A hypothesis or theory is clear, decisive, and positive,
but it is believed by no one but the person who created it.
Experimental findings, on the other hand, are messy, inexact things,
which are believed by everyone except the person
who did that work.

Harlow Shapley
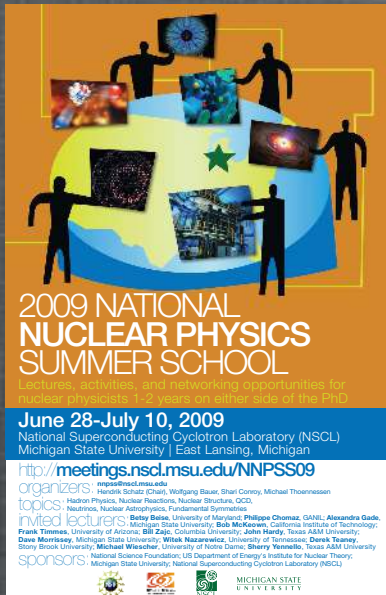Through Rugged Ways to the Stars

Nuclear Astrophysics: Reaction Networks

Frank Timmes

Outline for 30Jun2009

1. CNO cycles

2. Time integration

3. Jacobian formation

4. Alpha - chains

cococubed.asu.edu

www.jinaweb.org

Break-out reactions from the CNO cycles
www.iop.org/EJ/abstract/0954-3899/25/6/201

An Inexpensive Nuclear Energy Generation Network ...
www.iop.org/EJ/abstract/0067-0049/129/1/377/

Last Lecture

P + P $\xrightarrow{10^{10} \text{ yr}}$ PN + e⁺ + ν

produces
99.75%
²H

P + P + e⁻ $\xrightarrow{10^{13} \text{ yr}}$ PN + ν

produces
0.25%
²H

PN + P $\xrightarrow{6 \text{ sec}}$ PPN + γ ray

PP I branch
86% of ³He

PPN + PPN $\xrightarrow{3 \times 10^5 \text{ yr}}$ NPPN + P + P

PP II branch
14% of ³He

PPN + NPPN $\xrightarrow{1.4 \times 10^6 \text{ yr}}$ ⁷Be + γ ray

⁷Be + e⁻ $\xrightarrow{0.5 \text{ yr}}$ ⁷Li + ν

⁷Li + P $\xrightarrow{800 \text{ sec}}$ NPPN + NPPN

PP III branch
0.1% of ³He

PPN + NPPN $\xrightarrow{1.4 \times 10^6 \text{ yr}}$ ⁷Be + γ ray

⁷Be + P $\xrightarrow{95 \text{ yr}}$ ⁸B + γ ray

⁸B $\xrightarrow{1 \text{ sec}}$ ⁸Be + e⁺ + ν

⁸Be $\xrightarrow{10^{-8} \text{ sec}}$ NPPN + NPPN
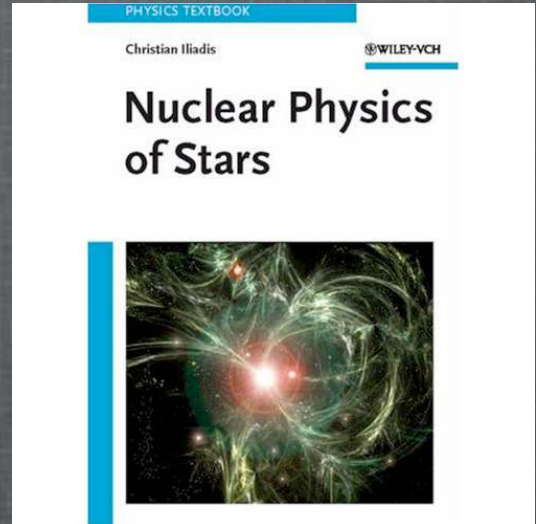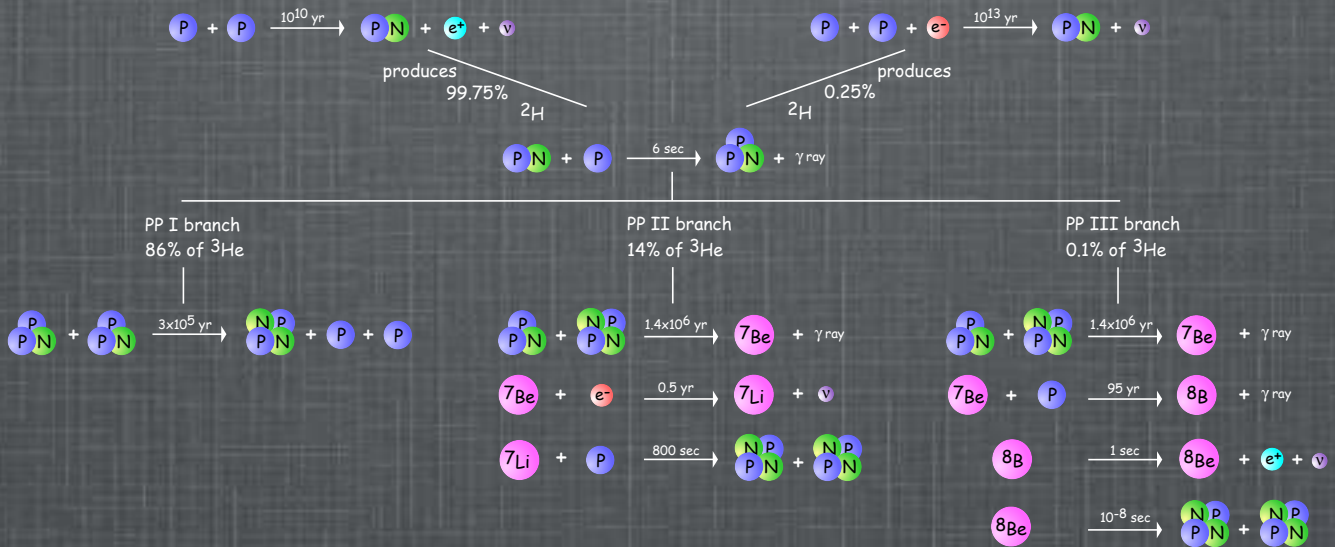
The weights of the reactions are given for conditions in the Sun.
The PP chains are the most important energy source in stars with masses less than 1.5 M$_{sun}$.

An answer to yesterday's task

* hydrostatic: btemp= 1.500E+07 bden= 1.600E+02
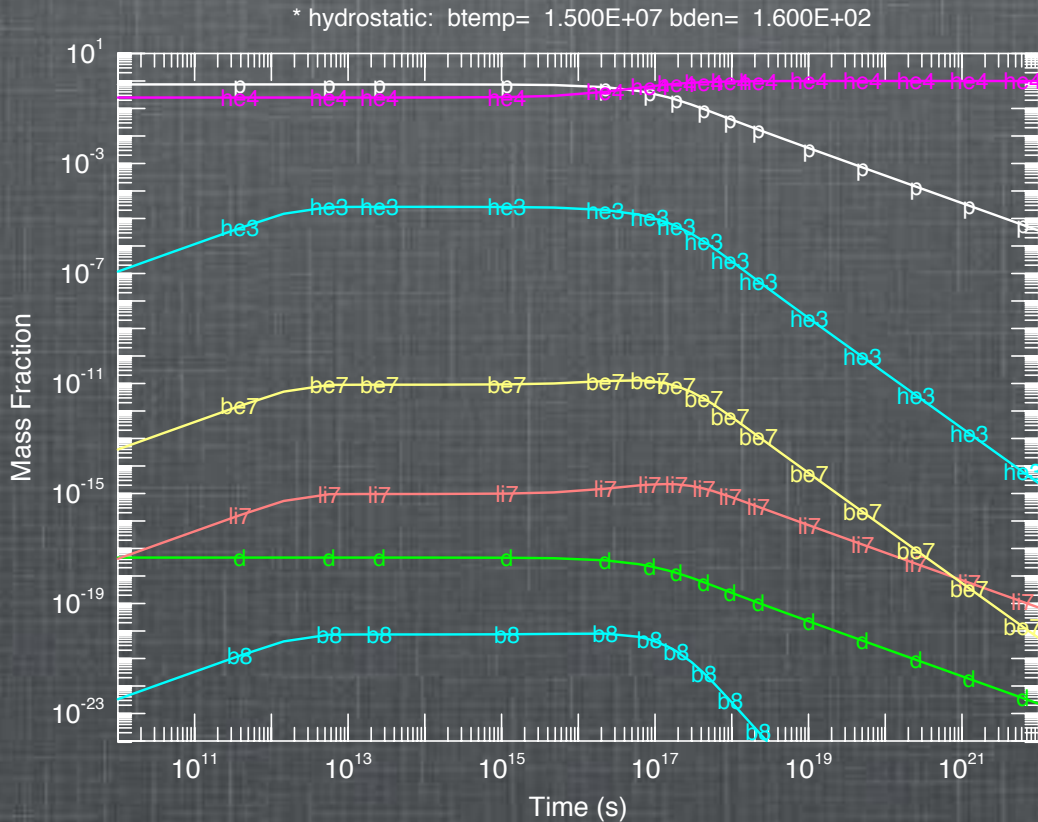
Some nomenclature

β^- decay : $n \rightarrow p + e^- + \overline{\nu_e}$
$$(Z, A) \rightarrow (Z + 1, A) + e^- + \overline{\nu_e}$$

β^+ decay : $p \rightarrow n + e^+ + \nu_e$
$$(Z, A) \rightarrow (Z - 1, A) + e^+ + \nu_e$$

electron capture : $p + e^- \rightarrow n + \nu_e$
$$(Z, A) + e^- \rightarrow (Z - 1, A) + \nu_e$$

positron capture : $n + e^+ \rightarrow p + \overline{\nu_e}$
$$(Z, A) + e^+ \rightarrow (Z + 1, A) + \overline{\nu_e}$$

CNO cycles

It was independently suggested by Bethe & von Weizsäcker in 1939 that reactions of protons with carbon and nitrogen would provide competition with the PP-chains.

They showed that the CNO cycle had the property that CNO nuclei served only as catalysts for the conversion of H into He.

The first CNO cycle is

$$^{12}C(p, \gamma)^{13}N(, e^+\nu)^{13}C$$

$$^{13}C(p, \gamma)^{14}N$$

$$^{14}N(p, \gamma)^{15}O(, e^+\nu)^{15}N$$

$$^{15}N(p, \alpha)^{12}C$$
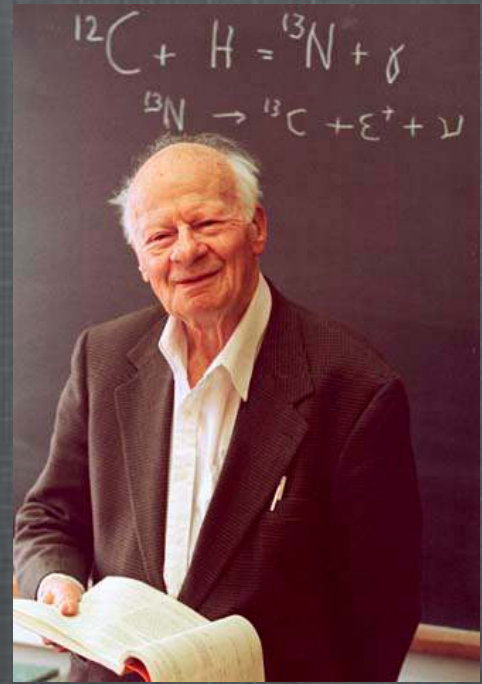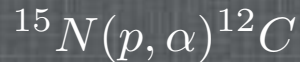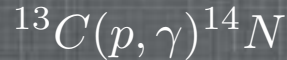
Summing the particles before and after the cycle one obtains

$$^{12}C + 4H \rightarrow^{12} C +^4 He + 2\beta^+ + 2\nu$$
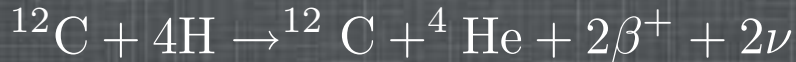
^{12}C only plays the role of a catalyst.

The cycle occurs with any of the four nuclei ^{12}C, ^{13}C, ^{14}N, ^{15}N as catalyst, or any mixture of them.

In fact, a mixture of those nuclei soon results regardless of the initial composition.
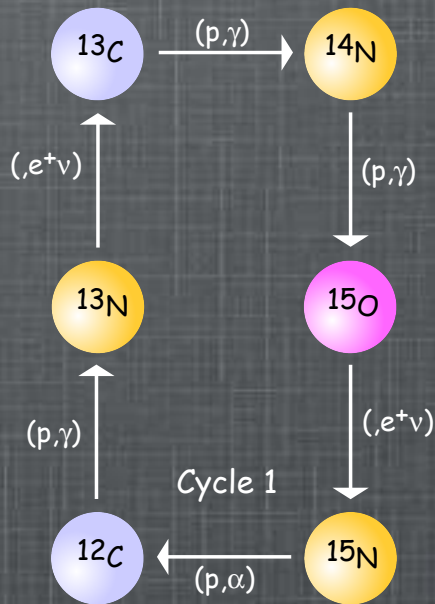
The energy generated is related to the reciprocal of the time it takes to go around the cycle multiplied by $(4M_H - M_{He4})c^2$ minus the energy loss in the two neutrinos.

It was later realized that all the stable oxygen isotopes provide additional cycles.
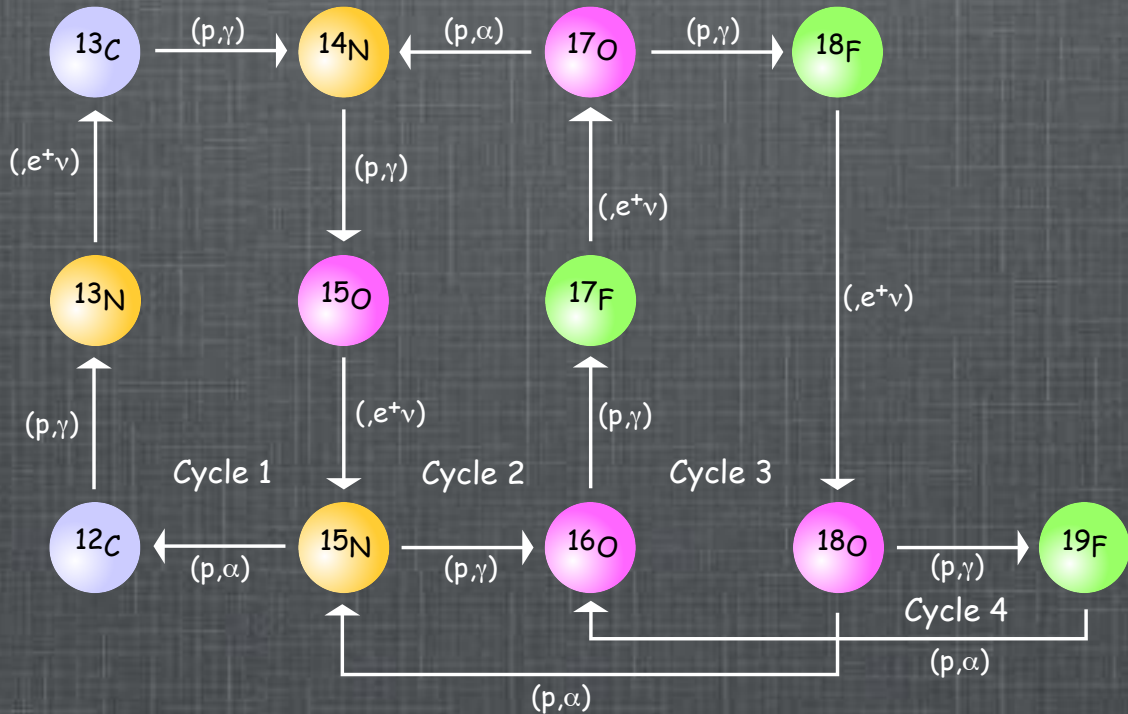
We have been assuming the β decay lifetimes are negligible.
For $0.2 < T_9 < 0.5$, the "hot" or "β-limited" CNO cycles dominate.
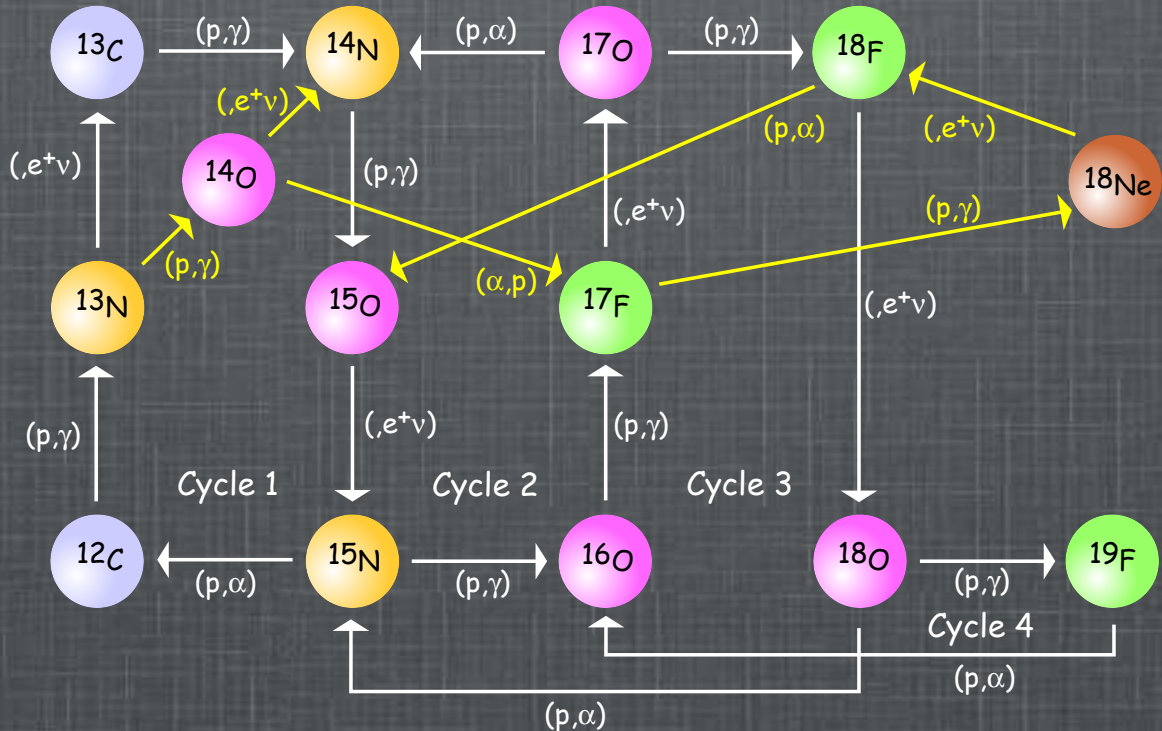
If $T_9 > 0.5$, then one breaks out of the β-limited CNO cycles and begins a journey on the rapid-proton capture process.
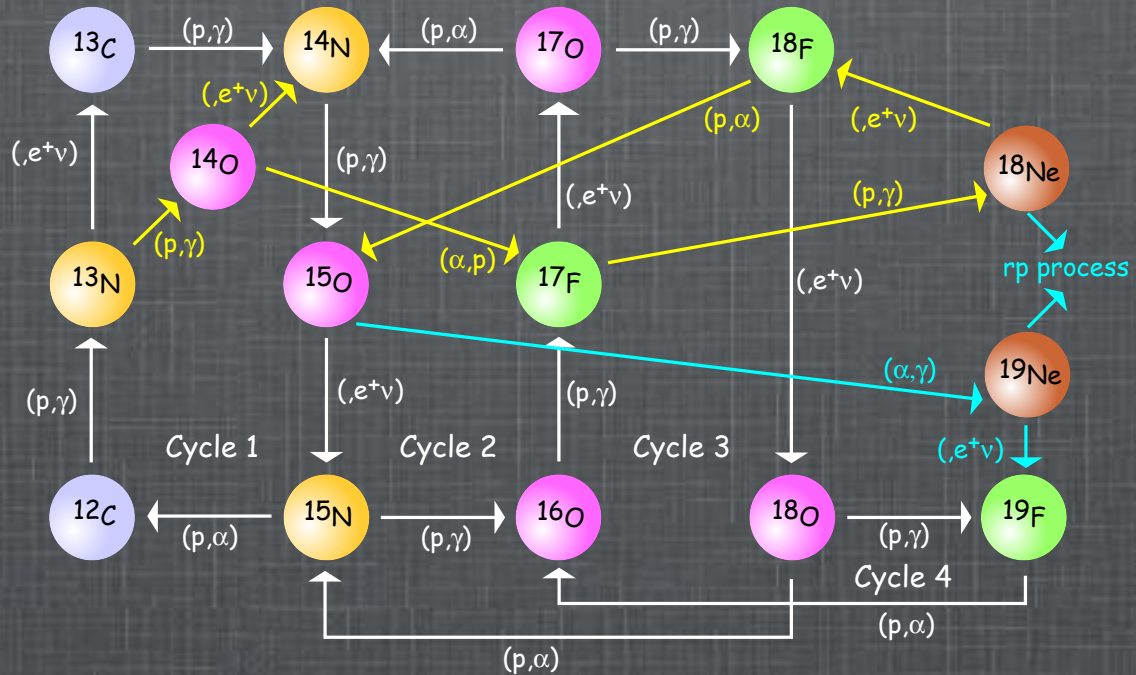
CNO: $T_9 < 0.2$ Hot CNO: $0.2 < T_9 < 0.5$ rp process: $T_9 > 0.5$

Prior to 1952 it was thought the CNO cycles generated most of the energy in the Sun. Edwin Salpeter showed the p(p,e⁺ν)d reaction was about an order of magnitude larger than previously believed.

Density=100 gr/cm^3 Z=Z$_{sun}$

Scan ©American Institute of Physics
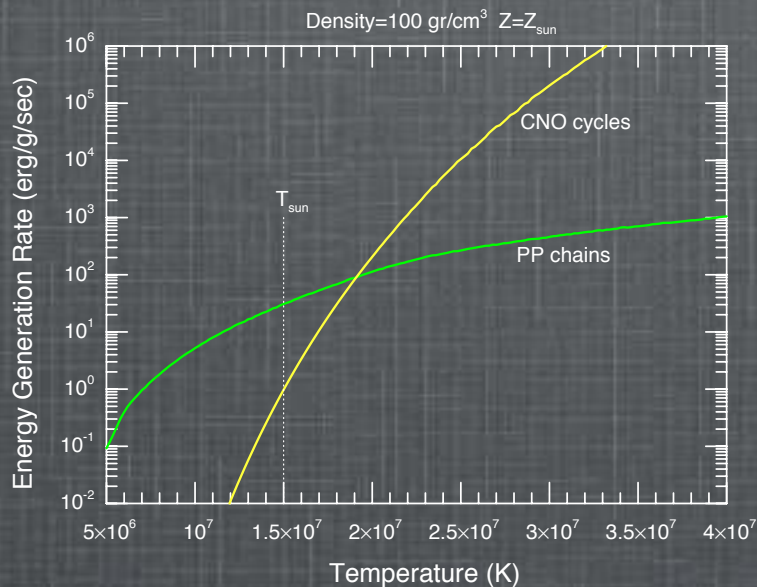
This brought about a reversal in the roles thought to be played by the two hydrogen burning mechanisms in the Sun.

Tasks for the day

Download, compile, and run the CNO cycle code from
www.cococubed.com/code_pages/burn.shtml

Verify the ODEs for the first CNO cycle.

Run the code for $T = 30 \times 10^6$ K, $\varrho = 100$ g/cm^3, and an initial
composition of $X(^{12}C) = X(^{16}O) = 0.1$.
Plot the abundance evolution.
What isotope is most abundant when the cycle is in equilibrium?
How long does it take for hydrogen to be depleted?

The Frontiers of Nuclear Science
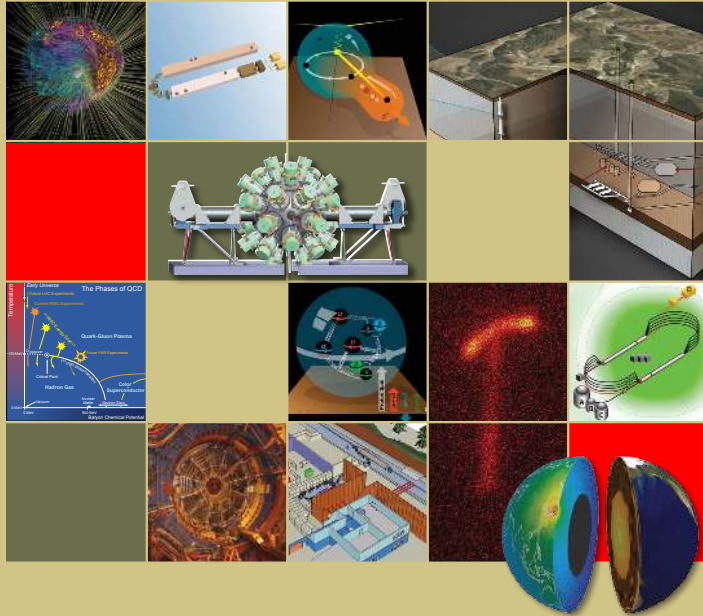
December 2007

The Frontiers of Nuclear Science

A LONG RANGE PLAN

The ODEs from nuclear reaction networks are nonlinear and stiff.

This means we'll be doing an implicit integration, which in turn means we'll be forming a Jacobian matrix and doing linear algebra.

Physically a stiff system of ODEs means some isotopes are changing on much faster timescales than other isotopes.
The hydrogen burning PPI chain is an excellent example.
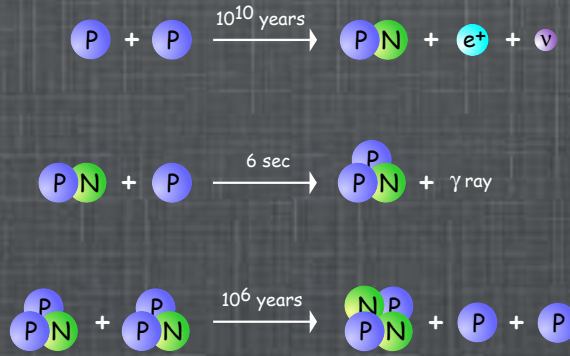
Mathematically, stiffness means the ratio of the maximum to the minimum eigenvalues λj of the Jacobian matrix are large.

$$\mathcal{S} = \frac{\max|\text{Re}(\lambda_j)|}{\min|\text{Re}(\lambda_j)|} \gg 1$$

$S > 10^{15}$ is not uncommon in nuclear astrophysics.

Pragmatically, stiffness means that an implicit time integration is typically needed to solve the initial value problem.

This means we'll be solving (large) systems of linear equations. As the linear algebra will generally dominate the time to obtain a solution, we'll want to use efficient solvers.

Our system of ODEs

$$\dot{Y}_i = \sum_j C_i R_j Y_j + \sum_{jk} \frac{C_i}{C_j! C_k!} R_{jk} Y_j Y_k + \sum_{jkl} \frac{C_i}{C_j! C_k! C_l!} R_{jk} Y_j Y_k Y_l$$

may be written in vector form as

$$\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$$

The Jacobian matrix is the derivative of the ODEs with respect to their dependent variables

$$\tilde{J} = \frac{\partial \mathbf{f}}{\partial \mathbf{y}}$$

Let's do an example of forming the Jacobian matrix ...

Consider the ^{12}C$(\alpha,\gamma)^{16}$O reaction proceeding at a rate R.

$$\dot{Y}(^4\text{He}) = -Y(^4\text{He})\ Y(^{12}\text{C})\ R + \ldots$$
$$\dot{Y}(^{12}\text{C}) = -Y(^4\text{He})\ Y(^{12}\text{C})\ R + \ldots$$
$$\dot{Y}(^{16}\text{O}) = +Y(^4\text{He})\ Y(^{12}\text{C})\ R + \ldots$$

Each right hand side contributes two Jacobian matrix elements:

$$J(^4\text{He},^4\text{He}) = \partial\dot{Y}(^4\text{He})/\partial Y(^4\text{He}) = -Y(^{12}\text{C})\ R + \ldots$$

$$J(^4\text{He},^{12}\text{C}) = \partial\dot{Y}(^4\text{He})/\partial Y(^{12}\text{C}) = -Y(^4\text{He})\ R + \ldots$$

$$J(^{12}\text{C},^4\text{He}) = \partial\dot{Y}(^{12}\text{C})/\partial Y(^4\text{He}) = -Y(^{12}\text{C})\ R + \ldots$$

$$J(^{12}\text{C},^{12}\text{C}) = \partial\dot{Y}(^{12}\text{C})/\partial Y(^{12}\text{C}) = -Y(^4\text{He})\ R + \ldots$$

$$J(^{16}\text{O},^4\text{He}) = \partial\dot{Y}(^{16}\text{O})/\partial Y(^4\text{He}) = +Y(^{12}\text{C})\ R + \ldots$$

$$J(^{16}\text{O},^{12}\text{C}) = \partial\dot{Y}(^{16}\text{O})/\partial Y(^{12}\text{C}) = +Y(^4\text{He})\ R + \ldots$$

The Jabobian matrix elements represent flows into (positive) or out of (negative) an isotope.

47 Isotopes
279 Rates
75.3% Sparse
Flows (#/sec):
1.85E+14
1.35E+11
9.77E+07
7.09E+04
5.15E+01
-2.67E+01
-3.68E+04
-5.07E+07
-6.98E+10
-9.62E+13
-1.32E+17
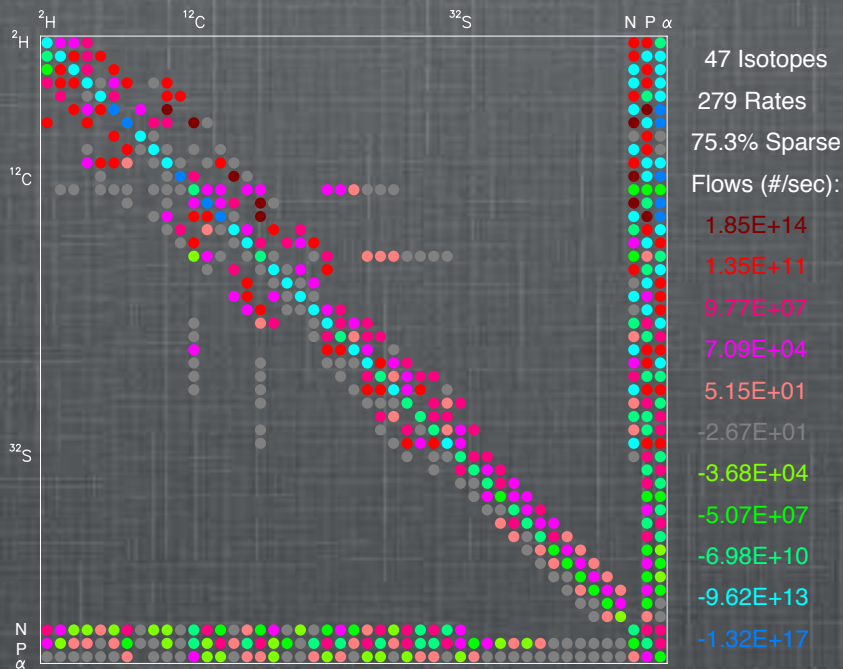
The matrix is not positive-definite or symmetric as reactions rates are not usually equal, but they are typically diagonally dominant.

The pattern of nonzeros doesn't change with time, but each matrix element may change in magnitude or sign as the temperature, density, or abundances change with time.

76 Isotopes
582 Rates
82.0% Sparse
Flows (#/sec):
3.05E+13
3.29E+10
0.56E+07
3.84E+04
4.15E+01
-2.23E+01
-2.07E+04
-1.91E+07
-1.77E+10
-1.64E+13
-1.52E+16
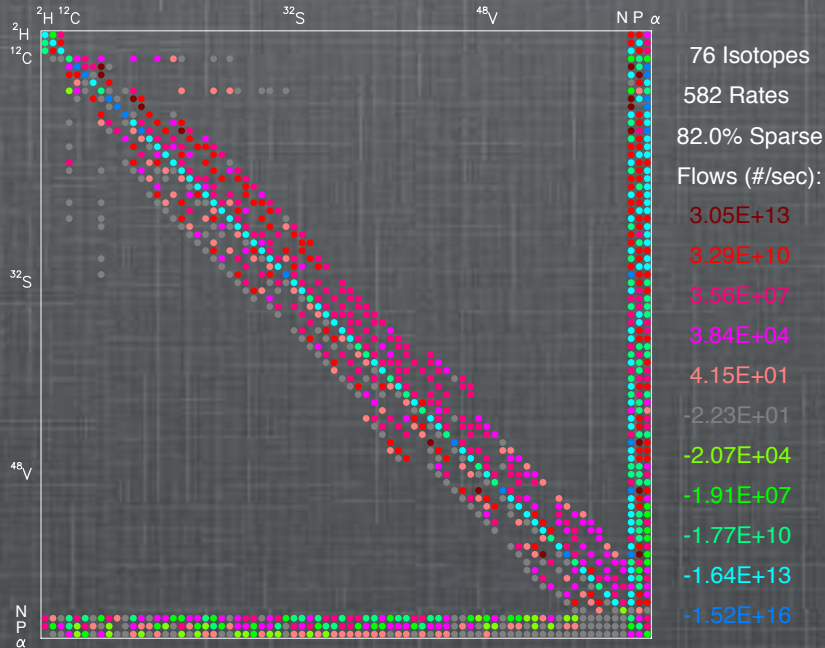
The matrices get sparser as the number of isotopes increase.

In principal every species reacts with every other species, resulting in a full, dense Jacobian matrix. In practice it is possible to neglect most of these reactions.

Captures of n, p, d, t, ^{3}He and α on heavy nuclei are easier than fusions of heavier nuclei because of the $Z_i\, Z_j$ dependence of the repulsive Coulomb term in the nuclear potential.

With the exception of the PP-chains and Big Bang nucleosynthesis, reactions involving d, t, and ^{3}He are negligible because their abundances are effectively zero.

Photodisintegrations tend to eject free nucleons or α-particles.

With a few important exceptions, we only need to consider twelve reactions linking a nucleus to its neighbors by the capture of an n, p, α or γ and release a different one of these four.

200 Isotopes
2134 Rates
91.9% Sparse
Flows (#/sec):
1.85E+14
1.34E+11
9.75E+07
7.07E+04
5.13E+01
-2.69E+01
-3.70E+04
-5.10E+07
-7.03E+10
-9.69E+13
-1.34E+17
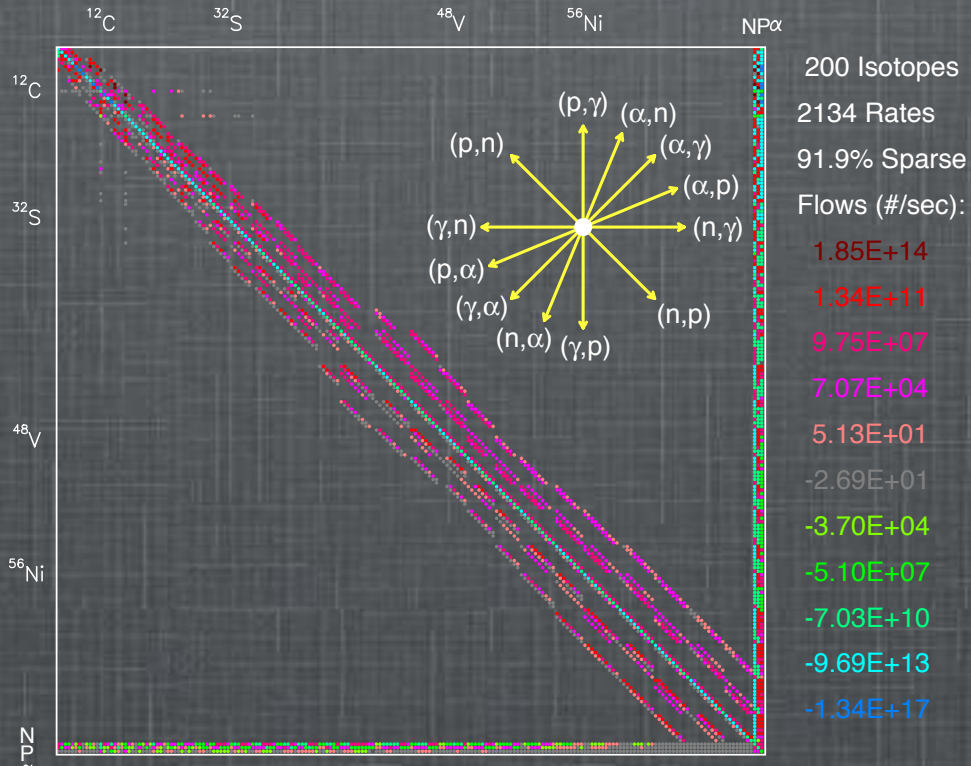
Interlude

The Medical Alchemist
Franz Christoph Janneck,
(1703 – 1761)
Oil on copper – 13" x 9"

Time Integration

$$\dot{y} = -y \longrightarrow y(t) = y(0)e^{-t}$$

In explicit methods, the state at the next time instant is computed as a function of the state at the previous time instant.

$$\frac{\Delta y}{\Delta t} = \frac{y(t + \Delta t) - y(t)}{\Delta t} = -y(t)$$

$$y(t + \Delta t) = y(t)(1 - \Delta t) \longrightarrow -\infty \text{ as } \Delta t \to \infty \qquad |1 - \Delta t| < 1$$

In implicit methods, the state at the next time instant is computed as a function of the state at the next time instant.

$$\frac{\Delta y}{\Delta t} = \frac{y(t + \Delta t) - y(t)}{\Delta t} = -y(t + \Delta t)$$

$$y(t + \Delta t) = \frac{y(t)}{1 + \Delta t} \longrightarrow 0 \text{ as } \Delta t \to \infty \qquad |1 + \Delta t| > 1$$

Given the initial conditions (temperature, density, composition), we wish to evolve the stiff ODEs that represent our reaction network.

$$\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$$

We'll take a look at several (but not all) implicit methods Nearly all of these methods are in active use among various researchers.

A good ODE integrator should exert some adaptive control over its own progress, making frequent changes in its stepsize.

The purpose adaptive stepsize control is to achieve a predetermined accuracy in the solution with minimum computational effort.

Many small steps should tiptoe through treacherous terrain,
while a few great strides should speed through smooth countryside.

The resulting gains in efficiency are not mere tens of percents or
factors of two; they can be factors of ten, a hundred, or more.

Sometimes accuracy may be demanded not directly in the solution
itself, but in some conserved quantity that can be monitored.

Implementation of adaptive stepsize control requires that the
stepping algorithm return information about its performance,
and most importantly, an estimate of its truncation error.

Obviously, calculation of this information will add to the overhead, but the investment will generally be repaid handsomely.
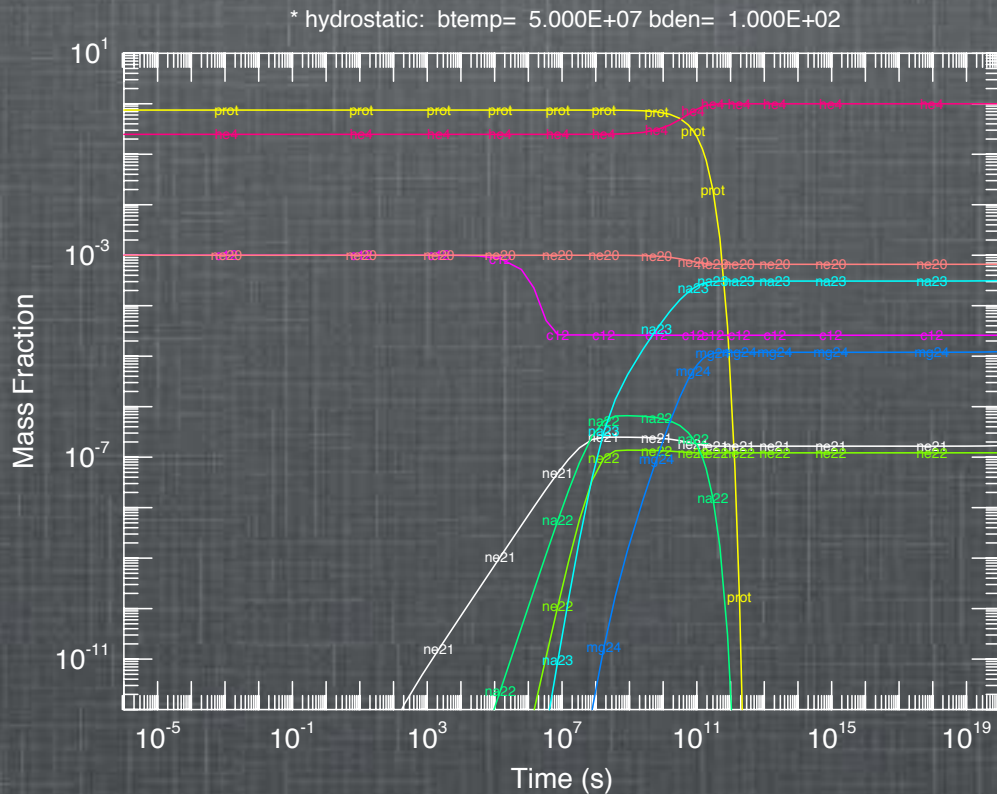
The simplest 1$^\text{rst}$ order Euler method advances over a time step h by

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta$$

where the change Δ is found by expanding $\mathbf{f}(\mathbf{y}_{n+1})$ about $\mathbf{f}(\mathbf{y}_n)$

$$(\tilde{\mathbf{1}}/h - \tilde{\mathbf{J}}) \cdot \Delta = \mathbf{f}(\mathbf{y}_n)$$

which is simply

$$\tilde{\mathbf{A}} \cdot \mathbf{x} = \mathbf{b}$$

This method costs 1 Jacobian and 1 right-hand side evaluation,
1 matrix reduction, and 1 backsubstitution.

This is the smallest possible cost per time step and is one of the
most common methods for evolving nuclear reaction networks.

This method is 1^{rst} order accurate, which as given provides no rigorous estimate of the truncation error over a given time step.

Heuristics, usually limiting the change in any abundance to be less than some small percentage, are often invoked to gain some sense of accuracy and to form the next time step.

One could implement "step doubling" to gain a formal accuracy estimate; take two half step and one full step. If the two solutions agree within some specified accuracy tolerance, accept the time step.

Step doubling is relatively expensive. Higher order methods obtain accuracy estimates by comparing solutions at different orders. We turn to two of these schemes next.

The 4th order Kaps-Rentrop method advances a time step h by

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \sum_{i=1}^{4} b_i \Delta_i$$

where the Δ_i are found from solving the staged equations

$$\tilde{\mathbf{A}} = (\tilde{\mathbf{1}}/\gamma h - \tilde{\mathbf{J}})$$

$$\tilde{\mathbf{A}} \cdot \Delta_1 = \mathbf{f}(\mathbf{y}_n)$$

$$\tilde{\mathbf{A}} \cdot \Delta_2 = \mathbf{f}(\mathbf{y}_n + a_{21}\Delta_1) + c_{21}\Delta_1/h$$

$$\tilde{\mathbf{A}} \cdot \Delta_3 = \mathbf{f}(\mathbf{y}_n + a_{31}\Delta_1 + a_{32}\Delta_2) + (c_{31}\Delta_1 + c_{32}\Delta_2)/h$$

$$\tilde{\mathbf{A}} \cdot \Delta_4 = \mathbf{f}(\mathbf{y}_n + a_{41}\Delta_1 + a_{42}\Delta_2 + a_{43}\Delta_3) + (c_{41}\Delta_1 + c_{42}\Delta_2 + c_{43}\Delta_3)/h$$

The b_i, γ, a_{ij}, and c_{ij} are fixed constants of the method.

The truncation error is estimated by comparing an embedded 3rd-order solution with the 4th-order solution.
This in turn, permits adaptive stepsize control.

This method costs 1 Jacobian, 3 right-hand side evaluations, 1 matrix reduction, and 4 backsubstitutions for a time step that meets the specified integration accuracy.

In this method not all of the right-hand sides are known in advance, Δ_4 depends on Δ_3 ... depends on Δ_1.

This general feature of higher-order integration methods impacts the optimal choice of a linear algebra package.

The variable order Bader-Deuflhard method advances a large time step H from y_n to y_{n+1} by forming

$$h = H/m \qquad \tilde{\mathbf{A}} = (\tilde{\mathbf{1}} - \tilde{\mathbf{J}})$$

$$\tilde{\mathbf{A}} \cdot \Delta_0 = h\mathbf{f}(\mathbf{y}_n) \qquad \mathbf{y}_1 = \mathbf{y}_n + \Delta_0$$

then for k=1,2 ... m-1 solving the staged equations

$$\tilde{\mathbf{A}} \cdot \mathbf{x} = h\mathbf{f}(\mathbf{y}_k) - \Delta_{k-1}$$

$$\Delta_k = \Delta_{k-1} + 2\mathbf{x}$$

$$\mathbf{y}_{k+1} = \mathbf{y}_k + \Delta_k$$

closure is obtained by the last stage

$$\tilde{\mathbf{A}} \cdot \Delta_m = h[\mathbf{f}(\mathbf{y}_m) - \Delta_{m-1}]$$

$$\mathbf{y}_{n+1} = \mathbf{y}_m + \Delta_m$$

The staged sequence is executed at least twice, yielding a 5th order method, or a maximum 7 times, yielding a 15th order method.

The exact number of times the staged sequence is executed depends on the accuracy requirements and the smoothness of the solution.

Accuracy estimates of a time step is made by comparing solutions from different orders. This in turn permits adaptive stepsize control.

Minimum cost is 1 Jacobian, 8 right-hand side evaluations, 2 matrix reductions, and 10 backsubstitutions for a time step that meets the specified integration accuracy.

Cost increases by 1 matrix reduction + m backsubstitutions for every order increase.

Cost/step is at least twice as large as the Euler or Kaps-Rentrop methods, but it may be more efficient if time steps at least twice as large can be taken.

The Bader-Deuflard method is used in the codes for these lectures.

Alpha-chain networks

Integrating the ODEs serves two functions for stellar models.

The primary function, as far as the hydrodynamics is concerned,
is to provide the magnitude and sign of the energy generation rate.
The second function is to describe the evolution of the abundances.

Obtaining accurate values for the energy generation rate is
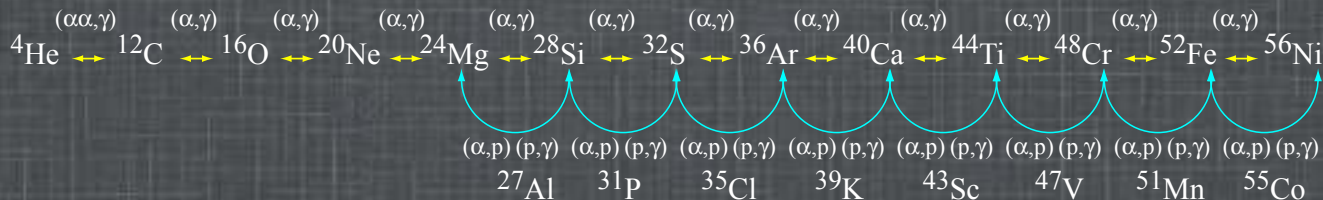expensive in terms of computer memory and CPU time.

The largest block of memory in a stellar hydrodynamic program
is reserved for storing the abundances at every grid point.

For a given set of resources usage one must choose between having fewer isotopes or having less spatial resolution.
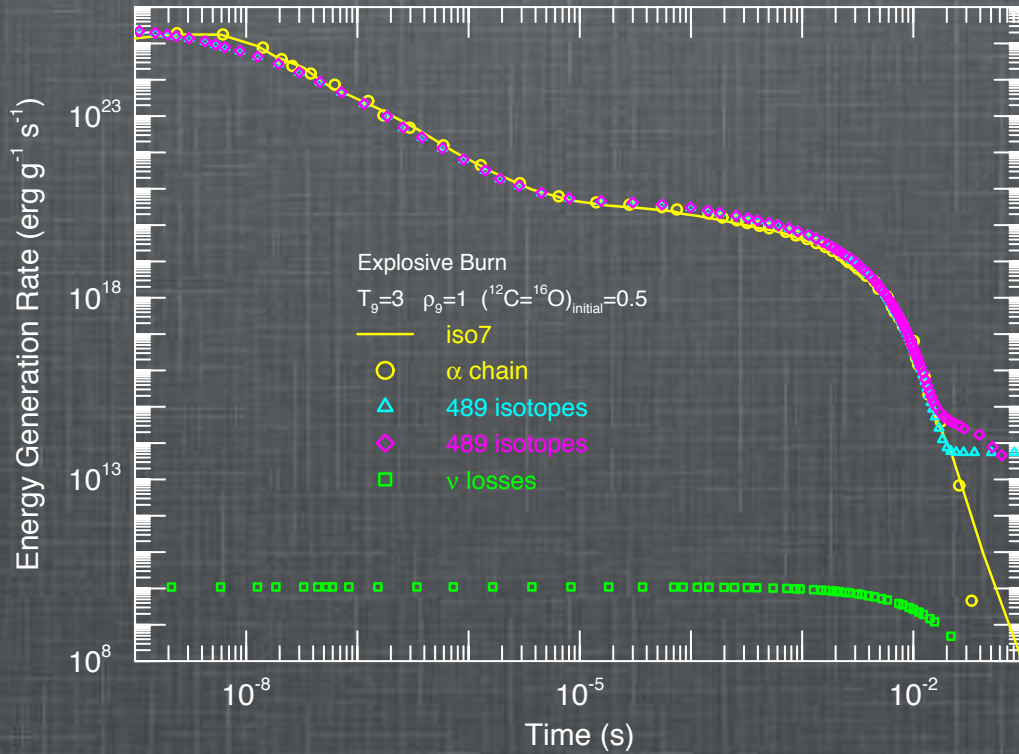
The general response to this tradeoff has been to evolve fewer isotopes, and thus calculate an approximate energy generation rate.

The set of 13 nuclei most commonly used for this purpose are ^{4}He, ^{12}C, ^{16}O, ^{20}Ne, ^{24}Mg, ^{28}Si, ^{32}S, ^{36}Ar, ^{40}Ca, ^{44}Ti, ^{48}Cr, ^{52}Fe, ^{56}Ni.

Alpha-chain Network

$$
\overset{(\alpha\alpha,\gamma)}{} \quad \overset{(\alpha,\gamma)}{} \quad \overset{(\alpha,\gamma)}{} \quad \overset{(\alpha,\gamma)}{} \quad \overset{(\alpha,\gamma)}{} \quad \overset{(\alpha,\gamma)}{} \quad \overset{(\alpha,\gamma)}{} \quad \overset{(\alpha,\gamma)}{} \quad \overset{(\alpha,\gamma)}{} \quad \overset{(\alpha,\gamma)}{} \quad \overset{(\alpha,\gamma)}{} \quad \overset{(\alpha,\gamma)}{}
$$

^{4}He $\leftrightarrow$ ^{12}C $\leftrightarrow$ ^{16}O $\leftrightarrow$ ^{20}Ne $\leftrightarrow$ ^{24}Mg $\leftrightarrow$ ^{28}Si $\leftrightarrow$ ^{32}S $\leftrightarrow$ ^{36}Ar $\leftrightarrow$ ^{40}Ca $\leftrightarrow$ ^{44}Ti $\leftrightarrow$ ^{48}Cr $\leftrightarrow$ ^{52}Fe $\leftrightarrow$ ^{56}Ni

$(\alpha,p)\,(p,\gamma)\ (\alpha,p)\,(p,\gamma)\ (\alpha,p)\,(p,\gamma)\ (\alpha,p)\,(p,\gamma)\ (\alpha,p)\,(p,\gamma)\ (\alpha,p)\,(p,\gamma)\ (\alpha,p)\,(p,\gamma)\ (\alpha,p)\,(p,\gamma)$

^{27}Al $\quad$ ^{31}P $\quad$ ^{35}Cl $\quad$ ^{39}K $\quad$ ^{43}Sc $\quad$ ^{47}V $\quad$ ^{51}Mn $\quad$ ^{55}Co

An α-chain network can give a energy generation rate that is generally within 20% of the energy generation rate given by larger reaction networks at a fraction of the cost.

Explosive Burn
$T_9=3$ $\rho_9=1$ $(^{12}C=^{16}O)_{initial}=0.5$
— iso7
○ α chain
△ 489 isotopes
◇ 489 isotopes
□ ν losses

A definition of what we mean by an α-chain network is prudent.

A strict α-chain only has (α,γ) and (γ,α) links among the 13 isotopes ^{4}He, ^{12}C, ^{16}O, ^{20}Ne, ^{24}Mg, ^{28}Si, ^{32}S, ^{36}Ar, ^{40}Ca, ^{44}Ti, ^{48}Cr, ^{52}Fe, and ^{56}Ni.

It is essential, though, to include $(\alpha,p)(p,\gamma)$ and $(\gamma,p)(p,\alpha)$ links in order to obtain reasonably accurate energy generation rates and abundances when the temperature exceeds $\sim 2.5 \times 10^9$ K.

At larger temperatures the flows through the $(\alpha,p)(p,\gamma)$ sequences are faster than the flows through (α,γ) channels. An $(\alpha,p)(p,\gamma)$ sequence is, effectively, an (α,γ) reaction through an intermediary.

In our α-chain network, we include 8 $(\alpha,p)(p,\gamma)$ sequences and their inverses by assuming steady-state proton flows through the intermediate isotopes ^{27}Al, ^{31}P, ^{35}Cl, ^{39}K, ^{43}Sc, ^{47}V, ^{51}Mn, and ^{55}Co.

Alpha-chain Network
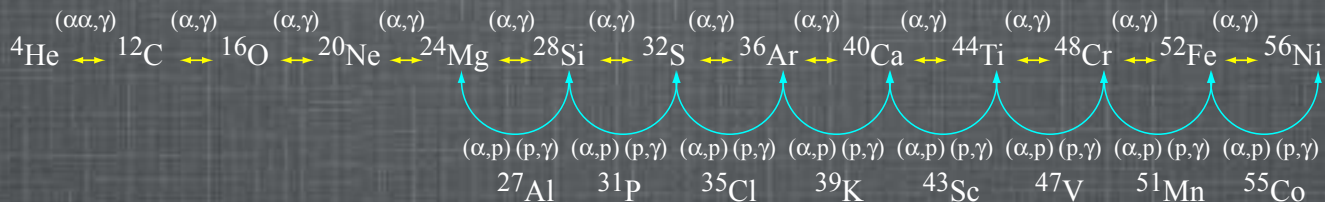
This strategy permits inclusion of $(\alpha,p)(p,\gamma)$ sequences without evolving the proton or intermediate isotope abundances.
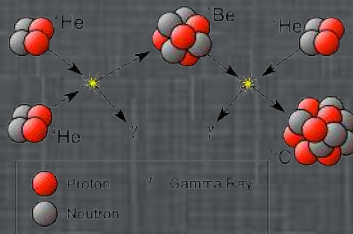
Tasks for the day

Download, compile, and run the 13 isotope α-chain code from
www.cococubed.com/code_pages/burn.shtml

Run the code in hydrostatic mode for the initial conditions
$T = 3\times10^9$ K, $\varrho = 10^9$ g/cm^3, $X(^4He) = 1.0$.
Plot the abundance evolution.
What isotope dominates when?
Run the code in explosive (adiabatic) mode (same initial conditions).
Compare and contrast the two results.