Nuclear Statistical Equilibrium:

Equilibrium of strong nuclear reactions due to photodisintegration i.e. reverse rates balancing forward rates.

For $T \lesssim 10^6\,K$: No reaction.

For $T \gtrsim 5\times 10^9\,K$: NSE

Governing Equations:

$$X_i = \frac{m_i}{\rho}\underbrace{(2J_i+1)}_{\text{total spin}}\underbrace{G(T)}_{\text{temperature-dependent nuclear partition function}}\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2}\exp\left\{\frac{\overbrace{Z_i\mu_p+N_i\mu_n}^{\text{chemical potential of free nucleon}}+\overbrace{B_i}^{\text{Binding Energy}}-\overbrace{\mu_i^C}^{\text{Coulomb contribution}}}{k_BT}\right\}$$

Note that the chemical potential of free nucleon

$$\mu_i = Z_i\mu_p + N_i\mu_n = Z_i(\mu_p^{kin}+\mu_p^C) + N_i(\mu_n^{kin})$$

Now the coulomb contribution term: μ_i^C, comes from plasma screening (electron)

An example comes from Chabrier & Potekhin (1998)

$$\frac{\mu_i^C}{k_BT} = A_1\left[\sqrt{\Gamma_i(A_2+\Gamma_i)} - A_2\ln\left(\sqrt{\frac{\Gamma_i}{A_2}}+\sqrt{1+\frac{\Gamma_i}{A_2}}\right)\right] + 2A_3\left(\sqrt{\Gamma_i}-\arctan\sqrt{\Gamma_i}\right)$$

where ion-specific Coulomb Coupling Parameter: $\Gamma_i = Z_i^{5/3}\Gamma_e$

with $\Gamma_e = \dfrac{e^2\left(\frac{4\pi}{3}n_e\right)^{1/3}}{k_BT}$, $A_1 = -0.9052$, $A_2 = 0.6322$, $A_3 = -\sqrt{3}/2 - \dfrac{A_1}{\sqrt{A_2}}$

Note note that electron screening: i.e. free-electrons surrounding ions reduces effective charge, thus lowering Coulomb barrier to fusion.

Consider reaction:

$$C_1 + C_2 + C_3 + \cdots \rightarrow B_1 + B_2 + B_3 \cdots$$

Then the reaction rate is enhanced by: $R_{scr} = R_{unscr} f$

$$f = \exp\left\{ \frac{u^C(Z_{c_1}) + \cdots + u^C(Z_{c_r}) - u^C(Z_{c_1} + \cdots Z_{c_r})}{k_B T} \right\}$$

Now note that Dewitt (1973) imposes the linear mixing rule for classical screening enhancement factor.

Consider reaction $R_1 + R_2 + R_3 \rightarrow P_1 + P_2 + \cdots$

we can consider an intermediate composite nuclei formed,

$$R_1 + R_2 + R_3 \longrightarrow O_{R_1+R_2} + R_3 \rightarrow P_1 + P_2 + \cdots$$

then the screening factor

$$f_{Z_1, Z_2, Z_3} = f_{Z_1, Z_2} f_{Z_1+Z_2, Z_3}$$

$$= \exp\left\{ \frac{u^C(Z_1) + u^C(Z_2) - u^C(Z_1+Z_2)}{k_B T} \right\} \exp\left\{ \frac{u^C(Z_1+Z_2) + u^C(Z_3) - u^C(Z_1+Z_2+Z_3)}{k_B T} \right\}$$

$$\stackrel{!}{=} \exp\left\{ \frac{u^C(Z_1) + u^C(Z_2) + u^C(Z_3) - u^C(Z_1+Z_2+Z_3)}{k_B T} \right\}$$

Note that free energy, $F = \frac{\mu^C}{k_B T}$, which is the expression given before

Now with μ_i^C calculated, the only two unknowns are μ_p and μ_n

It can be solved via root-finding algorithm with 2 constraints with input (ρ, T, Y_e)

$$\begin{cases} 1)\ \text{Conservation of Mass}: \sum_i X_i^{NSE} - 1 = \sum_i A_i Y_i^{NSE} - 1 = 0 = f_A \\ 2)\ \text{Conservation of charge}: \sum_i \frac{X_i^{NSE} Z_i}{A_i} - Y_e = \sum_i Z_i Y_i^{NSE} - Y_e = 0 = f_Z \end{cases}$$

Note that Y_e remains the same if no weak rates are present, if there are weak rates, one needs to predict $\dot{Y}_e$.

Also note since $n_e = \frac{\rho}{m_u} \sum_i \frac{X_i Z_i}{A_i}$, but μ_i^C depends on n_e, so just use the constraint that $\sum_i \frac{X_i Z_i}{A_i} = Y_e$ so that μ_i^C is a constant.

Now this system can be solved via root-finding algorithm. For NR method, we need to find the Jacobian of constraint eq.

$$J_{NSE} = \begin{bmatrix} \partial f_A / \partial \mu_p & \partial f_A / \partial \mu_n \\ \partial f_Z / \partial \mu_p & \partial f_Z / \partial \mu_n \end{bmatrix}$$

$$= \begin{bmatrix} \sum_i \frac{Z_i}{k_B T} X_i & \sum_i \frac{N_i}{k_B T} X_i \\ \sum_i \frac{Z_i}{A_i} \frac{Z_i}{k_B T} X_i & \sum_i \frac{Z_i}{A_i} \frac{N_i}{k_B T} X_i \end{bmatrix}$$

Newton-Raphson Method:

Consider we have M-constraint eqs with N-variables:

$$\vec{f}(\vec{x}) = \begin{bmatrix} f_1(x_1, x_2, \cdots, x_N) \\ \vdots \\ f_M(x_1, x_2, \cdots, x_N) \end{bmatrix} = 0$$

Now consider Taylor expanding $\vec{f}(\vec{x})$ about the point $\vec{x}_0$, which represents the initial guess of the parameter.

$$(m = 1, \cdots M) \quad 0 = f_m(\vec{x}) = f_m(\vec{x}_0) + \sum_{n=1}^{N} \frac{\partial f_m(x_0)}{\partial x_n}(x_n - x_{0,n}) + \mathcal{O}((\vec{x} - \vec{x}_0)^2)$$

$$\hookrightarrow \sim \vec{f}(\vec{x}_0) + \vec{J}(\vec{x}_0)(\vec{x} - \vec{x}_0) = 0$$

Case 1: $\underline{M = N}$, then $\vec{J}$ is a square matrix, then the inverse of the Jacobian is possible.

$$f(\vec{x}_n) + \vec{J}(\vec{x}_n)(\vec{x}_{n+1} - \vec{x}_n) = 0$$

$$\hookrightarrow \boxed{\vec{x}_{n+1} = \vec{x}_n \underbrace{- J^{-1}(\vec{x}_n) f(\vec{x}_n)}_{= +\Delta x}}$$

Case 2: $\underline{M > N}$, over-constrained system. No-exact solution but we can find an optimal solution that that it minimizes the error:

$$\epsilon = \frac{1}{2} || f(x) ||^2$$

But let's not worry about this case.

Derivations of NSE formula: (following pynucastro references):

First describe the EoS to start with:

Ideal Boltzmann Gas Approximation:

Assume non-degenerate, non-interacting, and non-relativistic regime for nuclei:

Consider grand canonical partition function (μ, V, T) for subsystems with N-identical particles, N goes from 0 to ∞, i.e. consider all N possibilities.

$$\mathcal{Z} = \sum_N z^N Z_N$$

grand canonical partition function

fugacity, $z = e^{\beta\mu}$

partition function, $Z_N = \frac{Z_1^N}{N!}$

assumed particles are classically indistinguishable.

where Z_1 is the partition function for only 1-particle.

Now

$$Z_1 = \sum_i d^3p \underbrace{d^3q}_{d^3q = V} e^{-\beta\varepsilon(i, p_i, q_i)}$$

internal degrees of freedom

For a spherically symmetric potential bounded particle, energy is given:

$$\varepsilon(i, p_i, q_i) = \frac{p^2}{2m} + \Delta_i + mc^2 + \mu^C$$

kinetic energy

discrete energy level i.e. energy of i-th level above ground state

rest mass

coulomb screening term

we can write $p^2/2m = \frac{\hbar^2 k^2}{2m}$, $p = \hbar k$ for plane wave

$g(k)dk = \frac{4\pi^2 k^2 dk}{(2\pi/L)^3}$

then

$$Z_1 = \sum_{l} (2J_l + 1) e^{-\beta\Delta_l} \int_0^\infty e^{-\beta\left(\frac{\hbar^2 k^2}{2m} + mc^2 + u^c\right)} g(k)dk$$

$2J_l + 1$: degeneracy due to $m_J = J, J-1 \cdots -J$

$$= \sum_{l} (2J_l + 1) e^{-\beta\Delta_l} \int_0^\infty e^{-\beta\left(\frac{\hbar^2 k^2}{2m} + mc^2 + u^c\right)} V \frac{k^2}{2\pi^2} dk$$

$$Z_1 \stackrel{!}{=} \sum_{l} (2J_l + 1) e^{-\beta\Delta_l} V \left(\frac{m k_B T}{2\pi\hbar^2}\right)^{3/2} e^{-\beta(mc^2 + u^c)}$$

Alternatively:

$$Z_1 = \sum_{l} (2J_l + 1) e^{-\beta\Delta_l} \frac{1}{h^3} \int d^3p \underbrace{d^3q}_{V} e^{-\beta\left(\frac{p^2}{2m} + mc^2 + u^c\right)}$$

$$\stackrel{!}{=} \sum_{l} (2J_l + 1) e^{-\beta\Delta_l} \frac{1}{(2\pi\hbar)^3} V \int_0^\infty 4\pi p^2 dp\, e^{-\beta\left(\frac{p^2}{2m} + mc^2 + u^c\right)}$$

$$\stackrel{!}{=} \sum_{l} (2J_l + 1) e^{-\beta\Delta_l} \frac{V}{2\pi^2\hbar^3} \sqrt{\frac{\pi}{2}} (m k_B T)^{3/2} e^{-\beta(mc^2 + u^c)}$$

$$Z_1 \stackrel{!}{=} \sum_{l} (2J_l + 1) e^{-\beta\Delta_l} V \left(\frac{m k_B T}{2\pi\hbar^2}\right)^{3/2} e^{-\beta(mc^2 + u^c)}$$

consider all configuration for N, i.e. $N = 0, 1, 2 \cdots, \infty$

$$\mathcal{Z} = \sum_{N=0}^{\infty} (e^{\beta\mu})^N \frac{Z_1^N}{N!}$$

$$\mathcal{Z} = \sum_{N=0}^{\infty} \frac{1}{N!} \left\{ \sum_l (2J_l + 1) e^{-\beta\Delta_l} V \left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2} e^{\beta(\mu - mc^2 - \mu^c)} \right\}^N$$

note $\quad e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$

Then the grand potential $\Phi_G = -k_BT \log \mathcal{Z}$

$$\Rightarrow \Phi_G = -k_BT \sum_l (2J_l + 1) e^{-\beta\Delta_l} V \left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2} e^{\beta(\mu - mc^2 - \mu^c)}$$

temperature-dependent partition function

Now with definition: $\boxed{(2J_0 + 1) G(T) = \sum_l (2J_l + 1) e^{-\beta\Delta_l}}$

ground-spin

Hence :

$$\boxed{\Phi_G = -k_BT (2J_0 + 1) G(T) V \left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2} e^{\beta(\mu - mc^2 - \mu^c)}}$$

And $\quad N = -\left(\frac{\partial \Phi_G}{\partial \mu}\right)_{T,V}$

$$\boxed{N = V (2J_0 + 1) G(T) \left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2} e^{\beta(\mu - mc^2 - \mu^c)}}$$

with $\quad n = N/V$

$$\boxed{\mu = \underbrace{k_BT \log\left[\frac{n}{(2J_0+1)G(T)} \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{3/2}\right]}_{\mu^{kin}\,:\ \text{kinetic term}} + mc^2 + \mu^c}$$

Now NSE condition is a statement of chemical equilibrium, i.e. the chemical potential needed to assemble the i-th nuclei is equal to the energy required for free nucleon via detailed balance.

i.e. $$\boxed{\mu_i = Z_i \mu_p + N_i \mu_n}$$

Now with: $\mu_i = \mu_i^{kin} + m_i c^2 + \mu_i^C$

$$\hookrightarrow \mu_i^{kin} + m_i c^2 + \mu_i^C = Z_i\left(\mu_p^{kin} + m_p c^2 + \mu_p^C\right) + N_i\left(\mu_n^{kin} + m_n c^2 + \cancelto{0}{\mu_n^C}\right)$$

since $B_i = (Z_i m_p + N_i m_n - m_i)c^2$ ← definition of binding energy

$$\hookrightarrow \boxed{\mu_i^{kin} = Z_i\left(\mu_p^{kin} + \mu_p^C\right) + N_i \mu_n^{kin} + B_i - \mu_i^C}$$

Now with definition of mass fraction: $X_i = \rho_i/\rho = \frac{m_i n_i}{\rho}$

$$X_i = \frac{m_i}{\rho}(2J_{0,i}+1)G_i(T)\left(\frac{m_i k_B T}{2\pi\hbar^2}\right)^{3/2} e^{\beta(\mu_i - m_i c^2 - \mu_i^C)}$$

with $\mu_i = \mu_i^{kin} + m_i c^2 + \mu_i^C$

$$\hookrightarrow \boxed{X_i = \frac{m_i}{\rho}(2J_i+1)G_i(T)\left(\frac{m_i k_B T}{2\pi\hbar^2}\right)^{3/2} \exp\left\{\frac{Z_i(\mu_p^{kin}+\mu_p^C) + N_i \mu_n^{kin} + B_i - \mu_i^C}{k_B T}\right\}}$$

or $Y_i = \frac{X_i}{A_i}$ and $m_i = A_{nuc}\, m_u = A_{nuc}/N_a$

$$\boxed{Y_i = \frac{1}{N_a \rho}\frac{(A_{nuc,i})^{5/2}}{A_i}(2J_i+1)G(T)\left(\frac{m_u k_B T}{2\pi\hbar^2}\right)^{3/2} \exp\left\{\frac{Z_i(\mu_p^{kin}+\mu_p^C) + N_i \mu_n^{kin} + B_i - \mu_i^C}{k_B T}\right\}}$$

Reverse Rates and Detailed Balance: following Pynucastro appendix and skynet paper.

Consider a nuclear reaction between a set of reactants $\{\tilde{R}_r\}$ and a set of products $\{\tilde{P}_j\}$ in equilibrium:

$$\sum_{\alpha \in \tilde{R}_r} [\alpha] \rightleftharpoons \sum_{\beta \in \tilde{P}_p} [\beta]$$

here r and p represent number of reactants and products.

It's important to stress $\{\tilde{R}_r\}$ and $\{\tilde{P}_p\}$ represent all nuclei, i.e. ${}^{12}C + {}^{12}C \rightleftharpoons {}^{20}Ne + {}^{4}He$, then $\tilde{R}_r = \{{}^{12}C, {}^{12}C\}$

Side Note:

For a two body reaction rate: $N_A A + N_B B \rightarrow N_C C + N_D D$

we have:
$$\frac{1}{N_A}\frac{d}{dt} n_A = \frac{1}{N_B}\frac{d}{dt} n_B = - n_A^{N_A} n_B^{N_B} \frac{\langle \sigma v \rangle}{N_A!\, N_B!}$$

$$\frac{1}{N_C}\frac{d}{dt} n_C = \frac{1}{N_D}\frac{d}{dt} n_D = + n_A^{N_A} n_B^{N_B} \frac{\langle \sigma v \rangle}{N_A!\, N_B!}$$

Here we assume $Y_i = \frac{n_i}{N_a \rho}$

or in molar fractions: $Y_i = \frac{m_u n_i}{\rho}\frac{A_{nuc;i}}{A_i} = \frac{n_i}{N_A \rho}\frac{A_{nuc;i}}{A_i}$

i.e.
$$\begin{cases} \frac{1}{N_A}\frac{d}{dt} Y_A = \frac{1}{N_B}\frac{d}{dt} Y_B = - \rho^{\nu} Y_A^{N_A} Y_B^{N_B} \frac{N_a \langle \sigma v \rangle}{N_A!\, N_B!} \\ \frac{1}{N_C}\frac{d}{dt} Y_C = \frac{1}{N_D}\frac{d}{dt} Y_D = \rho^{\nu} Y_A^{N_A} Y_B^{N_B} \frac{N_a \langle \sigma v \rangle}{N_A!\, N_B!} \end{cases}$$

$\lambda = N_A \langle \sigma v \rangle$

Here we assume $A \neq B$.

$\nu = N_A + N_B - 1$

Therefore, for the general reaction $\sum_{\tilde{\alpha} \in \tilde{R}_\alpha} [\alpha] \rightleftharpoons \sum_{\tilde{\beta} \in \tilde{P}_p} [\beta]$

we have:

$$\frac{1}{N_{R_1}} \frac{d}{dt} n_{R_1} = \cdots = \frac{1}{N_{R_r}} \frac{d}{dt} n_{R_r} = - \frac{\prod_{\tilde{\alpha} \in \tilde{R}_r} n_{\tilde{\alpha}}}{\prod_{\alpha \in R_r} N_\alpha !} \langle \sigma v \rangle_R + \frac{\prod_{\tilde{\beta} \in \tilde{P}_p} n_{\tilde{\beta}}}{\prod_{\beta \in P_p} N_\beta !} \langle \sigma v \rangle_P$$

and

$$\frac{1}{N_{P_1}} \frac{d}{dt} n_{P_1} = \cdots = \frac{1}{N_{P_p}} \frac{d}{dt} n_{P_p} = + \frac{\prod_{\tilde{\alpha} \in \tilde{R}_r} n_{\tilde{\alpha}}}{\prod_{\alpha \in R_r} N_\alpha !} \langle \sigma v \rangle_R - \frac{\prod_{\tilde{\beta} \in \tilde{P}_p} n_{\tilde{\beta}}}{\prod_{\beta \in P_p} N_\beta !} \langle \sigma v \rangle_P$$

Here we did $Y_i \simeq \frac{n_i}{N_a \rho}$

Or work with molar fractions: $Y_i = \frac{n_i m_i}{\rho} \frac{1}{A} = \frac{n_i}{N_a \rho} \frac{A_{nuc_i}}{A_i}$

$$\frac{1}{N_{R_{1\ldots r}}} \frac{d}{dt} Y_{R_{1\ldots r}} = - \rho^{r-1} \frac{\prod_{\tilde{\alpha} \in \tilde{R}_r} Y_{\tilde{\alpha}}}{\prod_{\alpha \in R_r} N_\alpha !} N_a^{r-1} \langle \sigma v \rangle_R + \rho^{P-1} \frac{\prod_{\tilde{\beta} \in \tilde{P}_p} Y_{\tilde{\beta}}}{\prod_{\beta \in P_p} N_\beta !} N_a^{P-1} \langle \sigma v \rangle_P$$

$$\frac{1}{N_{P_{1\ldots p}}} \frac{d}{dt} Y_{P_{1\ldots p}} = + \rho^{r-1} \frac{\prod_{\tilde{\alpha} \in \tilde{R}_r} Y_{\tilde{\alpha}}}{\prod_{\alpha \in R_r} N_\alpha !} N_a^{r-1} \langle \sigma v \rangle_R - \rho^{P-1} \frac{\prod_{\tilde{\beta} \in \tilde{P}_p} Y_{\tilde{\beta}}}{\prod_{\beta \in P_p} N_\beta !} N_a^{P-1} \langle \sigma v \rangle_P$$

Here $\{R_r\}$ and $\{P_p\}$ represent distinctive nuclei with their N-count appear in the reaction, i.e. $2\,{}^{12}C \rightleftharpoons {}^{20}Ne + {}^{4}He + \gamma$

Now if rate is in equilibrium i.e. forward rate balances the inverse rate, then the right-hand-side should be $\underline{\underline{0}}$.

This imposes detail-balance

i.e.

$$\frac{N_a^{p-1}\langle \sigma v\rangle_P}{N_a^{r-1}\langle \sigma v\rangle_R} = \rho^{r-p}\,\frac{\prod_{\tilde\alpha\in\tilde R_r} Y_{\tilde\alpha}}{\prod_{\tilde\beta\in\tilde P_p} Y_{\tilde\beta}} \times \frac{\prod_{\beta\in P_p} N_\beta !}{\prod_{\alpha\in R_r} N_\alpha !}$$

Now use molar fraction via Boltzmann Approximation.

$$Y_i = \frac{1}{N_a\rho}\frac{(A m_u c)^{5/2}}{A}(2J_0+1)G(T)\left(\frac{m_u k_B T}{2\pi\hbar^2}\right)^{3/2}\exp\left\{\frac{u - mc^2 - u^c}{k_B T}\right\}$$

$$\frac{\lambda_P}{\lambda_R} = \frac{N_a^{p-1}\langle \sigma v\rangle_P^{scn}}{N_a^{r-1}\langle \sigma v\rangle_R^{scn}} = \left(\frac{1}{N_a}\right)^{r-p}\left(\frac{m_u k_B}{2\pi\hbar^2}\right)^{\frac{3}{2}(r-p)} T^{\frac{3}{2}(r-p)} \times \frac{\prod_{\beta\in P_p} N_\beta !}{\prod_{\alpha\in R_r} N_\alpha !}$$

this bit should be screened.

$$\times \frac{\prod_{\tilde\alpha\in\tilde R_r}\frac{(A m_u c_{\tilde\alpha})^{5/2}}{A_{\tilde\alpha}}(2J_{\tilde\alpha}+1)G_{\tilde\alpha}(T)}{\prod_{\tilde\beta\in\tilde P_p}\frac{(A m_u c_{\tilde\beta})^{5/2}}{A_{\tilde\beta}}(2J_{\tilde\beta}+1)G_{\tilde\beta}(T)}$$

$$\times \exp\left\{-\frac{\left(\sum_{\tilde\alpha\in R_r} m_{\tilde\alpha} - \sum_{\tilde\beta\in P_p} m_{\tilde\beta}\right)c^2}{k_B T}\right\}$$

$$\times \exp\left\{\frac{\left(\sum_{\tilde\alpha\in R_r} u_{\tilde\alpha} - \sum_{\tilde\beta\in P_p} u_{\tilde\beta}\right)}{k_B T}\right\}$$

$$\times \exp\left\{-\frac{\sum_{\tilde\alpha\in R_r} u^c_{\tilde\alpha} - \sum_{\tilde\beta\in P_p} u^c_{\tilde\beta}}{k_B T}\right\}$$

Now the Q-value of a reaction rate is by definition, the energy release, i.e.

$$Q = \left(\sum_{\tilde{\alpha} \in R_r} m_{\tilde{\alpha}} - \sum_{\tilde{\beta} \in P_p} m_{\tilde{\beta}} \right) c^2$$

note that this is the Q-value of the forward rate.

And since forward and reverse rates are in equilibrium, chemical potential is the same.

$$\boxed{\sum_{\tilde{\alpha} \in \tilde{R}_r} \mu_{\tilde{\alpha}} = \sum_{\tilde{\beta} \in \tilde{P}_p} \mu_{\tilde{\beta}}}$$

This is basically the NSE condition

Note that with NSE condition $\mu_{\tilde{\alpha}} = Z_{\tilde{\alpha}} \mu_p + N_{\tilde{\alpha}} \mu_n$

$$\hookrightarrow \quad \mu_p^R \sum_{\tilde{\alpha} \in \tilde{R}_r} Z_{\tilde{\alpha}} + \mu_n^R \sum_{\tilde{\alpha} \in \tilde{R}_r} N_{\tilde{\alpha}} = \mu_p^P \sum_{\tilde{\beta} \in \tilde{P}_p} Z_{\tilde{\beta}} + \mu_n^P \sum_{\tilde{\beta} \in \tilde{P}_p} N_{\tilde{\alpha}}$$

since in NSE: $\mu_p^R = \mu_p^P$, $\mu_n^R = \mu_n^P$

and with only strong reactions: $\sum_{\tilde{\alpha}} Z_{\tilde{\alpha}} = \sum_{\tilde{\beta}} Z_{\tilde{\beta}}$

$$\sum_{\tilde{\alpha}} N_{\tilde{\alpha}} = \sum_{\tilde{\beta}} N_{\tilde{\beta}}$$

so By imposing $\sum_{\tilde{\alpha} \in \tilde{R}_r} \mu_{\tilde{\alpha}} = \sum_{\tilde{\beta} \in \tilde{P}_p} \mu_{\tilde{\beta}}$,

we're essentially using Y_{NSE} instead of general Y

* However, this only imposes condition where the sum cancels, so it doesn't guarantee $\mu = Z \mu_p + N \mu_n$.

Then we have:

$$\boxed{\begin{aligned}\frac{N_a^{p-1}\langle\sigma v\rangle_P^{scn}}{N_a^{r-1}\langle\sigma v\rangle_R^{scn}} &= \left(\frac{1}{N_a}\right)^{r-p}\left(\frac{m_u k_B}{2\pi\hbar^2}\right)^{\frac{3}{2}(r-p)} T^{\frac{3}{2}(r-p)}\exp\left\{\frac{-Q}{k_B T}\right\}\\ &\times \frac{\prod_{\tilde{\alpha}\in\tilde{R}_r}\frac{(A_{nuc\tilde{\alpha}})^{5/2}}{A_{\tilde{\alpha}}}(2J_{\tilde{\alpha}}+1)G_{\tilde{\alpha}}(T)}{\prod_{\tilde{\beta}\in\tilde{P}_p}\frac{(A_{nuc\tilde{\beta}})^{5/2}}{A_{\tilde{\beta}}}(2J_{\tilde{\beta}}+1)G_{\tilde{\beta}}(T)}\;\frac{\prod_{\beta\in P_p}N_\beta!}{\prod_{\alpha\in R_r}N_\alpha!}\\ &\times\exp\left\{-\frac{\left(\sum_{\tilde{\alpha}\in\tilde{R}_r}u^c_{\tilde{\alpha}}-\sum_{\tilde{\beta}\in\tilde{P}_p}u^c_{\tilde{\beta}}\right)}{k_B T}\right\}\end{aligned}}$$

note that it's screened rate.

Now we can techniquely just multiply the RHS to the λ of the forward rate, $\lambda = N_a^{p-1}\langle\sigma v\rangle$

we can also write things in terms of <u>unscreened forward rate</u>

$$N_a^{p-1}\langle\sigma v\rangle_p^{scn} = \left(\frac{1}{N_a}\right)^{r-p}\left(\frac{m_u k_B}{2\pi\hbar^2}\right)^{\frac{3}{2}(r-p)} T^{\frac{3}{2}(r-p)} \exp\left\{\frac{-Q}{k_B T}\right\}$$

$$\times \frac{\prod_{\tilde{\alpha}\in\tilde{R}_r} \frac{(A_{nuc\tilde{\alpha}})^{5/2}}{A_{\tilde{\alpha}}}(2J_{\tilde{\alpha}}+1)G_{\tilde{\alpha}}(T)}{\prod_{\tilde{\beta}\in\tilde{P}_p} \frac{(A_{nuc\tilde{\beta}})^{5/2}}{A_{\tilde{\beta}}}(2J_{\tilde{\beta}}+1)G_{\tilde{\beta}}(T)} \frac{\prod_{\beta\in P_p} N_\beta!}{\prod_{\alpha\in R_r} N_\alpha!}$$

$$\times \exp\left\{-\frac{\left(\cancel{\sum_{\tilde{\alpha}\in\tilde{R}_r} u^c_{\tilde{\alpha}}} - \sum_{\tilde{\beta}\in\tilde{P}_p} u^c_{\tilde{\beta}}\right)}{k_B T}\right\}$$

$$\times N_a^{r-1}\langle\sigma v\rangle^{uns} \exp\left\{\frac{\cancel{\sum_{\tilde{\alpha}\in\tilde{R}_r} u^c_{\tilde{\alpha}}(Z_{\tilde{\alpha}})} - u^c\left(\sum_{\tilde{\alpha}\in\tilde{R}_r} Z_{\tilde{\alpha}}\right)}{k_B T}\right\}.$$

Due to conservation of charge for strong reactions

$$\sum_{\tilde{\alpha}\in\tilde{R}_r} Z_{\tilde{\alpha}} = \sum_{\tilde{\beta}\in\tilde{P}_p} Z_{\tilde{\beta}}$$

$$\boxed{\frac{\lambda^{scn}_{rev}}{\lambda^{uns}_{for}} = \frac{N_a^{p-1}\langle\sigma v\rangle_p^{scn}}{N_a^{r-1}\langle\sigma v\rangle_R^{uns}} = \left(\frac{1}{N_a}\right)^{r-p}\left(\frac{m_u k_B}{2\pi\hbar^2}\right)^{\frac{3}{2}(r-p)} T^{\frac{3}{2}(r-p)} \exp\left\{\frac{-Q}{k_B T}\right\} \times \frac{\prod_{\tilde{\alpha}\in\tilde{R}_r} \frac{(A_{nuc\tilde{\alpha}})^{5/2}}{A_{\tilde{\alpha}}}(2J_{\tilde{\alpha}}+1)G_{\tilde{\alpha}}(T)}{\prod_{\tilde{\beta}\in\tilde{P}_p} \frac{(A_{nuc\tilde{\beta}})^{5/2}}{A_{\tilde{\beta}}}(2J_{\tilde{\beta}}+1)G_{\tilde{\beta}}(T)} \frac{\prod_{\beta\in P_p} N_\beta!}{\prod_{\alpha\in R_r} N_\alpha!} \times \exp\left\{\frac{\sum_{\tilde{\beta}\in\tilde{P}_p} u^c_{\tilde{\beta}}(Z_{\tilde{\beta}}) - u^c\left(\sum_{\tilde{\beta}\in\tilde{P}_p} Z_{\tilde{\beta}}\right)}{k_B T}\right\}}$$

standard screening factor. $\Rightarrow$

Since Reaclib works with format, each λ_j is a single set

$$\lambda_{tot} = \sum_j \lambda_j = \sum_j \exp\left(a_0 + \sum_{i=1}^{5} a_i T_9^{(2i-5)/3} + a_6 \log T_9\right)_j$$

we can rearrange the above equation and derive λ_{rev} in the Reaclib format by taking the log on both sides of $N_a^{P-1}\langle\sigma v\rangle_p$ and compare:

i.e. $\lambda^{rev}_{tot} = \lambda^{for}_{tot} F$ where F is the ratio between λ^{rev}_{tot} and λ^{for}_{tot}

since $\lambda_{tot} = \sum_j \lambda_j$

$$\sum_j \lambda_j^{rev} = \sum_j F \lambda_j^{for}$$

$$\hookrightarrow \quad \sum_j \left(\lambda_j^{rev} - F\lambda_j^{for}\right) = 0$$

so simply require each single set of the reverse rate to be a ratio of the forward rate single set.

$$\lambda_j^{rev} = F\lambda_j^{for}$$

$$\lambda_j^{rev} = \log\left(\exp\left\{a_0 + \sum_i a_i T_9^{\frac{2i-5}{3}} + a_6 \log T_9\right\}_j\right)$$

$$= \log\left\{\left(\frac{1}{N_a}\right)^{r-p}\left(\frac{m_u k_B}{2\pi\hbar^2}\right)^{\frac{3}{2}(r-p)} \times \frac{\prod_{\tilde{\alpha}\in\tilde{R}_r} \frac{(A_{\tilde{\alpha}}^{nuc})^{5/2}}{A_{\tilde{\alpha}}}(2J_{\tilde{\alpha}}+1)G_{\tilde{\alpha}}(T)}{\prod_{\tilde{\beta}\in\tilde{P}_p} \frac{(A_{\tilde{\beta}}^{nuc})^{5/2}}{A_{\tilde{\beta}}}(2J_{\tilde{\beta}}+1)G_{\tilde{\beta}}(T)} \frac{\prod_{\beta\in P_\beta} N_\beta!}{\prod_{\alpha\in R_\alpha} N_\alpha!}\right\}$$

$$- \frac{Q + \cancel{\left(\sum_{\tilde{\alpha}\in R_\alpha} \mu_{\tilde{\alpha}}^c - \sum_{\tilde{\beta}\in P_\beta} \mu_{\tilde{\beta}}^c\right)}}{k_B 10^9} T_9^{-1}$$

since charge is conserved for strong reaction

$\hookrightarrow \sum_{\tilde{\alpha}\in R_r} Z_{\tilde{\alpha}} = \sum_{\tilde{\beta}\in P_p} Z_{\tilde{\beta}}$

$$+ \frac{3}{2}(r-p)\left(\log T_9 + \log 10^9\right)$$

$$+ \underbrace{\log\left(\lambda_j^{for}\right)}$$

$$\log \lambda_{tot}^{scn} = \log\left(\exp\left(a_0 + \sum_{i=1}^{5} a_i T_9^{\frac{2i-5}{3}} + a_6 \log T_9\right)_j\right) + \frac{\cancel{\sum_{\tilde{\alpha}\in R_r} \mu_{\tilde{\alpha}}^c} - \mu^c\left(\sum_{\tilde{\alpha}\in R_r} Z_{\tilde{\alpha}}\right)}{k_B T}$$

Note that in reality, we work with unscreened forward rate to find unscreened reverse rate, so just set $\mu^c = 0$. After finding the unscreened reverse rate, we can simply do the usual screening routine, if screening routine follows linear mixing rule, i.e.

$$R^{scn} = R^{unscn} \exp\left\{\frac{\sum_{\tilde{\beta}\in P_p} \mu_{\tilde{\beta}}^c(Z_{\tilde{\beta}}) - \mu^c\left(\sum_{\tilde{\beta}\in P_p} Z_{\tilde{\beta}}\right)}{k_B T}\right\}$$

An example is the Chabrier & Potekhin 1998 screening.

Now by matching $\lambda_j = \exp\left\{ a_0 + \sum_{i=1}^{5} a_i T_9^{(2i-5)/3} + a_6 \log T_9 \right\}_j$

Each j-th single set of the derived rate is:

$$a^j_{0,rev} = a^j_0 + \log\left\{ \left(\frac{1}{N_a}\right)^{r-p} \left(\frac{m_u k_B 10^9}{2\pi\hbar^2}\right)^{\frac{3}{2}(r-p)} \times \frac{\prod_{\tilde{\alpha}\in\tilde{R}_\alpha} \frac{(A^{nuc}_{\tilde{\alpha}})^{5/2}}{A_{\tilde{\alpha}}} (2J_{\tilde{\alpha}}+1) G_{\tilde{\alpha}}(T)}{\prod_{\tilde{\beta}\in\tilde{P}_\beta} \frac{(A^{nuc}_{\tilde{\beta}})^{5/2}}{A_{\tilde{\beta}}} (2J_{\tilde{\beta}}+1) G_{\tilde{\beta}}(T)} \frac{\prod_{\beta\in P_\beta} N_\beta!}{\prod_{\alpha\in R_\alpha} N_\alpha!} \right\}$$

$$a^j_{1,rev} = a^j_1 + \Bigg[\underbrace{\left(\sum_{\tilde{\beta}\in P_\beta} \mu^c_{\tilde{\beta}} - \mu^c\left(\sum_{\tilde{\beta}\in P_\beta} Z_{\tilde{\beta}}\right)\right)}_{\text{This is screening term,}} - Q \Bigg] \Big/ (10^9 k_B)$$

we ignore to find unscreened reverse rate, the apply screening later.

$$a^j_{2\cdots5,rev} = a^j_{2\cdots5}$$

$$a^j_{6,rev} = a^j_6 + \frac{3}{2}(r-p)$$

NSE network pre-requisite:

1) Species must be connected. It's ok to have artificial end-points.

2) Must able to represent network in 2 species. proton and neutrons are exceptions.
If α-captures are involved, then 3-α should be connected.

Example: 1) α-capture rate, $A(\alpha,\gamma)B$

Detailed Balance requires: $\sum_{\tilde{\alpha}\in R_r} \mu_{\tilde{\alpha}} = \sum_{\tilde{\beta}\in P_p} \mu_{\tilde{\beta}}$

$$\mu_A + \mu_\alpha = \mu_B$$

NSE says $\mu_i = Z_i \mu_p + N_i \mu_n$, but there is ambiguity in detailed balance condition where we have the freedom to choose the value of μ_A and μ_α, hence NSE won't predict exactly.

Likewise since $\lambda_{reverse} \propto \left(\frac{Y_A Y_\alpha}{Y_B}\right)_{NSE} \lambda_{forward}$

so ambiguity between Y_A and Y_α

Now suppose we have 3-α: $3\mu_\alpha = \mu_{^{12}C}$

There is no ambiguity in the proportionality between α and ^{12}C.
So 3-α alone definitely gives accurate NSE prediction.

Now suppose we have

$$3\alpha \rightleftharpoons {}^{12}C \qquad \text{and} \qquad 2\,{}^{12}C \rightleftharpoons \alpha + {}^{20}Ne$$

i.e. $3\mu_\alpha = \mu_{12C}$ and $2\mu_{12C} = \mu_\alpha + \mu_{20Ne}$.

This network also predicts NSE since we can represent μ_{20Ne} in terms of μ_α. Likewise, standard α-chain networks will also work.

Example 2) proton and neutron capture rates:

$$A(p,\gamma)B \quad \text{or} \quad A(n,\gamma)B$$

suppose we do proton-capture, then $\mu_A + \mu_p = \mu_B$

Now even though there are 3 species, because μ_p is already in the form of $Z_i\mu_p + N_i\mu_n$, so there is no ambiguity in μ_p, or μ_n for neutron capture. Therefore, we again have the correct proportionality between A and B.

Example 3) $A(\alpha,p)B \rightarrow \mu_A + \mu_\alpha = \mu_p + \mu_B$

NSE won't predict correctly for this reaction since aside from proton, we also have μ_A, μ_α and μ_B.

An example is

$$\begin{tikzcd}[column sep=small] & {}^{19}F \arrow[dr, shift left, "{(p,\gamma)}"] \arrow[dl, shift left] & \\ {}^{16}O \arrow[ur, shift left, "{(\alpha,p)}"] \arrow[rr, shift left] & & {}^{20}Ne \arrow[ul, shift left] \arrow[ll, shift left, "{(\alpha,\gamma)}"] \end{tikzcd}$$

won't work

To make the above reaction cycle be compatible with NSE, simply connect via $3-\alpha$ so we can correctly eliminate μ_α.

$$\begin{tikzcd}[column sep=small] & & & {}^{19}F \arrow[dr, shift left, "{(p,\gamma)}"] \arrow[dl, shift left] & \\ {}^{4}He \arrow[r, shift left, "{(\alpha\alpha,\gamma)}"] & {}^{12}C \arrow[l, shift left] \arrow[r, shift left, "{(\alpha,\gamma)}"] & {}^{16}O \arrow[l, shift left] \arrow[ur, shift left, "{(\alpha,p)}"] \arrow[rr, shift left] & & {}^{20}Ne \arrow[ul, shift left] \arrow[ll, shift left, "{(\alpha,\gamma)}"] \end{tikzcd}$$

This works.

Example: 4) consider: ${}^{12}C(p,\gamma)\,{}^{13}N$, works since proton-capture.

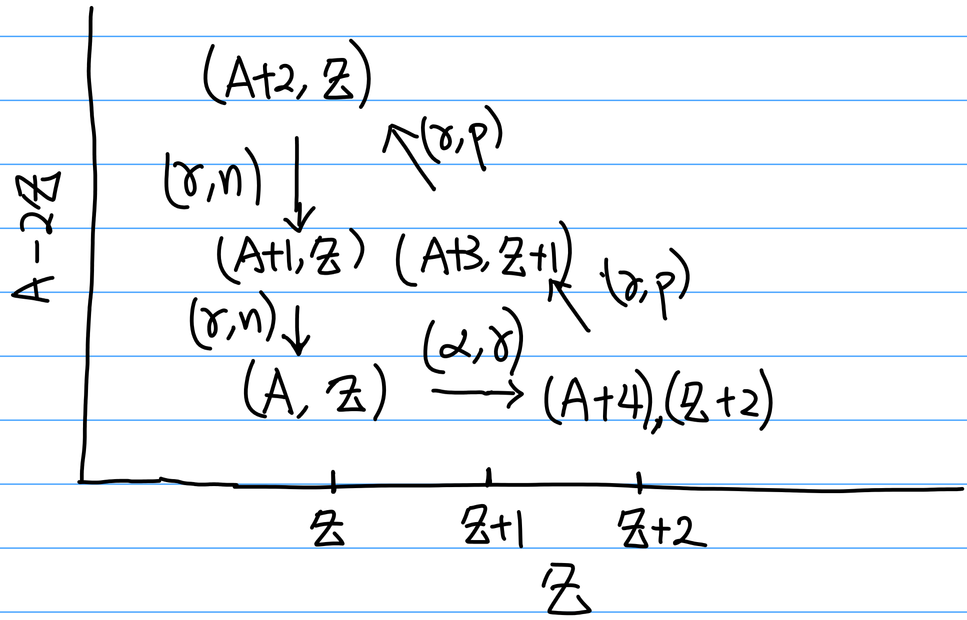
Now connect with ${}^{13}N(\alpha,p)\,{}^{16}O$, won't work since (α,p)

To make it work, connect with 3α:

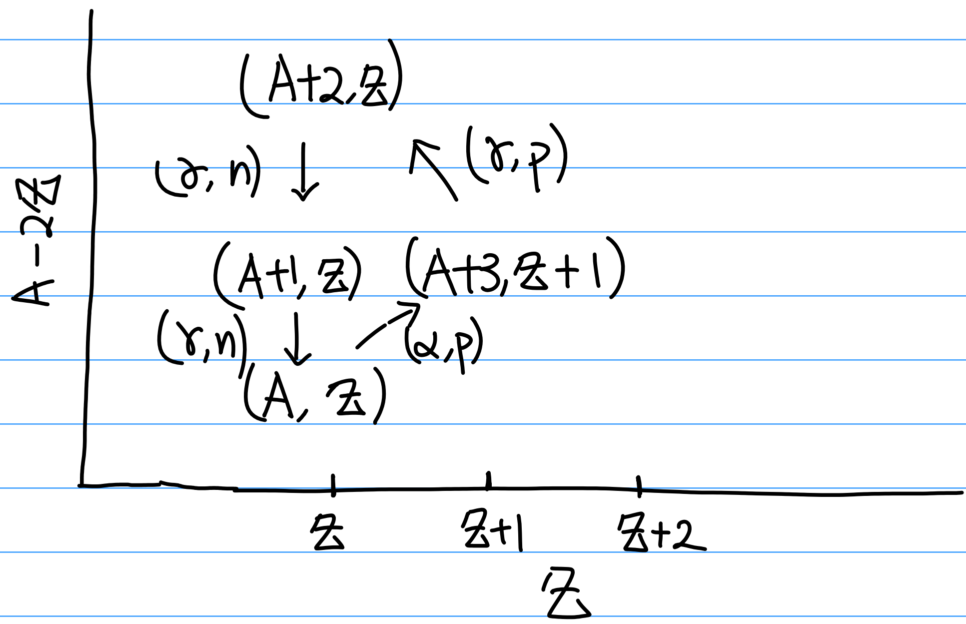
$$\underbrace{\underbrace{{}^{4}He(\alpha\alpha,\gamma)\,{}^{12}C}_{\checkmark}\underbrace{(p,\gamma)\,{}^{13}N}_{\checkmark}\underbrace{(\alpha,p)\,{}^{16}O}_{\times}}_{\checkmark}$$

Equilibrium cycle suggested by kushnir:

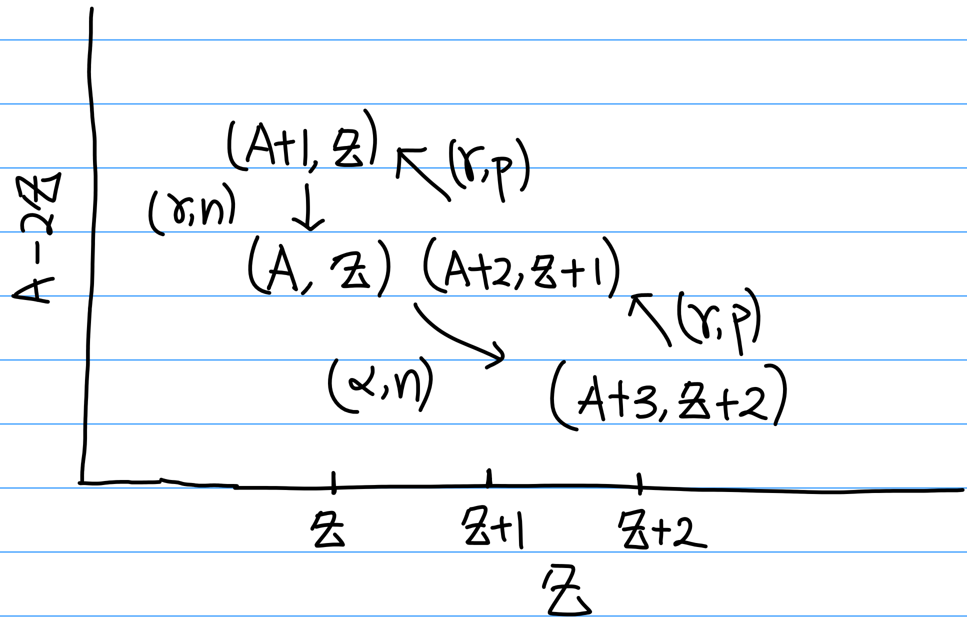
1) $1\ (\alpha,\gamma)\ ,\ \ 2\ (\gamma,p)\ ,\ \ 2(\gamma,n)$



2) $1\ (\alpha,p)\ ,\ \ 1\ (\gamma,p)\ ,\ \ 2\ (\gamma,n)$



3) 1 (α, n), 2 (γ, p), 1 (γ, n)



one example:

$$^{32}S(\gamma,p)\,^{31}P\,(\gamma,p)\,^{30}Si\,(\gamma,n)\,^{29}Si\,(\gamma,n)\,^{28}Si\,(\alpha,\gamma)\,^{32}S$$

Quasi equilibrium in small groups.

1) $24 \le A \le 45$: Si - group

2) $46 \le A \le 60$ (at least) : Iron Group.

^{24}Mg or below is not in NSE initially.

NSE EOS:

Note that for general eos, it needs 2-inputs and the massfractions of the state. If one of the input is not Temperature, T still needs to be initialized.

$$e = eos(\rho, T, X_k)$$

Now suppose we're given internal energy, e_{in}, instead of T, so to find the NSE massfractions we want:

$$X_k^{NSE} = X_k^{NSE}(\rho, \underset{\uparrow \text{ instead of } T.}{e}, Y_e)$$

This imposes an additional constraint on internal energy where we solve for T, i.e. now have 3 constraint eqs:

$$\vec{f}(u_p, u_n, T) = \begin{bmatrix} \sum_k X_k^{NSE}(u_p, u_n, T) - 1 \\ \sum_k \frac{Z_k}{A_k} X_k^{NSE}(u_p, u_n, T) - Y_e \\ \underbrace{e(u_p, u_n, T)} - e \end{bmatrix} = 0 \quad \begin{matrix} \text{Mass-conservation} \\ \text{Charge-conservation} \\ \text{Energy-conservation (?)} \end{matrix}$$

$$= e(\rho, T, X_k(u_p, u_n, T))$$

$$\overset{!}{=} e(\rho, T, \bar{A}(u_p, u_n, T), \bar{Z}(u_p, u_n, T))$$

In this case we have a 3×3 Jacobian, but let's first evaluate some derivatives:

with $$X_k^{NSE} = \frac{m_k}{\rho}(2J_k+1)G(T)_k\left(\frac{m k_B T}{2\pi\hbar^2}\right)^{3/2}\exp\left\{\frac{Z_k u_p + N_k u_n + B_k - u_k^c(T)}{k_B T}\right\}$$

$$\frac{u_k^c}{k_B T} = A_1\left[\sqrt{\Gamma_k(A_2+\Gamma_k)} - A_2\underbrace{\ln\left(\sqrt{\frac{\Gamma_k}{A_2}}+\sqrt{1+\frac{\Gamma_k}{A_2}}\right)}_{\text{arcsinh}\sqrt{\frac{\Gamma_k}{A_2}}}\right] + 2A_3\left[\sqrt{\Gamma_k} - \text{atan}\sqrt{\Gamma_k}\right]$$

where $\Gamma_k = Z_k^{5/3}\Gamma_e$, $\Gamma_e = e^2\left(\frac{4\pi n_e}{3}\right)^{1/3}\frac{1}{k_B T}$

Also $\bar{A} = \left(\sum_k \frac{1}{A_k} X_k\right)^{-1}$ $\quad \bar{Z} = \bar{A}\, Y_e$

1) $\frac{\partial}{\partial u_p} X_k^{NSE} = \frac{Z_k}{k_B T} X_k^{NSE}$

2) $\frac{\partial}{\partial u_n} X_k^{NSE} = \frac{N_k}{k_B T} X_k^{NSE}$

3) $\frac{\partial}{\partial T} X_k^{NSE} = X_k^{NSE}\left\{\left(\frac{\partial}{\partial T} G_k\right)\frac{1}{G} + \frac{1}{T}\left[\frac{3}{2} - \frac{Z_k u_p + N_k u_n + B_k}{k_B T}\right] - \frac{\partial}{\partial T}\left(\frac{u_k^c}{k_B T}\right)\right\}$

To evaluate $\frac{\partial}{\partial T}\left(\frac{u^c}{k_B T}\right)$, $\frac{\partial}{\partial T}\Gamma_e = -\frac{1}{T}\Gamma_e$, so $\frac{\partial}{\partial T}\Gamma = -\frac{1}{T}\Gamma$

$$\frac{\partial}{\partial T}\left(\frac{u^c}{k_B T}\right) = A_1\left\{\frac{A_2\Gamma' + 2\Gamma\Gamma'}{2\sqrt{\Gamma(A_2+\Gamma)}} - A_2\frac{\frac{\Gamma'}{2\sqrt{\Gamma A_2}} + \frac{\Gamma'/A_2}{2\sqrt{1+\Gamma/A_2}}}{\sqrt{\frac{\Gamma}{A_2}} + \sqrt{1+\frac{\Gamma}{A_2}}}\right\}$$

$$+2A_3\left[\frac{\Gamma'}{2\sqrt{\Gamma}} - \frac{1}{1+\Gamma}\frac{\Gamma'}{2\sqrt{\Gamma}}\right]$$

Mathematica

$$\stackrel{!}{=} \Gamma'\left\{\frac{A_3\sqrt{\Gamma}}{1+\Gamma} - \frac{A_1 A_2\sqrt{\frac{\Gamma}{A_2+\Gamma}}}{2\Gamma} + \frac{A_1(A_2+2\Gamma)}{2\sqrt{\Gamma(A_2+\Gamma)}}\right.$$

$$\stackrel{!}{=} \Gamma'\sqrt{\Gamma}\left\{\frac{A_3}{1+\Gamma} + \frac{A_1}{\sqrt{A_2+\Gamma}}\right\}$$

4) $\frac{\partial}{\partial u_p}\bar{A} = -\bar{A}^2\left(\sum_k \frac{1}{A_k}\frac{\partial}{\partial u_p}X_k^{NSE}\right) = -\bar{A}^2\left(\sum_k \frac{1}{A_k}\frac{Z_k}{k_BT}X_k^{NSE}\right)$

5) $\frac{\partial}{\partial u_n}\bar{A} = -\bar{A}^2\left(\sum_k \frac{1}{A_k}\frac{\partial}{\partial u_n}X_k^{NSE}\right) = -\bar{A}^2\left(\sum_k \frac{1}{A_k}\frac{N_k}{k_BT}X_k^{NSE}\right)$

6) $\frac{\partial}{\partial T}\bar{A} = -\bar{A}^2\left(\sum_k \frac{1}{A_k}\frac{\partial}{\partial T}X_k^{NSE}\right)$

7) $\frac{\partial}{\partial u_p}e(u_p,u_n,T) = \frac{\partial e}{\partial \bar{A}}\frac{\partial}{\partial u_p}\bar{A} + \frac{\partial e}{\partial \bar{Z}}\frac{\partial \bar{Z}}{\partial u_p} = \left\{\frac{\partial}{\partial \bar{A}}e + Y_e\frac{\partial}{\partial \bar{Z}}e\right\}\frac{\partial \bar{A}}{\partial u_p}$

8) $\frac{\partial}{\partial u_n}e(u_p,u_n,T) = \left\{\frac{\partial}{\partial \bar{A}}e + \left(\frac{\partial}{\partial \bar{Z}}e\right)Y_e\right\}\frac{\partial \bar{A}}{\partial u_n}$

9) $\frac{\partial}{\partial T}e(u_p,u_n,T) = \frac{\partial}{\partial T}e(\rho,T,\bar{A}(u_p,u_n,T),\bar{Z}(u_p,u_n,T))$

$$+\left\{\frac{\partial}{\partial \bar{A}}e(\rho,T,\bar{A},\bar{Z}) + Y_e\frac{\partial}{\partial \bar{Z}}e(\rho,T,\bar{A},\bar{Z})\right\}\left(\frac{\partial}{\partial T}\bar{A}\right)\Big|_{u_p,u_n}$$

* It is important to stress that on LHS, $e = e(u_p,u_n,T)$ but on RHS $e = e(\rho,T,\bar{A},\bar{Z})$, which is the eos interface.

With the above derivatives, the analytic Jacobian Matrix of the system is:

$$J_{NSE} = \begin{pmatrix} \frac{\partial}{\partial u_p}f_A = \sum_k \frac{\partial}{\partial u_p}X_k & \frac{\partial}{\partial u_n}f_A = \sum_k \frac{\partial}{\partial u_n}X_k & \frac{\partial}{\partial T}f_A = \sum_k \frac{\partial}{\partial T}X_k \\ \frac{\partial}{\partial u_p}f_Z = \sum_k \frac{Z_k}{A_k}\frac{\partial}{\partial u_p}X_k & \frac{\partial}{\partial u_n}f_Z = \sum_k \frac{Z_k}{A_k}\frac{\partial}{\partial u_n}X_k & \frac{\partial}{\partial T}f_Z = \sum_k \frac{Z_k}{A_k}\frac{\partial}{\partial T}X_k \\ \frac{\partial}{\partial u_p}f_e = \left(\frac{\partial}{\partial \bar{A}}e + Y_e\frac{\partial}{\partial \bar{Z}}e\right)\frac{\partial \bar{A}}{\partial u_p} & \frac{\partial}{\partial u_n}f_e = \left(\frac{\partial}{\partial \bar{A}}e + Y_e\frac{\partial}{\partial \bar{Z}}e\right)\frac{\partial \bar{A}}{\partial u_n} & \frac{\partial}{\partial T}f_e = \frac{\partial}{\partial T}e + \left(\frac{\partial}{\partial \bar{A}}e + Y_e\frac{\partial}{\partial \bar{Z}}e\right)\frac{\partial}{\partial T}\bar{A} \end{pmatrix}$$

Option #2

What we can do instead is to solve for X_k first using a guess T, then iterate through to find T such that it satisfies the energy constraint.

Note that the eos: $e(\rho, T, X_k) \longrightarrow e(\rho, T, \bar{A}, \bar{Z})$

where

$$Y_e = \sum_k \frac{Z_k}{A_k} X_k = \frac{1}{\mu_e}, \quad \bar{A} = \left(\sum_k \frac{1}{A_k} X_k \right)^{-1}, \quad \text{and } \bar{Z} = \bar{A} Y_e$$

Steps:

1) $X_{k,0}^{NSE} = X_k^{NSE}(\rho, T_0, Y_e)$

2) $e_0 = eos(\rho, T_0, X_{k,0}^{NSE})$

3) update via NR, where $f = e_0 - e_{in} = 0$

$$T_{n+1} = T_n - \underbrace{\left(\frac{de}{dT}\right)^{-1} f}_{dT} = T_n - \left(\frac{\partial e}{\partial T} + \frac{\partial e}{\partial \bar{A}} \frac{\partial \bar{A}}{\partial T} + \frac{\partial e}{\partial \bar{Z}} \underbrace{\left(Y_e \frac{\partial \bar{A}}{\partial T} \right)}_{\frac{\partial \bar{Z}}{\partial T}} \right)^{-1} f$$

This gets the temperature corresponding to $\underline{e_{in}}$

then $X_k^{NSE} = X_k^{NSE}(\rho, T, Y_e)$

Energy Generation in NSE Evolution:

To get 2nd order convergence do RK2 integration:

$$\frac{d}{dt} Y = f(t, Y) \quad \text{with} \quad Y(t_0) = Y_0$$

For 2^{nd} order RK:

$$Y_{n+1} = Y_n + \Delta t \, \dot{Y}\left[t_n + \tfrac{1}{2}\Delta t,\ Y_n + \tfrac{1}{2}\Delta t \, \dot{Y}(t_n, Y_n)\right]$$

want to update $\rho, \rho\vec{U}, \rho e$ and ρE

$$= Y_n + \Delta t \, \dot{Y}_{n+1/2}$$

Note that for simplified - SDC algorithm, we arrive at:

$$\frac{\partial}{\partial t} \mathcal{U} = \underbrace{\left[A(\mathcal{U})\right]^{n+1/2,(k)}}_{\text{This advection source term is already time-centered}} + \underbrace{R(\mathcal{U})}_{\text{Reaction Source.}}$$

We first update ρ and $\rho\vec{U}$, since they have no reactive sources

i.e. and

$$\begin{cases} \rho^{n+1} = \rho^n + \Delta t \, A(\rho)^{n+1/2} \\ (\rho U)^{n+1} = (\rho U)^n + \Delta t \, A(\rho U)^{n+1/2} \end{cases}$$

Now we need to find the derivative: $\dot{Y}(t_n, Y_n) = \frac{\partial}{\partial t}(\rho e)$
Since NSE depends on ρ, e and Y_e, we're interested in evolving ρ, e, and Y_e so that we can determine the correct thermo condition for getting X_k^{NSE} so that the correct energy generation rate is computed.

The calculation of $R(\rho e)$ is computed in "nse_derivs"

Given ρ, ρe and $\rho Y_e \rightarrow Y_e$

get the corresponding T and $\bar{A}$ from nse_eos using (ρ, e, Y_e). We can't just work with T because we evolve ρe so we only have source terms for ρe.

Now compute the NSE state $X_k^{NSE} = X_k^{NSE}(\rho, T, Y_e)$

With that compute thermal neutrino losses

i.e. $\text{sneut5}(T_0, \rho_0, \bar{A}, \bar{Z}, \epsilon_{\nu,\text{thermal}})$ accounts for plasma, photo-, pair-, recombination and Bremsstralung.

i.e. $\epsilon_{\nu,\text{thermal}}$

Now get $\dot{Y}_{weak}$ due to weak reactions.

With $\dot{Y}_{weak}$, there is a change in Y_e:

$$R(\rho Y_{e,weak}) = \rho \sum_k Z \dot{Y}_{weak} + \cancel{\underbrace{Y_e \frac{\partial}{\partial t}\rho}_{?}}$$

? but reaction doesn't change ρ

Then
$$\boxed{(\rho \dot{Y}_e)_{tot} = \underbrace{\sum_k \frac{Z_k}{A_k}(\rho X_k)_A}_{\text{advective source for } (\rho X_k)} + \underbrace{\rho \sum_k Z_k \dot{Y}_{k,weak}}_{\text{source due to weak reaction.}}}$$

Now we can compute $R(\rho e)$: this from sneut5

$$\boxed{R(\rho e) = \rho\epsilon = \rho\epsilon_{nuc} - \underbrace{\rho\epsilon_{\nu,\text{thermal}}}_{\substack{\text{thermal neutrino} \\ \text{due to plasma,} \\ \text{photo, pair,} \\ \text{recombination and} \\ \text{Bremsstralung}}} - \underbrace{\rho\epsilon_{\nu,\text{react}}}_{\substack{\text{neutrino loss due} \\ \text{to electron-captures} \\ \text{and beta-decays}}}}$$

neutrinos from weak reactions

Only weak reaction contribute since we're in NSE

specific energy generation rate

where $\epsilon_{nuc} = -N_A c^2 \sum_k \dot{Y}_k m_k = -\sum_k \dot{X}_k \frac{1}{A_k}\frac{1}{m_u} m_k c^2$

where nuclei mass :

$$\boxed{m_k c^2 = N_k m_n c^2 + Z_k(m_p + m_e)c^2 - B_k}$$

In tabular NSE, we write:

$$\epsilon_{nuc} = -N_A c^2 \sum_k \frac{1}{A_k}\dot{X}_k\left(\overset{A_k - Z_k}{N_k} m_n + Z_k(m_p + m_e) - B_k/c^2\right)$$

$$= \underbrace{N_A \sum_k \frac{B_k}{A_k}\dot{X}_k}_{\frac{d}{dt}\langle B/A\rangle} - N_A c^2 \sum_k \left(\underbrace{\dot{X}_k}_{=0} - \frac{Z_k}{A_k}\underbrace{(m_n - (m_p + m_e))}_{\Delta m_{np}}\right)$$

$$\boxed{\epsilon_{nuc} = N_A \frac{d}{dt}\langle B/A\rangle + N_A \Delta m_{np} c^2 \frac{d}{dt}\underbrace{Y_e}_{\sum_k \frac{Z_k}{A_k}\dot{X}_k}}$$

Tabular NSE form

$*$ { Note that the following doesn't seem to be required, since $R(\rho e)$ is already a completed source term, we just use that

Now we need to find the total reactive source term that not only has reaction influence, but also see advection.

$$R(\rho e)_{tot} = -N_a c^2 \sum_k \frac{m_k}{A_k} \frac{\left[(\rho X_k^{NSE})_1 - \tau A(\rho X_k) - (\rho X_k^{NSE})_0\right]}{\tau} - (\rho \epsilon_{v,thermal})_1 - (\rho \epsilon_{v,react})_1$$

Total Reaction source

To do that we need to find $(\rho X_k^{NSE})_1$

evolve for some τ, $\tau \ll \Delta t$

$$\left\{\begin{aligned} \rho_1 &= \rho_0 + \tau A(\rho) \\ (\rho e)_1 &= (\rho e)_0 + \tau\left(A(\rho e) + R(\rho e)\right) \\ (\rho Y_e)_1 &= (\rho Y_e)_0 + \tau\left(A(\rho Y_e) + R(\rho Y_e)\right) \end{aligned}\right\} \quad e_1 = \frac{(\rho e)_1}{\rho_1}, \quad Y_{e_1} = \frac{(\rho Y_e)_1}{\rho_1}$$

With updated thermo-quantities, get T_1 from ρ_1 and e_1, and $\Rightarrow$ $(X_k^{NSE})_1 = X_k^{NSE}(\rho_1, T_1, Y_{e_1})$