> Unknowingly, we plow the dust of stars, blown about us by the wind, and drink the universe in a glass of rain.
>
> Ihab Hassan

University of Notre Dame

JINA Lecture Series on
Tools and Toys in Nuclear Astrophysics

# Nuclear Reaction Network Techniques

Francis X. Timmes
fxt44@mac.com
cococubed.com/talk_pages/jina05.shtml

Los Alamos National Laboratory
Steward Observatory, University of Arizona

# Sites of the week

- nucleo.ces.clemson.edu/pages/nse/0.1/
- www.astro.ucla.edu/~wright/cosmology_faq.html
- www.astronomynotes.com/cosmolgy/chindex.htm
- www.cococubed.com/papers/meyer94.pdf
- www.cococubed.com/papers/wallerstein97.pdf

# Syllabus

| | | |
|---|---|---|
| 1 | June 20 | Purpose, Motivation, Forming a network, PP-chain code |
| 2 | June 21 | Jacobian formation, Energy generation, Time integration, CNO-cycle code |
| 3 | June 22 | Linear algebra, Thermodynamic trajectories, Alpha-chain code |
| 4 | June 23 | Nuclear Statistical Equilibrium code, Big-Bang code |
| 5 | June 24 | Networks in hydrodynamic simulations, General network code |

# Last Lecture

- The origin of this (LEQS) legacy routine is somewhat obscure, in use by at least 1962, and is probably the most common linear algebra package presently used for evolving reaction networks.
- LEQS is used in the codes I'm providing for the JINA lectures.

Ford-Seattle
1962

# Last Lecture

- MA28 is described by Duff, Erisman & Reid (1985) in their book "Direct Methods for Sparse Matrices". MA28 is the Coke classic of sparse matrix solves.

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

- In such packages one continuous real parameter sets the amount of searching done to locate the pivot element. When set to zero, no searching is done and the diagonal element is the pivot. When set to unity, complete partial pivoting is done.

# Last Lecture

- BiCG is described by Barret et al (1993) in their "Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods".

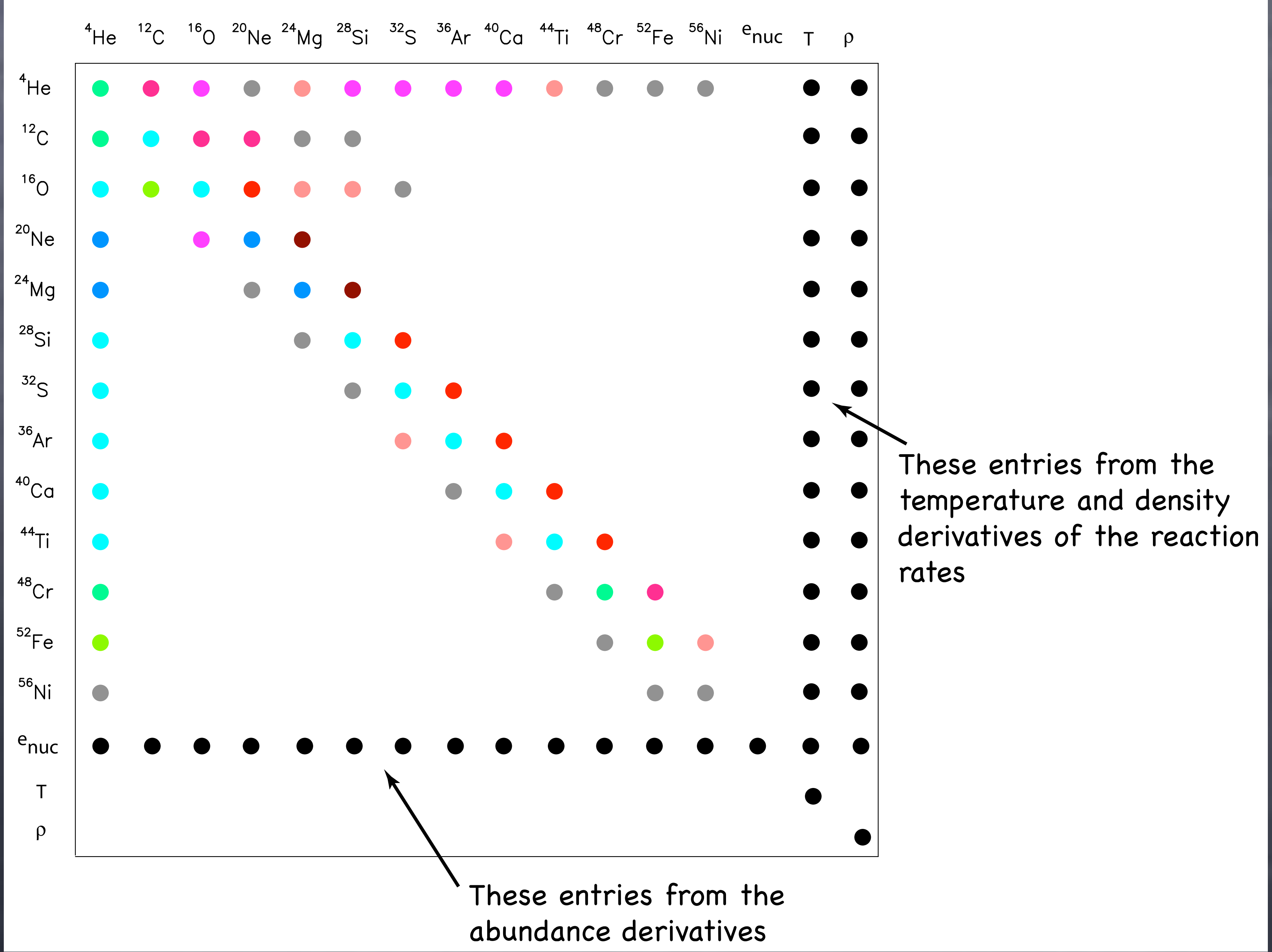
- SPARSKIT is a modern, iterative sparse matrix solver. www-users.cs.umn.edu/~saad/software/SPARSKIT/sparskit.html

- Both method generates a sequence of vectors for the matrix $\tilde{A}$ and another sequence for the transpose matrix $\tilde{A}^T$. These vector sequences are the residuals of the iterations and are made mutually orthogonal, or bi-orthogonal.

# Last Lecture

- Its usually improves mass and energy conservation to append the energy generation rate to our set of ODEs

$$\dot{\epsilon}_{\rm nuc} = -\sum_i N_A M_i c^2 \dot{Y}_i - \dot{\epsilon}_\nu$$



| | $^{4}$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 | $e_{nuc}$ | T | ρ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $^{4}$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 | ● | | | | | | | | | | | ● | ● | | ● | ● |
| $e_{nuc}$ | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● |
| T | | | | | | | | | | | | | | | ● | |
| ρ | | | | | | | | | | | | | | | | ● |

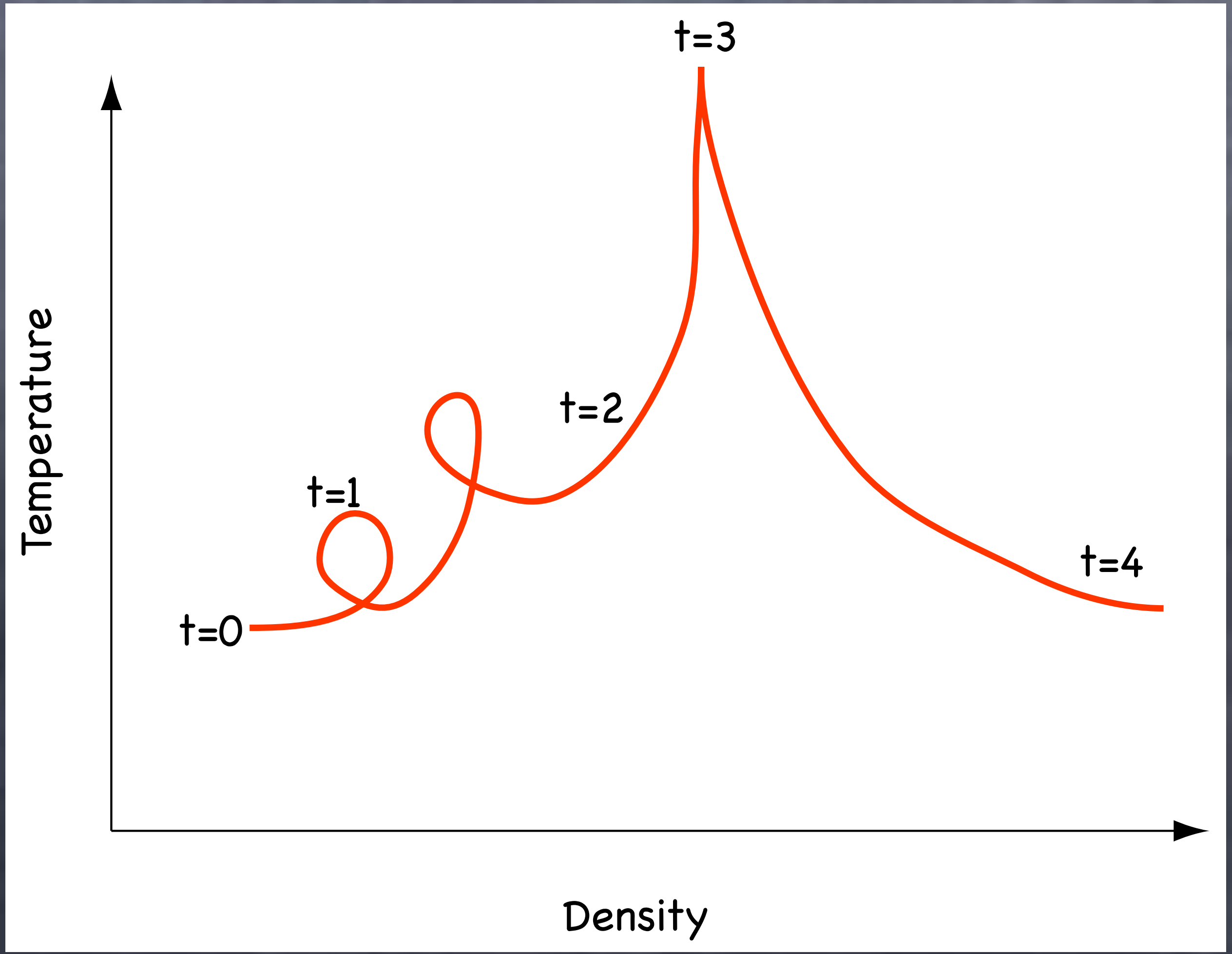
These entries from the temperature and density derivatives of the reaction rates

These entries from the abundance derivatives

# Last Lecture

- One also encounters cases where the post-processing of a previously calculated thermodynamic trajectory is desired.

- In this case one interpolates T(t) and ρ(t) for time point demanded by the integration, and one uses the hydrostatic ODEs dT/dt=0 and dρ/dt=0.



# Last Lecture

- To decrease the resources usage means making a choice between having fewer isotopes in the reaction network or having less spatial resolution.

- The general response to this tradeoff has been to evolve a limited number of isotopes, and thus calculate an approximate thermonuclear 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.

- This minimal set of nuclei, usually called an $\alpha$-chain network, can reasonably track the abundance levels from helium burning through nuclear statistical equilibrium.

# NSE

- At conditions of high temperature (T ≥ $3\times10^9$ K), the thermonuclear reaction rates may be sufficiently rapid to achieve equilibrium within the timescale set by the hydrodynamics of the astrophysical setting.

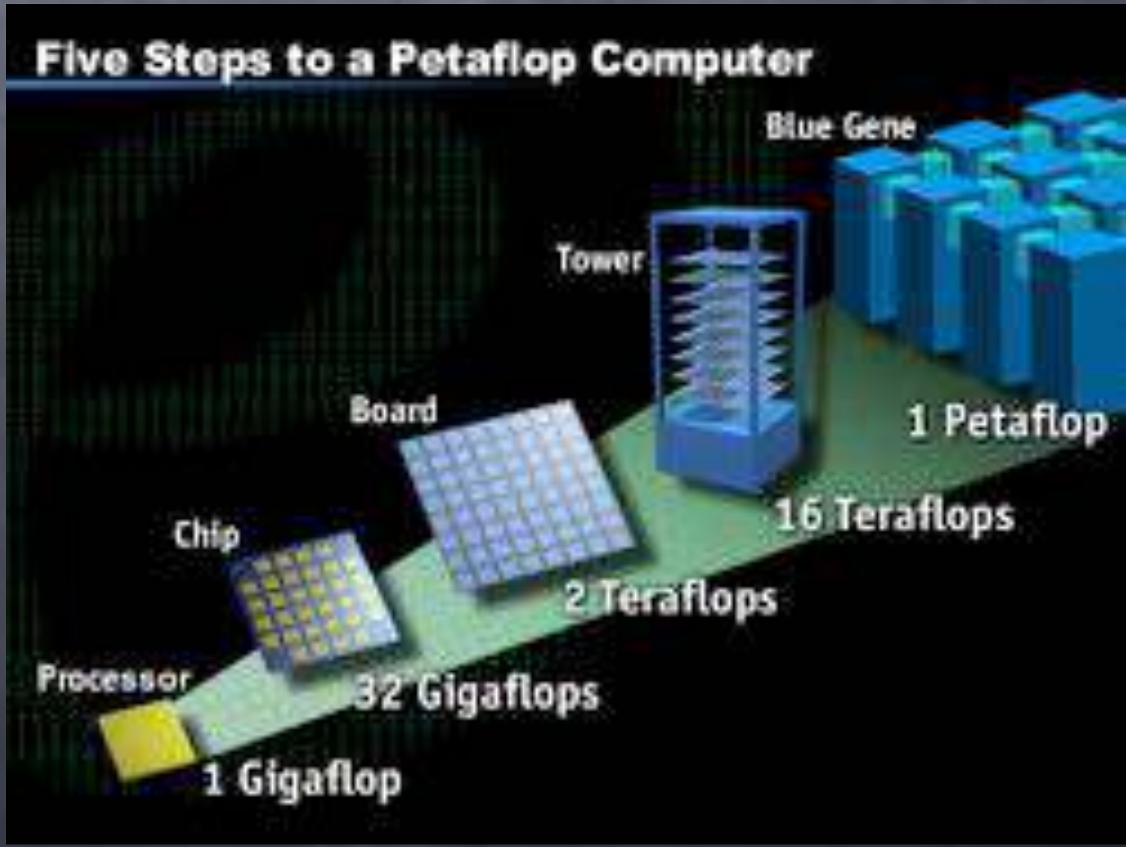
- In most such cases, the strong and electromagnetic reactions reach equilibrium while those involving the weak nuclear force do not. Thus, the resulting Nuclear Statistical Equilibrium (NSE) requires monitoring of weak reaction activity.

Meghnad Saha
1893-1956

# NSE

- NSE permits considerable simplification since calculation of the nuclear abundances are uniquely defined by the temperature T, density ρ, and the degree of neutronization $Y_e$.

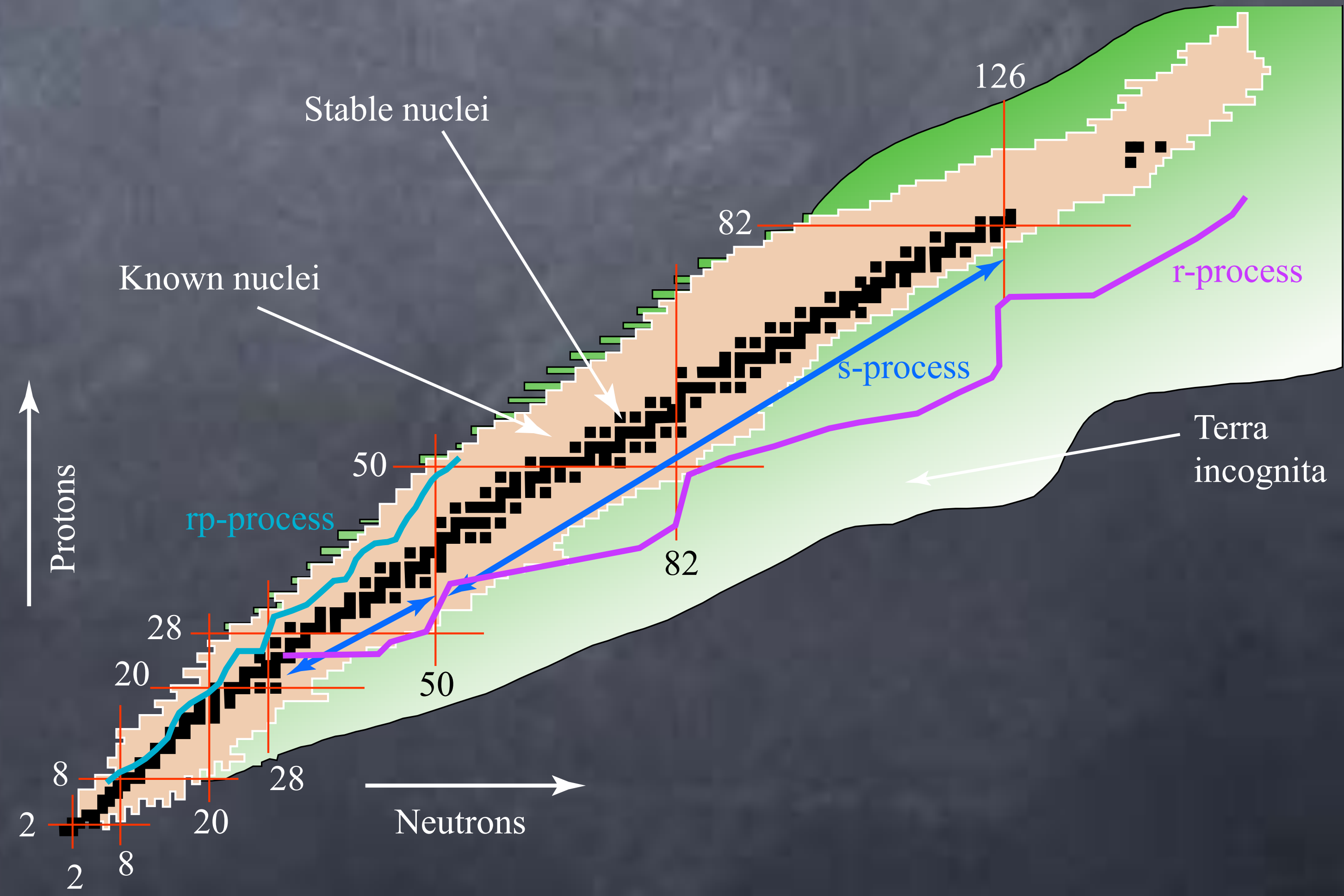
- This reduction in the number of independent variables greatly reduces the cost (CPU and memory) of nuclear abundance evolution, an issue of importance in modern multi-dimensional hydrodynamic models.



# NSE

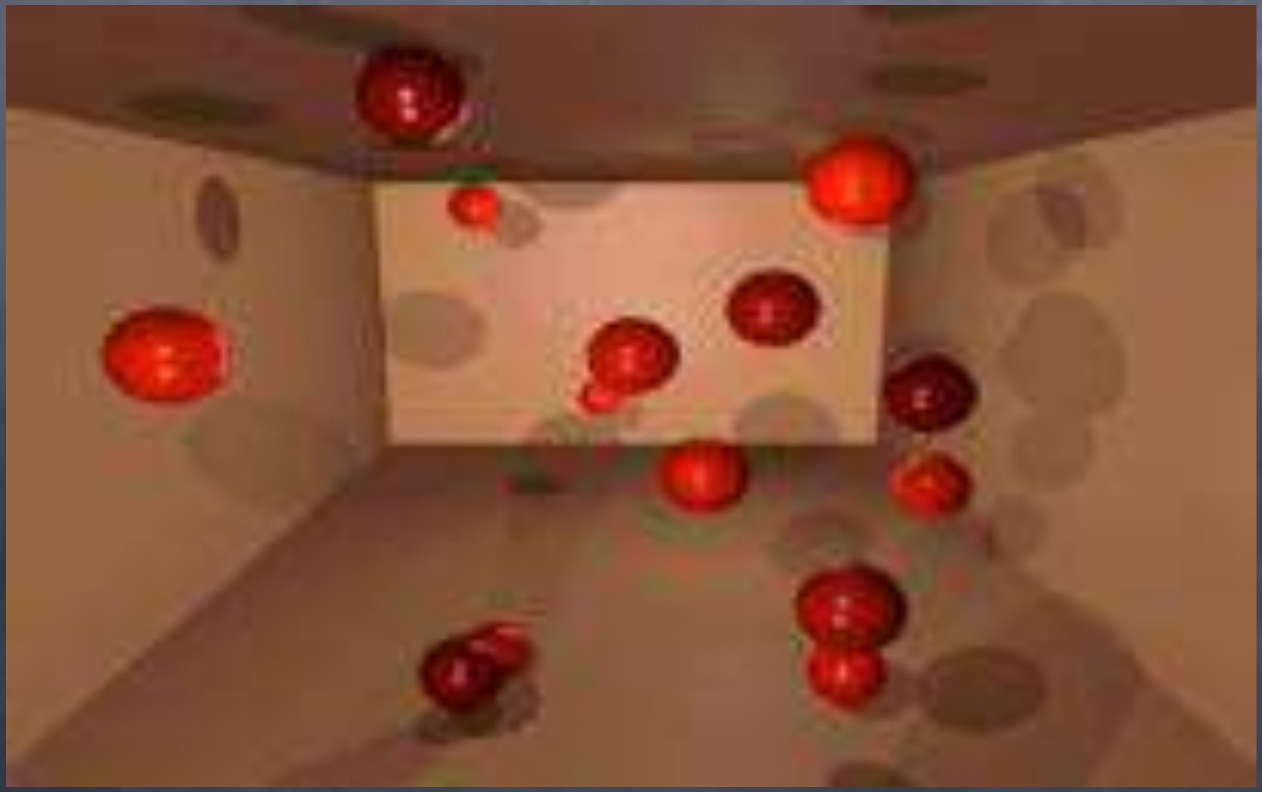
- NSE calculations depend on binding energies and partition functions, quantities which are better known than many reaction rates.

- This is particularly true for unstable nuclei and for conditions where the mass density approaches that of the nucleus itself, resulting in exotic nuclear structures.



# NSE

- All components of the system, electrons, nuclei, and free nucleons are assumed to be in thermal equilibrium at a given temperature. All strong and electromagnetic reactions occur at rates balanced by their inverses.



# NSE

- Assuming nuclei can be treated as an ideal, nonrelativistic, nondegenerate gas, the mass fraction of the nucleus $^{A}Z$ is given by the Maxwell-Boltzmann relation

$$X_i = \frac{A_i}{N_A \rho}\,\omega(T)\left(\frac{2\pi A_i m_{\rm amu}}{h^2 kT}\right)^{3/2} \exp\left(\frac{\mu_i + B_i}{kT}\right)$$

where ω(T) is the partition function and $\mu_i$ is the chemical potential of isotope i, which is related to the chemical potential of the neutrons and protons as

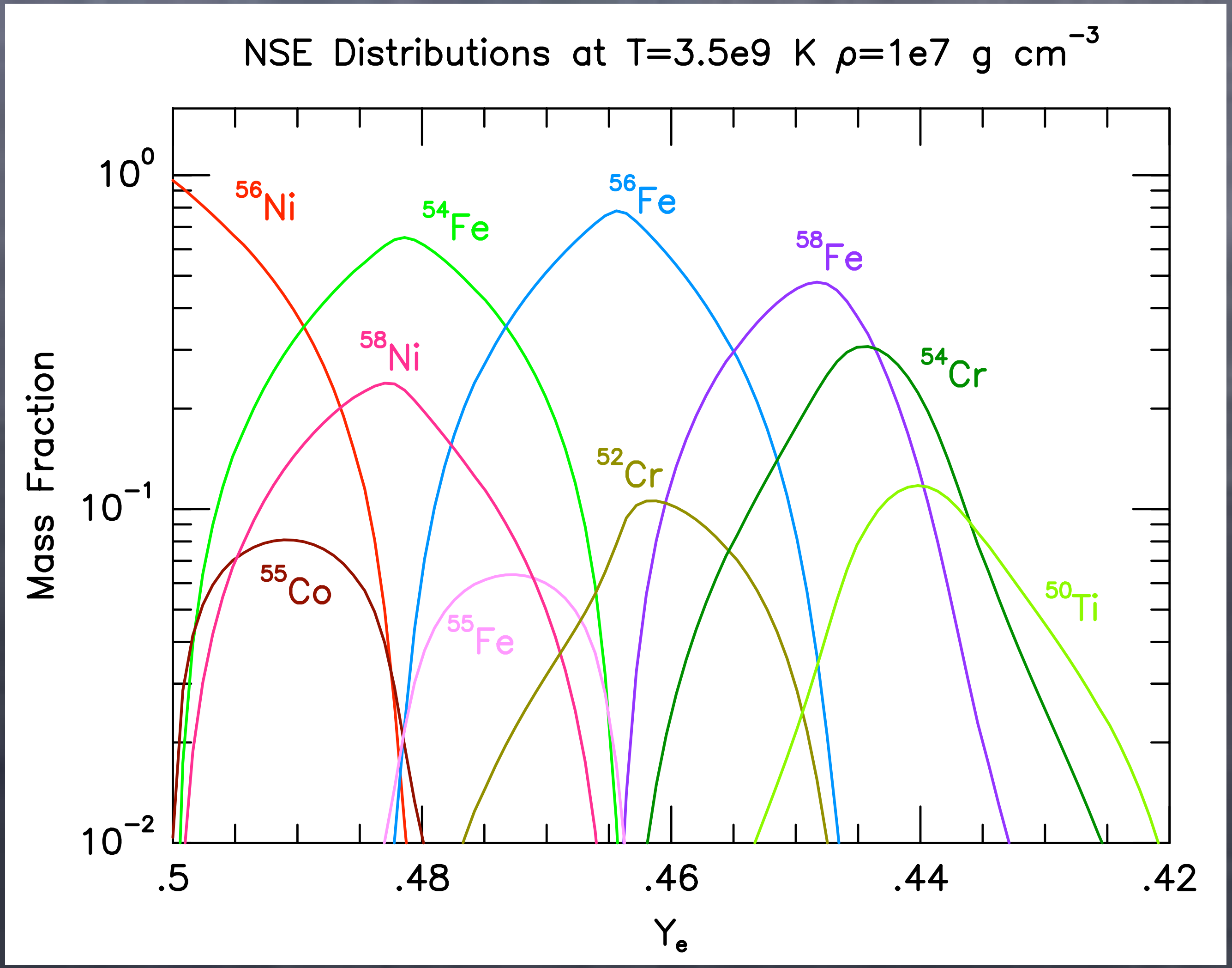
$$\mu_i = (A_i - Z_i)\mu_n + Z\mu_p$$

# NSE

- The constraints of mass and charge conservation

$$\sum_{i=1}^{n} X_i = 1 \qquad \sum_{i=1}^{n} Z_i Y_i = Y_e$$

give two equations for the two unknowns, $\mu_n$ and $\mu_p$.


NSE Distributions at T=3.5e9 K ρ=1e7 g cm$^{-3}$

# NSE

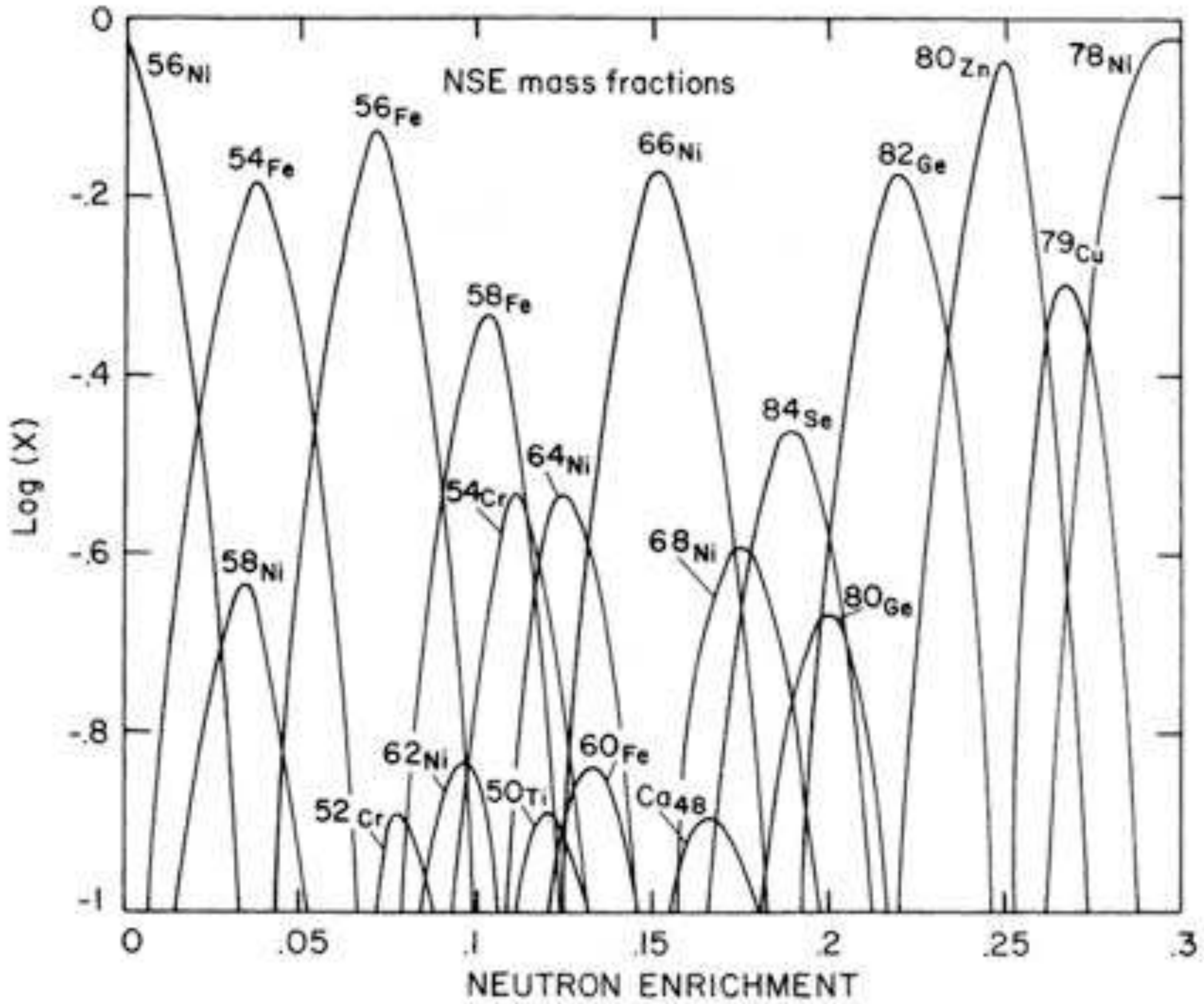


FIG. 2.—Mass fractions obtained in NSE as a function of neutron enrichment η for fixed temperature $T = 3.5 \times 10^9$ K and density $\rho = 10^7$ g cm$^{-3}$

Hartmann et al.
ApJ 297,837, 1985

# NSE

- Statistical equilibrium is the condition of maximum entropy maximum randomness. All allowed macroscopic states, all sets of abundance with a total energy E and satisfying our constraints are available to the system, and all are equally likely.

- How then are definite abundances possible?

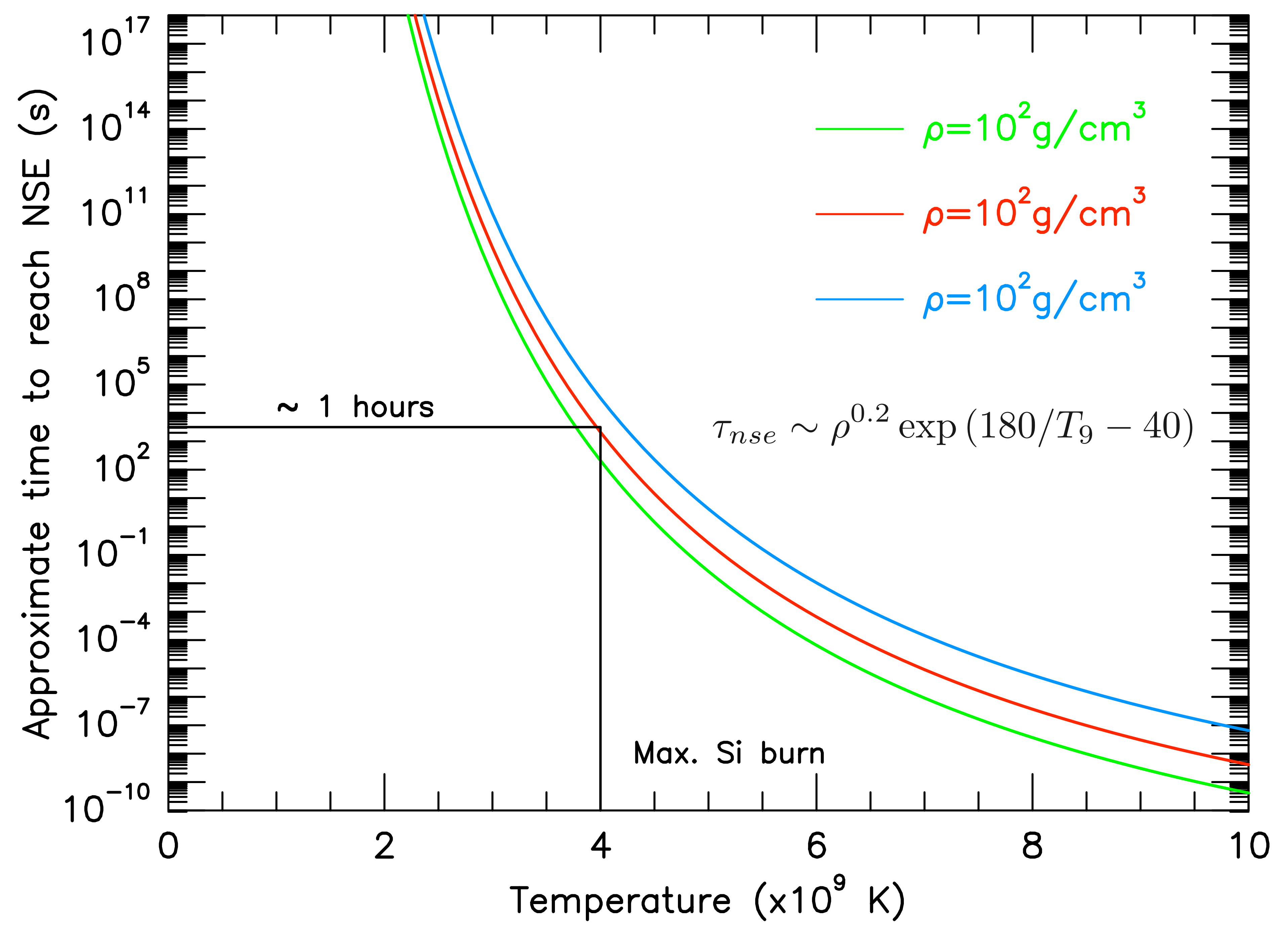
# NSE

- As with any equilibrium distribution, there are limitations on the applicability of NSE. For NSE to provide a good estimate of the nuclear abundances the temperature must be sufficient for the endoergic reaction of each reaction pair to occur.

- Usually the endothermic reactions are photodisintegrations, with typical Q-values among β stable nuclei of 8-12 MeV, or $T > 3 \times 10^9$ K.

- While this requirement is necessary, it is not sufficient. Time is needed for a composition to adjust to an NSE state.

# NSE

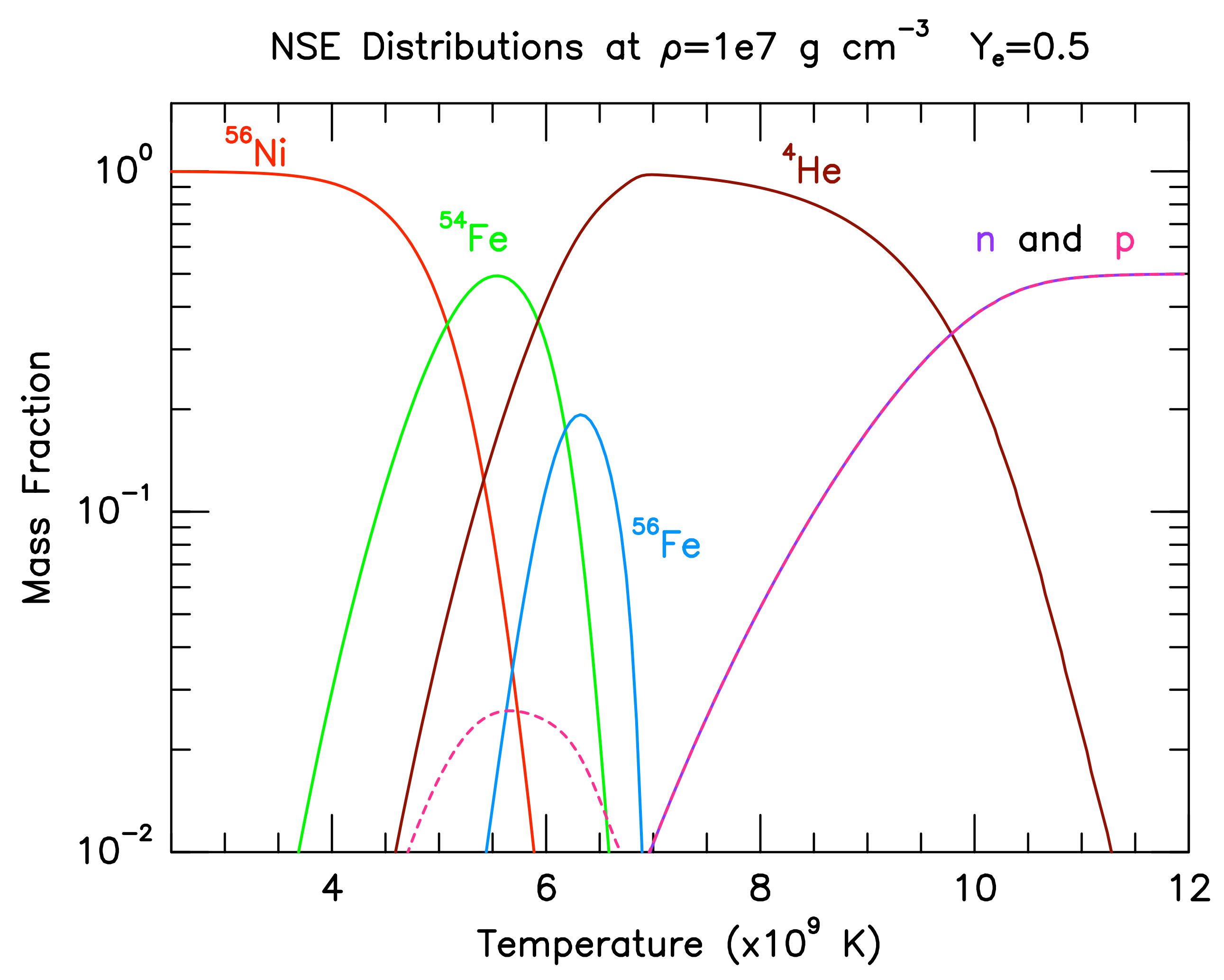


After Khokhlov, A&A 245, 114, 1991

- In the face of sufficiently rapid thermodynamic variations, NSE provides a poor estimate of the abundances.

# NSE

- If weak interactions are also balanced (e.g., neutrino capture occurring as frequently on the daughter nucleus as electron capture on the parent), then only two parameters, ρ and T, specify the abundances.



- This last occurred for T > $10^9$ K in the Big Bang.

# Interlude

The sower
1888.
Oil on canvas.
72.5 x 92 cm
Vincent van Gogh

# Big Bang Nucleosynthesis

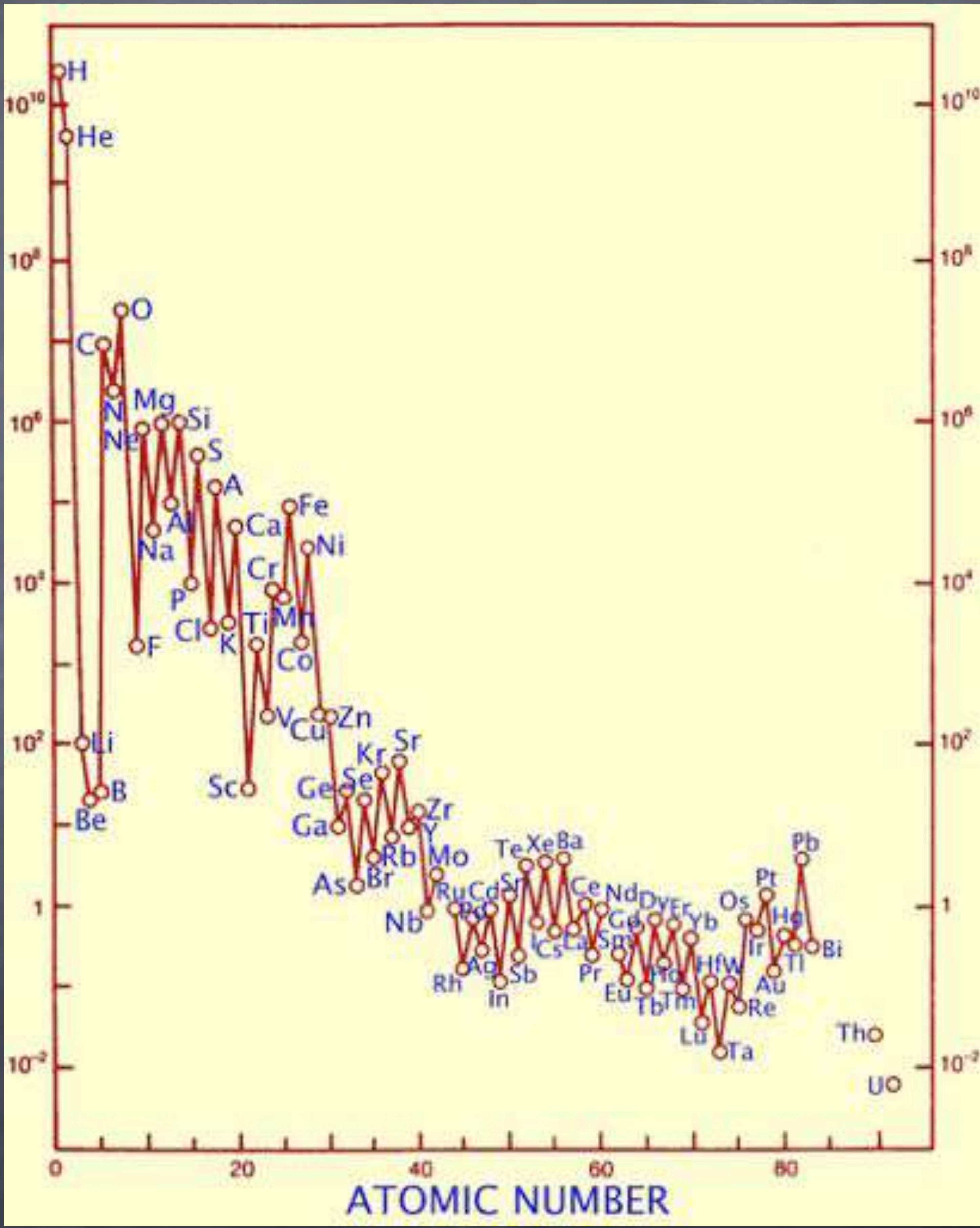
- When we look at the starry night ...

The Starry Night
over the Rhone,
1888.
Oil on canvas.
72.5 x 92 cm
Vincent van Gogh

# Big Bang Nucleosynthesis

- … we find hydrogen and helium are the dominant elements.

- Why is that?



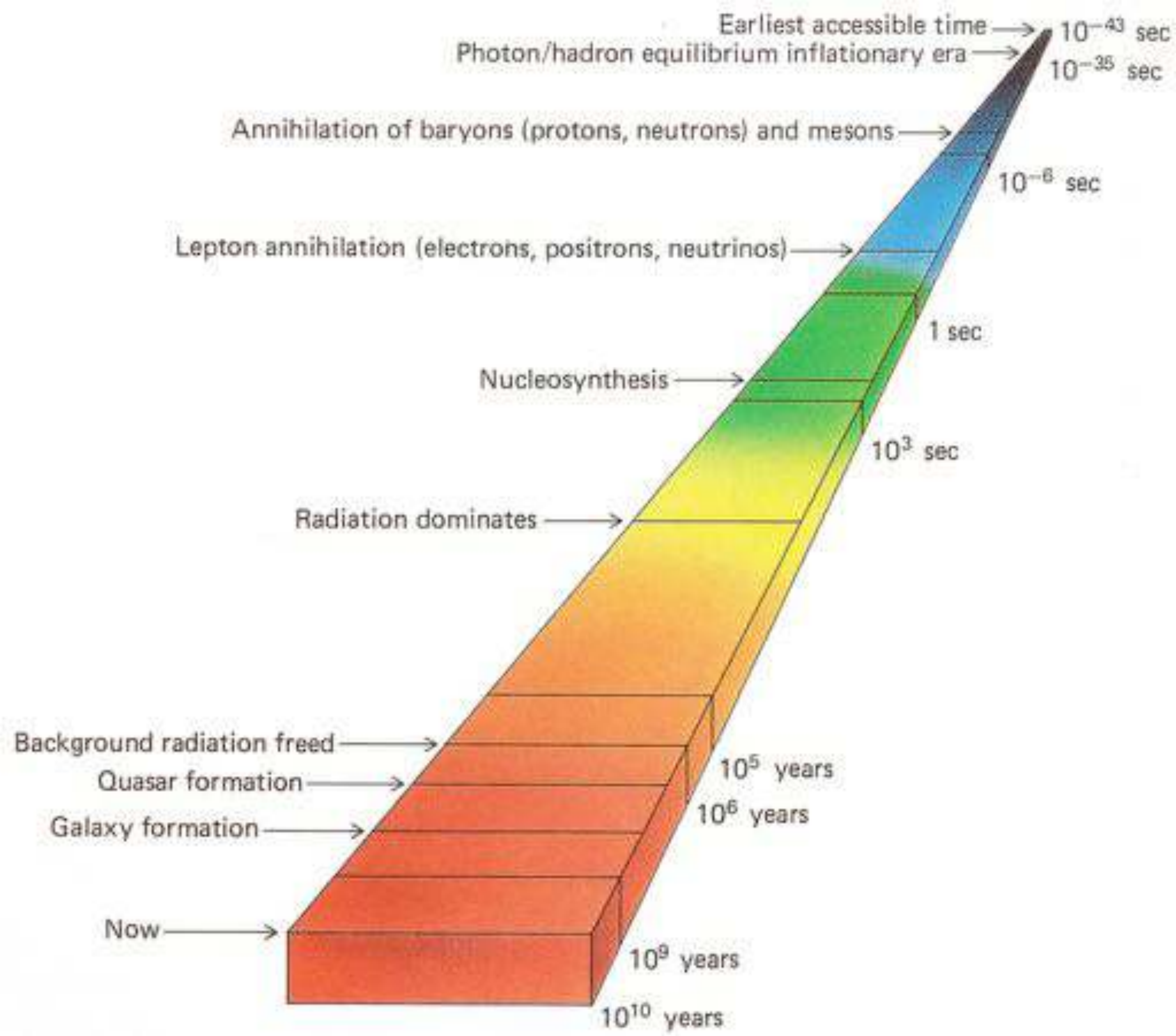
# Big Bang Nucleosynthesis

- The lovely story of how the universe became dominated by hydrogen and helium is called Big Bang nucleosynthesis.

Sunflowers
1889.
Oil on canvas.
73 x 95 cm
Vincent van Gogh

# Big Bang Nucleosynthesis

- While there are lots of interesting ideas to explore within the Big Bang paradigm, we'll focus on forging the elements.



# Big Bang Nucleosynthesis

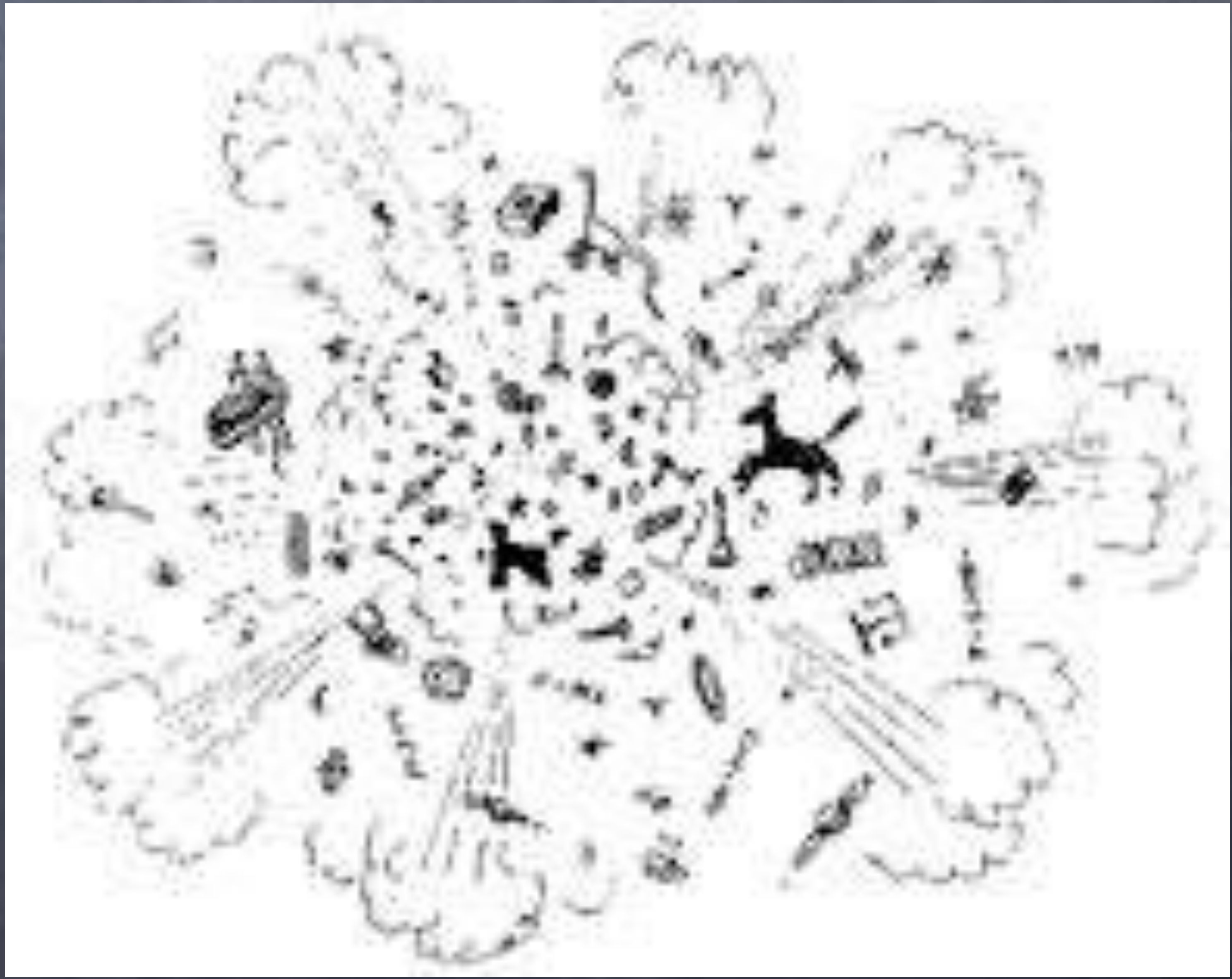
- Before we explore in detail how to cook up the elements, let’s take a broad overview look at the key events that occurred as the universe cooled down.

Illustration from
L'atmosphere: meteorologie populaire, 1888,
by Camille Flammarion

# Cool down

- When the temperature was above $10^{12}$ K, the universe contained a great variety of particles in thermal equilibrium, including photons, leptons, mesons, nucleons, and their antiparticles.

The strong interaction among nuclei and mesons (non-perturbative quantum chromodynamics) make this era difficult to study.



Big Bang, 1988, John C. Holden

# Cool down

- At the time when T ≈ $10^{12}$ K, the universe contained photons, muons, electrons, neutrinos and their antiparticles. There was a very small nucleonic contamination, with neutrons and protons in equal numbers.

  All these particles were in NSE.

Big Bang, 1998, Kerry Mitchell

# Cool down

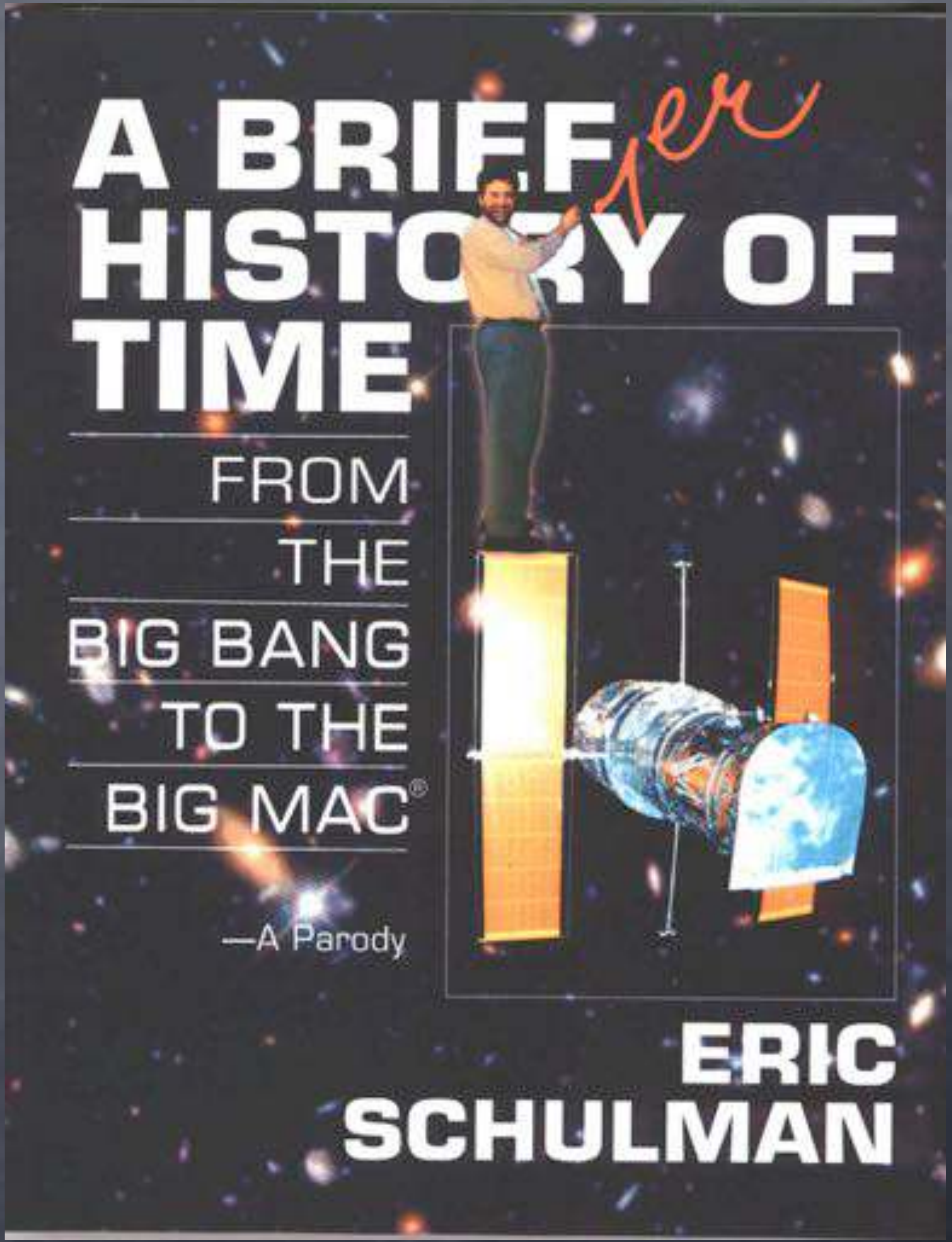
- As the temperature dropped below $10^{12}$ K, the muons and antimuons began to annihilate.

Billboard in Baton Rouge

- After almost all the muons were gone, at $T \approx 1.3 \times 10^{11}$ K, the neutrinos and antineutrinos decoupled from the other particles, leaving electrons, positrons, photons, and a few nucleons in thermal equilibrium, with $T \approx 1/R$.

# Cool down

- Below $10^{11}$ K ($t \approx 0.01$ sec), the neutron-proton mass difference began to shift the small nucleonic contamination toward more protons and fewer neutrons.

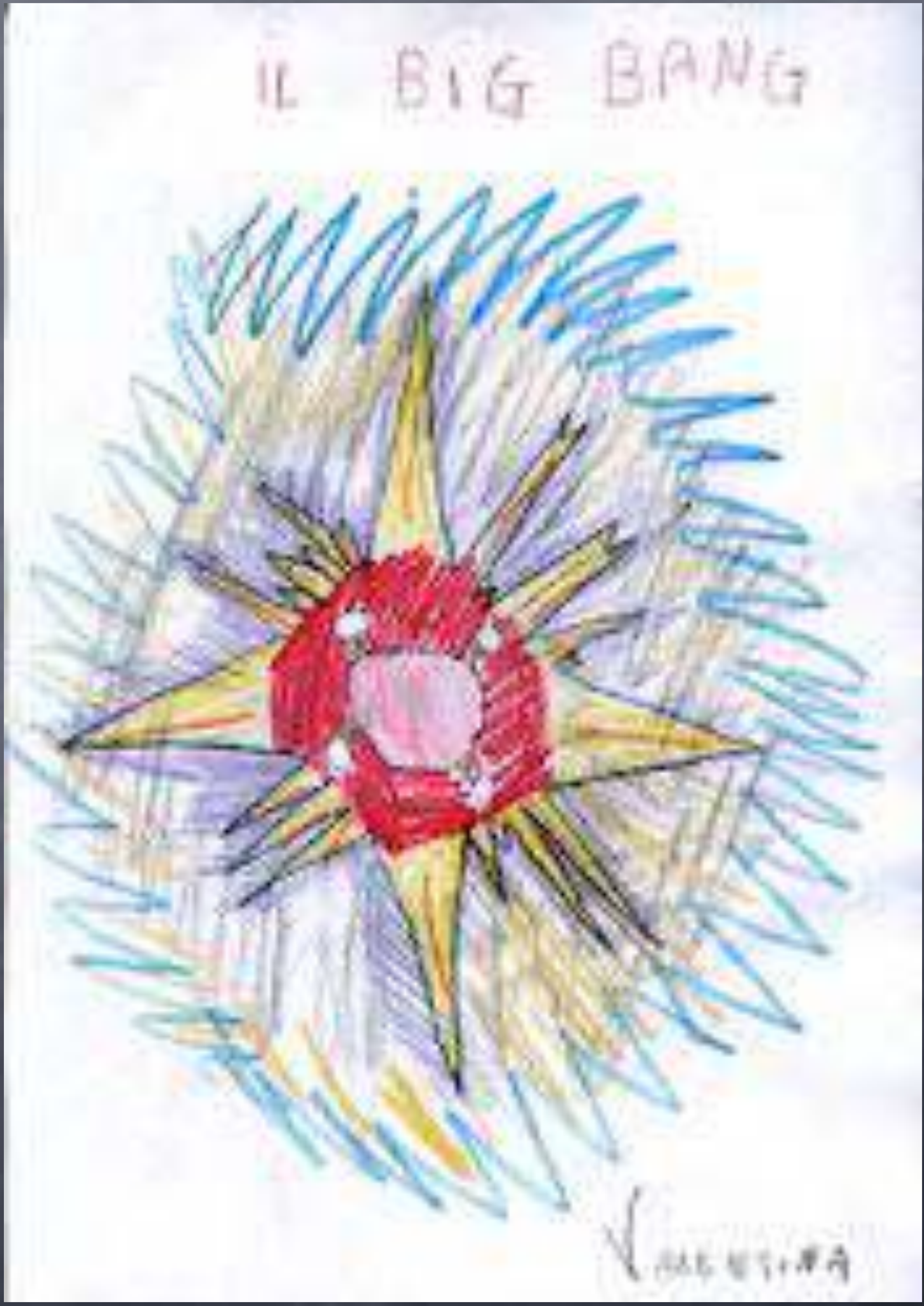


# Cool down

- Below 5 x 109 K (t ≈ 4 sec), the electron-positron pairs began to annihilate.

- This leaves photons, neutrinos and antineutrinos in essentially free expansion, with the $T_{photon}$ 40% higher than the $T_{neutrino}$.

- At the same time, the cooling froze the neutron-protons ratio at about 1:5.



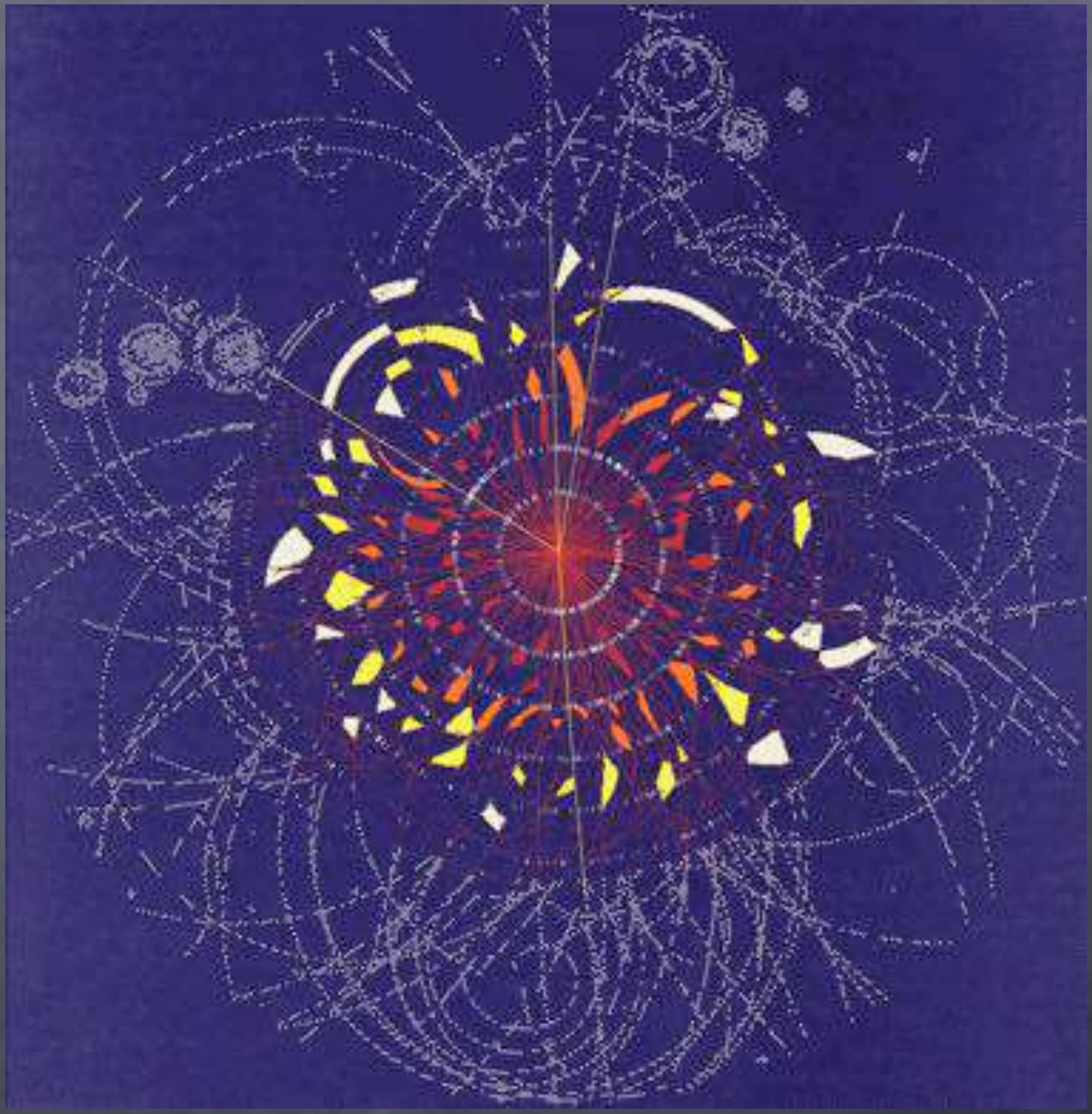
# Cool down

- At bout $10^9$ K ($t \approx 3$ min), the neutrons rapidly began to fuse with protons into heavier nuclei.

- This leaves an ionized gas of hydrogen and helium, with traces of deuterium $^2H$, $^3He$, and $^7Li$.

# Cool down

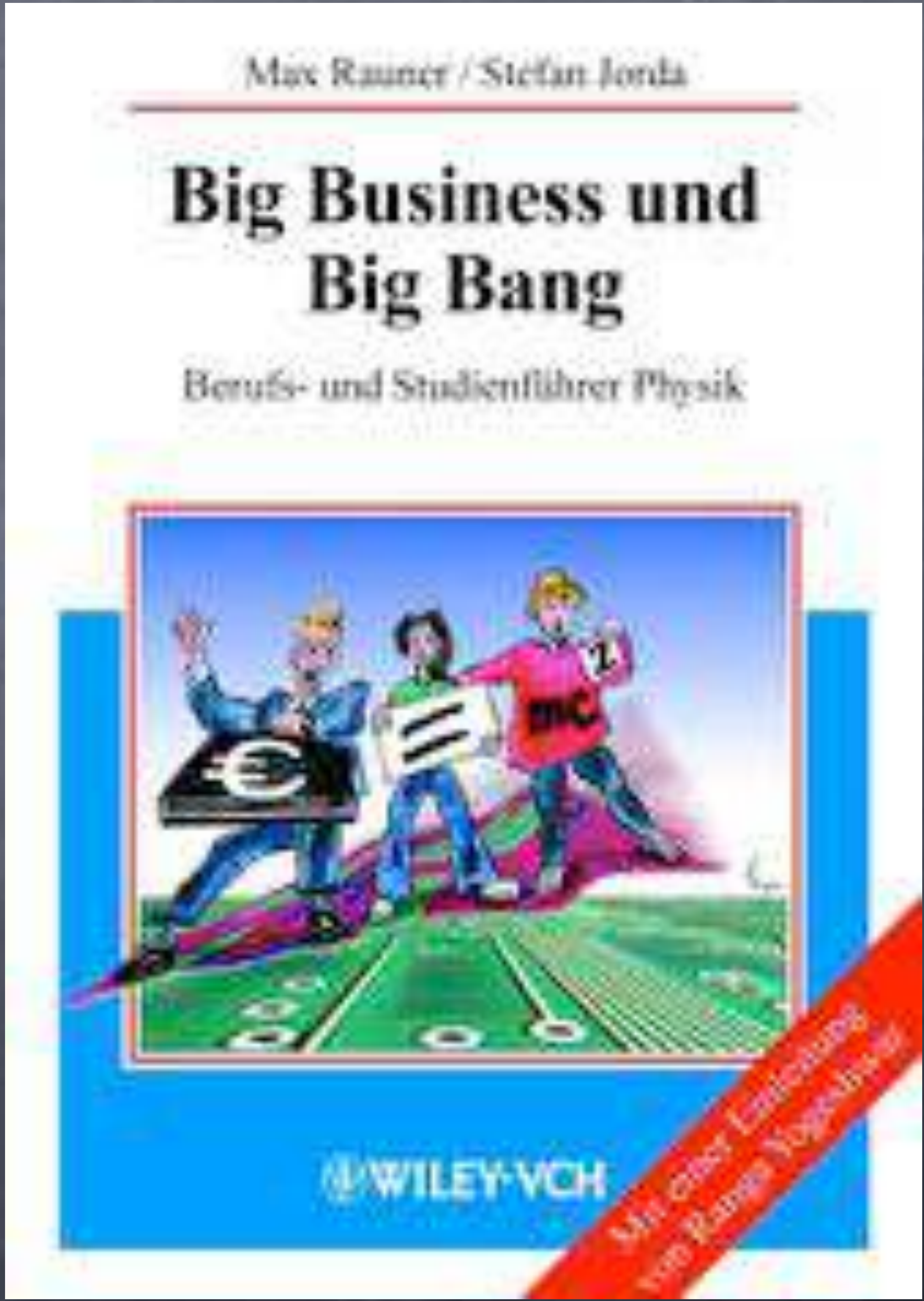
- The free expansion of the photons, neutrinos and antineutrinos continues, with $T_{photon} = 1.4\ T_{neutrino} \sim 1/R$.
- The ionized gas temperature remained locked to the photon temperature until the hydrogen atoms formed at T ~ 4000 K.



Wilson Synchrotron Lab

# Cool down

- Between 1000 and 10,000 K, the energy density of photons, neutrinos, and antineutrinos dropped below the rest-mass density of hydrogen and helium, and we entered the matter dominated era.



Max Rauner / Stefan Jonda

Big Business und Big Bang

Berufs- und Studienführer Physik

WILEY-VCH

Mit einer Einleitung von Ranga Yogeshwar

# Cool down

- Precisely how does the universe cool down?

$$\dot{R}^2 = \frac{8\pi G E}{3} R$$

How fast our universe expands

$$E = E_\gamma + E_{e-} + E_{e+} + \sum (E_\nu + E_{\overline{\nu}})$$

Energy density of
things in our universe

# Cool down

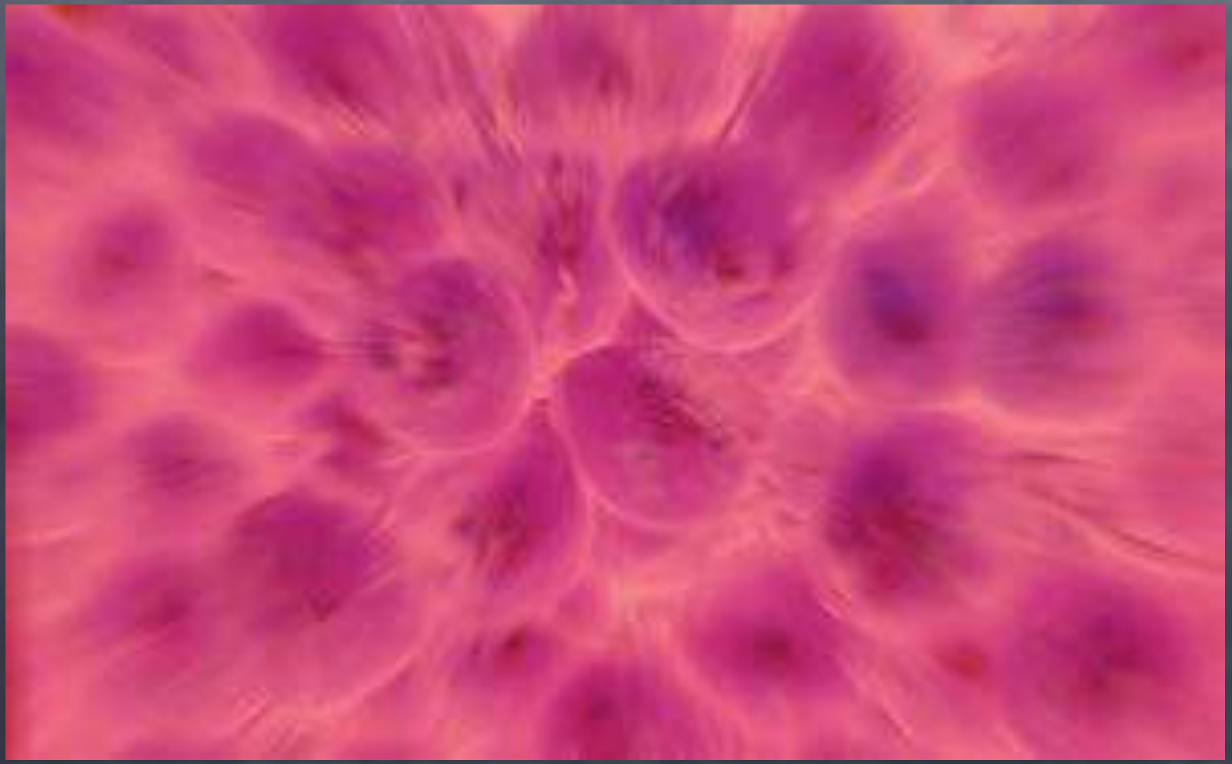
$$s = \frac{R^3}{T}\left[\rho(T) + P(T)\right] = \text{constant}$$

2nd law of thermodynamics

$$s = \frac{4}{3}a(RT)^3 f\left(\frac{m_e c^2}{kT}\right)$$

Entropy of things in our universe

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



Big Bang, 2002.
Photo, Jack Bishop

# Cool down

$$\frac{dT}{dt} = \frac{dR}{dt}\frac{dT}{dR}$$

We want an ODE for the temperature

$$\frac{R}{R_0} = \frac{T_{\gamma,0}}{T} f^{-1/3} \left(\frac{m_e c^2}{kT}\right)$$

How the temperature changes with the size of our universe

# Cool down

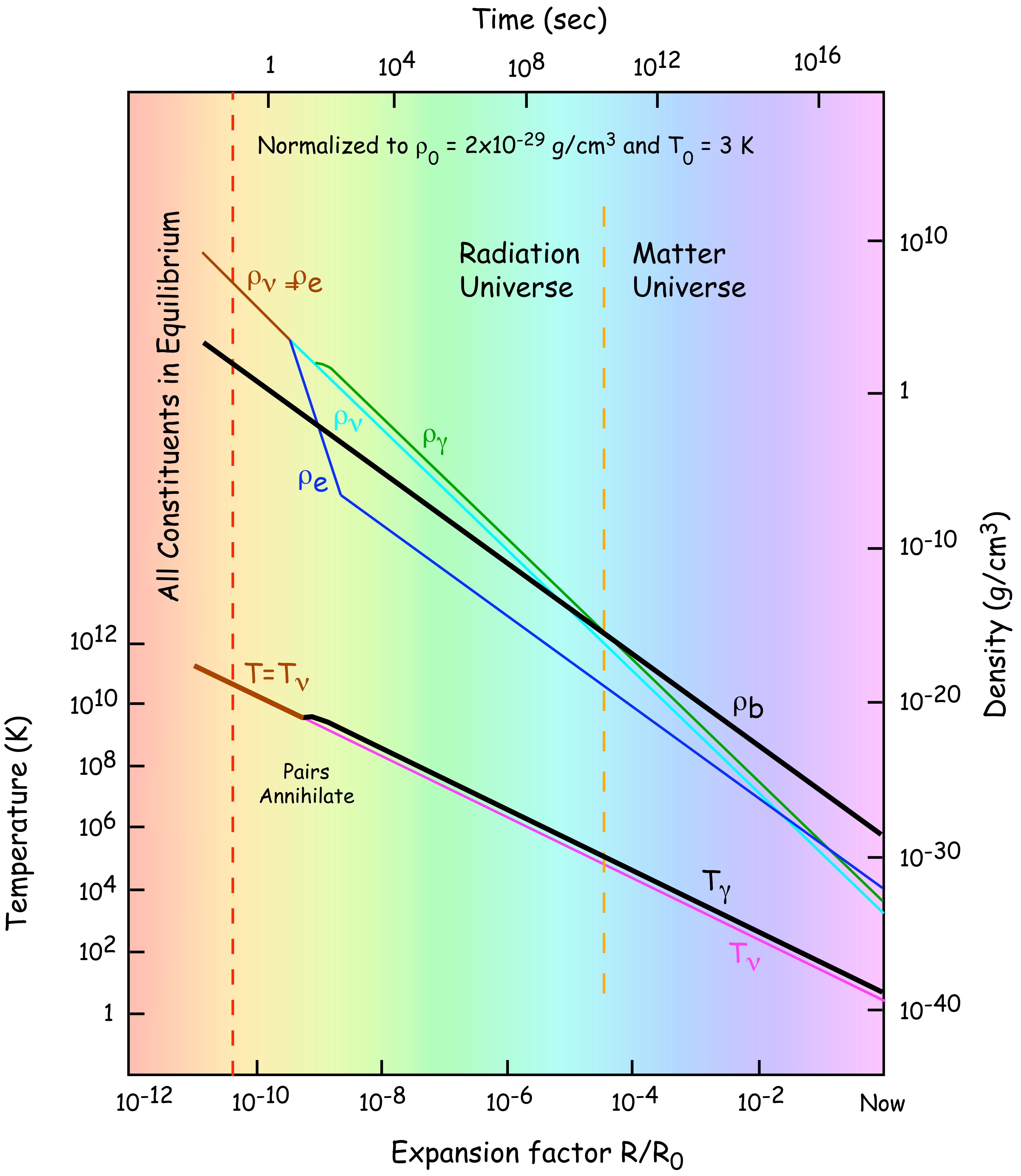
$$\frac{dT}{dt} = \sqrt{\frac{8\pi G a f(x)}{3c^2}}\, T^3 \; \left[x\frac{dg/dT}{3g} - 1\right]^{-1}$$

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

An ordinary differential equation for the photon temperature of the expanding universe.

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

- How our universe cools down as it expands.



# Cool down

- Simpler scaling relations:

$$T \approx 1.4 \frac{10^{10}}{\sqrt{t}}\ \mathrm{K} \quad \text{for } T < 10^9$$

$$T \approx \frac{10^{10}}{\sqrt{t}}\ \mathrm{K} \quad \text{for } 5 \times 10^9 < T < 10^{12}$$

BIG-BANG

NO MATCHES - NO POWDER

Can't Burst From Overcharge

HEAVY ARTILLERY

LIGHT FIELD GUN

Illustrated
Order Blank
and
Further Details
On Request

Permanent
Show Room
Room 461
Fifth Avenue
Building

ARMY TANK

NAVY GUN-BOAT

THE CONESTOGA CORPORATION BETHLEHEM, PA., U.S.A.

# Cool down

- We now know how hot the oven is at any given time. We can do this because the dominant constituents are either massless or moving very fast (relativistic).

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

# Cool down

- A common way to express the unknown baryon density is in terms of the baryon-to-photon ratio; how many photons there are for every particle.

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

Mass density and number density

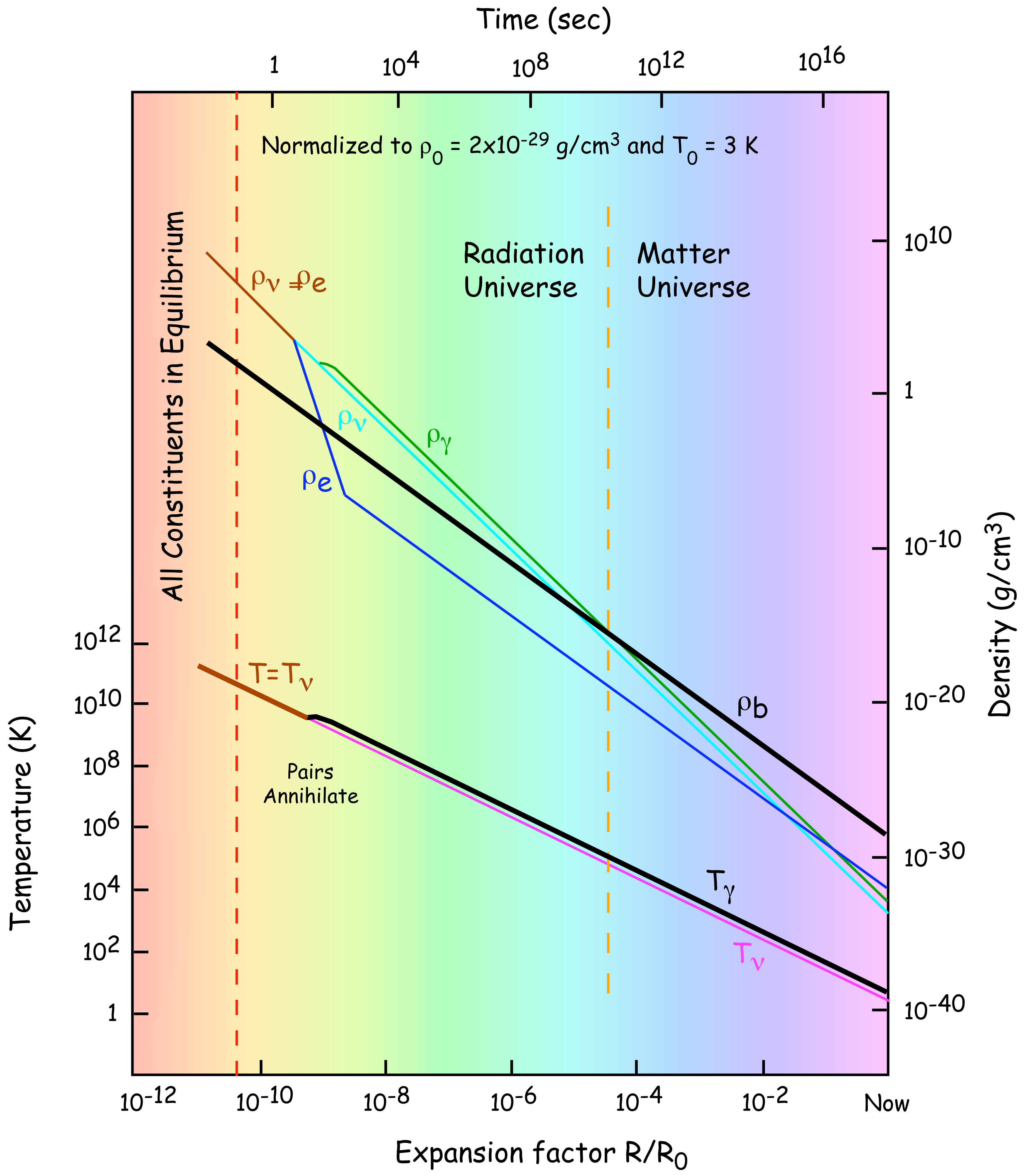
$$n_\gamma = \frac{30\zeta(3)}{\pi^4}\frac{aT_\gamma^3}{k}$$

Number of photons per cm$^3$

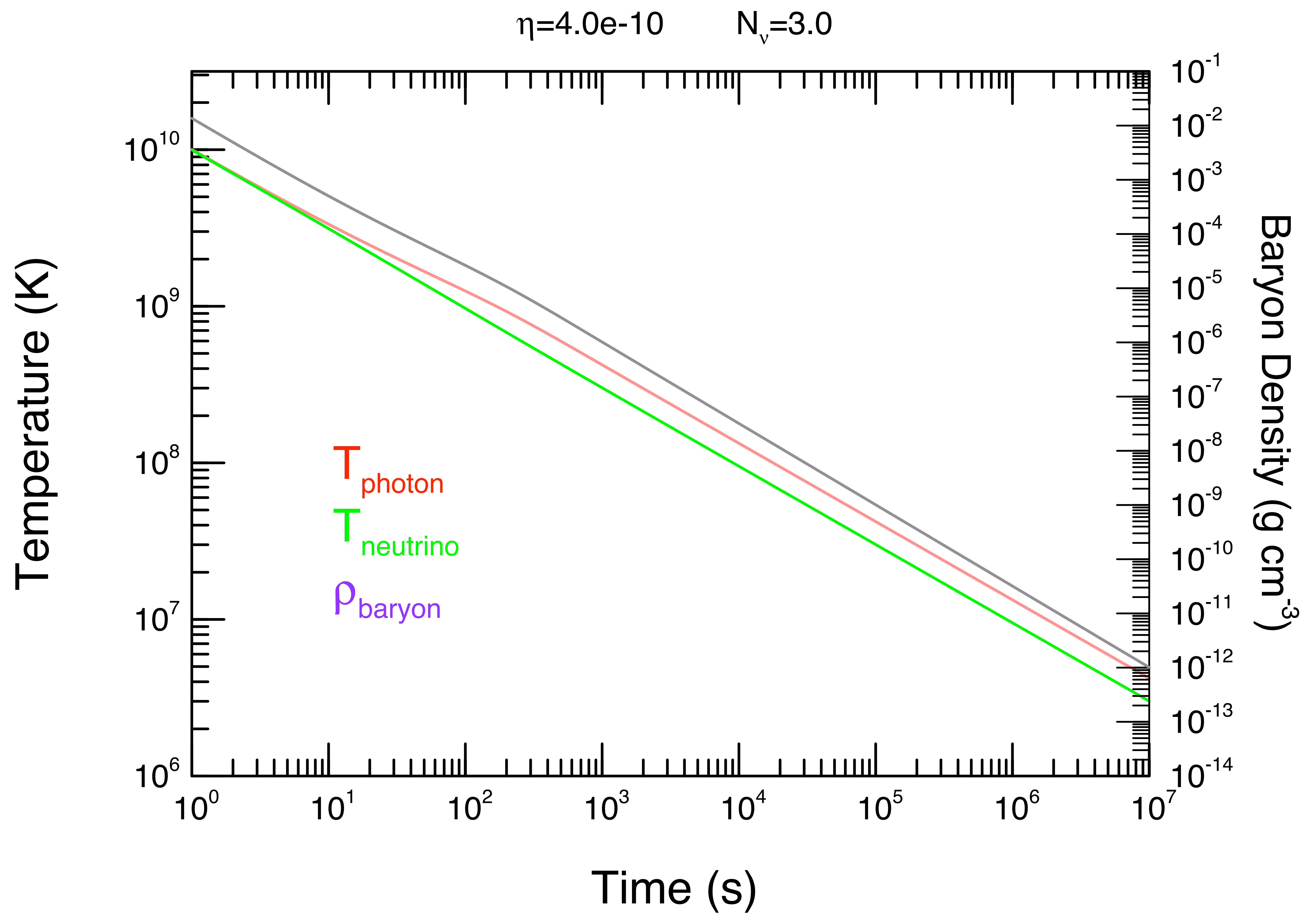
$$\rho_b = \frac{n_b}{n_\gamma} = \frac{30\zeta(3)}{\pi^4 k N_A} T_\gamma^3$$

Mass density in terms of the photon temperature and the free parameter $n_b/n_\gamma$

- How our universe gets less dense, for a chosen $n_b/n_\gamma$ ratio, as it expands.



# Cool down



$\eta$=4.0e-10
$N_\nu$=3.0
Temperature (K)
$10^{10}$
$10^{9}$
$10^{8}$
$10^{7}$
$10^{6}$
$T_{photon}$
$T_{neutrino}$
$\rho_{baryon}$
Baryon Density (g cm$^{-3}$)
$10^{-1}$
$10^{-2}$
$10^{-3}$
$10^{-4}$
$10^{-5}$
$10^{-6}$
$10^{-7}$
$10^{-8}$
$10^{-9}$
$10^{-10}$
$10^{-11}$
$10^{-12}$
$10^{-13}$
$10^{-14}$
$10^{0}$
$10^{1}$
$10^{2}$
$10^{3}$
$10^{4}$
$10^{5}$
$10^{6}$
$10^{7}$
Time (s)

# Colorful characters

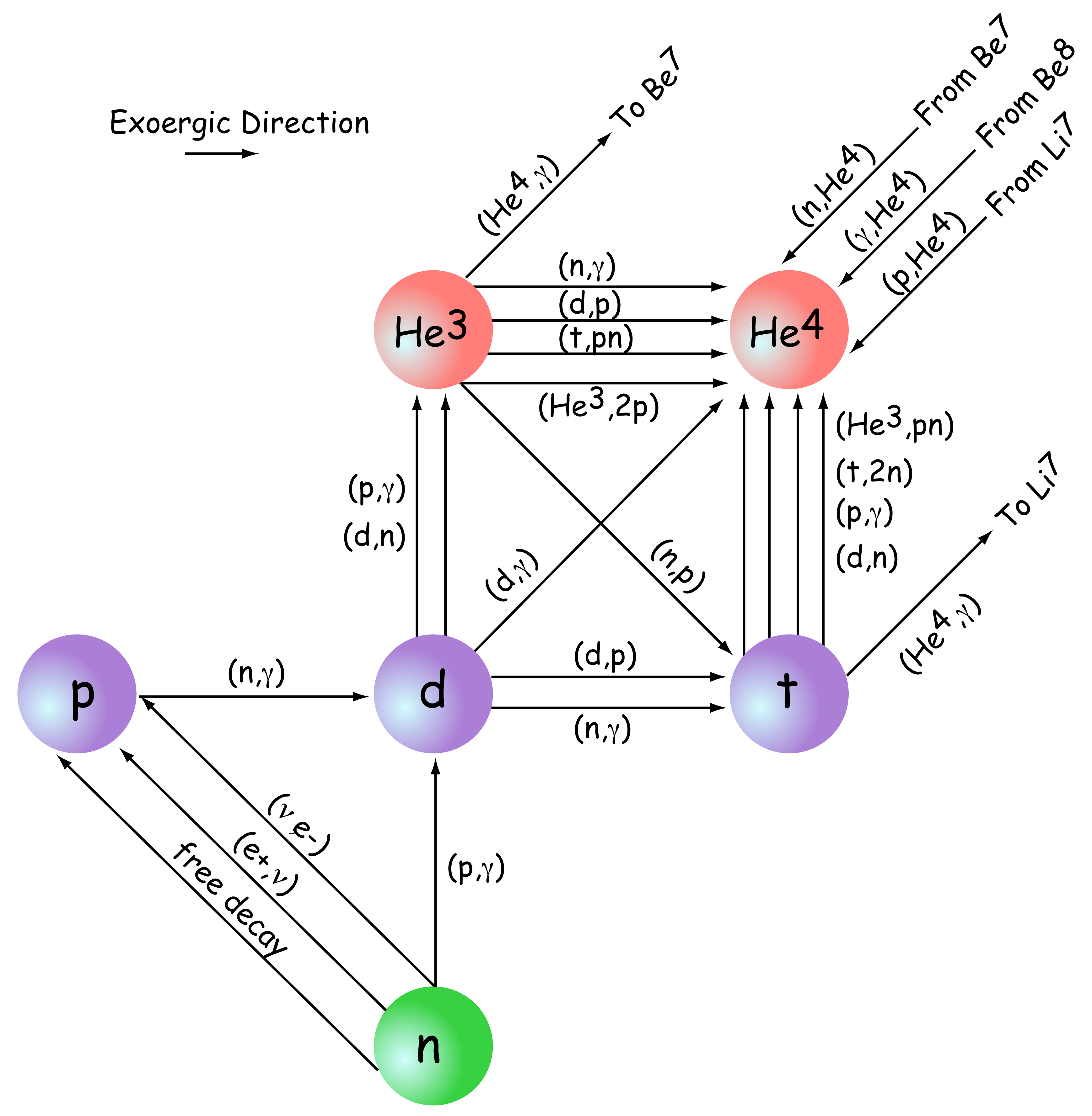
Fred Hoyle
1915 - 2001

Bob Wagoner
1967

David Schramm
1945 - 1997

# Big Bang Nucleosynthesis

- A typical Big Bang reaction network.



# Big Bang Nucleosynthesis

- Above 10 billion K, the ratio of neutrons to protons is kept in equilibrium by weak processes:

$$\nu_e + n \leftrightarrow e^- + p$$

$$\overline{\nu_e} + p \leftrightarrow e^+ + n$$

$$\overline{\nu_e} + e^- + p \leftrightarrow +n$$

$$\downarrow$$

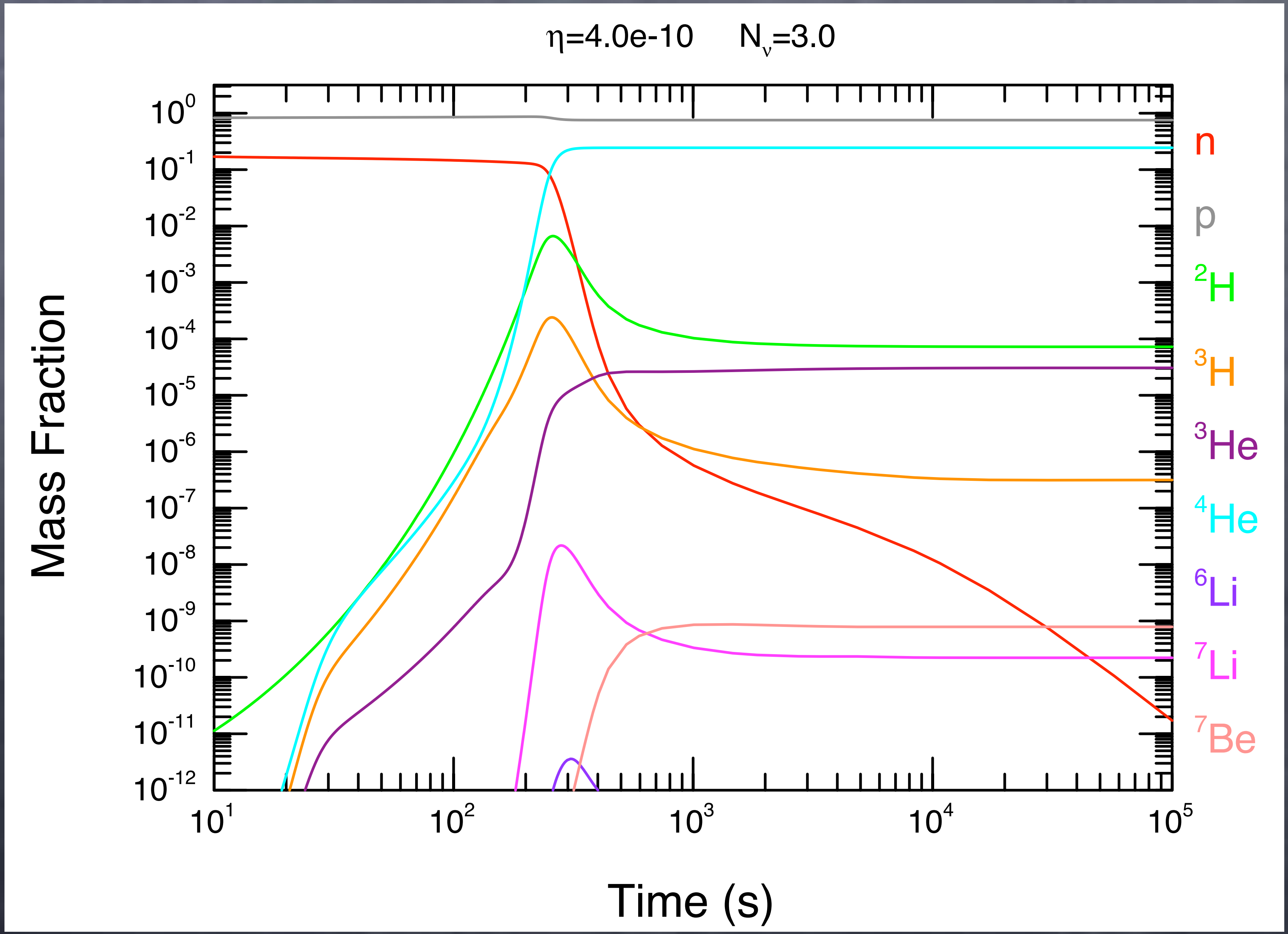
$$\frac{n_n}{n_p} = \exp\left(\frac{(m_p - m_n)c^2}{kT}\right)$$

All other abundances are negligible for T > $10^{10}$ K.

Big Bang, 1989,
Boris Valejo

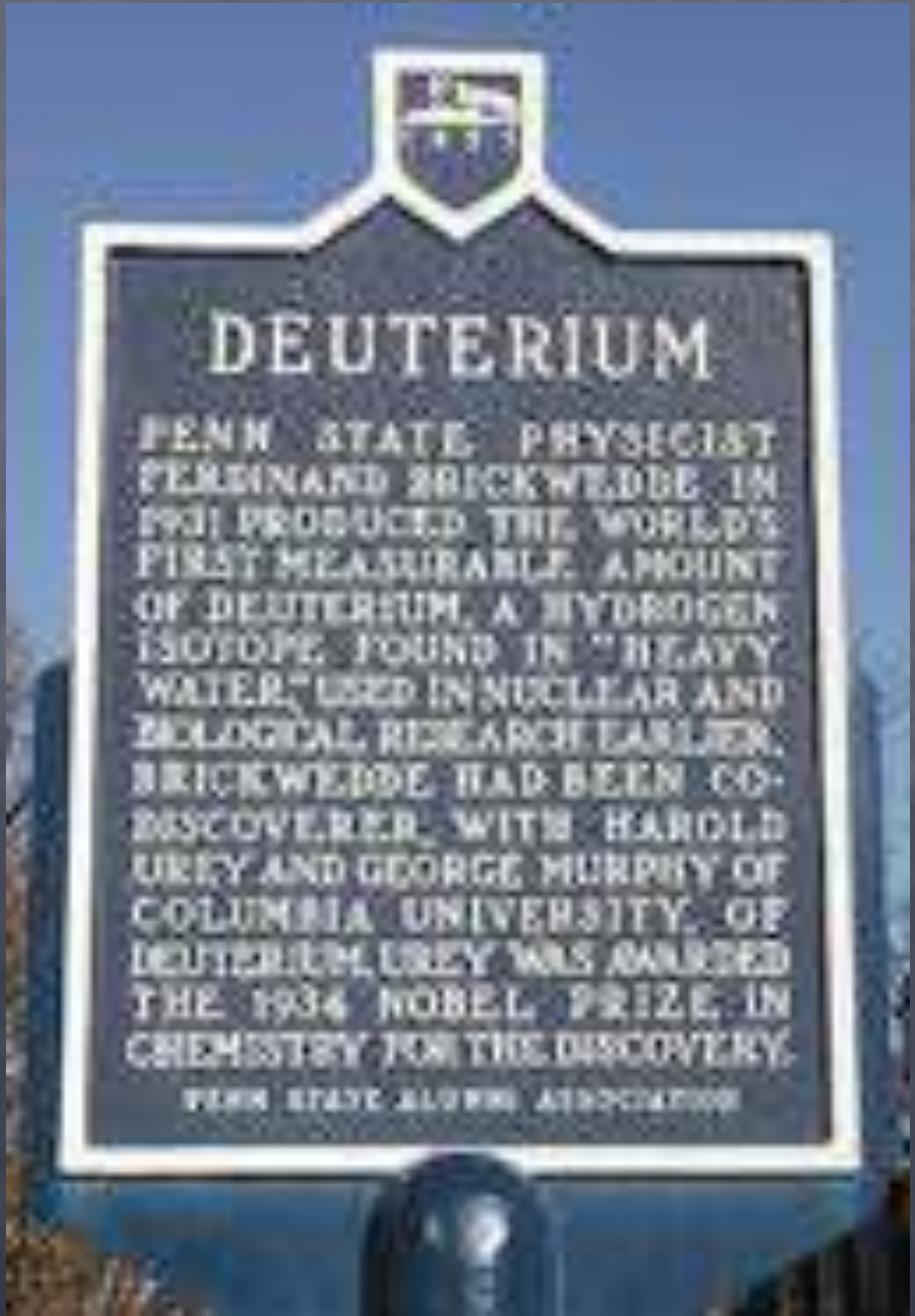
# Big Bang Nucleosynthesis

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



# Big Bang Nucleosynthesis

- Deuterium formation is crucial for triggering additional nuclear reactions. Without deuterium all the neutrons would decay and our universe would be pure hydrogen.



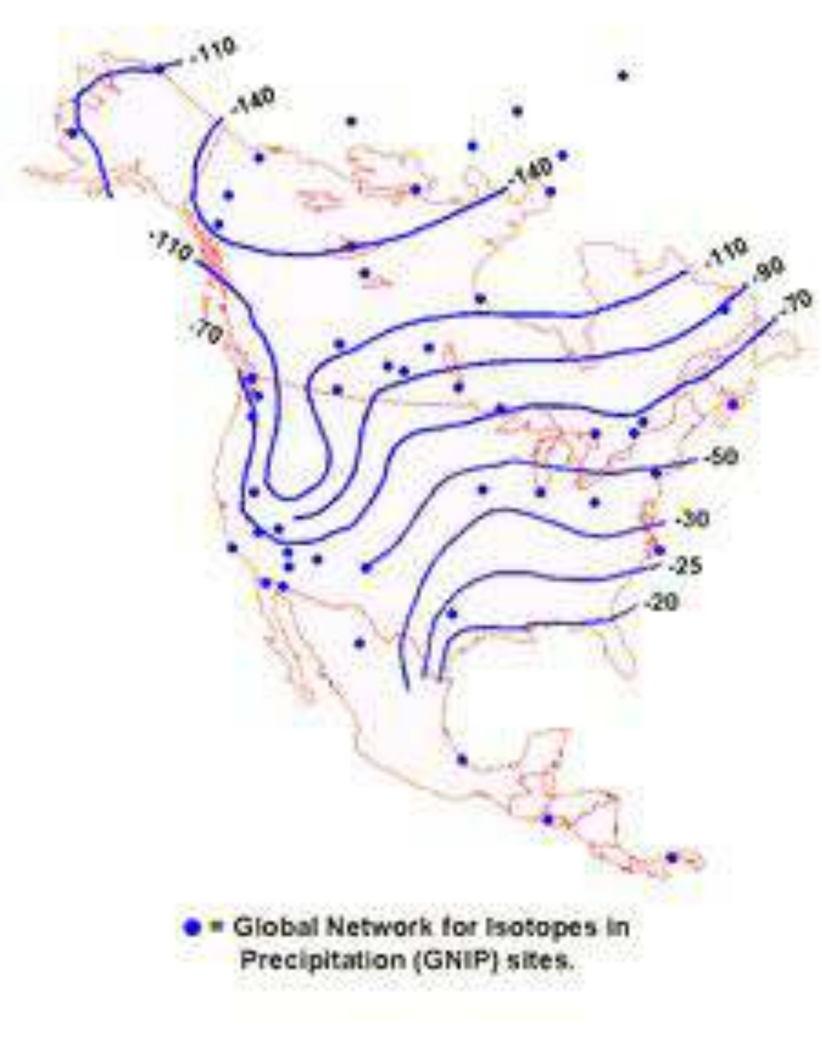
DEUTERIUM

PENN STATE PHYSICIST FERDINAND BRICKWEDDE IN 1931 PRODUCED THE WORLD'S FIRST MEASURABLE AMOUNT OF DEUTERIUM, A HYDROGEN ISOTOPE FOUND IN "HEAVY WATER," USED IN NUCLEAR AND BIOLOGICAL RESEARCH. EARLIER, BRICKWEDDE HAD BEEN CO-DISCOVERER, WITH HAROLD UREY AND GEORGE MURPHY OF COLUMBIA UNIVERSITY, OF DEUTERIUM. UREY WAS AWARDED THE 1934 NOBEL PRIZE IN CHEMISTRY FOR THE DISCOVERY.

PENN STATE ALUMNI ASSOCIATION

# Big Bang Nucleosynthesis

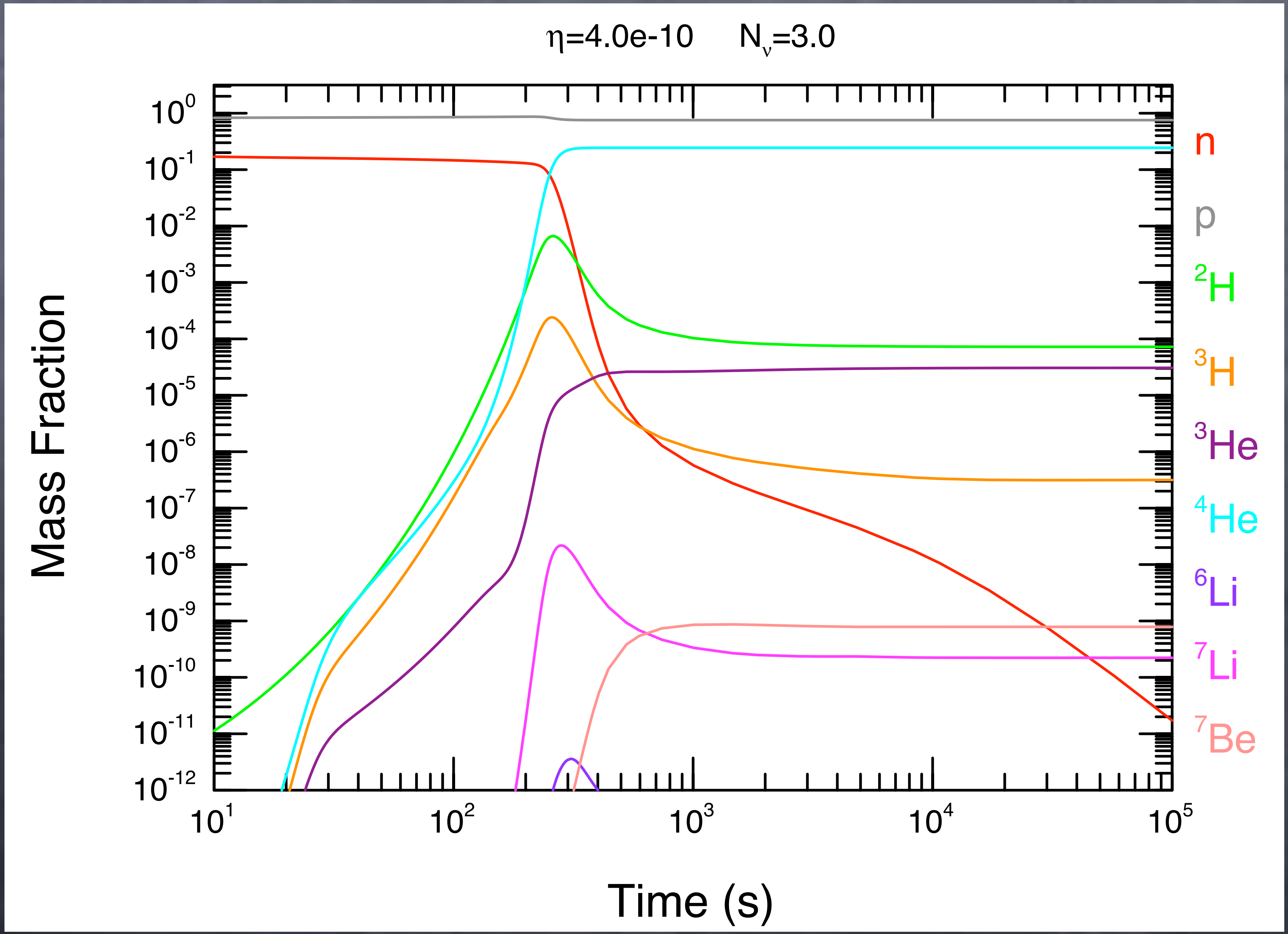
- Creation and destruction p(n,γ)d compete.
- One might expect that when the temperature drops below the 2.23 MeV binding energy of $^2$H, that the destruction process would become ineffective. However, there are too many photons!



2003, variation of deuterium with latitude. USGS

# Big Bang Nucleosynthesis

- By 3 min deuterium survives after it is fused and is quickly turned into helium. The whole process is slowed by a shortage of deuterium.



# Big Bang Nucleosynthesis

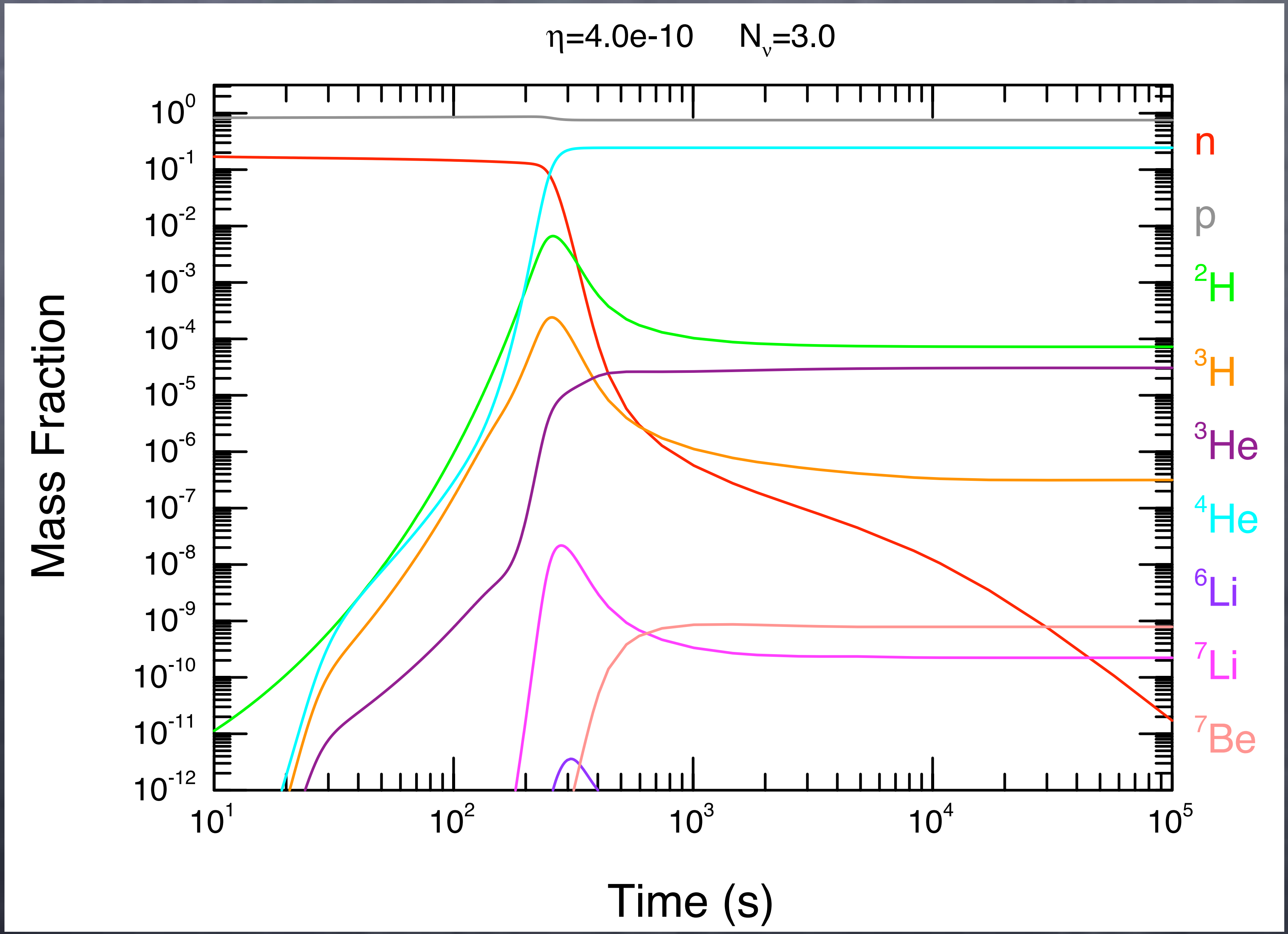
- Once deuterium is produced, $^4$He is rapidly formed, along with small fractions of $^3$H, $^3$He, $^6$Li, $^7$Li and $^7$Be.

- 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.

Big Bang, 2002 styrofoam and acrylics,
48" x 72" x 54”, Paul Kittelson.

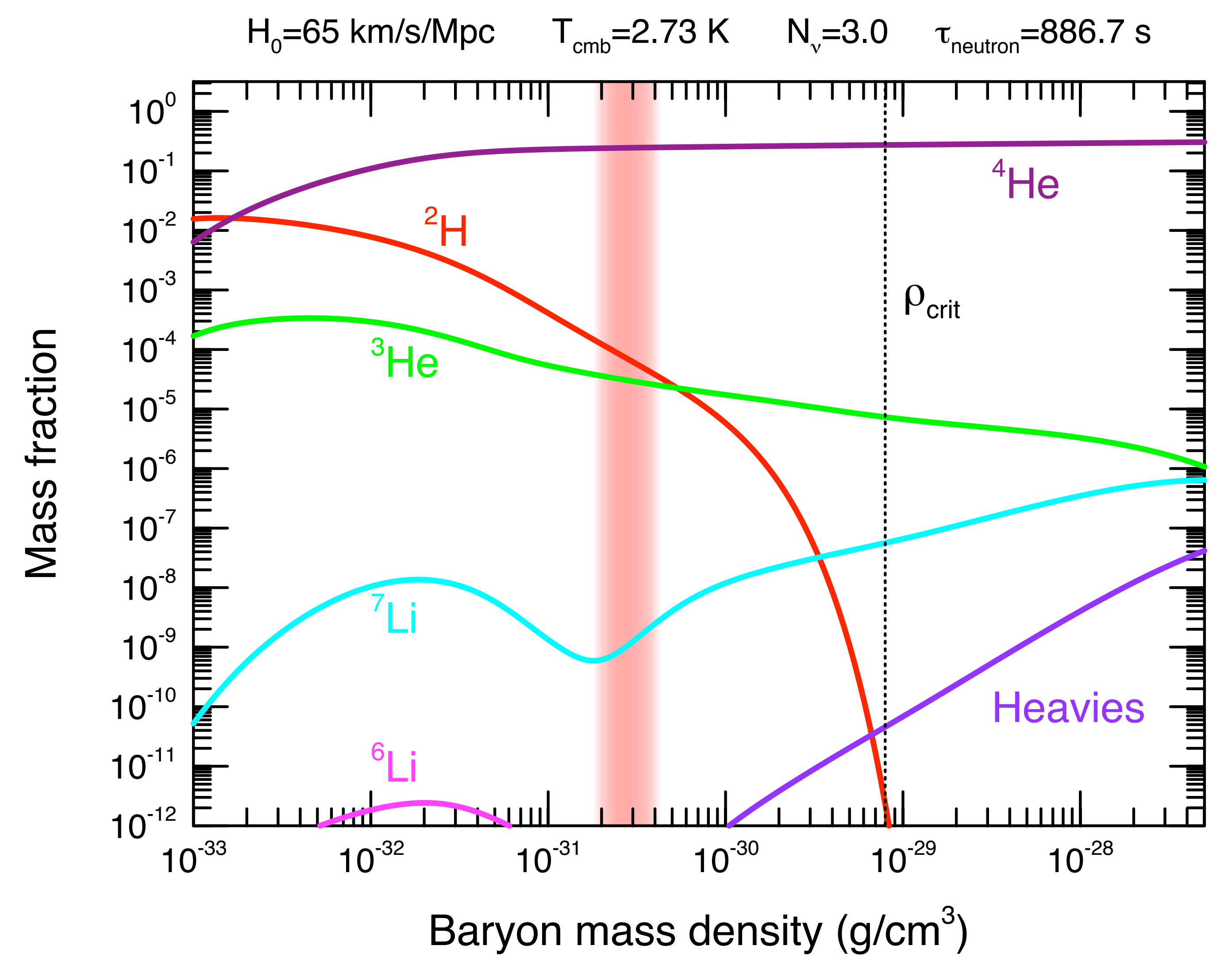
# Big Bang Nucleosynthesis

- By 35 min nucleosynthesis is essentially complete.



# Big Bang Nucleosynthesis

- A key unknown in big bang nucleosynthesis calculations is the density of ordinary matter.



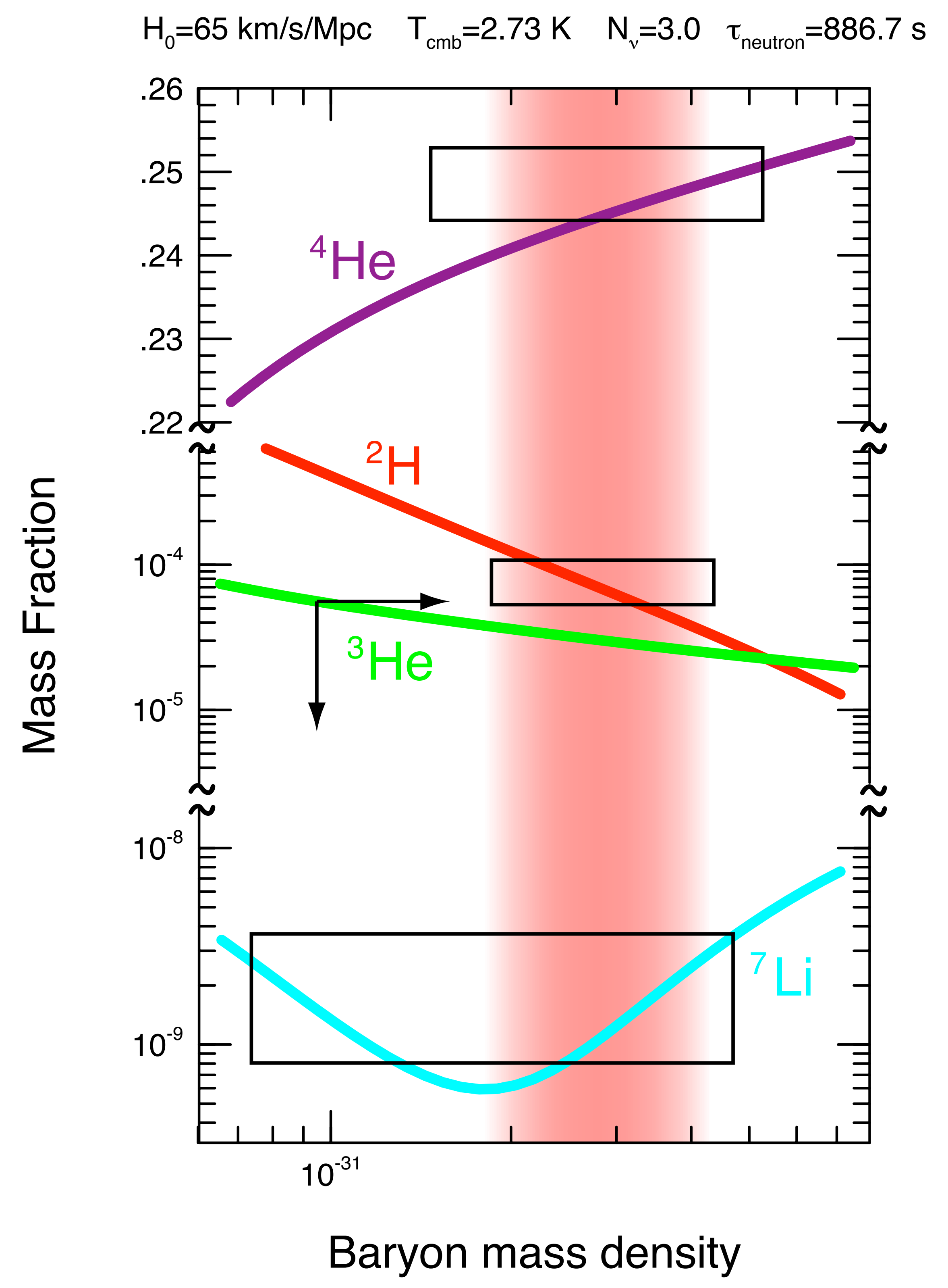
- Measurement of the light elements abundances constrains the present density of ordinary matter in the universe.

# Big Bang Nucleosynthesis

- The observed abundances of the light elements imply the density of normal matter in the universe is about 3.5 x $10^{-31}$ g/cm$^3$.

- Four independent measurements of four different elements lead to a consistent constraint.

- This gives us confidence that BBN provides a correct explanation of light element formation.



# Tasks for the day

- Answer the question posed on slide 19,
  “How then are definite (NSE) abundances possible?”

- Download, compile, and run the NSE code from
  www.cococubed.com/code_pages/nse.shtml
  Duplicate the two plots on the web page; slides 17 and 22.

- Add a realistic set of partition functions to the NSE code.
  Redo the plots above. What do you conclude?

# Tasks for the day

- Download, compile, and run the Big Bang thermodynamics code from www.cococubed.com/code_pages/burn.shtml
  Duplicate the plots on silde 46 and slide 45.

- Download, compile, and run the Big Bang nucleosynthesis code from www.cococubed.com/code_pages/burn.shtml
  Can you replicate the pplots on slides 55 - 57?

- Can you comment on inhomogeneous Big Bang nucleosynthesis by having (initially) some proton rich regions and some neutron rich regions?

# Tools and Toys in Nuclear Astrophysics

Uraniae,
1885,
Camille Flammarion