Quantifying the Sensitivity of Big Bang Nucleosynthesis to Isospin Breaking

Matthew Ramin Hamedani Heffernan
College of William and Mary

Follow this and additional works at: https://scholarworks.wm.edu/honorstheses

Part of the Nuclear Commons

Recommended Citation
https://scholarworks.wm.edu/honorstheses/974
Quantifying the Sensitivity of Big Bang Nucleosynthesis to Isospin Breaking

A thesis submitted in partial fulfillment of the requirement for the degree of Bachelor of Science in Physics from The College of William and Mary

by

Matthew Ramin Hamedani Heffernan

Accepted for [Signature]
(Honors or no-Honors)

André Walker-Loud, Physics

Henry Krakauer, Physics

Bruce Campbell, German Studies

Williamsburg, VA
May 4, 2016
Quantifying the Sensitivity of Big Bang Nucleosynthesis to Isospin Breaking

Matthew Heffernan

Advisor: André Walker-Loud

Abstract

We perform a quantitative study of the sensitivity of Big Bang Nucleosynthesis (BBN) to the two sources of isospin breaking in the Standard Model (SM), the splitting between the down and up quark masses, \( \delta_q \equiv \frac{1}{2}(m_d - m_u) \) and the electromagnetic coupling constant, \( \alpha_{f.s.} \). To very good approximation, the neutron-proton mass splitting, \( \Delta m \equiv m_n - m_p \), depends linearly upon these two quantities. In turn, BBN is very sensitive to \( \Delta m \). A simultaneous study of both of these sources of isospin violation had not yet been performed.

Quantifying the simultaneous sensitivity of BBN to \( \delta_q \) and \( \alpha_{f.s.} \) is interesting as \( \Delta m \) increases with increasing \( \delta_q \) but decreases with increasing \( \alpha_{f.s.} \). A combined analysis may reveal weaker constraints upon possible variations of these fundamental constants of the SM. To perform this study, we utilized the latest results from lattice QCD calculations of \( \Delta m \) to quantify the connection between \( \delta_q \), \( \alpha_{f.s.} \) and BBN.

In order to undertake this project, the existing BBN code, written in FORTRAN, has been updated to allow for string replacement from Python as well as by incorporating rates specifically designed for this variation. This has resulted in a more user-friendly implementation of the variation of various input parameters, such as \( \alpha_{f.s.} \) and \( \delta \), allowing future studies to be conducted much more easily than before possible and with a greater scope brought by the ability to vary parameters simultaneously.
Contents

1 Introduction 4

2 Groundwork and Theory: Identifying Varying Quantities in Standard Big Bang Nucleosynthesis (SBBN) 6
  2.1 Stages of SBBN ................................................................. 8
  2.2 Motivations for the variation of the fine structure constant $\alpha_{f.s.}$ .................. 12

3 Results and Analysis: Discovering the Constraints 16
  3.1 Independent Variation of Weak and Thermal Rates ............................. 17
  3.2 The $^4$He Case ......................................................................... 18
  3.3 The Deuterium Case ................................................................. 19
  3.4 Combining $^4$He and Deuterium for a Tight Constraint .................... 22

4 Conclusions 25

5 Future Work 25

6 Acknowledgements 26

References 27

A Python Code 29
  A.1 Grid Controls ................................................................. 29
  A.2 Parent Wrapper .............................................................. 29
  A.3 Basic Wrapper ............................................................... 32
  A.4 First Run Program ............................................................ 37
  A.5 Table Writer ................................................................. 41

List of Figures

1 Time evolution of nuclear abundances in the nominal case. ......................... 7
2 Network diagram of the 12 primary reactions in the processing of the light elements, reproduced from [25]. Note that our code uses a much more complex and extensive nuclear network, but this network contains the most important of these reactions. These are the fusion reactions which dominate after the breaking of the deuterium bottleneck. .......................................................... 10
3 Various mass fraction abundances with varying baryon-photon ratio. Note that horizontal bands represent measured abundances and uncertainties, lines represent the abundances produced at varying $\eta$, and the vertical band represents the constraint due to the measured Cosmic Microwave Background. ............................ 14
4 Various mass fraction abundances with variation in $2\delta q = m_d - m_u$. Again, mass fractions are given with respect to hydrogen. Note that the solid vertical line represents the middle value that is measured and the dashed vertical lines denote the error bounds on the current best measurement of $m_d - m_u$. ................. 15
\section*{List of Tables}

\begin{enumerate}
\item The impact of variation of thermal and weak rates independently. Note that for these, $\delta_q$ is held at its physical value. \hfill 17
\end{enumerate}
1 Introduction

If the Standard Model (SM) is a low-energy effective field theory (EFT) of some UV-complete\textsuperscript{1} extension, then the fundamental constants of the SM are derived quantities from this larger theory. Hence, at high energy - which corresponds to early times in the universe - these constants could vary from the values they are measured to be today, when additional beyond Standard Model (BSM) degrees of freedom were active. In summary, the SM may be a low-energy case of a more complex theory and by understanding the sensitivity of physical processes to variations in the SM constants, we can constrain the effects of BSM physics on measured and observed quantities. One useful time to look for new physics is $\sim$1-15 minutes after the Big Bang, during the production of light nuclei in an epoch known as Big Bang Nucleosynthesis (BBN).

One quantity which BBN is especially sensitive to is the proton-neutron mass splitting, $\Delta m \equiv m_n - m_p = 1.29333217(42)$ MeV. This is because this mass splitting controls the neutron to proton ratio before BBN when the universe was in approximate thermodynamic equilibrium. The $n \leftrightarrow p$ weak reaction rates are also very sensitive to this quantity. These $n \leftrightarrow p$ reactions also receive small corrections from radiative photons which are known [1]. At low energies, there are two sources of this isospin breaking; the mass splitting between the up and down quarks, $\delta_q \equiv \frac{1}{2}(m_d - m_u)$, and the electromagnetic coupling of these quarks to the photon field, $\alpha_{f.s.} \equiv \frac{e^2}{4\pi}$. The sensitivity of BBN to $\delta_q$ and $\alpha_{f.s.}$ through $\Delta m$ and the sensitivity of the nuclear reactions to $\alpha_{f.s.}$ can be used to constrain possible sources of new physics in terms of constraints upon allowed variations in $\delta_q$ and $\alpha_{f.s.}$. There have been numerous studies of BBN constraints on fundamental constants of the SM, such as $\alpha_{f.s.}$ and the average quark mass, $\frac{1}{2}(m_d + m_u)$, but there has not yet been a detailed study of BBN constraints on both sources of isospin breaking simultaneously [2].

The only rigorous tool to study the nucleon mass splitting as a function of isospin breaking $\Delta m(\delta_q, \alpha_{f.s.})$ is lattice QCD, a numerical non-perturbative solution of QCD, the fundamental

\textsuperscript{1}Renormalizable in the high-energy / short-distance regime
theory of the nuclear strong force. With the advances in computational power made in recent
times, we can now solve QCD and use this to evaluate the variation in the neutron-proton
mass splitting as the result of isospin violation.

To a very good approximation, $\Delta m$ depends linearly upon $\delta_q$ and $\alpha_{f.s.}$. We also know
that an increase in $\delta_q$ will cause an increase in $\Delta m$ while an increase in $\alpha_{f.s.}$ will cause a
decrease in $\Delta m$. Therefore, allowing for simultaneous variations in both isospin breaking
quantities may allow for a larger change in $\delta_q$ and $\alpha_{f.s.}$ than if they are varied independently.

Much research has been performed investigating BBN as a constraint on the amount and
nature of the variation of fundamental constants of the SM [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19], see Ref. [20] for a recent review. With all the nuclear reactions
taken from experimental measurements, BBN depends upon only a single parameter, the
primordial baryon-to-photon ratio, $\eta$. The baryon-to-photon ratio determined by comparing
predictions from BBN with observed abundances of light nuclei in low-metallicity gas clouds,
such as deuterium ($D$) and $^4$He, is in excellent agreement with the value of $\eta$ determined
independently from the cosmic microwave background (CMB) [21].

This provides a very precise constraint (within 1%) on these variational studies. Existing
research, particularly that of [15], also mentions various effects due to shifted light quark
masses at the time of BBN, when the universe was approximately three minutes old. As
also mentioned in [15], variation of quark masses are likely to be related to changes in other
quantities, the simplest of which would be the Higgs vev\footnote{This denotes “vacuum expectation value”, the expectation value of the Higgs field in a vacuum, which is 246 GeV [21]} which would result in linear mass
change, i.e. the masses of all subatomic fermions would change linearly in response to a
change in the Higgs vev. Therefore, studies involving the variation of SM constants has
included the variation of many quantities, particularly variation in the Higgs vev and the
electromagnetic coupling $\alpha_{f.s.}$.

The nucleon mass splitting $\Delta m$ is an input to BBN and is goverend by $\delta_q$ and $\alpha_{f.s.}$.
Refs. [15, 17] explored the variation of BBN with respect to the average light quark mass,
mostly due to the change in the $D$ binding energy and other reactions. An anthropic determination of the weak scale was determined in Ref. [19] by demanding a universe similar to our own. Given our recent quantitative knowledge of the dependence of $\Delta m$ upon $\delta_q$ and $\alpha_{f.s.}$, a natural next step in this line of investigation is to analyze the dependence of BBN upon a simultaneous variation of both sources of isospin breaking.

2 Groundwork and Theory: Identifying Varying Quantities in Standard Big Bang Nucleosynthesis (SBBN)

We will consider standard BBN, i.e. BBN without the inclusion of any exotic particles beyond the scope of the Standard Model. In this thesis, I identify how the variation of the fine structure constant $\alpha_{f.s.}$ and the quark mass splitting $\delta_q$ causes changes in the fundamental physics during SBBN through the change in $\Delta m$ and also the nuclear reactions, and identify ways of incorporating these quantities into the existing code.

Due to the importance of the processes involved, we include a summary of the interactions and stages of the physics. This is done below in similar divisions and much reference to [22, 23]. Additionally, in Sections 2.1 and 2.2, I identify changes caused by variation of the $\delta_q$, $\alpha_{f.s.}$, and reactions rates and determine ways to account for these changes in the code.

The code used, not attached due to length, is modified through the use of a simple Python wrapper on the original FORTRAN so that string replacement can be used to modify the mass splitting and the fine structure constant. This code, originally written by Wagoner in 1973 and upgraded by Kawano in 1992, calculates the evolution of primordially synthesized light elements with temperature. This time evolution is shown in Figure 1, which is produced from the calculations we performed. Additionally, temperature or energy scales may be used in place of time because this corresponds more directly to the thermal history of the early universe and therefore encodes more information. The cooling of the early universe is a function of its expansion, making this process involved, although both time and
Temperature are provided for each timestep of the evolution produced by Kawano’s code as modified for the purpose of this study. This bears out our expectations: early in the universe, the neutron-proton ratio is relatively stable. Several (order $10^0$) seconds in, weak freeze-out occurs (the expansion rate of the universe exceeds the weak reaction rate) and the neutrons begin to decay to protons. This then begins to plateau at approximately 20 seconds until the deuterium bottleneck, which takes place at approximately 200 seconds. As the universe further cools, the bottleneck is broken and the remaining available neutrons are nearly entirely converted to $^4$He. The dependence of the first 200 seconds on $\Delta m$ comes from its effect on the $n \rightarrow p$ rate. After 200s, fusion is the dominant force in BBN and the sensitivity to changes in isospin breaking is dominated by changes in $\alpha_{f.s.}$.

![Nuclear Evolution Over Time](image.png)

Figure 1: Time evolution of nuclear abundances in the nominal case.
2.1 Stages of SBBN

The first stage of SBBN takes place in the regime when temperature $T \gg 1 \text{ MeV}$, i.e. where time $t \ll 1 \text{ second}$. At this stage, the energy density is dominated by the relativistic electron, positron, neutrino, anti-neutrino, and photon. The choice of 3 neutrino flavors is governed by the strong agreement of theory and computational probing [20] as well as through independent experimental evidence for 3 “light” neutrino flavors. Due to the high densities of electrons, positrons and neutrinos, neutrons and protons are kept in chemical and thermal equilibrium via

\begin{align*}
    n + \nu_e &\leftrightarrow p + e^- \quad (1) \\
    n + e^+ &\leftrightarrow p + \bar{\nu}_e \quad (2) \\
    n &\leftrightarrow p + e^- + \bar{\nu}_e \quad (3)
\end{align*}

Assuming no lepton asymmetry, which is a central assumption of SBBN, the neutron-proton mass difference $\Delta m$ determines the ratio of neutrons to protons in this regime,

$$
\frac{Y_n}{Y_p} = e^{-\Delta m/T} \quad (4)
$$

where $Y_n$ and $Y_p$ are respectively the neutron and proton number abundances. This is one of the quantities that will be varied in this thesis and that will be constrained by astronomical observations of primordial abundances. Its prominence in the physics is mandated by its setting of this ratio, which goes on to later effect nuclei formation and relative abundances. At this temperature, the rate of weak reactions are faster than the expansion rate of the universe, as are the nuclear reaction rates which produce light elements. The combination of kinetic and chemical equilibrium that the light elements are in is known as Nuclear Statistical Equilibrium (NSE).

The second stage takes place with a freeze-out of the neutron-proton equilibrating inter-

---

3Note that all times are quoted as “time after the big bang”.
actions (in equations 1-3), which occurs at $T \sim 0.8$ MeV and $t \sim 2$ seconds. The expansion rate of the universe exceeds the weak interaction rate, resulting in the weak freeze-out. At this stage, neutrinos are decoupled from the rest of the matter thermally, but they continue to interact with neutrons and protons. In the next few hundred seconds after weak freeze-out, a third of the neutrons are converted to protons. This continues until the time that the so-called deuterium bottleneck is overcome, which marks the next stage of BBN. The deuterium bottleneck was a situation which prevented the formation of larger nuclei. Up to this stage, the temperature was high such that enough photons, with energies above the deuterium binding energy of 2.2 MeV, were present such that almost all of the D produced are immediately dissociated. As the universe continued to expand and cool, deuterium-photon interactions became less frequent and the photons became less energetic, and the deuterium was no longer immediately destroyed, allowing deuterium to form. This subsequently allowed $^4\text{He}$ and heavier nuclei to form.

The third stage is called light-element synthesis and takes place after the breaking of the deuterium bottleneck at approximately 0.08 MeV. At this stage, the neutron-proton ratio continues to decrease due to the decay of unbound neutrons - it is not until the end of this temperature range that neutrons are mostly bound in nuclei and therefore stop decaying. Additionally, at this stage, fusion reactions are dominant and control the interactions. This is also the regime in which strong nuclear interactions and electromagnetic interactions become relevant to the physics and thus the process of nucleosynthesis can begin. To visualize the reactions which produce various elements, Figure 2 is included.

To describe the nuclear network shown in Figure 2, we will refer to the figure heavily in order to provide both description and visualization of the complex processes in the nuclear network. We note first that $^4\text{He}$ is the most abundant nucleus and, save for a minor contribution from $^7\text{Li}$, is produced only by reactions of the mass-3 nuclei: $^3\text{He}$ and tritium ($t$ in the diagram)$^4$. It is only through reactions 6 and 9 that $^4\text{He}$ is kept in NSE [23]. In the

---

$^4$We differentiate this with time $t$ by the fact that time is italicized and based on context.
Figure 2: Network diagram of the 12 primary reactions in the processing of the light elements, reproduced from [25]. Note that our code uses a much more complex and extensive nuclear network, but this network contains the most important of these reactions. These are the fusion reactions which dominate after the breaking of the deuterium bottleneck.
temperature regime we consider for light-element synthesis, the reactions that maintain the NSE of $^4\text{He}$ become too slow and it instead becomes dependent on the NSE of $^3\text{He}$ and $t$, as the reactions that maintain the NSE of these are sufficiently fast. These reactions are stable until the temperature decreases to $T \sim 0.2 \text{ MeV}$, where the deuterium -mass-3 reactions are sufficiently slowed that now the mass-3 nuclei (and thus also $^4\text{He}$) are forced to become dependent on the deuterium ($D$) NSE. This is our first sign of a deuterium bottleneck, albeit this one is not as severe as the one which occurs later. Next, at $T \sim 0.08 \text{ MeV}$, the $^3\text{He}$ reaction freezes out and thus the mass-3 nuclei are no longer kept in NSE. Finally, at $T \sim 0.06 \text{ MeV}$, the famous “deuterium bottleneck” is encountered and the nuclear species evolve in a quasistatistical equilibrium which exists due to the limit of available $D$. This bottleneck is due to the fact that there are enough photons at the high energy tail of the spectra with energies above the D binding energy of 2.2 MeV even though $T \ll 2.2 \text{ MeV}$. The reason for this is the very high number of photons per baryon $\eta = 6.10(4) \times 10^{10}$. Once the bottleneck is broken, a rapid formation of the heavier light nuclei takes place.

Note that there are significant gaps at $A = 5$ and $A = 8$ as there are no corresponding bound nuclei for these atomic numbers. These gaps are responsible for the comparatively low production of Li, Be and the omission of higher elements. Elements beyond $A = 8$ are further reduced due to Coulomb barrier suppression. The total production ends with a fractional production of approximately 25% $^4\text{He}$ and 75% H, although the timescale for this to occur is dictated by Eq. 3 and is very sensitive to $\Delta m$.

It is worth emphasizing the strong role played in the above processes by $\Delta m$. Through the role in setting the neutron-proton ratio both in equilibrium and after equilibrium cannot be maintained, the value of $\Delta m$ has a direct impact on the production of deuterium. The main sensitivity of the $D$ abundance comes from the binding energy, which is abnormally small. If the $D$ binding energy per nucleon were similar to most nuclei, the bottleneck would not be nearly as severe. As the $D$ is an iso-scalar object, the binding energy is sensitive to isospin breaking at second order. We only consider leading order (linear) dependence upon
$\delta_q$ and $\alpha_{f.s.}$. The effect of $\Delta m$ on the $D$ abundance is in the number of free neutrons available after the bottle neck is broken to form $D$. If $\Delta m$ is larger, the neutrons will decay before they can form $D$, if $\Delta m$ is smaller, there will be more neutrons during the production time of $D$.

2.2 Motivations for the variation of the fine structure constant $\alpha_{f.s.}$

From the overview of nuclear processes and BBN, it is already clear that there is a strong dependence on $\Delta m$, the neutron-proton mass difference. As mentioned above, $\Delta m$ is a function of both $\delta_q$ and $\alpha_{f.s.}$. The sensitivity of BBN to $\delta_q$ resides only in $\Delta m$ while the rest of the BBN reaction network is further sensitive to $\alpha_{f.s.}$.

During stages 1 and 2 of SBBN, outside of $\Delta m$, there is a reduced dependence on $\alpha_{f.s.}$ due to the only important reactions being the weak reactions (all the $n \leftrightarrow p$ reactions in Eqs. 1-3 are sensitive to $\Delta m$ as this sets the available energy in the reactions). A variation in $\alpha_{f.s.}$ would also modify the Coulomb repulsion which affects the rate of nucleosynthesis. Previous work studying constraints on $\alpha_{f.s.}$ [23] used an old estimate of the electromagnetic self-energy contribution to $\Delta m$ [26, 27] providing the estimate

$$\Delta m = 2.05 - 0.76(1 + \Delta\alpha/\alpha) \text{MeV}$$

However, with lattice QCD, we now have a better understanding of $\Delta m(\delta_q, \alpha_{f.s.})$. At leading order in isospin breaking, we have

$$\Delta m = \delta M_{n-p}^\gamma + \delta M_{n-p}^{\delta q} = 1.29333217(42) \text{ MeV}$$ (5)

where [18]

$$\delta M_{n-p}^{\delta q} = 2.44(17) \text{ MeV},$$ (6)
\[ \delta M_{n-p} = -1.00(07)(14) \text{ MeV}. \] (7)

We can independently estimate the electromagnetic contribution by subtracting Eq. 6 from the experimentally measured value, arriving at

\[ \delta M_{n-p} = -1.14(17) \text{ MeV}, \] (8)

in good agreement with Eq. 7. The updated variation of \( \Delta m \) is then obtained by dividing these values by \( \delta_q \) and \( \alpha_{f.s.} \) respectively. We take \( \alpha_{f.s.}^{-1} = 137.04 \) and \( \delta_q = 2.52(15) \text{ MeV} \) from the FLAG review [29]. For the central values of our variation, this results in

\[
\Delta m_{central} = 2.44 \times \delta_q \frac{\alpha_{f.s.}}{\alpha_{phys}} - 1.14 \times \alpha_{f.s.} \text{ MeV}
\]

\[
= 0.968 \times \delta_q - 156 \times \alpha_{f.s.} \text{ MeV}.
\] (9)

During stage 3 of SBBN, the dependence on \( \alpha_{f.s.} \) is key. These are the primary motivations for our use of [23] and are incorporated into the FORTRAN code used for the calculation. The variations used are expressed to first-order in [23] and these are considered to be sufficient for the degree of accuracy currently available.

It is clear that the variation of the fine structure constant will result in many changes to the processes involved in SBBN, but we consider this in concert with the variation of the neutron-proton mass difference in order to provide a more representative constraint on the system. While variation of only one of these quantities will vary light element production and thus give limits based on astronomical observations, the compensating effect of varying both of these simultaneously will allow for more accurate limits to be placed on both quantities.

We note explicitly that we choose to ignore the so-called “Lithium problem” in which current models of BBN are not able to faithfully reproduce the expected \(^7\text{Li} \) abundances [20]. This is considered to be a possible avenue for further research and is beyond the scope
of this thesis.

As a result of all the processes detailed below, BBN can be used to calculate the mass fractions of various abundances by comparing the abundance of a given element to the abundance of Hydrogen. There are two particular instances which directly show the sensitivity of BBN to various parameters. In Figure 3, the sensitivity of BBN to varying baryon-photon ratio is shown. This is an input parameter to BBN and severely restricts the possibility for new physics.

![Figure 3: Various mass fraction abundances with varying baryon-photon ratio. Note that horizontal bands represent measured abundances and uncertainties, lines represent the abundances produced at varying $\eta$, and the vertical band represents the constraint due to the measured Cosmic Microwave Background.](image)

What is worth noting is the constraints placed on $m_d - m_u = 2\delta_q$ and therefore on new physics. While variation of the quantity $m_d - m_u$ can vary widely within the experimentally determined band, the CMB constraint combined with the constraint from astronomical
Figure 4: Various mass fraction abundances with variation in $2\delta_q = m_d - m_u$. Again, mass fractions are given with respect to hydrogen. Note that the solid vertical line represents the middle value that is measured and the dashed vertical lines denote the error bounds on the current best measurement of $m_d - m_u$.

observations of low metallicity gas clouds\(^5\) provide a strong constraint on the degree of variation. As a result, Figures 3 and 4 demonstrate the motivation behind the use of BBN and related constraints in the search for extensions to the Standard Model.

\(^5\)These are taken to represent primordial abundances as the presence of heavier elements is taken as a sign of stellar activity.
3 Results and Analysis: Discovering the Constraints

The first stage in computational advancement required modification of the FORTRAN code to allow for string replacement with a new dictionary of values supplied by the Python wrapper included in the appendices at the end of this thesis. The FORTRAN routine was originally produced by Wagoner (1973) and Kawano (1992) and only allows for modification of certain parameters, otherwise the code is set to the currently predicted or evaluated values from the Standard Model. In this study, our variance of \( \delta_q = \frac{1}{2}(m_d - m_u) \) and \( \alpha_{f.s.} \) necessitates first the calculation of \( \Delta m \equiv m_n - m_p \) as set out in the previous section. This is done at leading order in isospin breaking as Eq. 9. Higher order corrections are expected to be numerically insignificant for understanding the constraints on variations of \( \delta_q \) and \( \alpha_{f.s.} \). The FORTRAN code then proceeds to simulate the propagation of element formation through Big Bang Nucleosynthesis and provides end-state mass fractions, which may then be evaluated as outlined in Section 2. We compare the final time step’s abundances with the estimated primordial abundances in [20] in order to show the amount of variation possible while remaining within experimental bounds.

The Python codes reproduced in Appendix A perform two tasks: first, to perform the necessary string replacements to calculate different variational combinations and second to iterate over different combinations in a grid. The granularity of the grid can also be modified, thereby allowing for more detailed study of particular regions of the variational space; these variations are kept symmetric around the physical values.

This study incorporates a number of novel aspects in addition to the novelty of simultaneous variation of multiple parameters. The first of these is the use of string replacement, which allows for both simultaneous variation and for a numerical study with rigorous mapping to be undertaken. Next, we use the docopt Python library to allow for a simplified and more intuitive method of passing command line arguments into the body of the code, thereby also introducing a level of ease which can be seen in Appendix A as it bypasses more complicated structures required for the more traditional method using sys.argv. A final
novelty employed is the use of the HDF5 storage format for the database rather than raw text DAT or CSV. This allows for more efficient I/O and management of high volumes of data, although it is not readable directly in a command line or terminal interface. This was an important innovation in order to curate the thousands of computational runs conducted to produce the desired results. The storage in the HDF5 table allows for fast slicing and combining of the results and multiple keys can be used for data filtering. For example, it is trivial to query the results for all values of $\delta_q < 1.1$ and $\alpha_{f.s.} > 0.95$.

### 3.1 Independent Variation of Weak and Thermal Rates

A small investigation was conducted in order to determine the influence of $\alpha_{f.s.}$ in different reactions, thermal and weak. These were varied independently and it was found that the variation of the constant in the thermal rates alone produces an effect in the final $^4$He several times greater than the effect produced by the variation of the constant in the weak rates alone. This effect is even more pronounced in the deuterium mass fraction, although the $^4$He mass fractions alone are sufficiently illustrative of the effect.

<table>
<thead>
<tr>
<th></th>
<th>Thermal $\alpha_{f.s.}$</th>
<th>Weak $\alpha_{f.s.}$</th>
<th>$^4$He Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Physical Values</strong></td>
<td>1/137.0359</td>
<td>1/137.0359</td>
<td>0.2486</td>
</tr>
<tr>
<td><strong>10% Variation</strong></td>
<td>1/124.6</td>
<td>1/137.0359</td>
<td>0.2480</td>
</tr>
<tr>
<td></td>
<td>1/152.3</td>
<td>1/137.0359</td>
<td>0.2491</td>
</tr>
<tr>
<td></td>
<td>1/137.0359</td>
<td>1/124.6</td>
<td>0.2487</td>
</tr>
<tr>
<td></td>
<td>1/137.0359</td>
<td>1/152.3</td>
<td>0.2484</td>
</tr>
<tr>
<td><strong>20% Variation</strong></td>
<td>1/114.2</td>
<td>1/137.0359</td>
<td>0.2475</td>
</tr>
<tr>
<td></td>
<td>1/171.3</td>
<td>1/137.0359</td>
<td>0.2497</td>
</tr>
<tr>
<td></td>
<td>1/137.0359</td>
<td>1/114.2</td>
<td>0.2489</td>
</tr>
<tr>
<td></td>
<td>1/137.0359</td>
<td>1/171.3</td>
<td>0.2482</td>
</tr>
</tbody>
</table>

Table 1: The impact of variation of thermal and weak rates independently. Note that for these, $\delta_q$ is held at its physical value.
Once this was performed, the weak and thermal rates were fixed to each other in the wrapper code for the remainder of the study. There is no known physical way in which the value of $\alpha_{f.s.}$ could vary independently in the weak and thermal reaction rates, this study was conducted in order to clarify which variations were dominating the observed changes in final abundances and as such illuminate which dynamics were most relevant at the various stages of BBN.

### 3.2 The $^4$He Case

In accordance with our expectations in Section 2, we begin with considering the final-state $^4$He abundances. These values are extracted from the data file and are correlated to the respective values of $\alpha_{f.s.}$ and $\delta_q$ for each calculation. Figure 5 reveals the individual dependences of the final mass fractions through cross-sections of the 2-D grid at constant $\delta_q$ and $\alpha_{f.s.}$. As can be observed, there is a linear dependence of varying strength on the total abundance from these variations. These linear variations have opposing slopes, which is directly related to the way that these quantities effect $\Delta m$. As shown in Section 2, increasing $\delta_q$ reduces $\Delta m$ while the opposite is true in the case of $\alpha_{f.s.}$ variation. Also as expected, the slopes are different, again reflecting the close coupling of $^4$He mass fraction and $\Delta m$.

What can clearly be seen in Figure 5 is the different number of calculations performed in
the regions of the variational space. At particularly low or high ratios, we do not expect that
the abundances produced will be within a few sigma of the observation, but we calculate
them in order to map the space as fully as possible. A coarser grid is used to scan regions
of parameter space further from the most interesting region.

The full variational space was used to contour plot shown in Figure 6. This plot reveals
the clear dependence of the $^4$He mass fraction on changing $\Delta m$, represented by the grey line
through the valley of acceptable values. Additional contributions of $\alpha_{f.s.}$ and $\delta_q$ demonstrate
that the mass fraction is more sensitive to $\delta_q$ variation. The main effect of the variations is to
modify $\Delta m$, which the mass fraction carefully tracks and the additional changes due to the
variations are higher-order effects. Figure 6 demonstrates that the linear shifts seen in Figure
5 produces an “acceptable region” or set of “acceptable regions” where the two parameters
can be shifted in concert to produce the observed abundance of $^4$He. The various “islands
of stability” visible in Figure 6 are most likely due to insufficiently fine grained resolution of
the parameter variation.

We adopt the value of the $^4$He mass fraction and the value of $\Delta m$ given in the latest
Particle Data Group review of Big Bang Nucleosynthesis, which provides the recommended
value of $Y_p = 0.245 \pm 0.004$ and $\Delta m \equiv m_n - m_p = 1.29333217$ [21].

It is clear from Figure 6 that the $^4$He mass fraction variation allows for a large simulta-
neous variation in $\delta_q$ and $\alpha_{f.s.}$ provided $\Delta m$ is near the physical nucleon mass splitting. The
compensating effect introduced by the simultaneous variation serves to generally broaden
the acceptable range of the varied parameters to produce the desired abundance, as initially
anticipated. The $^4$He mass fraction is only sensitive to $\Delta m$.

3.3 The Deuterium Case

The production of $D$, unlike $^4$He, is sensitive to charged particle interactions and thus
Coulomb corrections due to variation in $\alpha_{f.s.}$. $D$ is also sensitive to $\Delta m$ through the abun-
dance of free neutrons to form $D$ when the deuterium bottleneck is broken. If $\Delta m$ is much
Figure 6: $^4$He mass fraction with variation in both parameters. Contours are placed at 1, 2, 3, 4, and 5 standard deviations from the measured value. The solid diagonal line is the line of constant $\Delta m = 1.29333217$, the physical nucleon mass splitting.
greater than its physical value, the free neutrons will all decay before they have a chance to be captures and form \( D \). The production of \( ^3\text{He} \) will be sensitive to \( \alpha_{f.s.} \) variation due to the Coulomb repulsion of \( D \) and \( p \). We therefore do not expect the \( D \) abundance to track lines of constant \( \Delta m \) as \( ^4\text{He} \) does.

In Fig. 7, we observe that the slope of \( D \) abundance with respect to independent variations of \( \delta_q \) and \( \alpha_{f.s.} \) is different as compared with the variations in \( ^4\text{He} \). Further, we observe curvature in the variations indicating non-linear dependence upon the variations. When combined with the variations of \( ^4\text{He} \), we anticipate a more stringent constraint on the possible variations of \( \alpha_{f.s.} \) and \( \delta_q \).

Continuing the study of deuterium mass fraction, the value of the deuterium abundance given in the latest Particle Data Group review of Big Bang Nucleosynthesis is adopted, providing the recommended value of \( \text{D/H} \big|_p = (2.53 \pm 0.04) \times 10^{-5} \) [21].

![Deuterium abundance with variation in \( \alpha_{f.s.} \) (left) and \( \delta_q \) (right).](image)

Figure 7: Deuterium abundance with variation in \( \alpha_{f.s.} \) (left) and \( \delta_q \) (right).

The contour plot for deuterium mass fraction shown in Figure 8 marks out the standard deviations of the final mass fraction for results of variational calculations. This clearly demonstrates the different dependence on \( \alpha_{f.s.} \) and \( \delta_q \). The line of constant \( \Delta m \) is approximately \( \pi/4 \) radians off axis from the line of constant \( D \) abundance.
3.4 Combining $^4$He and Deuterium for a Tight Constraint

In previous subsections, it is established that a combination of $^4$He and deuterium mass fractions are together sufficient to highly constrain the variation of our quantities. While other mass fractions calculated are not considered, several are calculated. These are $^7$Be, $^3$He, and tritium. These other mass fractions act in an analogous way in that they further constrain the permissible values of $\alpha_{f.s.}$ and $\delta_q$ through having different dependences. We add in quadrature the variation from the central value of each of these, producing a rigorously constrained result. While the plots preceding this section show

$$|\Delta X|/\sigma_X$$

\hfill (10)
where $X$ can refer to the mass fraction of a single quantity under study, we sum the mass fractions and uncertainties for quantities with quadrature addition:

$$\sqrt{\sum_X \Delta X^2 / \sigma_X^2}$$  \hspace{1cm} (11)

Figure 9 reveals the degree to which the abundances and their uncertainties constrain the variation of the two quantities under investigation. The results shown in Figure 9 allow for strong constraints on the variations of $\alpha_{f,s.}$ and $\delta_q$ explicitly, effectively demonstrating that with 68% confidence, the quantities may not vary more than approximately 0.5% from their currently established values. A single interval provides an uncorrelated 68% confidence interval.

It is worth noting the degree to which the abundances constrain the “permissible region” in which the universe as measured today is reproduced. The region of Figure 9 where the mass fraction variation is less than $1\sigma$ allows for less than a 0.5% variation in the value of $\alpha_{f,s.}$ and less than 1% in the value of $\delta_q$. While the higher confidence intervals are for obvious reasons less constraining, it is still worth noting that even at the $5\sigma$ boundary, variations in $\delta_q$ do not exceed 4% and variations in $\alpha_{f,s.}$ do not exceed 3%.

This degree of sensitivity is not entirely unexpected. Due to the way in which lighter quantities and charged particles are sensitive to variations in $\alpha_{f,s.}$ and heavier quantities are more sensitive to change in $\Delta m$, it was anticipated that the combination of the two would be very constraining. Our study, which allowed for simultaneous variation, provided a more rigorous treatment of these constraints than was previously performed and continues to agree with the accepted wisdom while also serving to more fully map the parameter space under investigation.
Figure 9: Contours with deviations for multiple mass fractions added in quadrature. 1, 2, 3, 4, and 5 standard deviation contours are shown where each of these is bounded by the deviation of any of the quantities added in quadrature.
4 Conclusions

Big Bang Nucleosynthesis, particularly standard Big Bang Nucleosynthesis without the inclusion of exotic particles, has been established as highly constraining in the search for new, beyond Standard Model physics. We have searched for new physics in the sources of isospin breaking at low energies, the fine structure (electromagnetic coupling) constant $\alpha_{\text{f.s.}}$ and the up/down quark mass splitting $\delta_q = \frac{1}{2}(m_d - m_u)$.

In order to perform this study, we have taken the most advanced available BBN code and have modified it with variational rates. We then performed a numerical study of the parameter space, evaluating many different combinations of the two main sources of isospin breaking in the search for constraints. We have demonstrated that comparison of the calculated $^4\text{He}$ mass fraction to astronomical observation was constraining but allowed for large simultaneous variations in $\alpha_{\text{f.s.}}$ and $\delta_q$, provided $\Delta m$ was held fixed. The $D$ mass fraction also allows for a large simultaneous variation in $\alpha_{\text{f.s.}}$ and $\delta_q$ but along an axis about $\pi/4$ radians shifted from the line of constant $\Delta m$. Therefore, using the combined constraints from the observed abundances of $^4\text{He}$ and $D$, the allowed variations in both $\alpha_{\text{f.s.}}$ and $\delta_q$ were $\lesssim 1\%$ each.

Through the new methods introduced in this investigation, we expanded on past work in exploring the variational space. For the first time, a quantitative study performing a simultaneous variation in both sources of isospin breaking was carried out. What allowed for this study was recent knowledge from lattice QCD about the precise ways in which the nucleon mass splitting varies with respect to $\delta_q$ and $\alpha_{\text{f.s.}}$.

5 Future Work

As was discussed in the theory section of this thesis, the so-called “Lithium Problem” was ignored as it is beyond the scope of this work. Resolution of this problem would increase the number of available constraints on the quadrature-added result. This is subject to
availabilities of primordial abundances and extrapolations from low-metallicity gas clouds.

More immediate work includes the updating of the Kawano code to a more modern computing format. The results of this thesis also point to a necessity for further work to be conducted in lattice QCD. This further work would be to reducing the error bars in any of the various theoretically predicted values, thereby allowing for more accurate calculations of Big Bang Nucleosynthesis and/or constraints on avenues for new physics.

6 Acknowledgements

Many thanks are owed to my advisor, André Walker-Loud for his help with getting to grips with the theory and with giving me a hand figuring out object-oriented programming and many other things. Projjwal Banerjee at the University of Minnesota, his expertise in BBN, and his skills in FORTRAN were invaluable to this project. Finally, George Vahala lent valuable computing resources in the form of the ESV stack to make my calculations possible. This work was supported in part through the U.S. Department of Energy Early Career Award Contract DE-SC0012180 awarded to André Walker-Loud.
References


A Python Code

A.1 Grid Controls

```python
# Overall grid writing script for bbn thesis

import os
import time  # will be used to time the script for general good purpose

t0 = time.time()

os.system('python bbn_mattalpha_docopt_firstrun.py')  # initialize the initial data files
os.system('python bbn_mattalpha_docopt_parent.py --A_ratio=0.9 --delta_ratio=0.9 --step=0.1')  # coarse grid
os.system('python bbn_mattalpha_docopt_parent.py --A_ratio=0.95 --delta_ratio=0.95 --step=0.01')  # finer grid
os.system('python bbn_mattalpha_docopt_parent.py --A_ratio=0.975 --delta_ratio=0.975 --step=0.001')  # finest grid

t1=time.time()
total = t1-t0
print('Overall Run Done')
print('Time elapsed = ',total)
```

A.2 Parent Wrapper

```
Usage: bbn_mattalpha_docopt_parent.py [--A_ratio=N] [--delta_ratio=N] [--step=N]

Options:
    --A_ratio=N  ratio to assign A.fine
    --delta_ratio=N  ratio to assign delta
    --step=N  ratio to assign step
```

```python
import os
import numpy as np
from docopt import docopt

'A_fine0':0.0072973525698
```
params2 = {'A_fine0': 1/137.035999139, 'A_ratio0': 1.000, 'A_ratio': 1.0000, 'delta0': 2.52, 'delta_ratio': 1.000, 'delta_ratio0': 1.000, 'step': 0.001}

arguments = docopt(__doc__)
print ('Replacements from Docopt')
print (arguments)

if arguments['--A_ratio'] != None:
    params2['A_ratio'] = float(arguments['--A_ratio'])
else:
    pass

if arguments['--delta_ratio'] != None:
    params2['delta_ratio'] = float(arguments['--delta_ratio'])
else:
    pass

if arguments['--step'] != None:
    params2['step'] = float(arguments['--step'])
else:
    pass

print ('New Parent Params')
print (params2)

def my_range(start, end, step):
    while start <= end:
        yield start
        start += step

if params2['A_ratio'] < 1:
    Aratio_start= params2['A_ratio']
    Aratio_step=params2['step']
    Aratio_end=2-params2['A_ratio']
elif params2['A_ratio'] > 1:
    Aratio_start= 2-params2['A_ratio']
    Aratio_step=params2['step']
    Aratio_end=params2['A_ratio']
elif params2['A_ratio'] == 1:
    print('Central value of A_ratio, so we will take a small band around unity')
    Aratio_start= 0.99
    Aratio_step=params2['step']
Aratio_end=1.01

if params2['delta_ratio'] < 1:
    deltaratio_start= params2['delta_ratio']
    deltaratio_step= params2['step']
    deltaratio_end= 2−params2['delta_ratio']
elif params2['delta_ratio'] > 1:
    deltaratio_start= 2−params2['delta_ratio']
    deltaratio_step= params2['step']
    deltaratio_end= params2['delta_ratio']
elif params2['delta_ratio'] == 1:
    print('Central value of delta ratio, so we will take a small band around unity')
    deltaratio_start= 0.99
    deltaratio_step= params2['step']
    deltaratio_end= 1.01

if (params2['A_weak_ratio']) == (params2['A_thermo_ratio']):
    A_ratio= params2['A_ratio']
    if (A_ratio != params2['A_ratio0']) and (params2['delta_ratio'] != params2['delta_ratio0']):
        for A_ratio in my_range(Aratio_start, Aratio_end, Aratio_step):
            for deltaratio in my_range(deltaratio_start, deltaratio_end, deltaratio_step):
                os.system('python bbn_mattalpha_docopt.py --A_ratio='+str(A_ratio)+' --delta_r='+str(deltaratio))

elif (params2['delta_ratio']) != params2['delta_ratio0'] and (A_ratio) == params2['A_ratio0']:
    for A_ratio in my_range(Aratio_start, Aratio_end, Aratio_step):
        for deltaratio in my_range(deltaratio_start, deltaratio_end, deltaratio_step):
            os.system('python bbn_mattalpha_docopt.py --A_ratio='+str(A_ratio)+' --delta_r='+str(deltaratio))

elif (params2['delta_ratio']) == params2['delta_ratio0'] and (A_ratio) != params2['A_ratio0']:
    for A_ratio in my_range(Aratio_start, Aratio_end, Aratio_step):
for delta_ratio in my_range(deltaratio_start, deltaratio_end, deltaratio_step):
    os.system('python bbn_mattalpha_docopt.py
              --A_ratio='+str(A.ratio)+' --delta_r='
              '+str(delta_ratio))

elif (A.ratio) == params2['A_ratio0'] and (params2['delta_ratio']) == params2['delta_ratio0']:
    print('Central Value')
    os.system('python bbn_mattalpha_docopt.py --A_ratio='+str
              (A.ratio)+' --delta_r='+str(delta_ratio))

A.3 Basic Wrapper

"""Usage: bbn_mattalpha_docopt.py [--A_ratio=N] [--delta_r=N]

Options:
    --A_ratio=N fine structure ratio
    --delta_r=N md_mns_mu ratio
"""

import os
import numpy as np
from docopt import docopt
import tables as h5
import bbn.h5_table_writer as bbn_w

#'MN_MNS_MP':1.29333317
#c_flag is the flag for choosing different coulomb correction 1
# for Smith2010 and 0 for Lopez 1999
#t9i0 is the initial temperature in units of 10^9 K
#inc0 controls the length of the output file. higher value means
#less frequent dumps
#tau0: latest PDG
params = {'delta_r':1.0, 'MN_PLS_MP':1877.837392, 'M_E'
          :0.510998910, 'tau_0':880.3, 'A_fine0':1.137.035999139, 'A_ratio '
          :1.0, 'delta_r0':2.52, 'MU_nue':0.000001, 'ETA':6.05E−10, 't9i0'
          :5.00E+01, 'c_flag':1, 'inc0':10}
tau0 = params['tau_0']

#### BEGIN DOCOPT IMPLEMENTATION ####
arguments = docopt(_doc_, version='why')
print ('Replacements from Docopt')
print (arguments)
if arguments['--delta_r'] != None:
    params['delta_r'] = float(arguments['--delta_r'])
else:
    pass

if arguments['--A_ratio'] != None:
    params['A_ratio'] = float(arguments['--A_ratio'])
else:
    pass

print ('New Params')
print (params)

### END DOCOPT IMPLEMENTATION ###

### BEGIN DEFINITIONS AND CLASS DECLARATIONS ###

m_e = 0.510998910
alpha_fs_0 = 1./137.035999139
dmN = 1.29333217
tau0 = 880.3 # latest PDG
md_mns_mu_0 = 2.52 # FLAG http://arxiv.org/abs/1310.8555
mn_mns_mp_mdu = 2.44 # Andre avg
mn_mns_mp_qed = dmN - mn_mns_mp_mdu

def mn_mns_mp(md_mns_mu, alpha_fs):
    n_p = mn_mns_mp_mdu * float(md_mns_mu) / md_mns_mu_0
    n_p += mn_mns_mp_qed * alpha_fs / alpha_fs_0
    return n_p

def tau_n(Q):
    Q0 = dmN
    a0 = Q0/m_e
    phase0 = (2*a0**4 - 9*a0**2 - 8) * np.sqrt(a0**2-1) / 15
    + a0 * np.log(a0 + np.sqrt(a0**2-1))
    a = Q/m_e
    phase = (2*a**4 - 9*a**2 - 8) * np.sqrt(a**2-1) / 15 + a
    * np.log(a + np.sqrt(a**2-1))
    return phase0/phase * tau0

def my_range(start, end, step):
    while start <= end:
        yield start
        start += step
delta = params['delta_r'] * params['delta_r0'] # extracting the new value of delta
A_fine = params['A_ratio'] * params['A_fine0'] # extracting new value of A_fine

# new params inputs
MN_MNS_MP = mn_mns_mp(delta, A_fine)
tau_new = tau_n(MN_MNS_MP)

##### END DEFINITIONS AND CLASS DECLARATIONS #####

##### BEGIN CHECKER IMPLEMENTATION #####

## Section: Reconstructing the ratios ##
A_ratio = params['A_ratio']
delta_ratio = params['delta_r']

## Section: Loading the data tables ##
debug_open=h5.open_file('bbn_results.h5','a')
datafile = h5.open_file('bbn_results.h5','r')
datafile_debug=datafile.get_node('/bbn_data')
datafile_debug2=datafile_debug.iterrows()

alpha_check=[0]
for i in datafile_debug.iterrows():
    if i['alpha_fs_r'] >= A_ratio-0.0001 and i['alpha_fs_r'] <= A_ratio+0.0001 and i['md_mns_mu_r'] >= delta_ratio -0.0001 and i['md_mns_mu_r'] <= delta_ratio+0.0001:
        alpha_check.append(i['alpha_fs_r'])

alpha_len = len(alpha_check)
datafile.close()

if alpha_len != 1:# and delta_len != 1:
    print('Already calculated, moving to next iteration')
else:
    ##### BEGIN CALCULATION OF RATES #####
    params_update= {'MN_MNS_MP':MN_MNS_MP,'MN_PLS_MP':1877.837392,'M_E':0.510998910,'tau_0':880.3,'A_fine0':0.0072973525698,'A_fine':A_fine,'MU_nue':0.000001,'
ETA':6.05E-10,'t9i0':5.00E+01,'c_flag':1,'inc0':10}

print ('')
print ('mn – mp [MeV] = ', MN_MNS_MP)
print ('New A_fine = ', A_fine)

f_in = open('bbn_new123_pythonalpha.f').read()
f_out = open('bbn.f','w')
f_out.write(f_in % params_update)
f_out.close()

print ('compiling')
print ('gfortran bbn.f –o bbn')

os.system('gfortran bbn.f –o bbn')#os.system('gfortran –g
−fcheck=all −Wall bbn.f')
print('running')

os.system('./bbn')

nuc_data = open('new123.dat').readlines()
n = 0; i=0
have_data = False

while not have_data:
    line = nuc_data[i]
    if 'Temp' in line:
        n += 1
    if n == 2:
        have_data = True
        l_info = i−2
        i += 1

I am using the output format of ProjJwals code, knowing that Temp appears twice, and the info we want is 2 lines before the second Writing of Temp

Tf = float(nuc_data[l_info].split()[0])
yp = float(nuc_data[l_info].split()[4])
yd = float(nuc_data[l_info].split()[5])
yHe3 = float(nuc_data[l_info].split()[7])
yH3 = float(nuc_data[l_info].split()[6])
yHe4 = float(nuc_data[l_info].split()[8])
yp = yp−yHe4*0.0072 # correction for finite temp
radiative correction etc

yHe4 = yHe4*1.0072
yli6 = float(nuc_data[l_info].split()[9])
yli7 = float(nuc_data[l_info].split()[10])
ybe7 = float(nuc_data[l_info].split()[11])
tau = float(nuc_data[7].split()[5])

if not os.path.exists('mn_mns_mp.docopt_indvar.dat'):  

35
fout = open('mn_mns_mp_docopt_indvar.dat','w')
print >> fout, "tau_0  tau  #mn–mp  Yp  Yd  Yh3  YHe3  YHe4  Yli6  Yli7  Ybe7  A_fine0  A_fine_th  A_fine_wk"
fout.close()

fout = open('mn_mns_mp_docopt_indvar.dat','a')
fout.write("%.1f  %.1f  %.8f  %.4f  %.3e  %.3e  %.3e  %.4f  %.3e  %.3e  %.5e  %.5e"
%(params['tau_0'],tau,
params_update['MN_MNS_MP'],yp,yd,yh3,yHe3,yHe4,yli6,
yli7,ybe7,params_update['A_fine0'],params_update['
A_fine']) + "\n")
fout.close()

### END CALCULATION OF RATES ###

### Table Writer implementation

h5_file = h5.open_file('bbn_results.h5','a')

#Below kept for legacy reasons
md_mns_mu = params['delta_r'] * params['delta_r0']
md_mns_mu physic = params['delta_r']
A_fine = params['A_ratio']*params['A_fine0']

#make dict and fill in keys
bbn_keys = dict()
bbn_keys['md_mns_mu_r'] = params['delta_r']
bbn_keys['alpha_fs_r'] = params['A_ratio']
bbn_keys['mn_mns_mp'] = mn_mns_mp(md_mns_mu,A_fine)
bbn_keys['tau_n'] = tau_n(mn_mns_mp(md_mns_mu,A_fine))

bbn_results = open('new123.dat').readlines()
data = []
i = 0
have_data = False
n_t = 48
while not have_data:
    line = bbn_results[i]
    if 'He4' in line:
        for t in range(n_t):
            try:
                if len(bbn_results[i+2+t].split()) > 0:
tmp = np.array([ 
    float(x) for x 
    in 
    bbn_results[i +2+t].split() 
]) 

except Exception:
    print('no data at t=%d' % t)

# print t, tmp
data.append(tmp)

have_data = True

i += 1
data = np.array(data)
bbn_row = bbn_w.SaveBBNData(n_t=n_t)
entries = bbn_row.bbn_output

for i,key in enumerate(entries):
    bbn_keys[key] = data[:,i]

bbn_row.save_row(h5_file,bbn_row(),bbn_keys)

h5_file.close()

print('Written to file!')

A.4 First Run Program

#!/usr/local/bin/python

import os
import numpy as np
from docopt import docopt
import tables as h5
import bbn_h5_table_writer as bbn_w

#'MN_MNS_MP':1.29333217
# c_flag is the flag for choosing different coulomb correction 1 for Smith2010 and 0 for Lopez 1999
#'t9i0' is the initial temperature in units of 10^9 K
#inc0 controls the length of the output file. higher value means less frequent dumps
#tau0: latest PDG
params = {'delta_r':1.0,'MN_PLS_MP':1877.837392,'M_E':0.510998910,'tau_0':880.3,'A_fine0':1.0/137.035999139,'A_ratio':1.0,'delta_r0':2.52,'MU_nue':0.000001,'ETA':6.05E−10,'t9i0'}
tau0 = params['tau_0']

### BEGIN DEFINITIONS AND CLASS DECLARATIONS ###

m_e = 0.510998910
alpha_fs_0 = 1./137.035999139
dmN = 1.29333217
tau0 = 880.3 # latest PDG
md_mns_mu_0 = 2.52 # FLAG http://arxiv.org/abs/1310.8555
mn_mns_mp_mdu = 2.44 # Andre avg
mn_mns_mp_qed = dmN - mn_mns_mp_mdu

def mn_mns_mp(md_mns_mu, alpha_fs):
    n_p = mn_mns_mp_mdu * float(md_mns_mu) / md_mns_mu_0
    n_p += mn_mns_mp_qed * alpha_fs / alpha_fs_0
    return n_p

def tau_n(Q):
    Q0 = dmN
    a0 = Q0/m_e
    phase0 = (2*a0**4 - 9*a0**2 - 8) * np.sqrt(a0**2-1) / 15
    + a0 * np.log(a0 + np.sqrt(a0**2-1))
    a = Q/m_e
    phase = (2*a**4 - 9*a**2 - 8) * np.sqrt(a**2-1) / 15 + a
    * np.log(a + np.sqrt(a**2-1))
    return phase0/phase * tau0

def my_range(start, end, step):
    while start <= end:
        yield start
        start += step

delta = params['delta_r'] * params['delta_r0'] # extracting the new value of delta
A_fine = params['A_ratio'] * params['A_fine0'] # extracting new value of A_fine

# new params inputs
MN_MNS_MP = mn_mns_mp(delta, A_fine)
tau_new = tau_n(MN_MNS_MP)

### END DEFINITIONS AND CLASS DECLARATIONS ###

### BEGIN CHECKER IMPLEMENTATION ###
Section: Reconstructing the ratios

A_ratio = params['A_ratio']
delta_ratio = params['delta_r']

Section: Loading the data tables

d.debug.open=h5.open_file('bbn_results.h5','a')
d.debug.open.close()

BEGIN CALCULATION OF RATES

params_update= {'MN_MNS_MP': MN_MNS_MP, 'MN_PLS_MP': 1877.837392, 'M_E': 0.510998910, 'tau_0': 880.3, 'A_fine0': 0.0072973525698, 'A_fine': A_fine, 'MU_nue': 0.000001, 'ETA': 6.05E-10, 't9i0': 5.00E+01, 'c_flag': 1, 'inc0': 10}
print ()
print ('mn - mp [MeV] = ', MN_MNS_MP)
print ('New A_fine = ',A_fine)
f_in = open('bbn_new123_pythonalpha.f').read()
f_out = open('bbn.f','w')
f_out.write(f_in % params_update)
f_out.close()
print ('compiling')
print ('gfortran bbn.f -o bbn')
os.system('gfortran bbn.f -o bbn')
print ('running')
os.system('./bbn')

nuc_data = open('new123.dat').readlines()
n = 0; i=0
have_data = False
while not have_data:
    line = nuc_data[i]
    if 'Temp' in line:
        n += 1
    if n == 2:
        have_data = True
        l_info = i-2
        i += 1
    
I am using the output format of Projjwals code, knowing that Temp appears twice, and the info we want is 2 lines before the second Writing of Temp

Tf = float(nuc_data[l_info].split()[0])
yp = float(nuc_data[1].split()[4])
yd = float(nuc_data[1].split()[5])
yHe3 = float(nuc_data[1].split()[7])
yh3 = float(nuc_data[1].split()[6])
yHe4 = float(nuc_data[1].split()[8])
yp = yp−yHe4*0.0072 # correction for finite temp radiative
correction etc
yHe4 = yHe4*1.0072
yli6 = float(nuc_data[1].split()[9])
yli7 = float(nuc_data[1].split()[10])
ybe7 = float(nuc_data[1].split()[11])
tau = float(nuc_data[7].split()[5])
if not os.path.exists('mn_mns_mp.docopt_indvar.dat'):
    fout = open('mn_mns_mp.docopt_indvar.dat','w')
    print >> fout, "tau_0 tau #mn−mp Yp Yd Yh3 YHe3 YHe4 Yli6 Yli7 Ybe7 A_fine0 A_fine_th A_fine_wk"
    fout.close()
    fout = open('mn_mns_mp.docopt_indvar.dat','a')
    fout.write("%.1f %.1f %.8f %.4f %.3e %.3e %.3e %.3e %.3e %.3e %.5e %.5e" % (params['tau_0'],tau,params_update['MN_MNS_MP'],yp,yd,yh3,yHe3,yHe4,yli6,yli7,ybe7,params_update['A_fine0'],params_update['A_fine']) + "\n")
    fout.close()

#### END CALCULATION OF RATES ####

#### Table Writer implementation

h5_file = h5.open_file('bbn_results.h5','a')

#Below kept for legacy reasons
md_mns_mu = params['delta_r'] * params['delta_r0']
md_mns_mu_phys = params['delta_r0']
A_fine = params['A_ratio']*params['A_fine0']
#make dict and fill in keys
bbn_keys = dict()
bbn_keys['md_mns_mu_r'] = params['delta_r']
bbn_keys['alpha_fs_r'] = params['A_ratio']
bbn_keys['mn_mns_mp'] = mn_mns_mp(md_mns_mu,A_fine)
bbn_keys['tau_n'] = tau_n(mn_mns_mp(md_mns_mu,A_fine))

bbn_results = open('new123.dat').readlines()
data = []
i = 0
have_data = False
n_t = 48
while not have_data:
    line = bbn_results[i]
    if 'He4' in line:
        for t in range(n_t):
            try:
                if len(bbn_results[i+2+t].split()) > 0:
                    tmp = np.array([float(x) for x in bbn_results[i +2+t].split()])
            except Exception:
                print('no data at t=%d' %t)
                #print t, tmp
data.append(tmp)
    have_data = True
i += 1
data = np.array(data)
bbn_row = bbn_w.SaveBBNDATA(n_t=n_t)
entries = bbn_row.bbn_output
for i,key in enumerate(entries):
    bbn_keys[key] = data[:,i]

bbn_row.save_row(h5_file,bbn_row(),bbn_keys)

h5_file.close()
print('Written to file!')

A.5 Table Writer

import sys
import tables as h5

class SaveBBNDATA:
    # initialize length of time steps
    def __init__(self,n_t=47):
        self.n_t = n_t
        self.bbn_input = [
            '#md_mns_mu_r','alpha_fs_r','alpha_weak_r','
alpthermo_r','
        md_mns_mu_r','alpha_fs_r','
         mn_mns_mp','tau_n']
```python
self.bbn_output = ['T_MeV', 'T_K9', 't_s',
                   'y_n', 'y_p', 'y_d', 'y_t', 'y_he3', 'y_he4',
                   'y_li6', 'y_li7', 'y_be7', 'y_xx', 'y_nT']

self.bbn_keys = self.bbn_input + self.bbn_output

# this function creates a description for the rows of the table
# when the class is called, it instantiates this description
# - see example below

def __call__(self):
    class DataEntries(h5.IsDescription):
        md_mns_mu_r = h5.Float32Col()  # ratio of (md - mu) / (md - mu)_phys
        alpha_fs_r = h5.Float32Col()  # ratio of alpha_fs / alpha_fs_phys

        # we add control of the ways alpha_fs can enter code
        # just to see how important different aspects are,
        # mn-mp, NP rates and thermodynamic rates
        alpha_weak_r = h5.Float32Col()  # same as alpha_fs but
                                      # only for radiative corrections to that go into N
                                      # <-> P rates
        alpha_thermo_r = h5.Float32Col()  # same as alpha_fs
                                         # but only for alpha which goes into other reactions
                                         # in BBN chain
        mn_mns_mp = h5.Float32Col()  # value of mn - mp [MeV]
                                    # that goes into code
        tau_n = h5.Float32Col()  # resulting value of neutron
                                  # lifetime in secs
        T_MeV = h5.Float32Col(shape=(self.n_t))  # time series
                                                   # Temp in MeV after BB
        T_K9 = h5.Float32Col(shape=(self.n_t))  # time series
                                                   # of Temp in 10^9 K
        t_s = h5.Float32Col(shape=(self.n_t))  # time series
                                               # of time in sec after BB
                                               # now define the time series mass fractions Y_X
        y_n = h5.Float32Col(shape=(self.n_t))  # free neutrons
        y_p = h5.Float32Col(shape=(self.n_t))  # protons
        y_d = h5.Float32Col(shape=(self.n_t))  # deuterium
        y_t = h5.Float32Col(shape=(self.n_t))  # tritium
        y_he3 = h5.Float32Col(shape=(self.n_t))  # 3He
        y_he4 = h5.Float32Col(shape=(self.n_t))  # 4He
        y_li6 = h5.Float32Col(shape=(self.n_t))  # Li6
        y_li7 = h5.Float32Col(shape=(self.n_t))  # Li7
```

```python
y_be7 = h5.Float32Col(shape=(self.n_t))  # Be7
y_xx = h5.Float32Col(shape=(self.n_t))  # Li8 and up
y_nT = h5.Float32Col(shape=(self.n_t))  # total

return DataEntries

# write the results into a row of an hdf5 pytables table

def save_row(self, h5_file, data_type, bbn.keys):
# if table exists, read it, else make it

    try:
        table = h5_file.get_node('/bbn_data')
    except:
        table = h5_file.create_table('/', 'bbn_data', data_type, "Test Example")

    # add bbn results to table from bbn.keys
    bbn_results = table.row
    good_row = True
    for key in self.bbn_keys:
        try:
            bbn_results[key] = bbn_keys[key]
        except:
            print('bad bbn_keys data entry %s' % key)
            good_row = False
            e = sys.exc_info()[0]
            print("<p>Error: %s</p>" % e)

    if good_row:
        bbn_results.append()
        table.flush()
    else:
        print('broken row of bbn data − not writing')

if __name__=='__main__':
    print('')

example use:
inside the equivalent of bbn_andre.py

import tables as h5
import numpy as np
import bbn_h5_table_writer as bbn_w

h5_file = h5.open_file('bbn_results.h5', 'a')
# Check h5_file table entries to make sure choices of md − mu, alpha_fs, etc not already recorded
# we can do this by making a new function in this class

43
```
if new choices then run bbn code, collect results and store in h5 table

#make dict and fill in keys
bbn_keys = dict()
bbn_keys['md_mns_mu_r'] = md_mns_mu / md_mns_mu_phys
bbn_keys['alpha_fs_r'] = alpha_fs / alpha_fs_phys

def mn_mns_mp(md_mns_mu, alpha_fs):
    return calc of mn-mp from md_mns_mu, alpha_fs
bbn_keys['mn_mns_mp'] = mn_mns_mp(md_mns_mu, alpha_fs)

bbn_results = open('new123.dat').readlines()
data = []
i = 0
have_data = False
while not have_data:
    line = bbn_results[i]
    if 'He4' in line:
        for t in range(47):
            data.append([float(x) for x in bbn_results[i+2+t].split()])
        have_data = True
    i += 1
data = np.array(data)
entries = ['T_MeV', 'T_K9', 't_s', 'y_n', 'y_p', 'y_d', 'y_t',
          'y_he3', 'y_he4', 'y_li6', 'y_li7', 'y_be7', 'y_xx', 'y_nT']
for i, key in enumerate(entries):
    bbn_keys[key] = data[:,i]

bbn_row = bbn_w.SaveBBNData(n_t=47)
bbn_row.save_row(h5_file, bbn_row, bbn_keys)
h5_file.close()