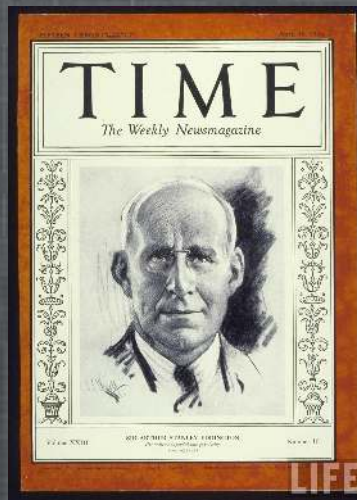


I ask you to look both ways. For the road to a knowledge of the stars leads through the atom; and important knowledge of the atom has been reached through the stars.

Arthur Eddington



Nuclear Astrophysics: Reaction Networks

Frank Timmes

Outline for 01Jul2009

1. Three Vignettes
 - a. Energy Generation
 - b. Linear Algebra
 - c. Thermodynamic trajectories
2. Big Bang Nucleosynthesis

2009 NATIONAL NUCLEAR PHYSICS SUMMER SCHOOL
 Lectures, activities, and networking opportunities for nuclear physicists 1-2 years on either side of the PhD
June 28-July 10, 2009
 National Superconducting Cyclotron Laboratory (NSCL)
 Michigan State University | East Lansing, Michigan

<http://meetings.nscsl.msu.edu/NNPSS09>

organizers: reproduced from slide
 Henrik Smitz (Chair), Wolfgang Bauer, Shail Conroy, Michael Thoennessen

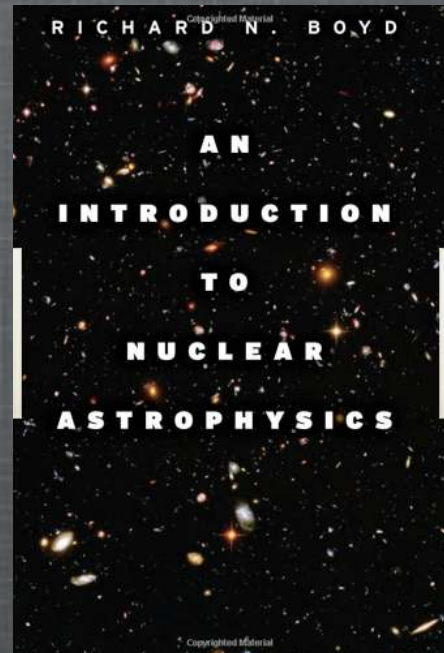
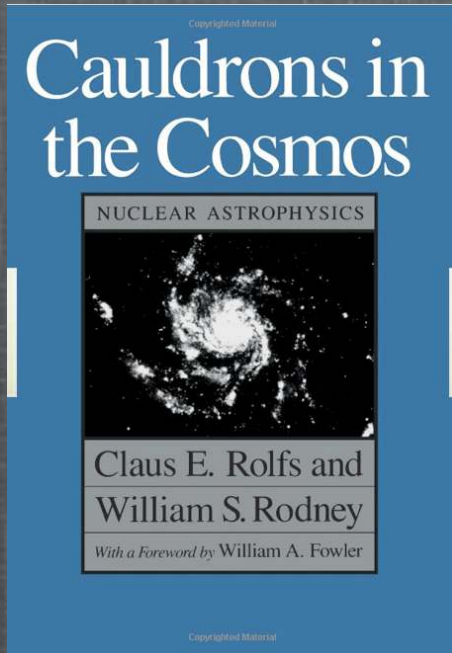
topics: Hadron Physics, Nuclear Reactions, Nuclear Structure, QCD, Neutrons, Nuclear Astrophysics, Fundamental Symmetries

invited lecturers: reproduced from slide
 Betty Bales, University of Maryland; Philippe Chomaz, GANIL; Alexandra Gadea, Michigan State University; Bob McKersie, California Institute of Technology; Frank Timmes, University of Arizona; Bill Zang, Columbia University; John Hardy, Texas A&M University; Dana Morley, Michigan State University; Witak Nazarewicz, University of Tennessee; Derek Teague, Stony Brook University; Michael Wiescher, University of Notre Dame; Sherry Yennello, Texas A&M University

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 National Science Foundation, US Department of Energy's Institute for Nuclear Theory, Michigan State University, National Superconducting Cyclotron Laboratory (NSCL)

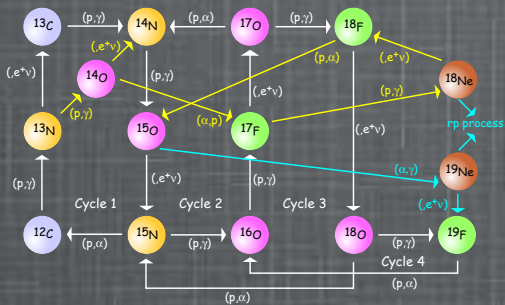


Stuff of the day



Synthesis of the elements in stars: forty years of progress
cococubed.asu.edu/papers/wallerstein97.pdf

An answer to yesterday's task

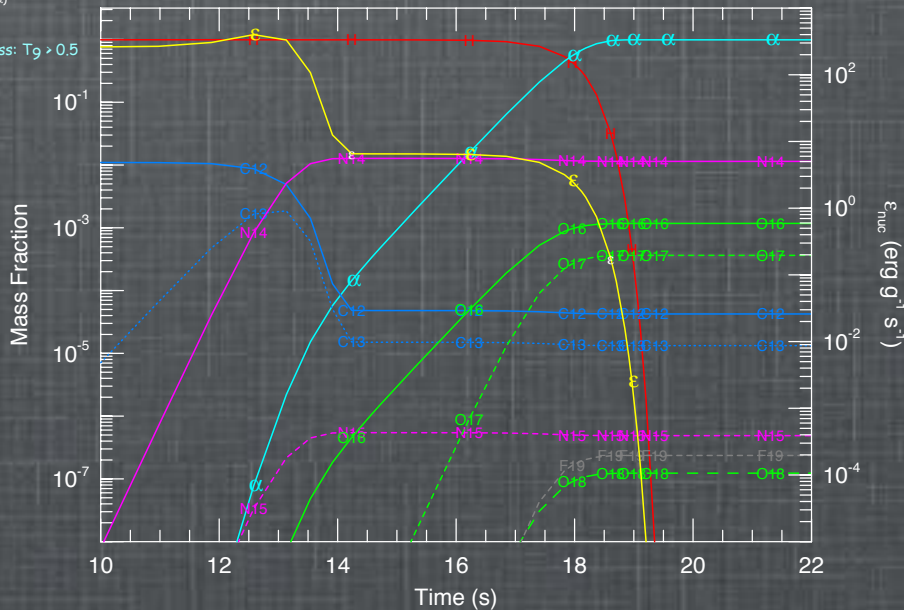


CNO: $T_9 < 0.2$

Hot CNO: $0.2 < T_9 < 0.5$

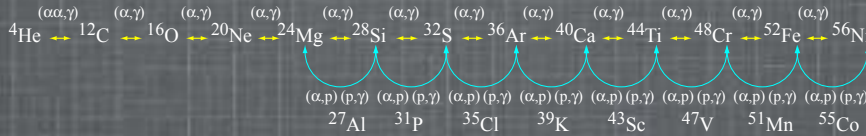
rp process: $T_9 > 0.5$

Cold CNO cycles, hydrostatic burn, $T=15 \times 10^6$ K $\rho=150$ g cm⁻³

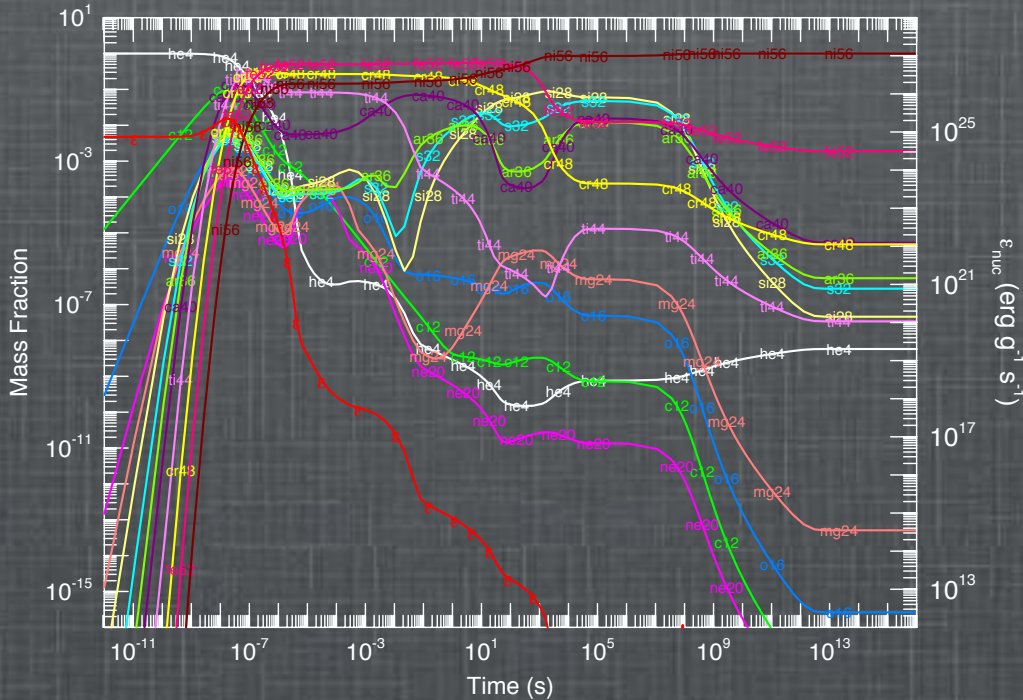


An answer to yesterday's task

Alpha-chain Network



* hydrostatic: btemp= 3.000E+09 bden= 1.000E+09



Energy Generation

An important consequence of changing the composition is the release (or absorption) of energy. The energy generation rate is

$$\dot{\epsilon}_{\text{nuc}} = - \sum_i N_A M_i c^2 \dot{Y}_i - \dot{\epsilon}_\nu \quad (\text{erg g}^{-1} \text{ s}^{-1})$$

where $M_i c^2$ is the rest mass energy of species i . Using

$$M_i = A_i m_\mu + M_{\text{ex},i}$$

$$M_{\text{ex},i} = Z_i M_{\text{ex},p} + N_i M_{\text{ex},n} - B_i/c^2$$

the energy generation rate is sometimes written as

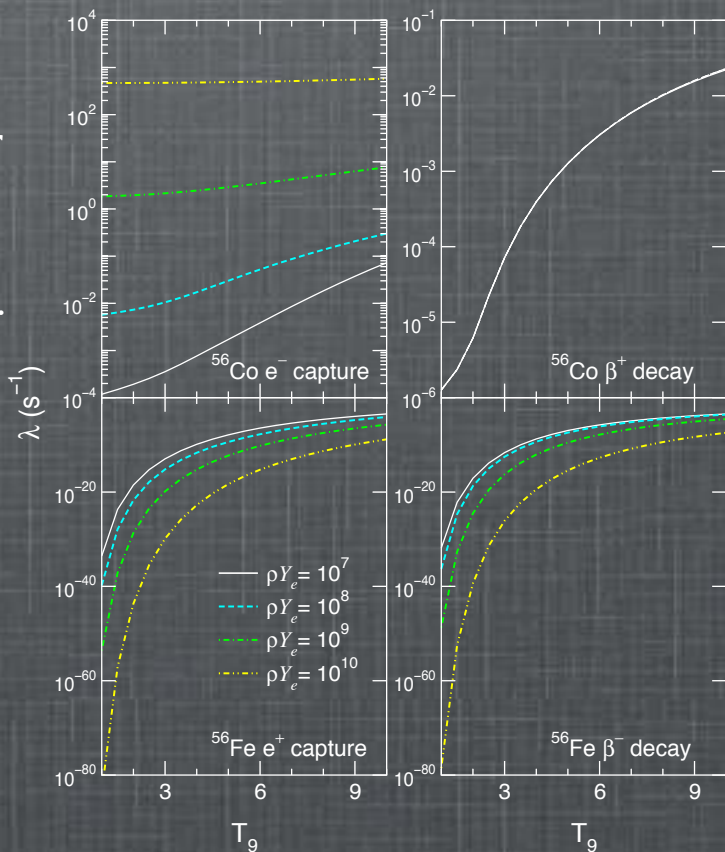
$$\dot{\epsilon}_{\text{nuc}} = \sum_i N_A E_{\text{bind},i} \dot{Y}_i - \sum_i N_A (Z_i M_{\text{ex},p} + N_i M_{\text{ex},n}) \dot{Y}_i - \dot{\epsilon}_\nu$$

The energy lost to the freely streaming neutrinos has two parts: weak reactions and neutrino thermal processes.

For weak reactions, average energy losses are calculated for each nucleus by considering the excited state distribution, Gamow-Teller distribution, etc.

The results are tabulated; see for example Langanke & Martinez-Pinedo (2000).

$$\dot{\epsilon}_\nu = \sum_i \langle E_\nu \rangle \dot{Y}_{i,weak}$$



Thermal neutrinos processes include

pair neutrino: $e^+ + e^- \rightarrow \nu + \bar{\nu}$

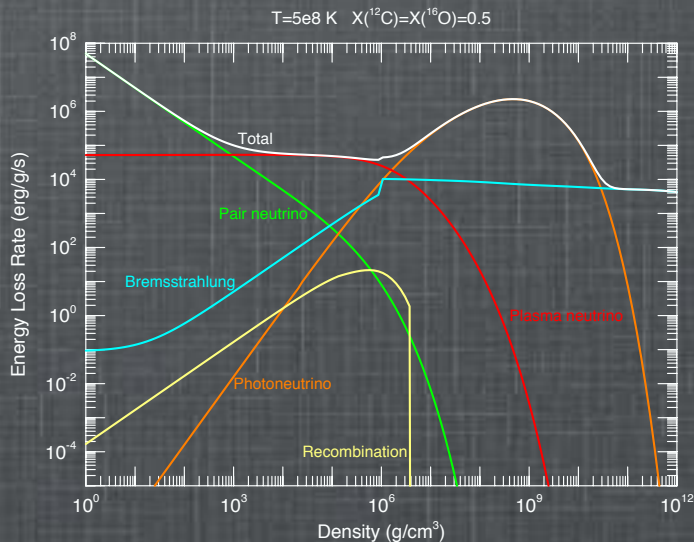
photoneutrino: $e^+ + \gamma \rightarrow e^- + \nu + \bar{\nu}$

plasma neutrino: $\gamma_{plasmon} \rightarrow \nu + \bar{\nu}$

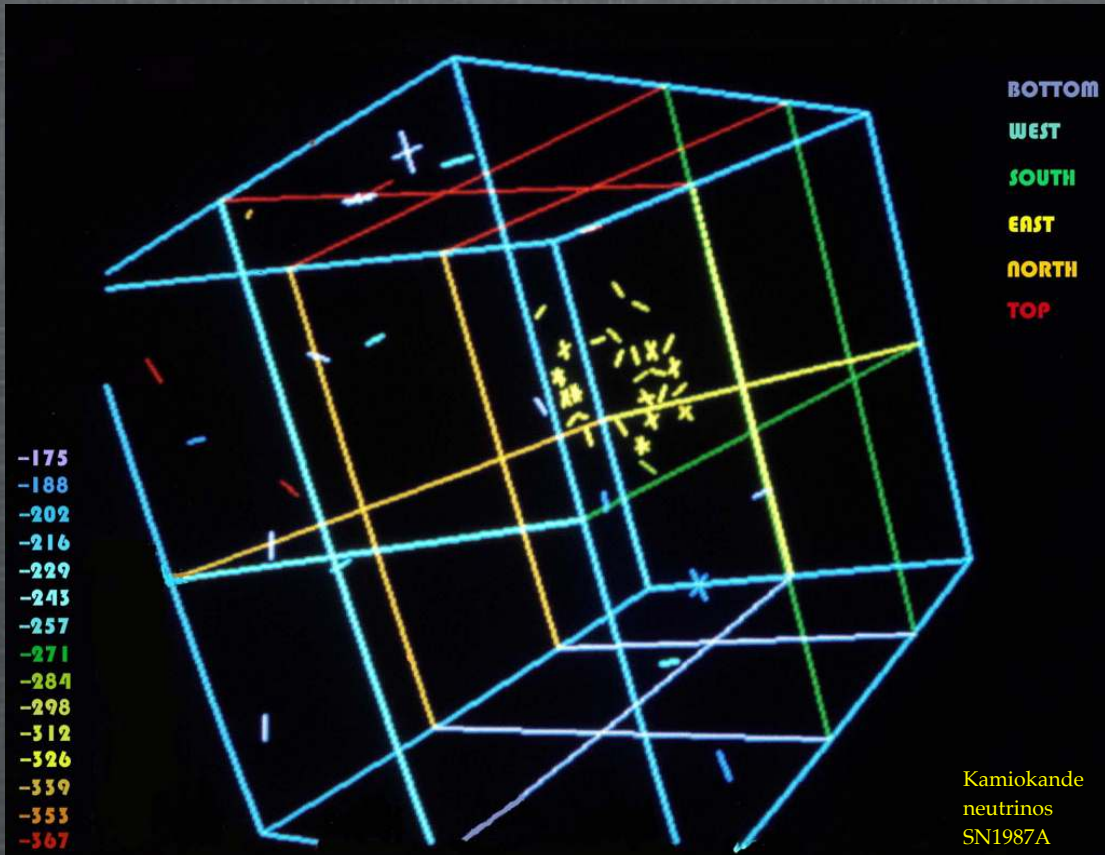
bremsstrahlung: $e^- + N(Z, A) \rightarrow e^- + N(Z, A) + \nu + \bar{\nu}$

recombination: $e^-_{continuum} \rightarrow e^-_{bound} + \nu + \bar{\nu}$

Results are typically expressed in tables or fitting formulas, for example, Itoh et al. 1996.



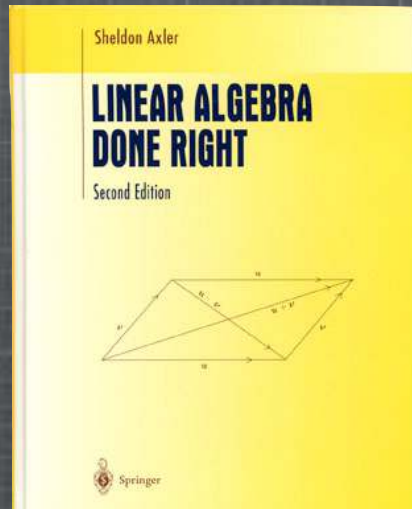
Interlude



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

Within our implicit integrations we're solving (large) systems of linear equations. As the linear algebra generally dominates the time to obtain a solution, we'll want to use efficient solvers.

We'll briefly look at dense, direct sparse, and iterative sparse solvers.



Matrix \tilde{A} is reduced to upper triangular form in tandem with a right-hand side b by Gaussian elimination, and backsubstitution on the upper triangular matrix yields the solution to $\tilde{A} \cdot x = b$.

$$\begin{bmatrix} 2 & -1 & 1 \\ -2 & 2 & -3 \\ 2 & -4 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ -7 \\ 3 \end{bmatrix}$$

$$\begin{bmatrix} 1 & -1/2 & 1/2 \\ -2 & 2 & -3 \\ 2 & -4 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3/2 \\ -7 \\ 3 \end{bmatrix}$$

This is the method you probably first learned.

$$\begin{bmatrix} 1 & -1/2 & 1/2 \\ 0 & 1 & -2 \\ 0 & -3 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3/2 \\ -4 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & -1/2 & 1/2 \\ 0 & 1 & -2 \\ 0 & 0 & -4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3/2 \\ -4 \\ -12 \end{bmatrix}$$

If the arithmetic is exact, then the answer computed in this manner will be exact, if no zeros appear on the diagonal.

$$\begin{bmatrix} 1 & -1/2 & 1/2 \\ 0 & 1 & -2 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3/2 \\ -4 \\ 3 \end{bmatrix}$$

$$x_3 = 3 \quad x_2 = 2 \quad x_1 = 1$$

But computer arithmetic is not exact, so there will always be some truncation and rounding error in the answer.

If a “small” number appears on the diagonal, then its use as the pivot may lead to computing differences between big numbers and little numbers with a subsequent loss of precision.

A way around this problem is to ensure small pivots are not used by swapping rows (partial pivoting) or rows and columns (full pivoting), so as to use a particularly desirable pivot element.

What is a desirable pivot? It is not completely known theoretically. It is known, both theoretically and in practice, that simply picking the largest available element as the pivot is a very good choice.

PIVOT POINT

Fact: Gauss elimination with no pivoting is numerically unstable in the presence of any roundoff error, even when a small pivot is not encountered. Never do Gauss elimination without pivoting!

LEQS is a dense matrix, Gaussian elimination routine.

The maximum element in each row serves as the pivot element, but no row or column interchanges are performed, so LEQS may be unstable on matrices that are not diagonally dominant.

A small amount of effort is expended to minimize calculations with matrix elements that are zero.

All Gaussian elimination routines have the disadvantage that for a sequence of right-hand sides, the entire matrix must be decomposed for each right-hand side.

The origin of LEQS is somewhat obscure, but circa 1962. It may be the most common linear algebra solver used for evolving nuclear reaction networks.



Ford-Seattle
1962

A frequently used form of Gauss Elimination is LU decomposition.

The basic idea is to find two matrices L and U such that $LU = \tilde{A}$, where L is a lower triangular matrix (zero above the diagonal) and U is an upper triangular matrix (zero below the diagonal).

$$\tilde{A} \cdot \mathbf{x} = (\tilde{L} \cdot \tilde{U}) \cdot \mathbf{x} = \tilde{L} \cdot (\tilde{U} \cdot \mathbf{x}) = \mathbf{b}$$

Once we have computed L and U we solve $L \cdot \mathbf{y} = \mathbf{b}$ then $U \cdot \mathbf{x} = \mathbf{y}$, a process that takes $O(n^2)$ operations.

While the factorization stage still requires $O(n^3)$ operations, it need be done only once. We can solve with as many right-hand sides as we care to, one at a time. This is a superior advantage.

A linear system is called sparse if only a relatively small number of its matrix elements a_{ij} are nonzero.

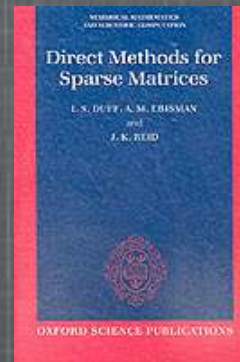
It is wasteful to use general methods on such problems, because most of storage the $O(n^3)$ operations involve zero operands.

Direct methods for sparse matrices are not that different from dense LU decomposition methods; they are just cleverly applied with due attention to the bookkeeping of zero elements.

The basic approach that all solvers use are

- 1) Symbolic decomposition
- 2) Numerical decomposition
- 3) Backsubstitution
- 4) Iterative polishing

MA28 is the Coke classic of sparse matrix solvers.
hsl.rl.ac.uk/archive/hslarchive.html



UMFPACK is a modern, direct sparse matrix solver.
www.cise.ufl.edu/research/sparse/umfpack



Iterative methods for sparse systems only reference the matrix $\tilde{\mathbf{A}}$ only through multiplication of a vector. “Matrix free” methods.

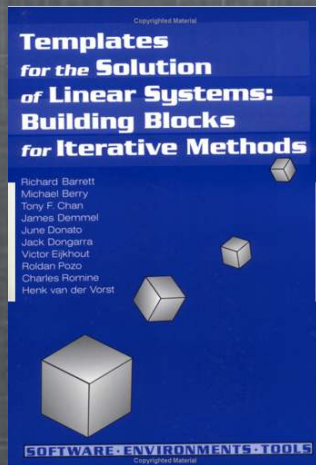
Iterative methods can be slow to converge and the number of iterations to reach a given level of accuracy is not known a priori.

A popular method, generalized minimum residuals, seeks a minimization of the function

$$f(\mathbf{x}) = \frac{1}{2} \mathbf{r} \cdot \mathbf{r} = \frac{1}{2} \left| \tilde{\mathbf{A}} \cdot \mathbf{x} - \mathbf{b} \right|^2 \quad \nabla f(\mathbf{x}) = \tilde{\mathbf{A}}^T \cdot \left(\tilde{\mathbf{A}} \cdot \mathbf{x} - \mathbf{b} \right)$$

One way to generate a good “guess” is to solve some portion of $\tilde{\mathbf{A}}$, call it matrix \mathbf{Z} , that is easy to solve. \mathbf{Z} is called the preconditioner.

BiCG is described by Barret et al in “Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods”.
netlib2.cs.utk.edu/linalg/html_templates/Templates.html



SPARSKIT is a modern, iterative sparse matrix solver.

www-users.cs.umn.edu/~saad/software/SPARSKIT/sparskit.html

Interlude

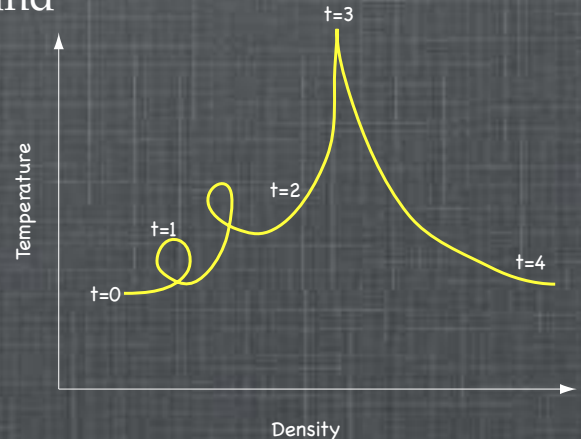


We've been holding the temperature and density constant;

$$\frac{dT}{dt} = 0 \quad \frac{d\rho}{dt} = 0$$

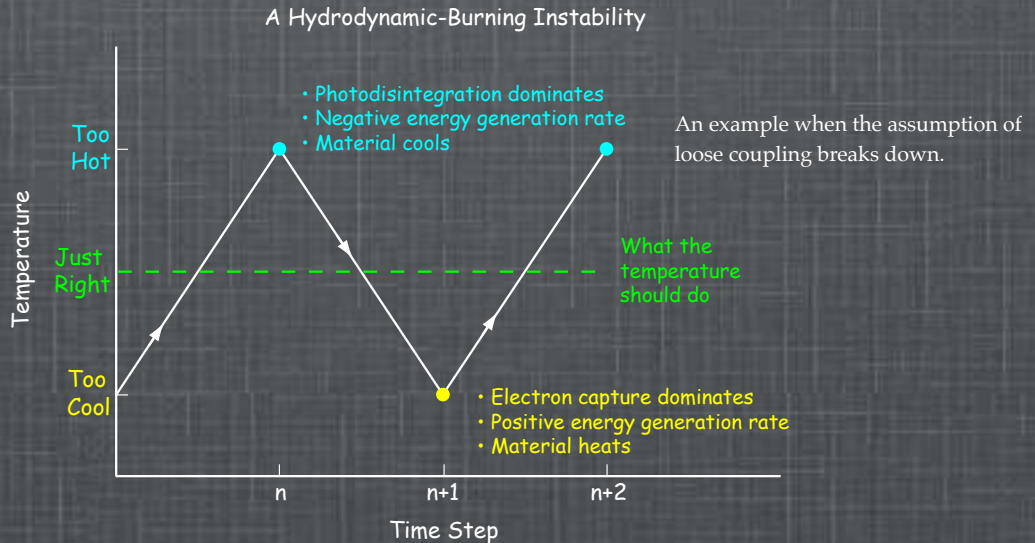
Such conditions are called “hydrostatic” burning, since the local energy release doesn't change the temperature or density, as during the hydrostatic phases of a star's evolution.

We will now relax these assumptions, and consider any thermodynamic profile.



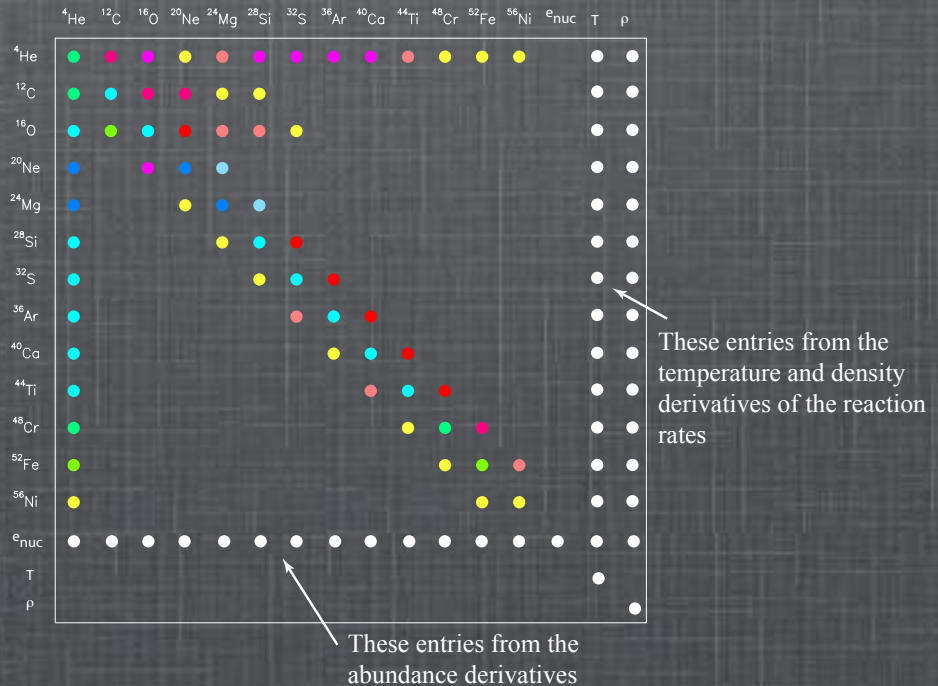
We could evolve temperature and density ODEs separately and then evolve the reaction network, or we can evolve the temperature and density ODEs simultaneously with the network.

The first is “operator splitting” and assumes a loose coupling between physical processes. Operator splitting is easy to implement and, by far, the most common choice.



The second is “unsplit”. It avoids the coupling issues, but is more difficult to implement, particularly for implicit integrations.

Our networks uses the unsplit method. Energy, temperature and density burning ODEs are appended to the reaction network.



As an example, during the Big Bang the photon temperature of the expanding universe obeys the ODE:

$$\frac{dT}{dt} = \sqrt{\frac{8\pi G a f(x)}{3c^2}} T^3 \left[x \frac{dg/dT}{3g} - 1 \right]^{-1}$$

where

$$f(x) = 1 + \frac{45}{2\pi^4} \int_0^\infty \left[\sqrt{x^2 + y^2} + \frac{y^2}{3\sqrt{x^2 + y^2}} \right] \exp \left[\sqrt{x^2 + y^2} + 1 \right]^{-1} y^2 dy$$

$$g(x) = 1 + N_\nu \frac{7}{8} \left[\frac{4}{11} f(x) \right]^{4/3} + \int_0^\infty \sqrt{x^2 + y^2} \left[\exp \left(\sqrt{x^2 + y^2} \right) + 1 \right]^{-1} y^2 dy$$

$$x = \frac{m_e c^2}{kT}$$



We can know the temperature at any given time because the dominant constituents are either massless or relativistic.

What we don't know a priori is the density ρ_b of ordinary matter in the expanding universe. How shall we parameterize our ignorance?

A common way to express the baryon density is in terms of a baryon-to-photon ratio; the number of photons for every particle.

$$\rho_b = \frac{n_b}{N_A}$$

Mass density and number density

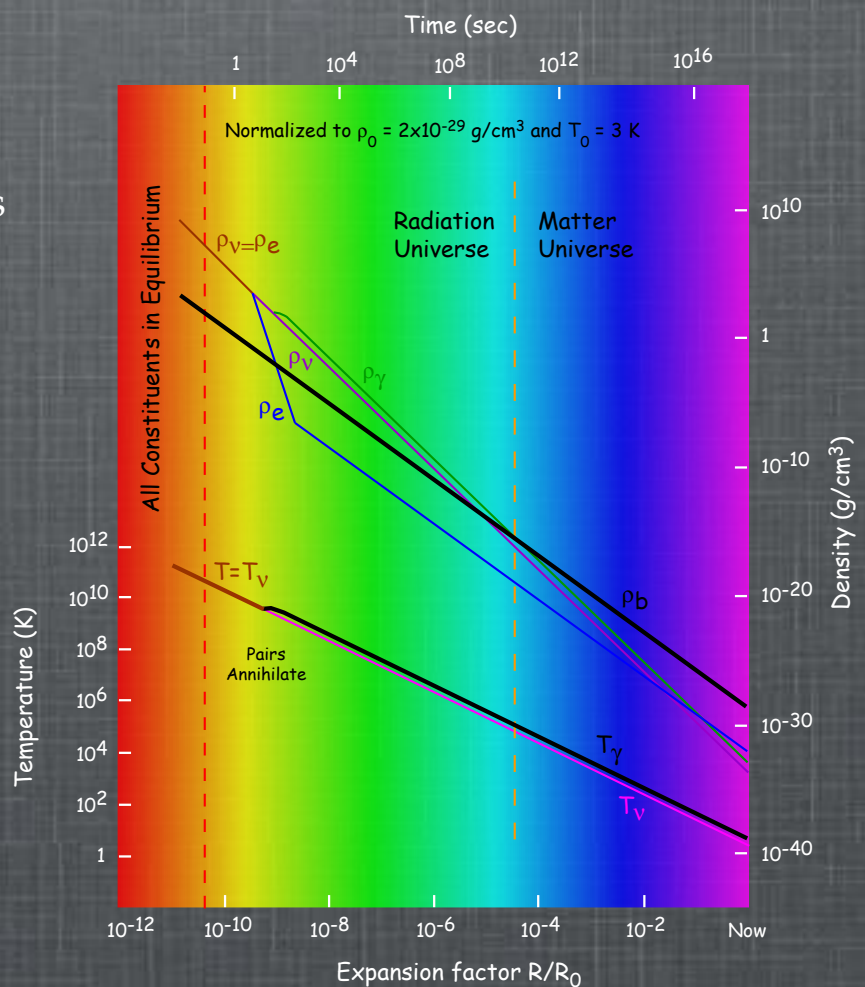
$$n_\gamma = \frac{30\zeta(3)}{\pi^4} \frac{aT_\gamma^3}{k}$$

Number density of photons

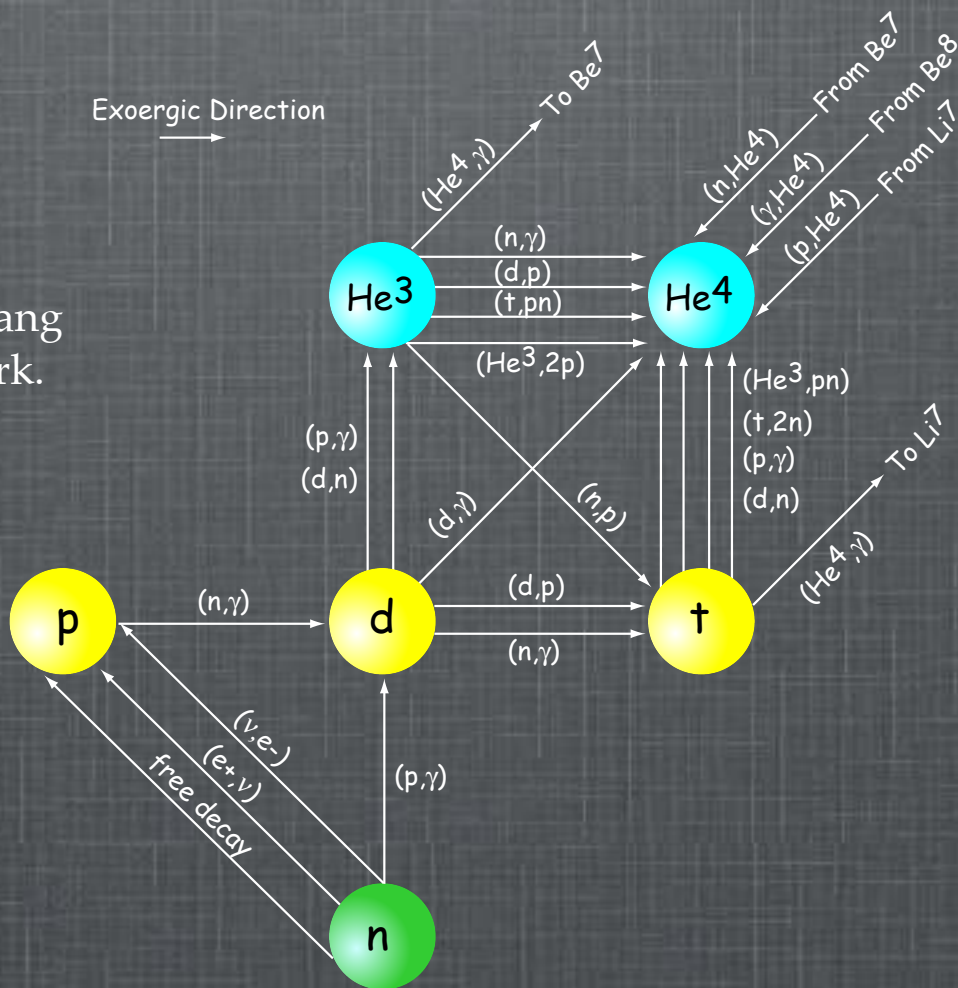
$$\rho_b = \frac{n_b}{n_\gamma} = \frac{30\zeta(3)}{\pi^4 k N_A} T_\gamma^3$$

Baryon density in terms of the photon temperature and the free parameter n_b/n_γ

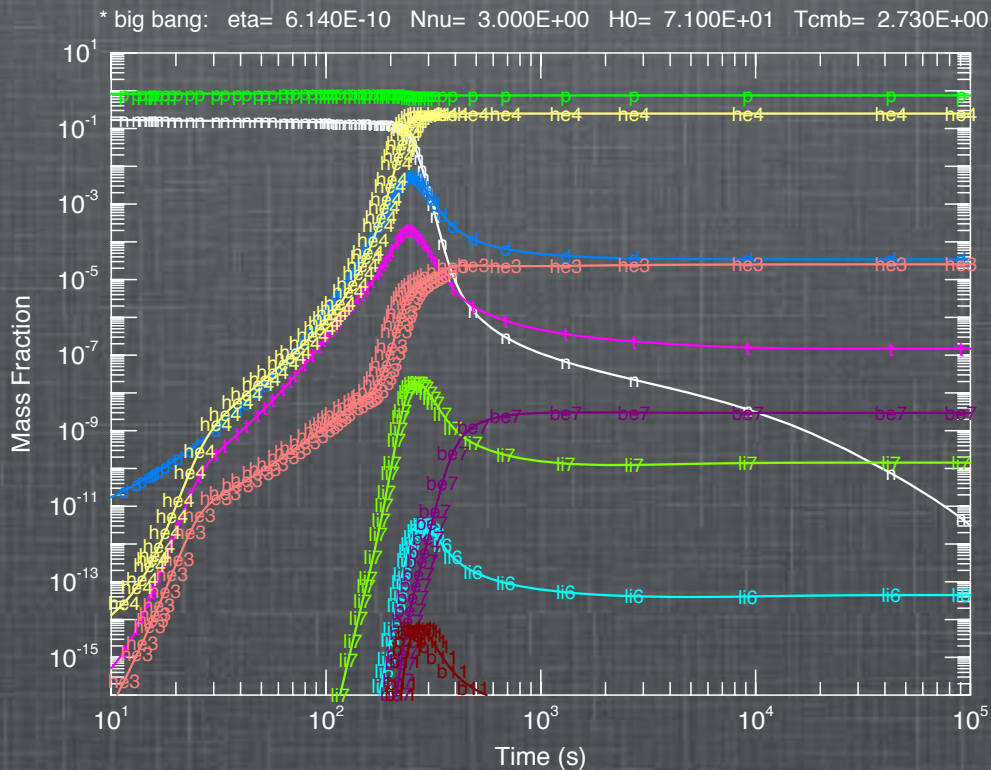
How our universe cools and gets less dense, for a given n_b/n_γ ratio.



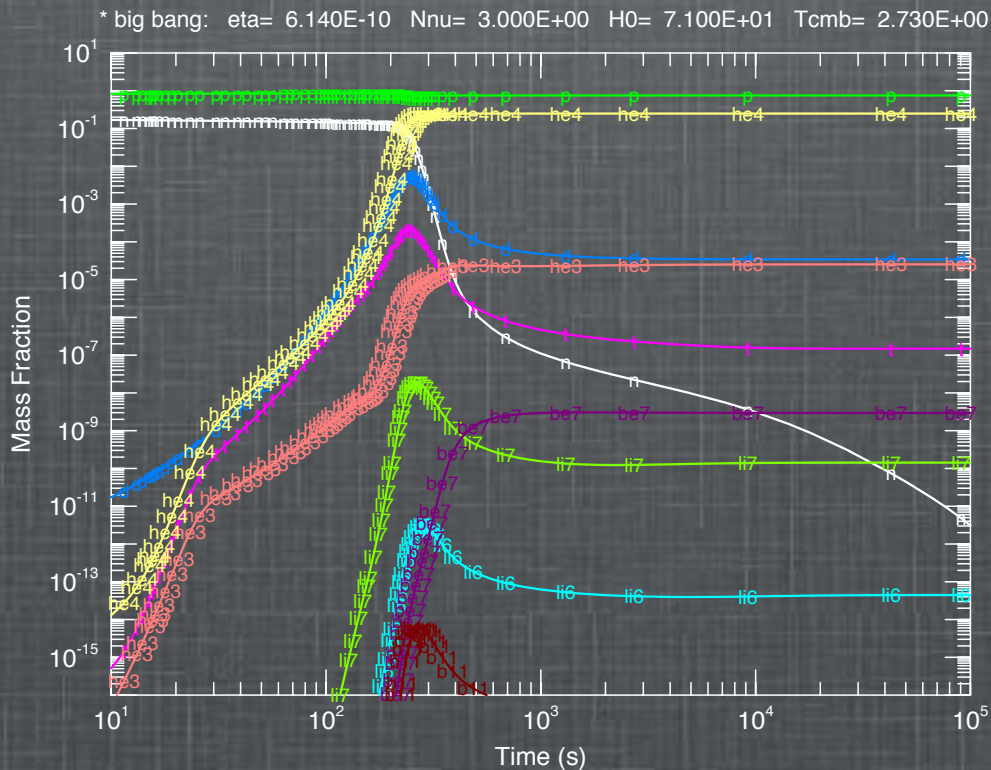
A typical Big Bang reaction network.



For times < 15 s the temperature > 3 billion K, and our universe is still a soup of protons, neutrons, electrons and more exotic matter. Anything more complex is blasted apart by high energy photons.



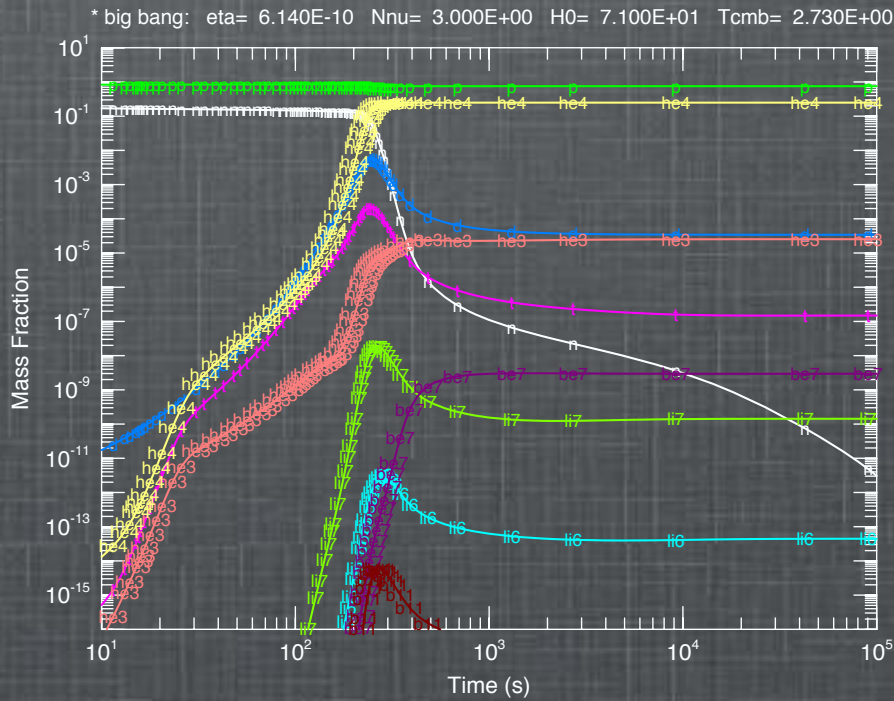
By 3 min deuterium survives after it is fused and is quickly turned into helium. Without deuterium all the neutrons would decay and our universe would be pure hydrogen.



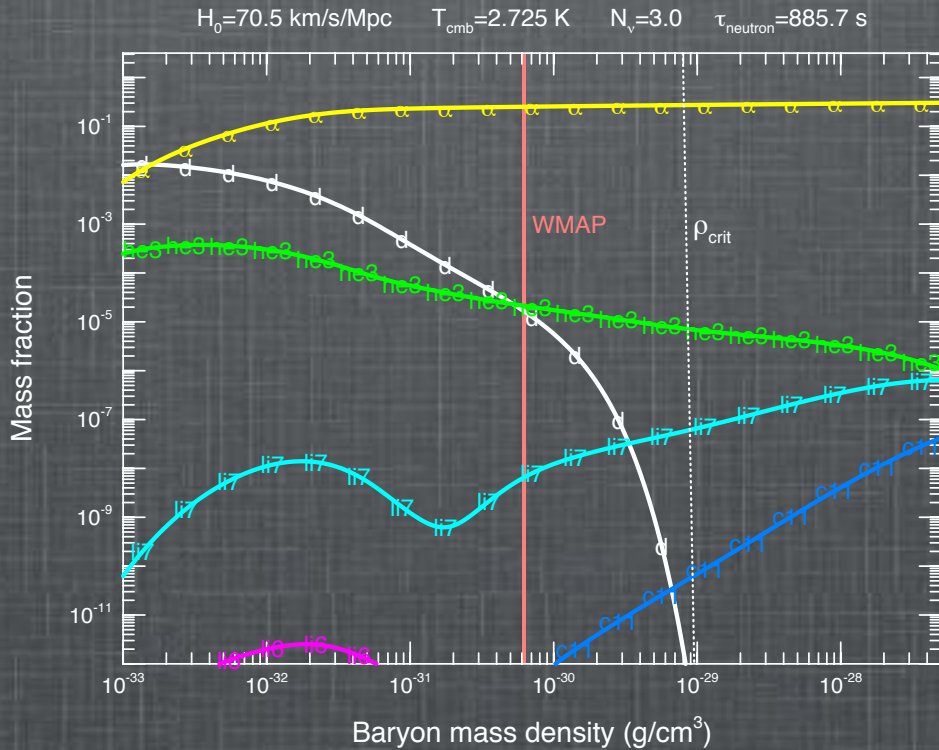
Carbon and oxygen are not produced since:

- (1) there are no stable isotopes with 5 or 8 nucleons,
- (2) the Coulomb barrier starts to be significant,
- (3) the low density suppresses the fusion of helium to carbon.

By 35 min
nucleosynthesis
is essentially
complete.

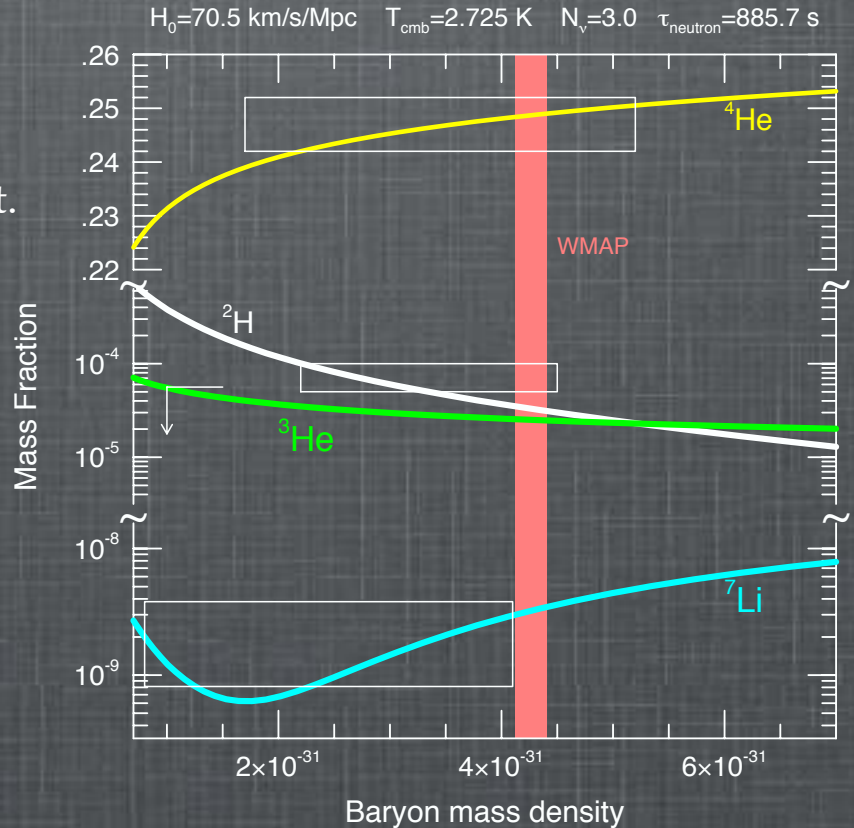


A key unknown in big bang nucleosynthesis had been the density of ordinary matter ρ_b . The cosmic microwave background provides by far the most precise determination.



The observed light element abundances is consistent with a WMAP determined baryon density, with the possible exception of ${}^7\text{Li}$.

Several independent measurements lead to a consistent constraint.



Tasks for the day

Download, compile, and run the Big Bang thermodynamics code from cococubed.asu.edu/code_pages/burn.shtml

Plot the evolution of the photon and neutrino temperatures.

Download, compile, and run the Big Bang nucleosynthesis code from cococubed.asu.edu/code_pages/burn.shtml

Plot the evolution of the abundances.

Questions and Discussion



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Hendrik Schatz (Chair), Wolfgang Bauer, Shari Conroy, Michael Thoennessen

topics: Hadron Physics, Nuclear Reactions, Nuclear Structure, QCD,
Neutrinos, Nuclear Astrophysics, Fundamental Symmetries

invited lecturers: **Betsy Beise**, University of Maryland; **Philippe Chomaz**, GANIL; **Alexandra Gade**,
Michigan State University; **Bob McKeown**, California Institute of Technology;
Frank Timmes, University of Arizona; **Bill Zako**, Columbia University; **John Hardy**, Texas A&M University;
Dave Morrissey, Michigan State University; **Witek Nazarewicz**, University of Tennessee; **Derek Teaney**,
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Michigan State University; National Superconducting Cyclotron Laboratory (NSCL)



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