The QSE-Reduced Network for Silicon Burning

Suzanne Parete-Koon

University of Tennessee
E-mail: `espresso@utk.edu`

W. Raphael Hix

Oak Ridge National Laboratory/University of Tennessee
E-mail: `raph@ornl.gov`

Christian Freiburghaus

University of Basel

Friedrich-Karl Thielemann

University of Basel
E-mail: `F-K.Thielemann@unibas.ch`

Iron and neighboring nuclei are formed in massive stars before core collapse and during supernova outbursts. Complete and incomplete silicon burning is responsible for the production of a wide range of nuclei with atomic mass numbers from 28 to 70. Because of the large number of nuclei involved, accurate modeling of silicon burning is computationally expensive. Examination of the physics of silicon burning reveals that the nuclear evolution is dominated by large groups of nuclei in mutual equilibrium. We present a hybrid equilibrium scheme, which takes advantage of this quasi-equilibrium (QSE) in order to reduce the number of independent variables calculated. This allows accurate prediction of the nuclear abundance evolution, deleptionization, and energy generation. During silicon burning the QSE-reduced network runs about an order of magnitude faster than the full network that it replaces and requires roughly a third as many variables without a significant loss of accuracy. These reductions in computational cost make the QSE-reduced network well suited for inclusion within hydrodynamic simulations, particularly in multi-dimensional applications.

1. Introduction

A nuclear reaction network serves two primary purposes in astrophysical models, first to accurately calculate the rate of thermonuclear energy generation and second to follow the evolution of the abundances of the nuclear species. At the heart of a nuclear reaction network is a matrix solution, so the computational cost of solving the network grows nonlinearly with the number of nuclei included in the calculation.

Because of the wide range of nuclei involved, from A =28 to A=70, the computational time needed to model silicon burning during stellar evolution often exceeds that of all other burning stages [1]. For this reason, hydrodynamic models of supernovae often employ a limited set of nuclei, such as an α-network, to achieve the necessary speed to calculate the nuclear energy generation during silicon burning. However, α-networks exclude many of the reaction channels important for iron formation, making them a partial solution at best for following the energy generation during silicon burning [2], [3].

Silicon burning proceeds from silicon to iron peak nuclei through a long chain of competing photodisintegrations and light particle captures. The final state of silicon burning is a nuclear statistical equilibrium (NSE) where the photodisintegrations are balanced by the light particle capture reactions. Modelers of the core collapse supernova mechanism trace the composition only during NSE, largely ignoring the elemental composition at lower temperatures [4],[5]. To allow models to better match observations, an efficient but more complete scheme for modeling iron formation *in situ* in hydrodynamic supernova simulations is needed.

2. The QSE-Reduced Network

NSE grows from several small groups of nuclei, which reach mutual equilibrium among themselves. These are called quasi-statistical equilibrium (QSE) groups. The abundances of all nuclei within a QSE group can be calculated if the abundance of one member of the group is known. This greatly reduces the number of variables that must be tracked in a nucleosynthesis calculation without sacrificing accuracy even at temperatures too low to maintain NSE [6][7][8]. For nuclei in quasi equilibrium with ^{28}Si the individual abundances can be calculated by :

$$Y_{QSE,Si}(^{A}Z) = \frac{C(^{A}Z)}{C(^{28}Si)} Y(^{28}Si) Y_{p}^{Z-14} Y_{n}^{N-14}$$

$$C(^{A}Z) = \frac{G(^{A}Z)}{2^{A}} \left(\frac{\rho N_{A}}{\theta}\right)^{A-1} A^{3/2} \exp\left(\frac{B(^{A}Z)}{k_{B}T}\right)$$

$$\theta = \left(\frac{m_{v} k_{B} T}{2\pi \hbar^{2}}\right)^{3/2}$$

Where A is the atomic number, Z, is the proton number. G(^{A}Z) and B(^{A}Z) are the partition function and the binding energy of the nucleus ^{A}Z, N$_{A}$ is Avogadro's number, k_{B} is Boltzmann's constant, and ρ and T are the density and temperature of the plasma. Y_{p} and Y_{n} are the abundances of free protons and neutrons and the integers $(N-14)$ and $(Z-14)$ are the number

of such nucleons needed to construct the nucleus $^A Z$ from ^{28}Si. A similar expression can be written for each QSE group using its focal nucleus in place of ^{28}Si.

We compare a full network composed of 299 independently evolved nuclei with a QSE-reduced network that utilizes three QSE groups: one centered around ^{28}Si, one centered around ^{56}Ni, and one formed by the lightest nuclei, which are held in equilibrium with each other by the balance of reactions among the members of the other two QSE groups. The focal abundances for each QSE group and the nuclei that must still be evolved independently form the reduced set of abundance.

For the purpose of showing the accuracy and speed of the QSE network compared to the full network, we test the QSE network with two definitions of group membership. The first has smaller QSE groups, here after SQSE, and uses 119 variables to evolve 299 nuclei. For the second form, LQSE, larger QSE groups are used so that only 82 variables are required to evolve 299 nuclei. To compare the full network and the QSE network under realistic conditions, we have used the prescription introduced by Fowler and Hoyle [9], an adiabatic expansion, to approximate the evolution of the density and temperature during the explosion. Both networks use the same LU decomposition routines to solve the matrix. In both networks the method of calculating the new time step for each iteration is the same.

3. Silicon Burning

Initial conditions of 5 GK coupled with a peak density of 10^9 g cm^{-3} lead to incomplete silicon burning. Figure 1a shows that the large abundances freeze out just after 3.5 GK. Figure 1b shows that the reduced networks reproduce the energy generation rate of the full network. Subfigures 1c and 1d show the details of the equilibrium at its lower temperature limit. For both LQSE and SQSE most of the nuclei agree to 12% down to 3.5 GK. By 3.0 GK most SQSE nuclei agree to within 50% and nuclei with mass fractions greater than 10^{-3} agree to 20%. Similar results were achieved for initial conditions of T_i =7 GK and ρ_i =10^9 g cm^{-3}, which lead to complete silicon burning.
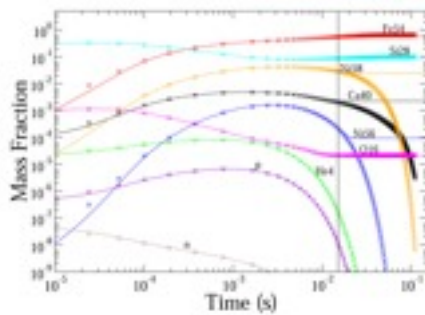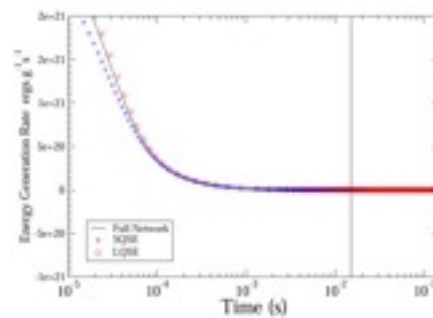
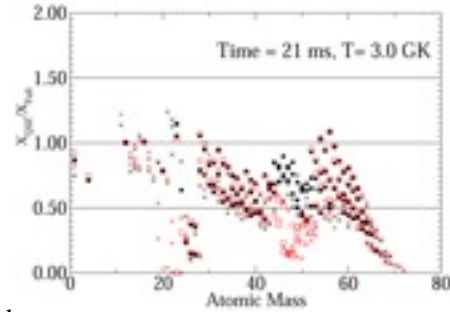1a   1b
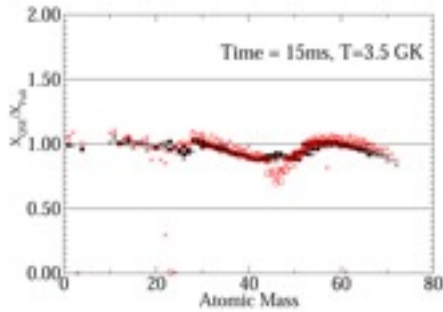
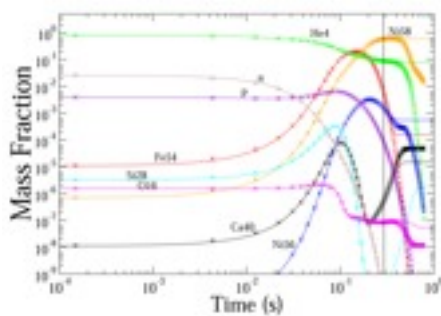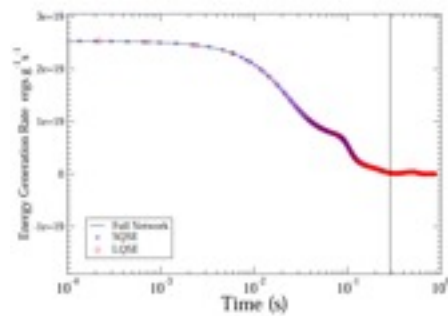1c   1d

Subfigure a shows the mass fractions of several nuclei plotted as a function of time. Solid lines are the full network, X's represent the LQSE results. Subfigure b shows the energy generation rate as a function of time. For a and b, a vertical black line marks 3.5 GK. Subfigures c and d show the ratio of mass fractions (QSE/Full network) for all nuclei. Black indicates SQSE and red indicates LQSE. Circles are dominant nuclei with mass fractions larger than 10^{-6}. The squares are mass fractions between 10^{-6} and 10^{-12}. The X's are mass fractions between 10^{-12} and 10^{-20}.

4. Silicon Burning with Alpha-Rich Freezeout

Initial conditions of $T_i = 7$ GK and $\rho_i = 10^7$ g cm^{-3} lead to silicon burning with an alpha-rich freezeout. For most iron peak nuclei both LQSE and SQSE agree to 20% down to a temperature of 3.0 GK. However, alpha-rich freezeout conditions are the most challenging for QSE-reduced networks, due to small abundances in the region around Si and the resulting breakdown in this QSE group. Figure 3c shows large deviations for a number of nuclei already at 3.5 GK. However, the dominant nuclei, n, p, alpha and iron/nickel nuclei are well reproduced for both LQSE and SQSE. Figure 3b shows that the reduced networks still reproduce the energy generation of the full network.

3a   3b
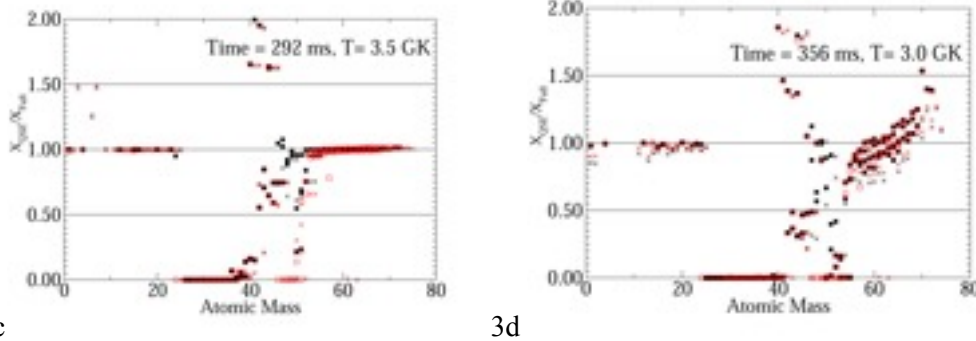
3c   3d

Subfigure a shows the mass fractions of several nuclei plotted as a function of time. Solid lines are the full network, X's represent the LQSE results. Subfigure b shows the energy generation rate as a function of time. For a and b, a vertical black line marks 3.5 GK. Subfigures c and d show the ratio of mass fractions (QSE/Full network) for all nuclei. Black indicates SQSE and red indicates LQSE. Circles are dominant nuclei with mass fractions larger than 10^{-6}. The squares are mass fractions between 10^{-6} and 10^{-12}. The X's are mass fractions between 10^{-12} and 10^{-20}.

5. Network Speed

Run	CPU Time Case 1	Matrix Solve Time Case 1	CPU Time Case 2	Matrix Solve time Case 2	CPU Time Case 3	Matrix Solve time Case 3	Time Step Count	Iteration Count
Incomplete Si Burning								
SQSE	3.74	0.87	8.71	1.47	10.49	2.88	529	1878
LQSE	1.92	0.26	4.07	0.45	4.62	0.73	404	1379
FULL	9.78	9.73	26.37	22.39	181.81	177.70	457	1423
Complete Si Burning								
SQSE	3.36	0.74	7.82	1.39	10.45	3.71	511	1370
LQSE	1.86	0.25	3.95	0.44	4.34	0.7	386	1311
FULL	11.38	10.09	21.6	18.2	136.75	135.86	365	1381
α-rich Freezeout								
SQSE	4.06	0.92	9.5	1.7	11.09	3.08	598	2184
LQSE	2.04	0.32	4.88	0.57	5.15	0.8	455	1640
FULL	17.04	15.22	39.77	30.75	167	200.85	529	1451

Table 1. Time comparisons (in sec.) for the QSE-reduced networks and the full network. Cases: 1=LAPACK, Itanium2; 2=LAPACK, Pentium4; 3=Numerical Recipes, Pentium4.

Table 1 shows that depending on the solver and processor used, the conservative SQSE network runs 3 to 17 times faster than the full network and the LQSE network runs 5 to 31 times faster than the full network. For LQSE, the LAPACK matrix solve was on average 100 times faster than the full network and for SQSE it was on average 30 times faster than the full network. The effect of the faster matrix solve in the reduced network is mitigated by the longer

time that is required to build the reduced Jacobian matrix. The QSE-reduced network is still under development and the speed of the Jacobian build is expected to improve. For each case, all networks ran from the peak temperature down to a temperature of 3.5 GK.

6. Conclusion

We have demonstrated the ability of QSE to greatly reduce the number of independent nuclear species that need to be evolved to accurately track nucleosynthesis during silicon burning. A network reduced in this fashion provides a good estimate of the nuclear energy generation and elemental production even in cases where thermodynamic variations result in incomplete silicon burning or α-rich freezeout. We envision two applications for the QSE-reduced network. First, as a replacement for α networks, the QSE-reduced network allows much more accurate modeling of the nuclear energy generation, making post-processing results more reliable. Second, as a bridge between NSE and a conventional network operating above 3.5 GK, the QSE-reduced network will enable fully consistent, *in situ* calculations of the nuclear evolution. Both of these applications will be aided by future improvements in the construction of the reduced Jacobian and the implementation of dynamic QSE groups. The latter enhancement will greatly aid accuracy as the groups fragment at lower temperatures while further improving speed at higher temperatures.

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