Following Stellar Nucleosynthesis

The calculation of stellar nucleosynthesis requires the simultaneous solution for a set of coupled differential equations, each of which has the form

$$\begin{aligned}\frac{dN_X}{dt} &= -N_a N_X f \lambda_{aX} - \frac{N_X}{\tau_\beta} + N_b N_Y f \lambda_{bY} + \frac{N_Z}{\tau_p} + \ldots \\ &= -\frac{N_X}{\tau_{aX}} - \frac{N_X}{\tau_\beta} + \frac{N_Y}{\tau_{bY}} + \frac{N_Z}{\tau_p} + \ldots \qquad (13.1.1)\end{aligned}$$

To appreciate the problem, let's examine the individual terms.

- Term 1 represents the loss of species X in reactions with particle a; the value τ_{aX} (defined through (12.2.5)) is a function of temperature (through the reaction rate, λ_{aX}) and particle number density a. The former is known through the equations of stellar structure (which have already been solved); an estimate of the latter is also known from the previous model.

- Term 2 gives the loss of N_X due to radioactivity; specifically, beta-decay. The decay constant τ_β is a constant of physics.

- Term 3 behaves like term 1; it computes the creation of X due to nuclear reactions between b and Y. Again, the τ_{bY} depends on temperature and the number density of b.

- Term 4 shows the creation of X by positron decay of species Z; like the second term, τ_p comes from atomic physics.

Like the equations of stellar structure, the nuclear reaction equations constitute a network of first-order, non-linear differential equations. Unlike the stellar structure equations, however, these are not two-point boundary problems. Instead, they are initial value problems, where all the abundances at $t = 0$ are known. Thus, a Henyey-type analysis is not required.

Simplifications for the Solving Nuclear Reaction Network

The entire network of nuclear reaction equations does not always have to be solved numerically. Many reactions quickly come to "equilibrium" and their rates can be expressed analytically. For example, consider a set of reactions where element X reacts with a proton to give element Y, and element Y reacts with another proton to yield element Z. The differential equations for these reactions would be

$$\frac{dN_X}{dt} = -N_p N_X f \lambda_{pX} \tag{13.1.2}$$

$$\frac{dN_Y}{dt} = +N_p N_X f \lambda_{pX} - N_p N_Y f \lambda_{pY} \tag{13.1.3}$$

$$\frac{dN_Z}{dt} = +N_p N_Y f \lambda_{pZ} \tag{13.1.4}$$

These could be solved simultaneously via the Runge-Kutta integration. However, suppose the reaction rate λ_{pY} is extremely high (or, equivalently, the lifetime of element Y against protons is extremely short). Suppose also that the initial abundance of Y was rather high. In this case, the derivative of (13.1.3) would be negative, and the abundance of Y would decrease rapidly. Eventually, the abundance of Y would fall enough so that the second term of (13.1.3) would no longer dominate. Equilibrium would then be reached, with $dN_Y/dt = 0$. When this occurs, (13.1.3) can be re-written to yield

$$N_Y = N_X \left(\frac{\lambda_{pX}}{\lambda_{pY}} \right)$$

Equation (13.1.3) can then be removed from the network, and N_Y replaced by its equilibrium value in the rest of the equations.

Nuclear Reactions in Main Sequence Stars

The temperatures and densities in the core of a star are conducive to nuclear reactions. However, in main sequence stars, the reactions that occur do so at a rather modest rate. The reason is that the two most abundant species in main sequence stars (by far) are $^{1}\mathrm{H}$ and $^{4}\mathrm{He}$, yet collisions between these nuclei rarely result in a reaction. Specifically, the species $^{2}\mathrm{He}$, $^{5}\mathrm{Li}$, and $^{8}\mathrm{Be}$ are all spectacularly unstable. (The most stable of these nuclei is $^{8}\mathrm{Be}$, which has a mean lifetime of 9.7×10^{-17} sec.) Thus

$$^{1}\mathrm{H} + {}^{1}\mathrm{H} \longrightarrow {}^{2}\mathrm{He} \longrightarrow {}^{1}\mathrm{H} + {}^{1}\mathrm{H}$$

$$^{1}\mathrm{H} + {}^{4}\mathrm{He} \longrightarrow {}^{5}\mathrm{Li} \longrightarrow {}^{1}\mathrm{H} + {}^{4}\mathrm{He}$$

$$^{4}\mathrm{He} + {}^{4}\mathrm{He} \longrightarrow {}^{8}\mathrm{Be} \longrightarrow {}^{4}\mathrm{He} + {}^{4}\mathrm{He}$$

Consequently, all nucleosynthesis must occur using species which are relatively rare, or proceed through low-probability events.

When one considers all the possible reactions that can occur, one finds that only a few are important. Most can be ignored, either because their cross section is very small, or because the reactants are extremely rare. For example

$$^{2}\mathrm{H} + {}^{2}\mathrm{H} \longrightarrow {}^{4}\mathrm{He}$$

is a reaction that has a very high cross section, but can be ignored because the abundance of $^{2}\mathrm{H}$ is so low, that the probability of a single $^{2}\mathrm{H}$ encountering another ion of $^{2}\mathrm{H}$, rather than proton is negligible. If we restrict ourselves to the non-negligible reactions, then one is left with three sets of reactions that change hydrogen to helium: the proton-proton chain, the CNO bi- (or tri-)cycles, and the neon-sodium cycle.

The Proton-Proton Chains

The PP chain can be broken down into 3 subchains:

PP-I

$$^{1}\mathrm{H} + {}^{1}\mathrm{H} \longrightarrow {}^{2}\mathrm{H} + \mathrm{e}^{+} + \nu_e \tag{13.2.1}$$

$$^{2}\mathrm{H} + {}^{1}\mathrm{H} \longrightarrow {}^{3}\mathrm{He} + \gamma \tag{13.2.2}$$

$$^{3}\mathrm{He} + {}^{3}\mathrm{He} \longrightarrow {}^{4}\mathrm{He} + {}^{1}\mathrm{H} + {}^{1}\mathrm{H} \tag{13.2.3}$$

PP-II

$$^{3}\mathrm{He} + {}^{4}\mathrm{He} \longrightarrow {}^{7}\mathrm{Be} + \gamma \tag{13.2.4}$$

$$^{7}\mathrm{Be} + \mathrm{e}^{-} \longrightarrow {}^{7}\mathrm{Li} + \nu_e + \gamma \tag{13.2.5}$$

$$^{7}\mathrm{Li} + {}^{1}\mathrm{H} \longrightarrow {}^{4}\mathrm{He} + {}^{4}\mathrm{He} \tag{13.2.6}$$

PP-III

$$^{7}\mathrm{Be} + {}^{1}\mathrm{H} \longrightarrow {}^{8}\mathrm{B} + \gamma \tag{13.2.7}$$

$$^{8}\mathrm{B} \longrightarrow {}^{8}\mathrm{Be} + \mathrm{e}^{+} + \nu_e \tag{13.2.8}$$

$$^{8}\mathrm{Be} \longrightarrow {}^{4}\mathrm{He} + {}^{4}\mathrm{He} \tag{13.2.9}$$

The net result of each chain is to change two protons into two neutrons (and two neutrinos) and bind them up with two other protons in an atomic of ^{4}He. Since each hydrogen atom has an atomic mass excess of 7.28899 MeV, while the mass excess of ^{4}He is 2.42475 MeV, the result of these chains is to liberate 26.73 MeV, or 0.7% of the rest mass of the proton (936.86 MeV). Most of this energy will go directly into the star via kinetic energy, but a few percent will be lost via the neutrinos.

Of the reactions listed above, (13.2.1) is by far the slowest. It involves the weak nuclear force, and an induced positron decay of a proton (the rate of which must be calculation via quantum theory). Although it is fundamentally a different type of reaction from that of the strong force, its reaction rate is usually expressed in a form similar to the other non-resonant, strong-force nuclear reactions, *i.e.,* through a value of $S(E)$ and $\frac{dS}{dE}$.

Reactions involving ^{2}H, Li, Be, and B go extremely quickly, as these nuclei are relatively brittle. Li, for example, can be destroyed by cosmic-ray spallation on the surfaces of stars, and can be burned in the lower envelopes of stars, far outside the core, where most nuclear reactions occur. Moreover, the lifetime of ^{8}B to positron decay is 0.78 seconds, so, for all intents and purposes, equations (13.2.8) and (13.2.9) can be combined into

$$^{7}\mathrm{Be} + {}^{1}\mathrm{H} \longrightarrow {}^{4}\mathrm{He} + {}^{4}\mathrm{He} + \mathrm{e}^{+} + \nu_e + \gamma \tag{13.2.10}$$

COMPUTING PP CHAIN NUCLEOSYNTHESIS

The abundances of the various proton-proton chain elements are described by a set of differential equations.

$$\frac{dN_{^1\mathrm{H}}}{dt} = -2\lambda_{(^1\mathrm{H},^1\mathrm{H})}\left(\frac{N^2_{^1\mathrm{H}}}{2}\right) - \lambda_{(^1\mathrm{H},^2\mathrm{H})}N_{^1\mathrm{H}}N_{^2\mathrm{H}} + 2\lambda_{(^3\mathrm{He},^3\mathrm{He})}\left(\frac{N^2_{^3\mathrm{He}}}{2}\right) - \lambda_{(^1\mathrm{H},^7\mathrm{Be})}N_{^1\mathrm{H}}N_{^7\mathrm{Be}} - \lambda_{(^1\mathrm{H},^7\mathrm{Li})}N_{^1\mathrm{H}}N_{^7\mathrm{Li}} \qquad (13.2.11)$$

$$\frac{dN_{^2\mathrm{H}}}{dt} = +\lambda_{(^1\mathrm{H},^1\mathrm{H})}\left(\frac{N^2_{^1\mathrm{H}}}{2}\right) - \lambda_{(^1\mathrm{H},^2\mathrm{H})}N_{^1\mathrm{H}}N_{^2\mathrm{H}} \qquad (13.2.12)$$

$$\frac{dN_{^3\mathrm{He}}}{dt} = +\lambda_{(^1\mathrm{H},^2\mathrm{H})}N_{^1\mathrm{H}}N_{^2\mathrm{H}} - 2\lambda_{(^3\mathrm{He},^3\mathrm{He})}\left(\frac{N^2_{^3\mathrm{He}}}{2}\right) - \lambda_{(^3\mathrm{He},^4\mathrm{He})}N_{^3\mathrm{He}}N_{^4\mathrm{He}} \qquad (13.2.13)$$

$$\frac{dN_{^4\mathrm{He}}}{dt} = +\lambda_{(^3\mathrm{He},^3\mathrm{He})}\left(\frac{N^2_{^3\mathrm{He}}}{2}\right) - \lambda_{(^3\mathrm{He},^4\mathrm{He})}N_{^3\mathrm{He}}N_{^4\mathrm{He}} + 2\lambda_{(^1\mathrm{H},^7\mathrm{Be})}N_{^1\mathrm{H}}N_{^7\mathrm{Be}} + 2\lambda_{(^1\mathrm{H},^7\mathrm{Li})}N_{^1\mathrm{H}}N_{^7\mathrm{Li}} \qquad (13.2.14)$$

$$\frac{dN_{^7\mathrm{Be}}}{dt} = +\lambda_{(^3\mathrm{He},^4\mathrm{He})}N_{^3\mathrm{He}}N_{^4\mathrm{He}} - \lambda_{(^7\mathrm{Be},\mathrm{e}^-)}N_eN_{^7\mathrm{Be}} - \lambda_{(^1\mathrm{H},^7\mathrm{Be})}N_{^1\mathrm{H}}N_{^7\mathrm{Be}} \qquad (13.2.15)$$

$$\frac{dN_{^7\mathrm{Li}}}{dt} = +\lambda_{(^7\mathrm{Be},\mathrm{e}^-)}N_eN_{^7\mathrm{Be}} - \lambda_{(^1\mathrm{H},^7\mathrm{Li})}N_{^1\mathrm{H}}N_{^7\mathrm{Li}} \qquad (13.2.16)$$

where the reaction rate $r_{i,j} = N_iN_j\lambda_{i,j} = N_i/\tau_j(i)$.

These are non-linear, coupled differential equations, which may be solved numerically with Runge-Kutta integration. However, several simplifications are possible, which take advantage of the fact that some reactions are fast enough to set up equilibrium conditions. Consider the individual reaction rates tabulated below.

PP Chain Reaction Rates

	Q	ϵ_n	S_0	$\frac{dS}{dE}$	τ
Reaction	(MeV)	(MeV)	KeV-barns	barns	(years)
$^1\mathrm{H}(p,\beta^+\nu)^2\mathrm{H}$	1.442	0.263	3.78×10^{-22}	4.2×10^{-24}	7.9×10^{9}
$^2\mathrm{H}(p,\gamma)^3\mathrm{He}$	5.493		2.5×10^{-4}	7.9×10^{-6}	4.4×10^{-8}
$^3\mathrm{He}(^3\mathrm{He},2p)^4\mathrm{He}$	12.859		5.0×10^{3}		2.4×10^{5}
$^3\mathrm{He}(^4\mathrm{He},\gamma)^7\mathrm{Be}$	1.586		4.7×10^{-1}	-2.8×10^{-4}	9.7×10^{5}
$^7\mathrm{Be}(e^-,\nu)^7\mathrm{Li}$	0.861	0.80			3.9×10^{-1}
$^7\mathrm{Li}(p,^4\mathrm{He})^4\mathrm{He}$	17.347		1.2×10^{2}		1.8×10^{-5}
$^7\mathrm{Be}(p,\gamma)^8\mathrm{B}$	0.135		4.0×10^{-2}		6.6×10^{1}
$^8\mathrm{B}(\beta^+,\nu)^8\mathrm{Be}^*(,^4\mathrm{He})^4\mathrm{He}$	18.074	7.2			3×10^{-8}

These numbers are from Clayton, *Principles of Stellar Evolution and Nucleosynthesis,* 1968, so are slightly out of date. The lifetimes, of course, are condition dependent. The values quoted here are appropriate for $\rho = 100$, $T_6 = 15$, and $X = Y = 0.5$.

The first thing to notice is the extremely short lifetime of deuterium. Under these (solar-type) conditions, ^{2}H will last $\sim$ 1 hour. As a result, ^{2}H quickly achieves its equilibrium abundance,

$$N_{^2\mathrm{H}} \longrightarrow \frac{N_{^1\mathrm{H}}\lambda_{(^1\mathrm{H},^1\mathrm{H})}}{2\lambda_{(^1\mathrm{H},^2\mathrm{H})}}$$

and $N_{^2\mathrm{H}}$ can be eliminated from the equations.

Similarly ^{7}Li and ^{7}Be have typical lifetimes against hydrogen of $\sim$ 1 year, so they, too, will attain their equilibrium abundance. If we add (13.2.15) and (13.2.16), then

$$\frac{d(N_{^7\mathrm{Be}} + N_{^7\mathrm{Li}})}{dt} = +\lambda_{(^3\mathrm{He},^4\mathrm{He})} N_{^3\mathrm{He}} N_{^4\mathrm{He}} - \lambda_{(^1\mathrm{H},^7\mathrm{Be})} N_{^1\mathrm{H}} N_{^7\mathrm{Be}} - \lambda_{(^1\mathrm{H},^7\mathrm{Li})} N_{^1\mathrm{H}} N_{^7\mathrm{Li}} \approx 0$$

so, while ^{2}H tracks the abundance of ^{1}H, ^{7}Be and ^{7}Li will follow the build up of He. If we then substitute this result into (13.2.14), we are then left with only three coupled equations

$$\frac{dN_{^1\mathrm{H}}}{dt} = -\frac{3}{2}\lambda_{(^1\mathrm{H},^1\mathrm{H})} N^2_{^1\mathrm{H}} + \lambda_{(^3\mathrm{He},^3\mathrm{He})} N^2_{^3\mathrm{He}} - \lambda_{(^3\mathrm{He},^4\mathrm{He})} N_{^3\mathrm{He}} N_{^4\mathrm{He}} \tag{13.2.17}$$

$$\frac{dN_{^3\mathrm{He}}}{dt} = +\frac{1}{2}\lambda_{(^1\mathrm{H},^1\mathrm{H})} N^2_{^1\mathrm{H}} - \lambda_{(^3\mathrm{He},^3\mathrm{He})} N^2_{^3\mathrm{He}} - \lambda_{(^3\mathrm{He},^4\mathrm{He})} N_{^3\mathrm{He}} N_{^4\mathrm{He}} \tag{13.2.18}$$

$$\frac{dN_{^4\mathrm{He}}}{dt} = +\frac{1}{2}\lambda_{(^3\mathrm{He},^3\mathrm{He})} N^2_{^3\mathrm{He}} + \lambda_{(^3\mathrm{He},^4\mathrm{He})} N_{^3\mathrm{He}} N_{^4\mathrm{He}} \tag{13.2.19}$$

Note that although these equations are more compact, they still are non-linear, and must be solved numerically.

Finally, depending on the star, ^{3}He may achieve equilibrium. (The time it takes to do this depends sensitively on the precise reaction rates. At temperatures $T_6 < 8$ K, equilibrium will take $> 10^9$ years, so equilibrium is usually not a good assumption in low mass stars. In more massive, stars, however, the time for equilibrium can be as short as $\sim 10^5$ years for burning temperatures of $T_6 \sim 20$ K.) If this equilibrium is achieved, then setting (13.2.18) to zero results in a simple quadratic equation in $N_{^3\mathrm{He}}$, which has the solution

$$N_{^3\mathrm{He}} = \frac{\sqrt{\lambda^2_{(^3\mathrm{He},^4\mathrm{He})} N^2_{^4\mathrm{He}} + 2\lambda_{(^3\mathrm{He},^3\mathrm{He})}\lambda_{(^1\mathrm{H},^1\mathrm{H})} N^2_{^1\mathrm{H}}} - \lambda_{(^3\mathrm{He},^4\mathrm{He})} N_{^4\mathrm{He}}}{2\lambda_{(^3\mathrm{He},^3\mathrm{He})}}$$

If you then plug this into (13.2.17) and (13.2.19), you get

$$\frac{dN_{^1\mathrm{H}}}{dt} = -\lambda_{(^1\mathrm{H},^1\mathrm{H})} N^2_{^1\mathrm{H}} - 2\lambda_{(^3\mathrm{He},^4\mathrm{He})} N_{^3\mathrm{He}} N_{^4\mathrm{He}}$$

$$\frac{dN_{^4\mathrm{He}}}{dt} = \frac{1}{4}\lambda_{(^1\mathrm{H},^1\mathrm{H})} N^2_{^1\mathrm{H}} - \frac{1}{2}\lambda_{(^3\mathrm{He},^4\mathrm{He})} N_{^3\mathrm{He}} N_{^4\mathrm{He}}$$

or

$$\frac{dN_{^4\mathrm{He}}}{dt} = -\frac{1}{4}\frac{dN_{^1\mathrm{H}}}{dt}$$

Thus, the equations are consistent.

Energy Production in the PP Chain

Although it is possible to simplify the PP-I, PP-II, and PP-III into just three (or one) equation, it is important to keep track of just how many reactions are occurring in each chain. Each chain helps turn hydrogen to helium and produces a neutrino in the process, but the energy carried away by the neutrino is different between the 3 chains. The neutrino produced in the PP-I chain (13.2.1) carries away 0.263 MeV. Thus, if ^{4}He is synthesized entirely through PP1, then 2% ($2 \times 0.263/26.73$), of the energy is lost from the system. Alternatively, if ^{3}He is fused into ^{4}He via PP-II, then a 0.80 MeV neutrino is produced, and $0.263 + 0.80/26.73 \Longrightarrow 4\%$ of the energy is lost. Finally, if ^{3}He is fused via PP-III, then a highly energetic 7.2 MeV neutrino is created. (This is the neutrino detected in ^{37}Cl experiments.) With the PP-III chain, 27.9% of the energy is lost from the system. Thus, the rate of usable energy generation is

$$\rho\epsilon_n = \frac{dN_{^4\mathrm{He}}}{dt} = (4m_p - m_{^4\mathrm{He}})c^2 \times$$
$$(0.980F_{\mathrm{PP-I}} + 0.960F_{\mathrm{PP-II}} + 0.721F_{\mathrm{PP-III}})$$

where F, the fraction of ^{4}He produced via the 3 chains, is computed via the reaction rate ratios, *i.e.*,

$$F_{\mathrm{PPI}} = \frac{r_{(^3\mathrm{He},^3\mathrm{He})}}{r_{(^3\mathrm{He},^3\mathrm{He})} + r_{(^3\mathrm{He},^4\mathrm{He})}} = \frac{N_{^3\mathrm{He}}\lambda_{(^3\mathrm{He},^3\mathrm{He})}}{N_{^3\mathrm{He}}\lambda_{(^3\mathrm{He},^3\mathrm{He})} + 2N_{^4\mathrm{He}}\lambda_{(^3\mathrm{He},^4\mathrm{He})}}$$

$$F_{\mathrm{PPII}} = (1 - F_{\mathrm{PPI}})\frac{r_{(^7\mathrm{Be},\mathrm{e}^-)}}{r_{(^7\mathrm{Be},\mathrm{e}^-)} + r_{(^7\mathrm{Be},^1\mathrm{H})}} = \frac{(1 - F_{\mathrm{PPI}})N_e\lambda_{(^7\mathrm{Be},\mathrm{e}^-)}}{N_e\lambda_{(^7\mathrm{Be},\mathrm{e}^-)} + N_{^1\mathrm{H}}\lambda_{(^7\mathrm{Be},^1\mathrm{H})}}$$

$$F_{\mathrm{PPIII}} = 1 - F_{\mathrm{PPI}} - F_{\mathrm{PPII}}$$

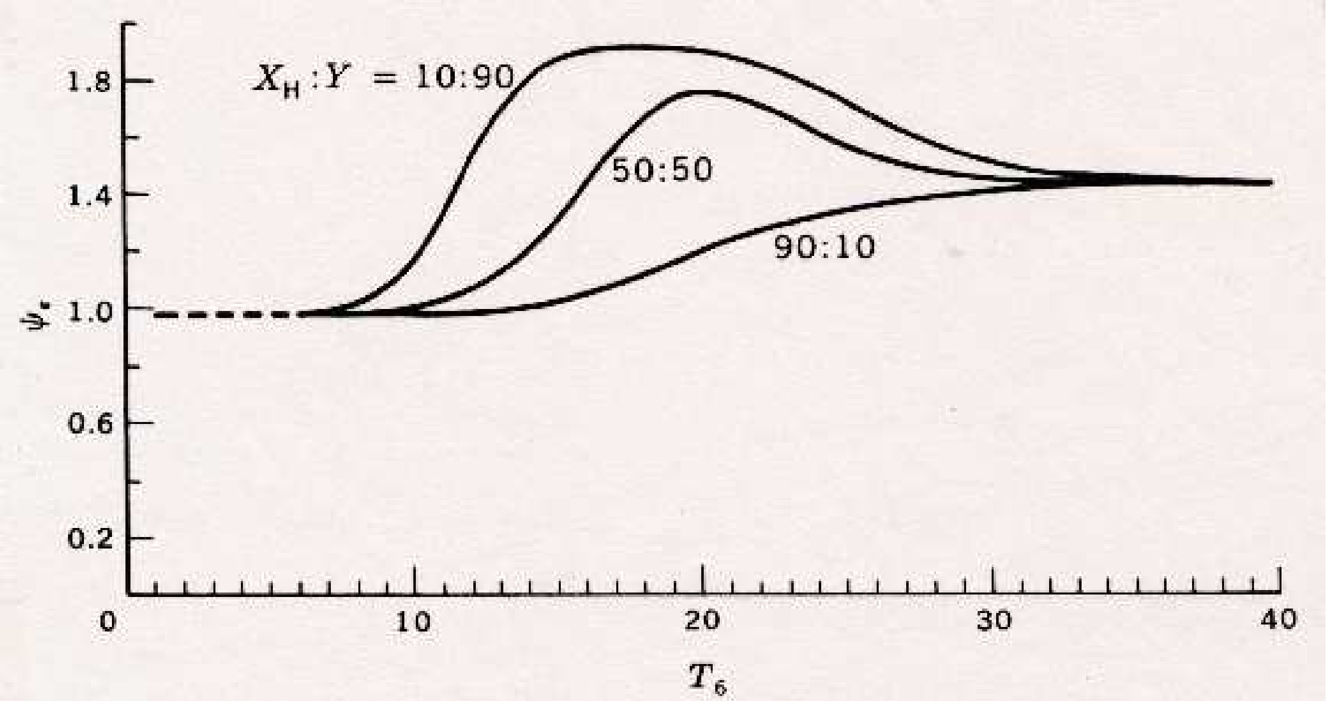
In equilibrium, the energy generation rate of the proton-proton chain is approximately

$$\epsilon_{\rm pp} = 2.38 \times 10^6 \, \psi \, f_{\rm pp} \, g_{\rm pp} \, \rho \, X^2 T_6^{-2/3} \, e^{-33.80/T_6^{1/3}} \, {\rm ergs \; s^{-1} \; cm^{-3}}$$

where $f_{\rm pp}$ is the electron shielding factor for hydrogen, ψ is the correction for PPII and PPIII reactions, and

$$g_{\rm pp} = 1 + 0.0123 \, T_6^{1/3} + 0.0109 \, T_6^{2/3} + 0.0009 \, T_6$$

The proton-proton chain has the least sensitivity to temperature of any fusion reaction. At temperatures of $T_6 \sim 5$, $\nu = d \ln \langle \sigma v \rangle / d \ln T \sim 6$, while at $T_6 \sim 20$, $\nu \sim 3.5$.



Correction for neutrino energy losses due PP II and PP III chain for 3 different compositions.

Solving Initial Value Problems

A "standard" way to solve a set of differential equations with known initial values is through fourth-order Runge-Kutta integration. To appreciate the method, let us solve the simple differential equation

$$\frac{dy}{dx} = f(x,y) = x + y, \qquad\qquad y(0) = 1 \tag{A1.1}$$

using a Taylor expansion. If we expand $y(x)$ about $x_0 = 0$, the expression for the function becomes

$$y(x) = y(x_0) + y'(x_0)\Delta x + \frac{y''(x_0)}{2!}\Delta x^2 + \frac{y'''(x_0)}{3!}\Delta x^3 + \ldots \tag{A1.2}$$

where $\Delta x = (x - x_0)$. From the boundary condition, we know that $y(x_0) = 1$, hence from (A1.1),

$$y'(x_0) = f(x_0, y_0) = x_0 + y(x_0) = 0 + 1 = 1 \tag{A1.3}$$

Next, we take the derivative of both sides of (A1.1), to get

$$\frac{d^2y}{dx^2} = \frac{dx}{dx} + \frac{dy}{dx} \quad\Longrightarrow\quad y'' = 1 + y' \tag{A1.4}$$

From (A1.3) we know that $y'(x_0) = 1$, hence (A1.4) gives us

$$y''(x_0) = 1 + 1 = 2 \tag{A1.5}$$

Similarly, if we take the next derivative of the function,

$$y''' = 0 + y''$$

and evaluate it at $x = x_0$ using (A1.5), we get $y'''(x_0) = 2$. This process can be extended as far out as needed. In the present case, the evaluation of $y(x)$ yields

$$y(x) = 1 + \Delta x + (\Delta x)^2 + \frac{1}{3}(\Delta x)^3 + \mathcal{O}^4 \tag{A1.6}$$

where $\mathcal{O} \sim \Delta x$ is the error term.

Note here, that had we stopped the expansion after the first term (*i.e.*, keeping the relation linear), the expression for $y(x)$ would have been

$$y(x) = y(x_0) + y'(x_0)\Delta x = y(x_0) + f(x_0, y_0)\Delta x + \mathcal{O}^2 \qquad (A1.7)$$

This is just simple forward-differencing solution (or Euler's method). Obviously, from (A1.7), we can expect the errors associated with the technique to be $\sim (\Delta x)^2$ *per step.* If the entire interval is divided into $1/\Delta x$ steps, then we expect the total error in the numerical integration to be $\sim \Delta x$.

It is easy to see why Euler's method is not very accurate — the slope used to determine the new value of y always comes from the beginning of the interval, and thus is always wrong. A better estimate would come from using the slope of the function at the middle of the interval, *i.e.*,

$$y(x) = y(x_0) + \frac{y'(x_0) + y'(x)}{2}\Delta x \qquad (A1.8)$$

Of course this function cannot be evaluated, since we cannot evaluate $y'(x)$ without knowing $y(x)$. However, we can *estimate* $y(x)$ from Euler's method, and then use the predicted value of $y'(x)$ to produce a "corrected" value of $y(x)$. In other words

$$y'(x_0) = f(x_0, y_0)$$

$$y_{\rm est}(x) = y(x_0) + y'(x_0)\Delta x$$

$$y'_{\rm est}(x) = f(x, y_{\rm est})$$

$$y(x) = y(x_0) + \frac{y'(x_0) + y'_{\rm est}(x)}{2}\Delta x \qquad (A1.9)$$

(This procedure can be repeated again if necessary, although after a while, it's better just to cut down the step size.) The accuracy of this modified Euler technique is $\sim (\Delta x)^3$. To see this, simply compare (A1.8) with the Taylor series expansion (A1.2), while substituting a forward-differencing expression for $y''(x_0)$, *i.e.*,

$$\begin{aligned} y(x) &= y(x_0) + y'(x_0)\Delta x + \frac{1}{2}\left(\frac{y'(x) - y'(x_0)}{\Delta x}\right)\Delta x^2 + \mathcal{O}^3 \\ &= y(x_0) + y'(x_0)\Delta x + \frac{y'(x)}{2}\Delta x - \frac{y'(x_0)}{2}\Delta x + \mathcal{O}^3 \\ &= y(x_0) + \frac{y'(x) + y'(x_0)}{2}\Delta x + \mathcal{O}^3 \qquad (A1.10) \end{aligned}$$

As above this error is per step; the total error of the integration is Δx^2.

The next improvement comes by combining the results of several estimates along the interval and weighting each one differently. For instance, suppose we generalize (A1.8) to

$$\begin{aligned} &y(x) = y(x_0) + ak_1 + bk_2 \qquad \text{where} \\ &k_1 = y'(x_0, y_0)\Delta x \qquad k_2 = y'(x_0 + \alpha\Delta x, y_0 + \beta k_1)\Delta x \qquad (A1.11) \end{aligned}$$

where a and b are the weights of the two estimates, α describes where on the interval the estimates are made, and β is a correction factor for the estimate made using k_1. When written out fully with the substitution $f(x, y) = y'$, (A1.11) becomes

$$y(x) = y(x_0) + af(x_0, y_0)\Delta x + bf(x_0 + \alpha\Delta x, y_0 + \beta f(x_0, y_0)\Delta x)\Delta x$$

If we expand the last term as a two-dimensional Taylor series about x_0, y_0, then

$$\begin{aligned} y(x) &= y(x_0) + af(x_0, y_0)\Delta x + b\Big\{f(x_0, y_0) + \\ &\qquad \frac{\partial f(x_0, y_0)}{\partial x}\alpha\Delta x + \frac{\partial f(x_0, y_0)}{\partial y}\beta f(x_0, y_0)\Delta x\Big\}\Delta x \\ &= y(x_0) + (a+b)f(x_0, y_0)\Delta x + \alpha b\frac{\partial f(x_0, y_0)}{\partial x}\Delta x^2 + \\ &\qquad \beta b\frac{\partial f(x_0, y_0)}{\partial y}f(x_0, y_0)\Delta x^2 \end{aligned} \tag{A1.12}$$

This expression can then be compared to the Taylor expansion for $y(x)$ given in (A1.2)

$$\begin{aligned} y(x) &= y(x_0) + f(x_0, y_0)\Delta x + \frac{1}{2}f'(x_0, y_0)\Delta x^2 \\ &= y(x_0) + f(x_0, y_0)\Delta x + \frac{\Delta x^2}{2}\left\{\frac{\partial f(x_0, y_0)}{\partial x} + \frac{\partial f(x_0, y_0)}{\partial y}\frac{dy}{dx}\right\} \\ &= y(x_0) + f(x_0, y_0)\Delta x + \frac{\Delta x^2}{2}\left\{\frac{\partial f(x_0, y_0)}{\partial x} + \frac{\partial f(x_0, y_0)}{\partial y}f(x_0, y_0)\right\} \end{aligned} \tag{A1.13}$$

Thus, $a + b = 1$, $\alpha\, b = 1/2$, and $\beta\, b = 1/2$. These are the coefficients for the second-order Runge-Kutta method; note that since there are three equations and four unknowns, more than one set of coefficients will work.

The fourth-order Runge-Kutta method works the same way, except that four intermediate estimates are made. The equations for this method are

$$
\begin{aligned}
y(x) &= y(x_0) + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} \qquad \text{where} \\
k_1 &= y'(x_0, y_0)\Delta x \\
k_2 &= y'(x_0 + \frac{\Delta x}{2}, y_0 + \frac{k_1}{2})\Delta x \\
k_3 &= y'(x_0 + \frac{\Delta x}{2}, y_0 + \frac{k_2}{2})\Delta x \\
k_4 &= y'(x_0 + \Delta x, y_0 + k_3)\Delta x \qquad (A1.14)
\end{aligned}
$$

In general, the method gives results with accuracies of the order of $(\Delta x)^5$ per step, and $(\Delta x)^4$ over the entire integration range. Because of its accuracy, and relatively few computational steps, it is perhaps the most widely used technique for solving initial-value differential equations.

A final improvement, given by Press in *Numerical Recipes,* is to use fourth-order Runge-Kutta with an adaptive step size. In this scheme, each integration is performed twice, with two different step sizes. For example, if you compute $y(x)$ first using a stepsize of Δx_1 and then using a stepsize of $\Delta x_1/2$, the difference in the results, ϵ_1, should be a measure of the local accuracy. Moreover, since the local error term on fourth-order Runge-Kutta integration goes as $(\Delta x)^5$,

$$\frac{\Delta x_0}{\Delta x_1} = \left(\frac{\epsilon_0}{\epsilon_1}\right)^{1/5}$$

where ϵ_0 is some *desired* accuracy, and Δx_0 is the stepsize that will yield that accuracy. Thus, to gain additional accuracy from a Runge-Kutta method, you can compare your estimate of the local accuracy with some desired accuracy. If it is too large, you can try again with a smaller stepsize; if it is too small, you can speed things up by increasing Δx for the next step of the integration.