Comparison of Two Distinct BBN Codes

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Abstract. This paper compares the results of two SBBN codes developped independently by different teams of physicists. These two codes have significant differences that lead to a discrepency between their final mass fractions of ^{4}He of 0.003. This paper shows that the mass fractions of each code had different orders of convergence, and how the number of timesteps affects the accuracy of the mass fractions. At the end, the paper shows how to modify both codes so that their ^{4}He mass fractions agree to around 0.0001.

1. Introduction

In 1993 I started working on a Big Bang Nucleosynthesis code once used by UT-Austin Professors Tony Rothman and Richard Matzner (hereafter known as the Texas code) for some papers between 1982 and 1984.[1] Two years later Mr. David Thomas e-mailed me a different BBN code (hereafter known as the Thomas et al code) which he used with Profs. David Schramm, Keith Olive, and Mr. Brian Fields for a series of papers starting in 1993.[2] But these two different codes calculated different final mass fractions of their isotopes, as shown in Table (1). In particular, the values of $X_{^4He}$ disagreed by about 0.003. So I went about determining the differences between the codes that could explain this discrepency.

A Big Bang Nucleosythesis code starts with free neutrons and protons plus photons, electrons and the three neutrino species, all at a high value of the electron/photon temperature T. Then in timesteps of value Δt the code calculates the current abundances $Y(i)$ of each isotope as determined by the reactions between the isotopes and other particles, as well as the temperatures and energy densities of the non-baryonic particles, which affect the reaction rates. The Thomas et al code featured some details like the Coulomb factor correction to the neutron-proton conversion rates that I had to add to the Texas code. Also the codes had several differences in calculating various thermal quantities.[3] The Thomas et al code would for instance calculate T via the Runge-

[1] The papers dealt with anisotropic models, but the code used for them had the option to turn the anisotropies off. Also I expanded this code's original number of 9 isotopes to the other code's 68.

[2] These papers lead up to a 1994 paper on an inhomogenous model, which could be compared to the standard model of the Thomas et al code.

[3] Kawano (1992) describes the details of a code similar to the Thomas et al code.

isotope	Thomas et al X	Texas X
d	$0.1203806246 \times 10^{-3}$	$0.1239148256 \times 10^{-3}$
^{3}H	$0.5791818972 \times 10^{-6}$	$0.5993673829 \times 10^{-6}$
^{3}He	$0.3616593549 \times 10^{-4}$	$0.364445127 \times 10^{-4}$
^{4}He	0.2369001572	0.2397015878
^{7}Li	$0.3349991579 \times 10^{-9}$	$0.3496296345 \times 10^{-9}$
^{7}Be	$0.286454318 \times 10^{-9}$	$0.2679050102 \times 10^{-9}$
^{9}Be	$0.1036417579 \times 10^{-16}$	$0.1126556133 \times 10^{-16}$
^{10}B	$0.8927007279 \times 10^{-18}$	$0.9643350569 \times 10^{-18}$
^{11}B	$0.9314884547 \times 10^{-16}$	$0.91442805 \times 10^{-16}$
^{12}C	$0.2898262833 \times 10^{-13}$	$0.3048347851 \times 10^{-13}$
^{14}N	$0.1275229996 \times 10^{-12}$	$0.1326174221 \times 10^{-12}$
^{16}O	$0.7290963822 \times 10^{-17}$	$0.7730848001 \times 10^{-17}$
^{21}Ne	$0.6698206755 \times 10^{-21}$	$0.5517307027 \times 10^{-23}$

Table (1): Mass Fractions X from each code. The results are for $\eta_{10} = 3.0$, but the codes have the same discrepency between the values of $X_{^4He}$ for all interesting values of η_{10}.

Kutta method and then plug in T to equations for energy densities and pressures. The Texas code would use R-K to calculate density $\rho_{e+\gamma}$ of the electrons and photons and then determine T from there. I wondered which differences caused the disagreements between the codes. This paper details two differences in the way each code goes about its evolution that made the accuracy of each code's results questionable.

2. Convergence of the codes

At each timestep n the BBN codes use the Second-Order Runge-Kutta method to calculate the isotope abundances $Y_{n+1}(i)$.:

$$Y_{n+1}(i) \quad = \quad Y_n(i) + \frac{1}{2}\left[\frac{dY(i)}{dt}(t, Y_n) + \frac{dY(i)}{dt}(t+\Delta t, Y_{n+1})\right]\Delta t \qquad (1)$$

Wagoner (1969, p. 253) lists the complicated equation for $\dot{Y}(i)$, which depends on the other abundances and on the reaction rates that destroy ($[ij]$) and create ($[kl]$) isotope i. But at the highest temperatures the total destruction rate of each isotope is nearly equal to its creation rate. So the codes calculate $\dot{Y}(i)$ using an equation linearized in terms of $Y_{n+1}(i)$

$$\frac{dY(i)}{dt}(t, Y_n) \quad = \quad A_{ij}(Y_n, [ij](T_n), [kl](T_n)) \times Y_{n+1}(j)$$

where the matrix A_{ij} is written out in Wagoner (1969, p. 294). The codes pair off the right hand side of this equation with an implicit expression of $\dot{Y}(i)$ leading to a matrix equation for $Y_{n+1}(i)$.

$$
\begin{aligned}
Y_n(i) &= Y_{n+1}(i) - \frac{dY(i)}{dt}[t+\Delta t_n, Y_{n+1}(i)]\Delta t_n + \cdots \\
\frac{dY(i)}{dt}[t+\Delta t_n, Y_{n+1}(i)] &= \frac{Y_{n+1}(i) - Y_n(i)}{\Delta t_n} && (2) \\
Y_n(i) &= Q_{ij}(Y_n, [ij](T_n), [kl](T_n)) \times Y_{n+1}(j) && (3)
\end{aligned}
$$

($Q_{ij} = 1_{ij} - A_{ij}\Delta t_n$) The codes solve for $Y_{n+1}(i)$ and plug it back in to get $\dot{Y}(i)$.

This R-K method should produce mass fractions that have second-order convergenge as the timestep values get smaller. I tested the convergences of mass fraction $X_{^4He}$ the Thomas et al code and the Texas code by starting with an array of timestep values Δt_n that naturally arise from a run, and then dividing those values by two, four, and so on. The Thomas el al code turned out to have the expected convergence:

$$
X_{^4He} = 0.2392602277 - (0.2474541681 \times 10^{-2})d^2
$$

where d equals one over the number of divisions of each timestep. But the Texas code had only first order convergence, and so needed to be fixed.

$$
X_{^4He} = 0.2394509836 + (0.3832102957 \times 10^{-3})d
$$

I traced each code to find out exactly how in step # n each went about calculating $Y_{n+1}(i)$. In the first Runge-Kutta step the Thomas et al code used the previous $Y_{n-1}(i)$ on the left hand side of matrix equation (3), and $Y_n(i)$ in matrix Q_{ij}.

$$
\begin{aligned}
Y_{n-1}(i) &= Q_{ij}(Y_n, [ij](T_n), [kl](T_n)) \times Y_{n\alpha}(j) \\
\frac{dY(i)}{dt}(t, Y_n(i)) &= \frac{Y_{n\alpha}(i) - Y_{n-1}(i)}{\Delta t_{n-1}}
\end{aligned}
$$

I'm calling the equation solution $Y_{n\alpha}(i)$ for the first step (and then $Y_{n\beta}(i)$ for the second step). Then this code used an expression for $\dot{Y}(i)$ that clearly matched up with Equation (2) for $\dot{Y}(i)[t, Y_n(i)]$, with $Y_{n-1}(i)$ in the numerator and Δt_{n-1} in the denominator. So $Y_{n\alpha}(i)$ appears to be an approximation of Y_n. The Thomas et al code then uses $\dot{Y}(i)[t, Y_n(i)]$ and a new timestep Δt_n to get the value $\tilde{Y}_n(i)$

$$
\tilde{Y}_n(i) = Y_n(i) + \frac{Y_{n\alpha}(i) - Y_{n-1}(i)}{\Delta t_{n-1}}\Delta t_n
$$

an approximation of $Y_{n+1}(i)$ to be used in the matrix of the second Runge-Kutta step.

$$
\begin{aligned}
Y_n(i) &= Q_{ij}\left(\tilde{Y}_n, [ij](\tilde{T}_n), [kl](\tilde{T}_n)\right) \times Y_{n\beta}(j) \\
\frac{dY(i)}{dt}(t+\Delta t_n, Y_{n+1}(i)) &= \frac{Y_{n\beta}(i) - Y_n(i)}{\Delta t_n} \\
Y_{n+1}(i) &= Y_n(i) + \frac{1}{2}\left[\frac{Y_{n\alpha}(i) - Y_{n-1}(i)}{\Delta t_{n-1}} + \frac{Y_{n\beta}(i) - Y_n(i)}{\Delta t_n}\right]\Delta t_n && (4)
\end{aligned}
$$

And this codes used $Y_n(i)$ in its matrix equation. So one could say that $Y_{n\beta}$ was an approximation of $Y_{n+1}(i)$, and this second time derivative corresponded to $\dot{Y}(i)[t + \Delta t_n, Y_{n+1}(i)]$ according to Equation (2). Plugging them into Equation (1) we get Equation (4) for our actual value of $Y_{n+1}(i)$. Note the Δt_n as a factor and the Δt_{n-1} in one of the denominators.

The first R-K step of the Texas code, though, has $Y_n(i)$ on the left-hand side, and Δt_n in the denominator for $\dot{Y}(i)$.:

$$\begin{aligned} Y_n(i) &= Q_{ij}(Y_n, [ij](T_n), [kl](T_n)) \times Y_{n\alpha}(j) \\ \frac{dY(i)}{dt}(t, Y_n) &= \frac{Y_{n\alpha}(i) - Y_n(i)}{\Delta t_n} \end{aligned}$$

That would imply that this code's $Y_{n\alpha}(i)$ is an approximation of $Y_{n+1}(i)$, and that $\dot{Y}(i)(t, Y_n)$ has been determined explicitly instead of implicitly. The second R-K step,

$$\begin{aligned} Y_n(i) &= Q_{ij}(\tilde{Y}_n, [ij](T_{n+1}), [kl](T_{n+1})) \times Y_{n\beta}(j) \\ \frac{dY(i)}{dt}(t + \Delta t_n, \tilde{Y}_n) &= \frac{Y_{n\beta}(i) - Y_n(i)}{\Delta t_n} \end{aligned}$$

implies that $Y_{n\beta}$ is also an approximation of Y_{n+1}, and when the Texas code plugs in our expressions for the $\dot{Y}(i)$'s.:

$$\begin{aligned} Y_{n+1}(i) &= Y_n(i) + \frac{1}{2}\left[\frac{Y_{n\alpha}(i) - Y_n(i)}{\Delta t_n} + \frac{Y_{n\beta}(i) - Y_n(i)}{\Delta t_n}\right]\Delta t_n \\ Y_{n+1}(i) &= \frac{1}{2}(Y_{n\alpha}(i) + Y_{n\beta}(i)) \qquad (5) \end{aligned}$$

the Δt_n factor cancels out the Δt_n's in the denominators. So the final $Y_{n+1}(i)$ is the average of the two first-order Euler approximations $Y_{n\alpha}$ and $Y_{n\beta}$, calculated from solving the matrix equations alone.

So I modified the Texas code to follow the Thomas et al code's more consistent scheme of calculating Y_{min}. The Texas code's $X_{^4He}$ then acquired the second-order convergence it should've had.:

$$X_{^4He} = 0.2394508633 - (0.1509902093 \times 10^{-3})d^2$$

For $d = 1$, $X_{^4He}$ fell from 0.23970 to 0.23929. Still far from the other code's 0.23690. But $X_{^4He}$ in the Texas code converged to the same value as it did with first-order.

3. The value of Y_{min}

$Y(i)$ of the Texas code could go all the way down to 0.0. But the Thomas et al code put a lower limit $Y_{min} = 10^{-25}$. That code used Y_{min} in its equation for Δt_n

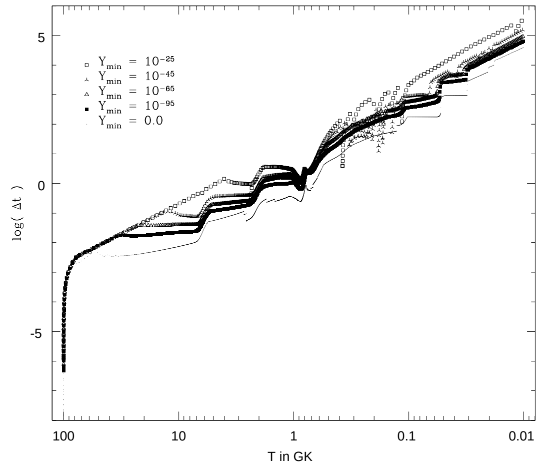

Figure 1a: Timesteps Δt_n of the Thomas et al code for various values of minimum abundance Y_{min}. The number of timesteps greatly increases with decreating Y_{min}. The linear portions of the graphs correspond to when the code uses temperature T to determine Δt_n.

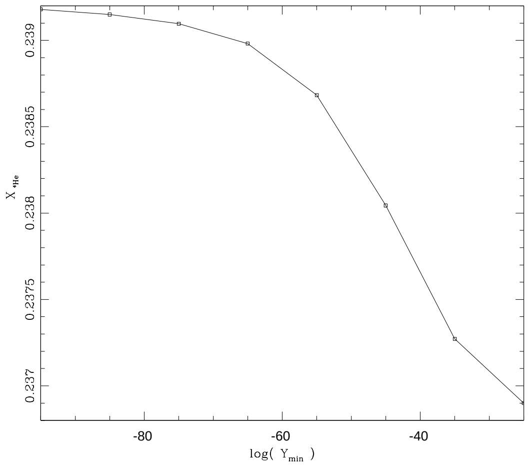

Figure 1b: Mass fraction $X_{^4He}$ of the Thomas et al code as a function of Y_{min}. The total number of timesteps varies from 323 for $Y_{min} = 10^{-25}$ up to 1020 for $Y_{min}=10^{-95}$.

$$
\begin{aligned}
\Delta t_n &= dk \min\left[\frac{Y_n(i)}{\dot{Y}(i)} dk_{fac}, \frac{T_n}{\frac{dT}{dt}}\right] \\
dk_{fac} &= \left(1 + \left(-\frac{\log Y_n(i)}{dt_{fac}}\right)^2\right) \\
dt_{fac} &= -\frac{\log Y_{min}}{\frac{dk_{max}}{dk} - 1}
\end{aligned}
$$

The Thomas et al code compared the ratio of T to $\dot{T}$ to the $Y(i)/\dot{Y}(i)$ ratios to pick the smallest ratio times $dk = 0.1$ as the value of Δt_n, so that the code could evolve stably. But to the $Y(i)/\dot{Y}(i)$ ratio the code also put a factor dk_{fac}, designed to prevent the code from picking a $Y(i)$ whose value was close to Y_{min}. But this factor lead to larger values of Δt_n than in the Texas code, and hence much fewer timesteps. At $\eta_{10} = 3.0$, the

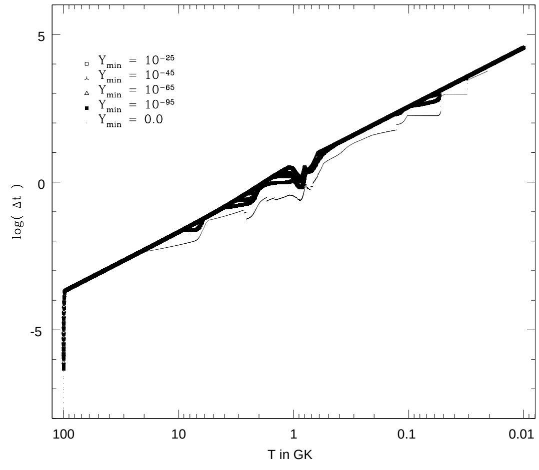

Figure 2a: The Thomas et al code Δt_n now with the temperature ratio T/ $\dot{T}$ lowered by a factor of 0.1. This ratio now determines the value of Δt_n for nearly the entire run, regardless of Y_{min}

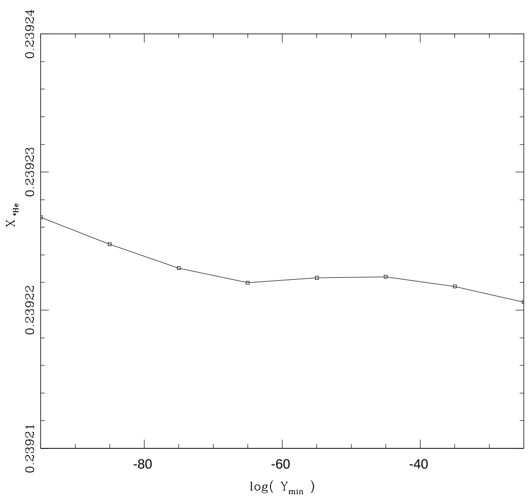

Figure 2b: With this new 0.1 factor, the dependence of $X_{^4He}$ on Y_{min} is greatly reduced in the Thomas et al code. Graphs very similar to Figures (1 – 2) can be made from the Texas code.

Thomas et al code would run in only 323 timesteps, whereas the Texas code needed 2772. Figure (1a) graphs Δt_n for various values of Y_{min}. Varying Y_{min} from 10^{-25} to 10^{-95} would vary the number of timesteps from around 300 to 1000. And $X_{^4He}$ would vary from 0.257 to 0.259, as shown in Figure (1b).

The linear sections in Figure (1a) corresponded to when the code chose $T/\dot{T}$ to determine Δt_n. So I got the idea of putting on $T/\dot{T}$ a second factor 0.1. Figure (2a) shows that this 0.1 factor lowered the $T/\dot{T}$ ratio to the point that the code would choose that ratio nearly all of the time. So in Figure (2a) the number of timesteps varied only from 1000 to 1300. And Figure (2b) shows that the 0.1 factor eliminated the influence of Y_{min} on $X_{^4He}$. So the number of timesteps instead of Y_{min} itself really determined the accuracy of $X_{^4He}$.

The Texas code uses this equation to determine the timestep.

$$\Delta t_{n+1} = dk \min \left[\frac{Y_{n+1}(i)}{\frac{dY(i)}{dt}}, \frac{(lnR)_{n+1}}{\frac{\dot{R}}{R}}, \frac{(\rho_{e+\gamma})_{n+1}}{\dot{\rho}_{e+\gamma}} \right]$$

No dk_{fac} factor. So the code could run with Y_{min} set at zero. I modified the Texas code to have a dk_{fac} for a non-zero Y_{min}. I also wanted to put in a 0.1 factor, but instead of T the Texas code used $\rho_{e+\gamma}$, which depended on T^4 for most of a run. So I put in a 0.4 factor instead. And indeed the Texas code exhibited the same behavior as the Thomas et al code with these new conditions, though $X_{^4He}$ tended to vary more here than in the other code.

I'd still prefer to not have a non-zero Y_{min} at all. But the Texas code's old way of calculating Δt_n would have that large number of steps in that case. So for $Y_{min} = 0.0$ I put in both codes the following dt_{fac} factor.:

$$dk_{fac} = \left(1 + \left(-\frac{\log Y_n(i)}{dt_{fac}} \right)^2 \right)$$

$$dt_{fac} = -\frac{\log 10^{-99}}{\frac{dk_{max}}{dk} - 1}$$

This factor set the number of timesteps at 1320 for both codes. A number on the order of 1000 seemed sufficient to get a value of $X_{^4He}$ that didn't depend very much on the timestep number.

4. Final results

Table (2) shows the final mass fractions for each code with the modifications put in, for the case of $\eta_{10} = 3.0$. The codes now have close agreement with each other, especially for ^{4}He where the mass fractions are within 0.0001 of each other. These results are for $Y_{min} = 0.0$, but I got similar results for $Y_{min} = 10^{-25}$ as well.

As for the thermal quantities, those differences seemed very confusing. But I checked these thermal quantities and determined them to be nearly equal between the codes after I put the changes in. So the number of timesteps and the convergences were the most signficant reasons for disagreement between the codes.

isotope	Thomas et al X	Texas X
d	$0.1214409373 \times 10^{-3}$	$0.1222110665 \times 10^{-3}$
^{3}H	$0.5869118485 \times 10^{-6}$	$0.5905659297 \times 10^{-6}$
^{3}He	$0.3615054989 \times 10^{-4}$	$0.3624197334 \times 10^{-4}$
^{4}He	0.2392346716	0.2393288161
^{7}Li	$0.3424567551 \times 10^{-9}$	$0.3445304655 \times 10^{-9}$
^{7}Be	$0.2810372859 \times 10^{-9}$	$0.277271461 \times 10^{-9}$
^{9}Be	$0.1078010758 \times 10^{-16}$	$0.1091991775 \times 10^{-16}$
^{10}B	$0.9337145278 \times 10^{-18}$	$0.9425546233 \times 10^{-18}$
^{11}B	$0.9855540716 \times 10^{-16}$	$0.9595478082 \times 10^{-16}$
^{12}C	$0.3026820198 \times 10^{-13}$	$0.30138561 \times 10^{-13}$
^{14}C	$0.6519717631 \times 10^{-13}$	$0.6515513573 \times 10^{-13}$
^{14}N	$0.1322155965 \times 10^{-12}$	$0.1320911107 \times 10^{-12}$
^{16}O	$0.7673887093 \times 10^{-17}$	$0.7632076774 \times 10^{-17}$
^{21}Ne	$0.5388613183 \times 10^{-23}$	$0.5374132790 \times 10^{-23}$

Table (2): Mass Fractions for Modified Codes Here, $Y_{min} = 0.0$ and $\eta_{10} = 3.0$. But the codes still agree for the range of 1 to 10 for η_{10} and Y_{min} up to 10^{-25}.

And finally, I took convergence tests of the codes again after all the changes had been added. The Thomas et al code obeyed:

$$X_{^4He} = 0.2392673182 - (0.3253724834 \times 10^{-4})d^2$$

while the Texas code obeyed.

$$X_{^4He} = 0.2394508628 - (0.1203603394 \times 10^{-3})d^2$$

The codes still converged to the same values that they've converged before. So the remaining differences between the codes result in these final values disagreeing by 0.0002.

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