dimensional space that all carry the same coordinate time. The slices can then be evolved over time [15–17]. The dynamics of a 3+1 split space-time are evolved by a system of dynamical and constrained differential equations dependent on the metric (spatial part, lapse function and shift vectors separately) extrinsic curvature, Ricci tensor, and the energy-momentum tensor. This formalism provides an evolution mechanism for the space-time coordinates independent of the energy-momentum distribution.

B. Relativistic Hydrodynamics

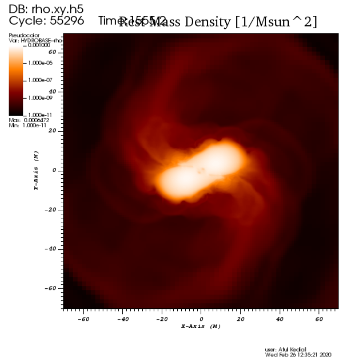
The hydrodynamics of neutron star material is evolved by imposing conservation of relativistic generalized momenta, internal energy, particle number density, and magnetic fields. These are performed for each grid point on each spatial slice [18].

C. Equations of State

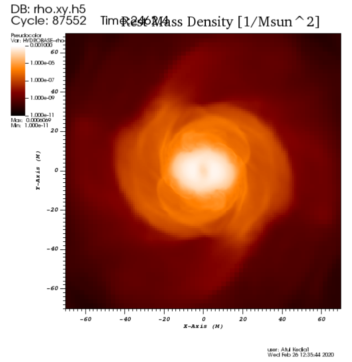
To describe the evolution of matter exactly, the hydrodynamics equations require an additional condition that relates the various state variables of the matter, i.e. pressure, density, electron fraction, chemical potentials, etc in a neutron star [19, 20]. Finding the nuclear equation of state (EoS) and is an active area of research in nuclear physics. Constraints on the EoS were placed by LIGO based upon the post-Newtonian corrections for the induced quadrupole moments of the stars as the inspiral. An aspect of this proposal is to constrain the nuclear EoS by analyzing GWs emitted during simulated BNSMs.



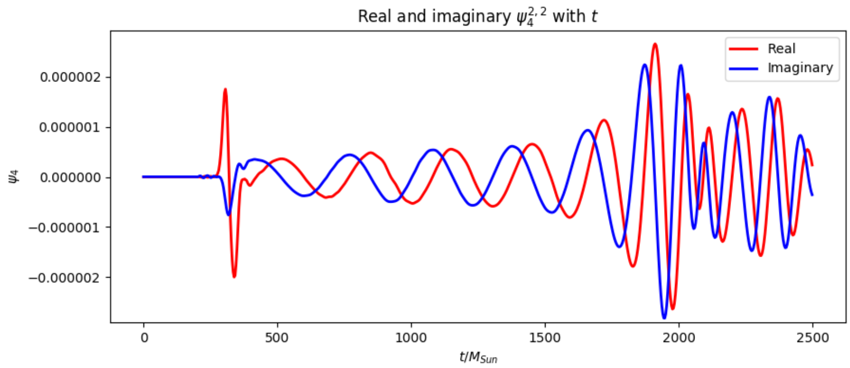
(a) The placement of the Neutron stars as the simulation starts.



(b) The Neutron stars at merger.



(c) The remnant during ringdown.



(d) Multipole moment of the Weyl scalar ($\Psi_4^{l=2,m=2}$) at simulation boundary ($r = 300units$).

FIG. 2: Progression ((a) to (c)) of an equal mass ($M_{tot} = 3.4M_{Sun}$) binary neutron star merger for Polytropic EoS, along with a sample gravitational wave signal generated by this merger.

D. Einstein Toolkit

At the heart of this part of my thesis will be an application of the Einstein Toolkit (ET). This is a collection of state-of-the art codes built to run and analyze numerical relativity problems within the Cactus code framework [21].

Cactus is a highly modular platform built for high performance computing in numerical relativity. The different modules in Cactus are called Thorns. A user gets access to a vast library of pre-written thorns that can perform various physics calculations for analysis and visualization, and can write their own thorns for specific needs. Cactus thorns support C, C++, F90, and Mathematica giving the user sufficient freedom for programming.

ET capitalizes on the versatility of Cactus and combines it with a highly sophisticated Adaptive Mesh Refinement system called Carpet. ET includes Simulation factory which executes and manages the computational details of running the ET codes on a system. Simulation Factory works on encapsulating the best coding practices employed by programmers so that physicists don't have to spend time understanding them. It also takes care of distributing the tasks according to the architectural differences of different computers ranging from personal computers to all the way to supercomputers.

E. Gravitational wave extraction

The gravitational waves (GW) emitted during the BNSM lead to miniscule (1 in 10^{21}) distortions in spacetime. Thus afar from the source these distortions can be mathematically modelled by the linearized Einstein's equations,

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2\right)\tilde{h}^{\alpha\beta} = 0 \quad . \tag{3}$$

Here, $\tilde{h}^{\alpha\beta}$ is the reverse traceless part of the metric and is a measure of the deviations of the metric from the Euclidean-flat space metric ($|\tilde{h}^{\alpha\beta}| \ll |\eta^{\alpha\beta}| \sim 1$).

Far from the source the ET determines the GW emission from the BNSM in the Newman-Penrose formalism and gives output in the form of multipole moments of the Weyl curvature scalar $\Psi_4^{l,m}$ [22, 23]. These are the spherical modes of the Weyl scalar related by

$$\Psi_4(r,t,\theta,\phi) = \sum_{l=2}^{\infty}\sum_{m=-l}^{l} \Psi_4^{l,m}(r,t)_{-2}Y^{l,m}(\theta,\phi) \qquad (4)$$

The Weyl scalar is related to the GW strain by

$$\Psi_4 = \ddot{h}_+ - i\ddot{h}_x \quad , \qquad (5)$$

I will use the multipole moments of the Weyl scalar to the extract strain in spacetime.

F. $f(R)$ Gravity

As a final section of this thesis I plan to place constraints on $f(R)$ gravity. This is a extended theory of Einstein's formulation of general relativity [24, 25]. Since the discovery of the theory of relativity there has been an ongoing debate whether the equations are precise or whether there are higher order terms that are being ignored. The Einstein equations can be modified slightly to have Ricci scalar and tensor be slightly deviated to either $R + \alpha R^2$ and $R^{1+\epsilon}$ to form the $f(R)$ gravity equations. Currently a collaborator is working on the neutron star stability analysis for an $f(R)$ theory and has some preliminary results. As part of my thesis I will complete that calculation.

G. Conclusion of binary neutron star merger simulations

Some of the preliminary runs using ET to simulate the BNSM for an equal mass binary is shown in Fig. 2. From (a) through (c) the panels show the progression of the state of the mergers over the range of the simulation. Panel (d) displays the GW emitted from this merger.

We plan to use the features available to us via ET to perform BNSM simulations for different EoS, including the NDL EoS [20], and by analyzing the GW emitted during these processes and those observed by LIGO constrain the nuclear EoS. Another long term goal of this project is to add the conformally flat approximation to ET to compare its results with that of the BNSM codes written in by Notre Dame and Lawrence-Livermore National Lab collaboration.

IV. TIMELINE

A proposed timeline for the completion of this dissertation is given in Table II. Many of the proposed calculations have already been started. I propose to finish my dissertation by Spring of 2022.

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TABLE II: Timeline of my Ph.D. progress.

Academic stage	Year	Ph.D Work
1^{st} year	2016-17	Course work
2^{nd} year	2017-18	Literature review on BBN and course work
Fall 3^{rd} year	Fall 2018	Research on BBN, i.e. building simulation tool.
Spring 3^{rd} year	Spring 2019	Running simulation tool for BBN case. Started writing BBN paper.
Fall 4^{th} year	Fall 2019	Writing Simulations techniques paper. Literature review on BNSM and running ET.
Spring 4^{th} year	Spring 2020	Refining simulations paper. Running BNSM for Polytropic EoS. Work on gravitational wave extraction.
Fall 5^{th} year	Fall 2020	Running BNSM for NDL and other tabulated EoS, followed by analyzing gravitational waves.
Spring 5^{th} year	Spring 2021	Write paper on constraining EoS. Add additional thorns on ET to improve the physics, i.e. conformally flat condition or neutrino diffusion.
Fall 6^{th} year	Fall 2021	Research on $f(R)$ gravity calculation. Apply for numerical relativity post-doc positions. Writing thesis.
Spring 6^{th} year	Spring 2022	Write paper on $f(R)$ gravity. Defend by March.