SIMPLIFYING SILICON BURNING: APPLICATION OF QUASI-EQUILIBRIUM TO α NETWORK NUCLEOSYNTHESIS

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Simplifying Silicon Burning: Application of Quasi-Equilibrium to α Network Nucleosynthesis

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Abstract. While the need for accurate calculation of nucleosynthesis and the resulting rate of thermonuclear energy release within hydrodynamic models of stars and supernovae is clear, the computational expense of these nucleosynthesis calculations often force a compromise in accuracy to reduce the computational cost. To redress this trade-off of accuracy for speed, we present an improved nuclear network which takes advantage of quasi-equilibrium in order to reduce the number of independent nuclei, and hence the computational cost of nucleosynthesis, without significant reduction in accuracy. In this paper we will discuss the first application of this method, the further reduction in size of the minimal α network. The resultant *QSE-reduced* α network is twice as fast as the conventional α network it replaces and requires the tracking of half as many abundance variables, while accurately estimating the rate of energy generation. Such reduction in cost is particularly necessary for future generation of multi-dimensional models for supernovae.

1. Introduction

Examination of the process of silicon burning reveals that the nuclear evolution is dominated by large groups of nuclei in mutual equilibrium. During silicon burning, these quasi-equilibrium (QSE) groups, first discussed by Bodansky *et al* (1968), form well

in advance of the global Nuclear Statistical Equilibrium (NSE) The QSE groups also persist after hydrodynamic changes have fragmented NSE (see Hix & Thielemann 1998, Meyer *et al* 1998). The existence of these groups greatly reduces the number of independent abundances, suggesting a way to reduce the computational cost of silicon burning without significant loss of accuracy

Tracking the nuclear evolution from helium burning through to NSE requires a network that includes nuclei from α-particles to Zn. Silicon burning presents a particular problem as material proceeds from silicon to the iron peak nuclei not via heavy ion captures but via a chain of photodisintegrations and light particle captures. The minimal nuclear set which can follow this evolution is the set of α-particle nuclei; α, ^{12}C, ^{16}O, ^{20}Ne, ^{24}Mg, ^{28}Si, ^{32}S, ^{36}Ar, ^{40}Ca, ^{44}Ti, ^{52}Fe, ^{56}Ni, ^{60}Zn. For convenience we will name this set $\mathcal{F}$ and refer to its abundance as $\vec{Y}^{\mathcal{F}}$. Silicon burning in fact presents a larger problem as the nuclear flow from silicon to the iron peak nuclei does not proceed through nuclei with N=Z, especially when significant neutronization has occurred (Hix & Thielemann 1996). However, for nucleosynthesis calculations within hydrodynamic models, such compromise is often made necessary by the computational limitations. Furthermore, the small size of the α network (14 nuclei and 17 reactions) makes application of QSE to α-chain nucleosynthesis a pedagogically useful example

2. Network Basics

From a set of nuclear abundances, $\vec{Y}(=\vec{n}/\rho N_A)$ and the rates for the reactions which link them, one can calculate the time derivatives of the abundances, $\dot{\vec{Y}}$. With these derivatives, the abundances of the included nuclei are evolved, at time t, and over timestep Δt, according to the implicit prescription

$$\frac{\vec{Y}(t+\Delta t)-\vec{Y}(t)}{\Delta t}=\dot{\vec{Y}}(t+\Delta t) \tag{1}$$

Solving Eq. 1 is equivalent to finding the zeros of the set of equations

$$\vec{\mathcal{Z}}(t+\Delta t)\equiv\frac{\vec{Y}(t+\Delta t)-\vec{Y}(t)}{\Delta t}-\dot{\vec{Y}}(t+\Delta t)=0\ . \tag{2}$$

This is done using the Newton-Raphson method (see, e.g Press, *et al* 1992), which is based on the Taylor series expansion of $\vec{\mathcal{Z}}(t+\Delta t)$, with the trial change in abundances given by

$$\Delta\vec{Y}=\left(\frac{\partial\vec{\mathcal{Z}}(t+\Delta t)}{\partial\vec{Y}(t+\Delta t)}\right)^{-1}\vec{\mathcal{Z}}\ , \tag{3}$$

where $\partial\vec{\mathcal{Z}}/\partial\vec{Y}$ is the Jacobian of $\vec{\mathcal{Z}}$. Iteration continues until $\vec{Y}(t+\Delta t)$ converges.

3. The QSE-reduced α Network

The objective of the QSE-reduced α network is to evolve $\vec{Y}^{\mathcal{F}}$ (and calculate the resulting energy generation) in a more efficient way. Under conditions where QSE applies, the

existence of the silicon and iron peak QSE groups allows calculation of these 14 abundances from 7. For the members of the silicon group (^{28}Si, ^{32}S, ^{36}Ar, ^{40}Ca, ^{44}Ti) and the iron peak group (^{48}Cr, ^{52}Fe, ^{56}Ni, ^{60}Zn) the individual abundances can be calculated by

$$Y_{QSE,\mathrm{Si}}(^AZ) = \frac{C(^AZ)}{C(^{28}\mathrm{Si})} Y(^{28}\mathrm{Si}) Y_\alpha^{\frac{A-28}{4}} \quad \text{and} \quad Y_{QSE,\mathrm{Ni}}(^AZ) = \frac{C(^AZ)}{C(^{56}\mathrm{Ni})} Y(^{56}\mathrm{Ni}) Y_\alpha^{\frac{A-56}{4}}, \quad (4)$$

where we have defined

$$C(^AZ) = \frac{G(^AZ)}{2^A} \left(\frac{\rho N_A}{\theta}\right)^{A-1} A^{\frac{3}{2}} \exp\left(\frac{B(^AZ)}{k_B T}\right) \quad \text{and} \quad \theta = \left(\frac{m_u k_B T}{2\pi\hbar^2}\right)^{3/2}. \quad (5)$$

$G(^AZ)$ and $B(^AZ)$ are the partition function and binding energy of the nucleus ^AZ, N_A is Avagadro's number, k_B is Boltzmann's constant, and ρ and T are the density and temperature of the plasma. $(A-28)/4$ and $(A-56)/4$ are the numbers of α-particles needed to construct ^AZ from ^{28}Si and ^{56}Ni, respectively.

Thus, where QSE applies, $\vec{Y}^{\mathcal{F}}$ is a function of $\vec{Y}^{\mathcal{R}}$, where the reduced nuclear set $\mathcal{R}$ is defined as α, ^{12}C, ^{16}O, ^{20}Ne, ^{24}Mg, ^{28}Si, ^{56}Ni, and we need only evolve $\vec{Y}^{\mathcal{R}}$. It should be noted that Woosley *et al* (1973) and Hix & Thielemann (1996) have shown that ^{24}Mg is ordinarily a member of the silicon QSE group, but for easier integration with a conventional nuclear network, we evolve ^{24}Mg independently.

While $\vec{Y}^{\mathcal{R}}$ is a convenient set of abundances for calculating $\vec{Y}^{\mathcal{F}}$, it is not the most efficient set to evolve, primarily because of the non-linear dependence on Y_α. Instead we define $\vec{Y}^{\mathcal{G}} = [Y_{\alpha G}, Y(^{12}\mathrm{C}), Y(^{16}\mathrm{O}), Y(^{20}\mathrm{Ne}), Y(^{24}\mathrm{Mg}), Y_{SiG}, Y_{FeG}]$ where

$$\begin{aligned} Y_{\alpha G} &= Y_\alpha + \sum_{i \in Si\ group} \frac{A_i - 28}{4} Y_i + \sum_{i \in Fe\ group} \frac{A_i - 56}{4} Y_i, \\ Y_{SiG} &= \sum_{i \in Si\ group} Y_i, \\ Y_{FeG} &= \sum_{i \in Fe\ group} Y_i. \end{aligned} \quad (6)$$

Physically, $Y_{\alpha G}$ represents the sum of the abundances of free α-particles and those α-particles required to build the members of the QSE groups from ^{28}Si or ^{56}Ni, while Y_{SiG} and Y_{FeG} represent the total abundances of the silicon and iron peak QSE groups.

Corresponding to this reduced set of abundances $\mathcal{G}$ is a reduced set of reactions, with quasi-equilibrium allowing one to ignore the reactions among the members of the QSE groups. Unfortunately, the rates of these reactions are functions of $\vec{Y}^{\mathcal{F}}$, and are not easily expressed in terms of $\vec{Y}^{\mathcal{G}}$. Thus, for each $\vec{Y}^{\mathcal{G}}$, one must solve for $\vec{Y}^{\mathcal{R}}$ and, by Eq. 4, $\vec{Y}^{\mathcal{F}}$, in order to calculate $\dot{\vec{Y}}^{\mathcal{G}}$ which is needed to evolve $\vec{Y}^{\mathcal{G}}$ via Eq. 1. Furthermore, Eq. 3 requires the calculation of the Jacobian of $\vec{\mathcal{Z}}$, which can not be calculated directly since $\dot{\vec{Y}}^{\mathcal{G}}$ can not be expressed in terms of $\vec{Y}^{\mathcal{G}}$. Instead we find it sufficient to use the chain rule,

$$\frac{\partial \dot{\vec{Y}}^{\mathcal{G}}}{\partial \vec{Y}^{\mathcal{G}}} = \frac{\partial \dot{\vec{Y}}^{\mathcal{G}}}{\partial \vec{Y}^{\mathcal{R}}} \frac{\partial \vec{Y}^{\mathcal{R}}}{\partial \vec{Y}^{\mathcal{G}}} \quad (7)$$

to calculate the Jacobian. Analytically, the first term of this chain rule product is easily calculated from the sums of reaction terms, while the second term requires implicit differentiation using Eq. 6.

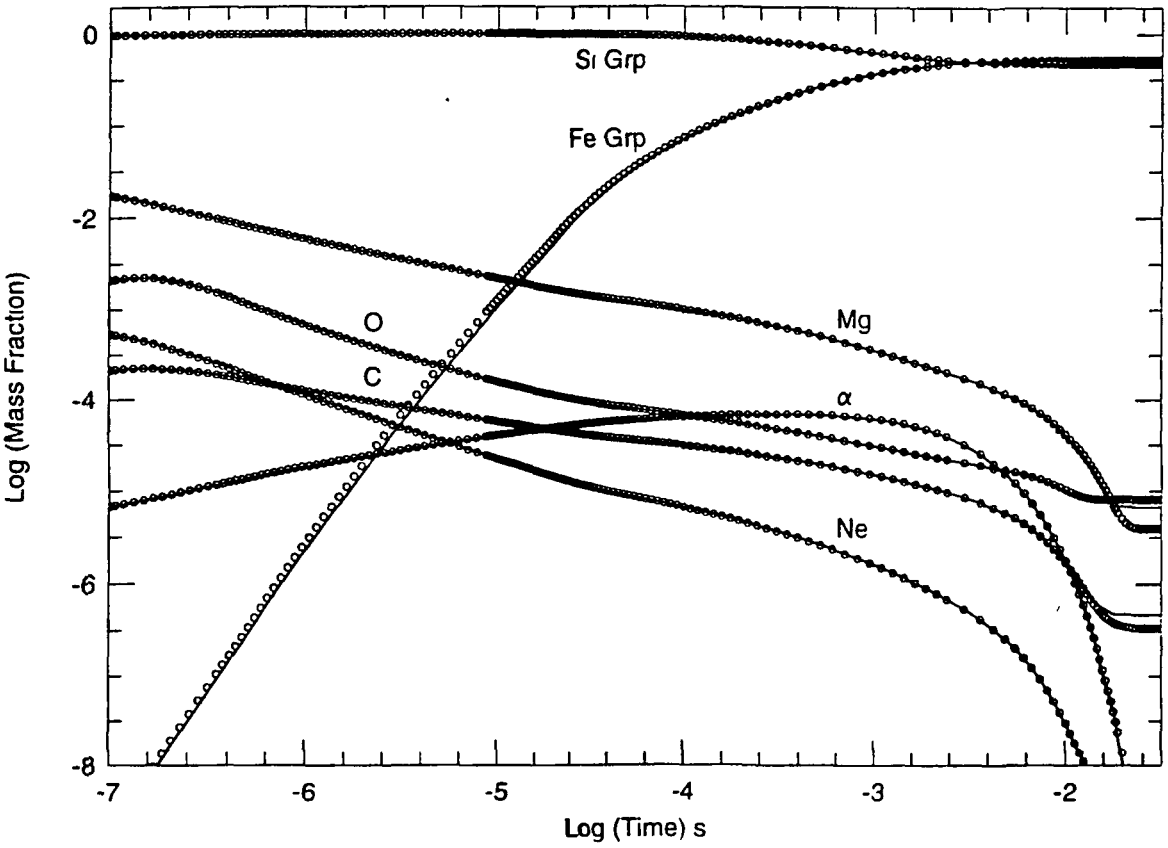

Figure 1. Temporal evolution of the group mass fractions for $T_{9i} = 5$ and $\rho_i = 10^9\,\mathrm{g\,cm^{-3}}$.

4. Explosive Silicon burning with the QSE-reduced α network

Because the products of hydrostatic silicon burning are trapped deep in the potential well of their parent star, it is only by explosion that the interstellar medium is enriched in intermediate mass and iron peak elements. Thus the ability to model explosive silicon burning is of particular importance, as even material which reaches NSE undergoes significant changes as it cools. For brevity sake, we will here concentrate on explosive burning, and refer the reader to Hix, Khokhlov, Wheeler & Thielemann (1998) for a more complete discussion of the application of this method.

To model silicon burning occurring as a result of shock heating, we will follow the approximation introduced by Fowler & Hoyle (1964). Therein a mass zone is instantaneously heated by a passing shock to some peak initial temperature, T_{9i}, and density, ρ_i, and then expands and cools adiabatically, with the timescale for the expansion given by the free fall timescale, $\tau_{\mathrm{HD}} = (24\pi G\rho)^{-1/2} = 446\rho_6^{-1/2}\mathrm{ms}$.

Figure 1 follows the evolution of the group mass fractions for an example of this explosive burning model starting from $T_{9i} = 5$ and $\rho_i = 10^9\,\mathrm{g\,cm^{-3}}$. Adiabatic cooling, which drops T_9 below 4 after 9.4 ms and below 3 after 21.6 ms, freezes out the nuclear reactions before NSE is reached, resulting in *incomplete silicon burning*, as discussed by Woosley *et al* (1973). The evolution of the mass fractions by the QSE-reduced network matches well with those evolved by its conventional counterpart, until T_9 approaches 3. Comparison of columns 2 & 3 of Table 1 reveals that the individual abundances also agree quite well With T_9=4, the individual abundances, even those as small as 10^{-9}, agree to within 5%.

Table 1. Comparison of network abundances for T_{9i}=5 0 and $\rho_i = 10^9\,\mathrm{g\,cm^{-3}}$.

Time (ms)	8.77		17 7		255
T_9	4.07		3.29		0.01
Nucleus	Y_{net}	Y_{qse}	Y_{net}	Y_{qse}	Y_{net}
^{4}He	7.90×10^{-7}	7.82×10^{-7}	1.04×10^{-8}	1.01×10^{-8}	1.94×10^{-14}
^{12}C	1.96×10^{-7}	1.96×10^{-7}	3.99×10^{-8}	3.23×10^{-8}	3.90×10^{-8}
^{16}O	7.34×10^{-7}	7.39×10^{-7}	$5\,26\times10^{-7}$	5.07×10^{-7}	$5\,27\times10^{-7}$
^{20}Ne	2.63×10^{-9}	2.63×10^{-9}	1.69×10^{-10}	1.48×10^{-10}	$9\,88\times10^{-11}$
^{24}Mg	$2\,24\times10^{-6}$	2.26×10^{-6}	2.88×10^{-7}	2.98×10^{-7}	2.80×10^{-7}
^{28}Si	$7\,65\times10^{-3}$	7.76×10^{-3}	7.58×10^{-3}	7.86×10^{-3}	7.58×10^{-3}
^{32}S	4.93×10^{-3}	4.96×10^{-3}	5.16×10^{-3}	5.15×10^{-3}	$5\,16\times10^{-3}$
^{36}Ar	1.43×10^{-3}	$1\,42\times10^{-3}$	1.27×10^{-3}	1.21×10^{-3}	1.27×10^{-3}
^{40}Ca	$1\,32\times10^{-3}$	$1\,30\times10^{-3}$	1.32×10^{-3}	1.22×10^{-3}	1.32×10^{-3}
^{44}Ti	7.07×10^{-6}	$6\,90\times10^{-6}$	1.96×10^{-6}	1.72×10^{-6}	1.69×10^{-6}
^{48}Cr	$5\,89\times10^{-5}$	5.58×10^{-5}	4.40×10^{-5}	1.19×10^{-5}	4.40×10^{-5}
^{52}Fe	7.17×10^{-4}	$6\,93\times10^{-4}$	$6\,33\times10^{-4}$	3.05×10^{-4}	$6\,33\times10^{-4}$
^{56}Ni	8.63×10^{-3}	8.60×10^{-3}	8.73×10^{-3}	9.04×10^{-3}	8.73×10^{-3}
^{60}Zn	6.18×10^{-8}	$6\,06\times10^{-8}$	3.26×10^{-9}	3.23×10^{-9}	4.38×10^{-10}

As the matter continues to cool, many of the photodisintegrations responsible for QSE freezeout between $T_9 = 3.5$ and 3, fragmenting the large QSE groups into smaller grouplets and individual nuclei as the remaining free α-particles are captured. This reduces the viability of a QSE based approach. While at T_9=3.3, the group abundances of the silicon and iron peak groups (which account for 99.9% of the mass) calculated by the QSE-reduced α network differ by less than 1% from the freezeout abundances of the conventional network, individual abundances are beginning to show larger variations. Comparison of columns 4 & 5 of Table 1 reveals that these variations are largest near the group boundaries. However, among the dominant nuclei the abundances are good to $\sim$ 10%. Comparison of the full network abundances at T_9=3.3 (column 4) with those at freezeout (column 6) reveals that only the free α-particle abundance, and those abundances comparable in size, are strongly affected by these final α-particle captures. Since the post-freezeout captures do not strongly affect the abundances, the abundances of the QSE-reduced network, frozen when $T_9 \sim 3.5$, provide reasonable estimates of the final abundances.

Figure 2 displays the evolution of another example of this explosive silicon burning model with $T_{9i} = 6$ and $\rho = 10^7\,\mathrm{g\,cm^{-3}}$. The lower density in this case results in a slower expansion, with T_9 reaching 5, 4, and 3 after 77, 172, and 293 milliseconds, respectively. Though the rate of cooling is relatively slow, the temperature drops too quickly for the large α-particle abundance to be completely incorporated into heavier nuclei, resulting in the *α-rich freezeout* of Woosley *et al* (1973). Even with this large over abundance of α-particles, the QSE-reduced network reliably tracks the group abundances until T_9 approaches 3.

As the material cools, the large α-particle abundance and resulting flow upward into the silicon group prevents the abundances within the silicon group from declining as rapidly as QSE requires, disrupting the QSE groups. Comparison of abundances calculated by the conventional α-particle network, at T_9=4, with those of its QSE-reduced

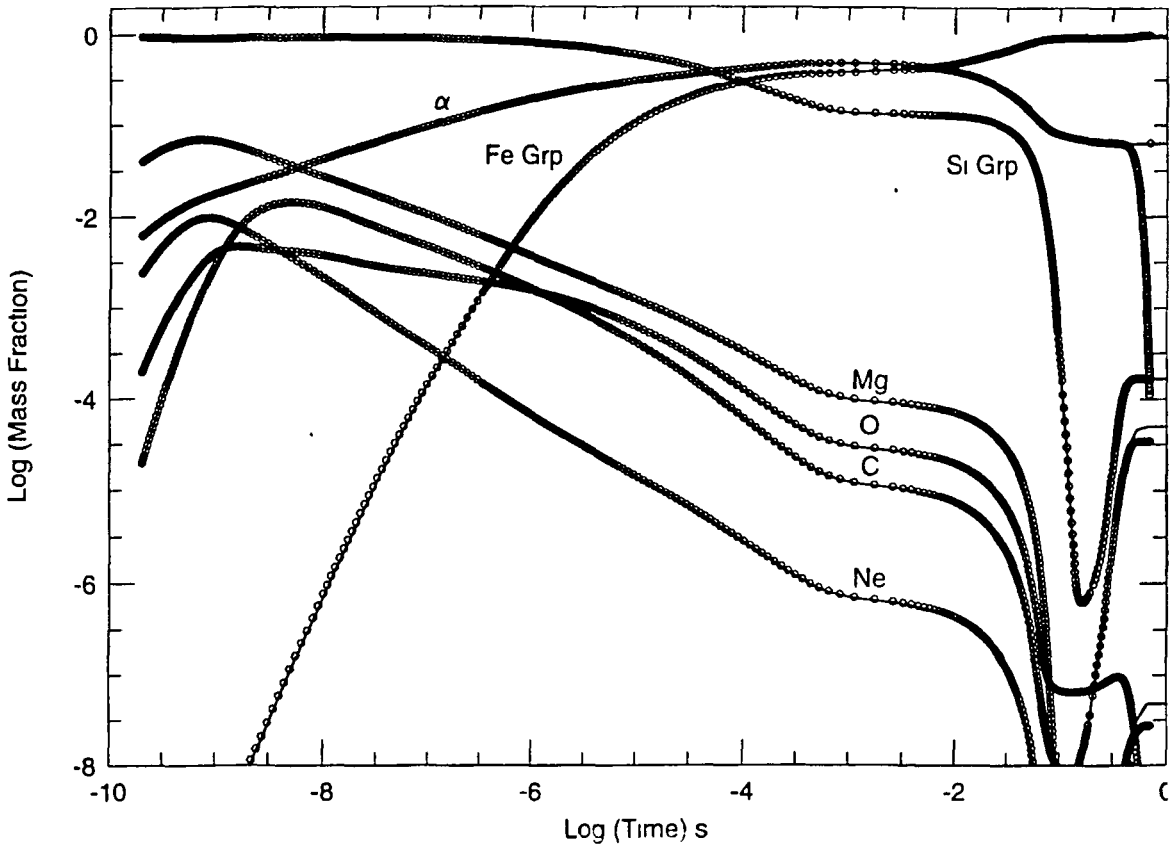

Figure 2. Temporal evolution of the group mass fractions for $T_{9_i} = 6$ and $\rho_i = 10^7\,\mathrm{g\,cm^{-3}}$.

counterpart (columns 2 & 3 of Table 2) shows the beginning of this process, with the abundances of ^{28}Si and ^{32}S much larger than QSE would predict. In spite of this breakdown in QSE, the abundances predicted for the more abundant members of the group agree well. As temperature continues to drop, the disruption of the QSE groups by the large α abundance continues. By the time T_9 drops to 3 (columns 4 & 5 of Table 2), the under prediction by QSE of the smaller group abundances also affects the iron peak group. However the abundances of the dominant nuclei, and hence the energy production, are still in good agreement. As the remaining photodisintegrations freezeout, the continued capture of the large abundance of α-particles results in significant abundances changes (column 6 of Table 2). However, even the conversion of 1.5% of the ^{56}Ni abundance to ^{60}Zn over several hundred milliseconds does not significantly affect the energy release of silicon burning.

5. Conclusion

We have shown that a QSE-reduced α network can be used as a replacement for full 14 element α network when modeling silicon burning without significant errors in energy generation or nucleosynthesis. Such an approach offers a significant reduction in the computational time spent on nucleosynthesis, a factor of 2 for this small system of equations. It also offers a reduction in the number of nuclear variables which must be included within a hydrodynamic model, a matter of concern for models with large numbers of zones or grid points. We plan to apply this method of QSE-reduction to

Table 2. Comparison of network abundances for T_{9i}=6 0 and ρ_i=10^7 g cm^{-3}.

Time (s)	.174		.290		2.67
T_9	3 98		3.02		0.01
Nucleus	Y_{net}	Y_{qse}	Y_{net}	Y_{qse}	Y_{net}
^{4}He	$1\ 73\times10^{-2}$	1.71×10^{-2}	1.62×10^{-2}	1.61×10^{-2}	1.57×10^{-2}
^{12}C	1.60×10^{-9}	$1\ 58\times10^{-9}$	9.76×10^{-8}	9.62×10^{-8}	4.18×10^{-6}
^{16}O	4.24×10^{-9}	4.19×10^{-9}	5.51×10^{-9}	5.45×10^{-9}	2.16×10^{-10}
^{20}Ne	8.55×10^{-12}	8.46×10^{-12}	7.05×10^{-11}	6.96×10^{-11}	2.92×10^{-10}
^{24}Mg	4.38×10^{-12}	4.33×10^{-12}	3.25×10^{-11}	$3\ 21\times10^{-11}$	2.00×10^{-9}
^{28}Si	1.92×10^{-11}	$6\ 39\times10^{-14}$	1.92×10^{-10}	8.10×10^{-22}	2.95×10^{-9}
^{32}S	4.94×10^{-11}	$4\ 42\times10^{-12}$	5.34×10^{-10}	2.14×10^{-17}	2.08×10^{-8}
^{36}Ar	2.60×10^{-10}	$1\ 26\times10^{-10}$	2.46×10^{-9}	1.73×10^{-13}	1.59×10^{-7}
^{40}Ca	1.19×10^{-8}	$1\ 12\times10^{-8}$	1.90×10^{-8}	6.44×10^{-9}	4.18×10^{-7}
^{44}Ti	4.73×10^{-9}	4.68×10^{-9}	1.71×10^{-7}	$1\ 69\times10^{-7}$	3.26×10^{-6}
^{48}Cr	$1\ 88\times10^{-8}$	1.51×10^{-8}	2.19×10^{-8}	1.26×10^{-14}	$2\ 55\times10^{-6}$
^{52}Fe	1.59×10^{-5}	1.61×10^{-5}	9.26×10^{-7}	1.35×10^{-8}	4.50×10^{-6}
^{56}Ni	1.66×10^{-2}	1.66×10^{-2}	1.67×10^{-2}	1.67×10^{-2}	1.64×10^{-2}
^{60}Zn	6.50×10^{-6}	$6\ 39\times10^{-6}$	4.23×10^{-5}	4.15×10^{-5}	2.97×10^{-4}

larger nuclear networks, where the potential for improvement in speed and size is even greater. For larger networks, reduction in the number of nuclei by a factor of 2-4 could result in a increases in network speed of a factor of 5-10 because of the nonlinear relation between matrix size and the length of time to solve a matrix equation.

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