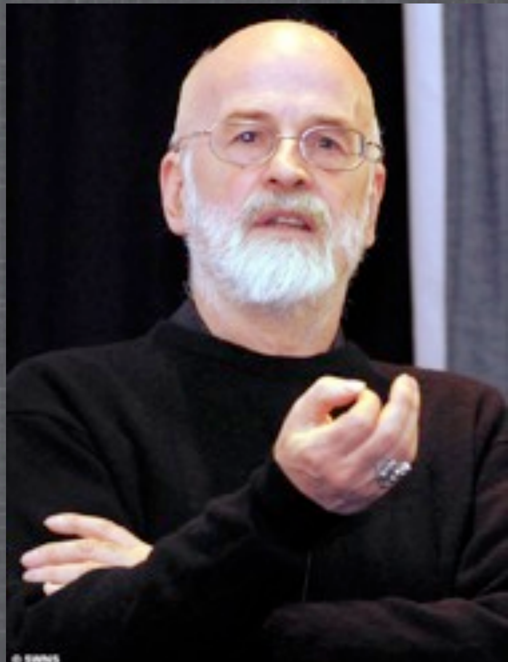
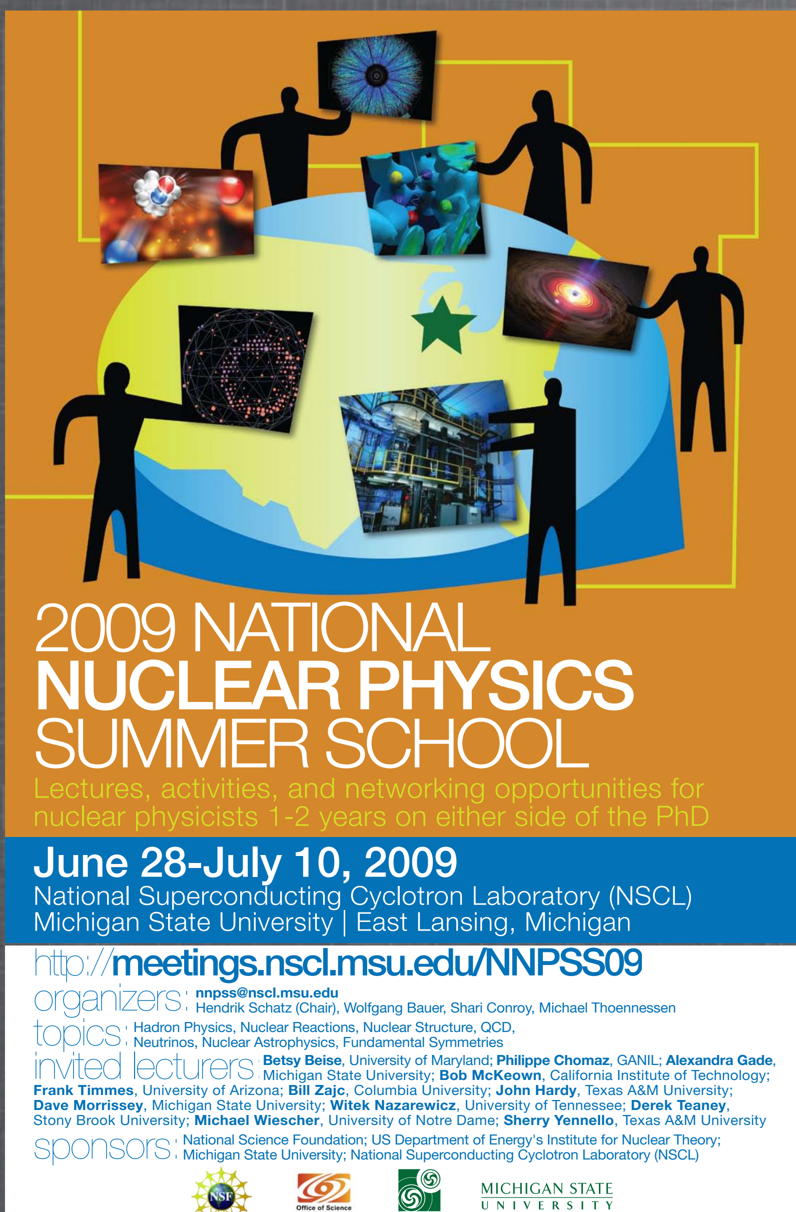
Granddad was superstitious about books.
He thought that if you had enough of them around,
education leaked out, like radioactivity.

Terry Pratchett



Nuclear Astrophysics: Reaction Networks

Frank Timmes



Outline for 29Jun2009

1. Overall theme: putting research tools in your hands
2. Some nomenclature
3. Forming a nuclear reaction network
4. Proton-proton chains

My overall purpose is to put a research level, nuclear reaction network toolkit in your hands.

By the end of my 4 lectures you will (hopefully) have these networks under your control and in your knowledge base:

Hydrogen burners: PP chains, CNO cycles
Alpha chains: 13 isotopes, 19 isotopes
Big Bang nucleosynthesis
General reaction network

These reaction networks are written in Fortran 90, so you will need a suitable compiler: gfortran, g95, ifort, xlf, absoft, portland, etc.

Reaction networks are an key tool in nuclear astrophysics and other areas of physics, astronomy, chemistry, biology, and geology.

Networks are relevant for modeling nucleosynthesis processes and their associated energy generation in stars.

STELLAR INTERIORS
SINS
& NUCLEOSYNTHESIS

These talks will provide an overview of the nuclear astrophysics, mathematics, and computational techniques of reaction networks. In only 4 talks, however, they will not be complete.

Stuff of the day

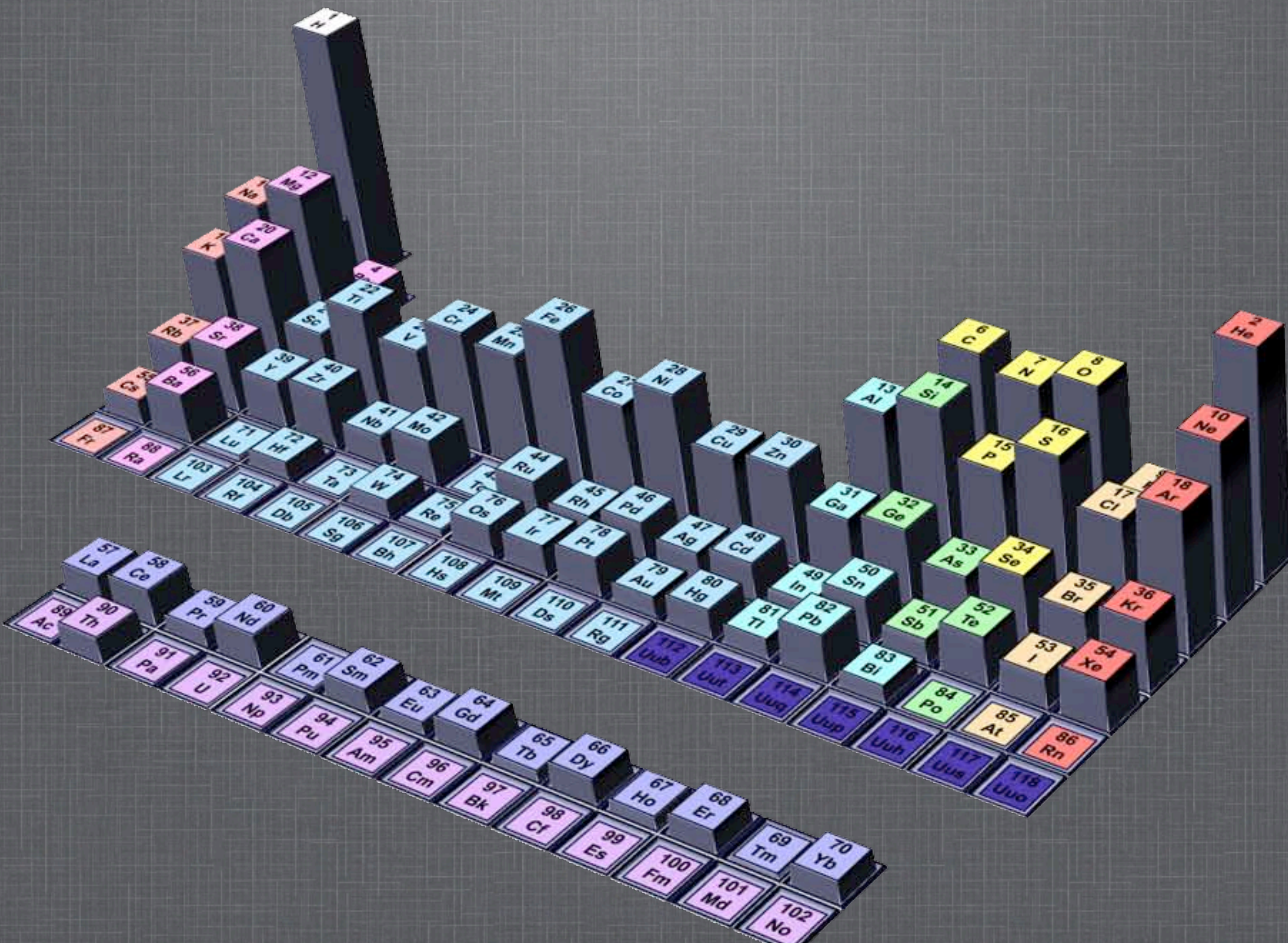
cococubed.asu.edu
click on “some astronomy codes” and/or “some astronomy talks”

How the Sun Shines
nobelprize.org/physics/articles/fusion/index.html

Thermonuclear Kinetics in Astrophysics
cococubed.asu.edu/papers/hix_meyer.pdf

Integration of Nuclear Reaction Networks...
www.iop.org/EJ/abstract/0067-0049/124/1/241/

Interlude



1 H
12 Mg
20 Ca
22 Ti
24 Cr
26 Fe
6 C
2 He
7 N
8 O
13 Al
14 Si
28 Ni
37 Rb
38 Sr
56 Ba
39 Y
40 Zr
41 Nb
42 Mo
10 Ne
15 P
16 S
29 Cu
30 Zn
87 Fr
88 Ra
71 Lu
72 Hf
103 Lr
104 Rf
105 Db
106 Sg
107 Bh
108 Hs
109 Mt
110 Ds
111 Rg
112 Uub
113 Uut
114 Uuq
115 Uup
116 Uuh
117 Uus
118 Uuo
73 Ta
74 W
44 Ru
45 Rh
46 Pd
75 Re
76 Os
77 Ir
78 Pt
47 Ag
48 Cd
79 Au
80 Hg
31 Ga
32 Ge
17 Cl
18 Ar
33 As
34 Se
35 Br
36 Kr
49 In
50 Sn
81 Tl
82 Pb
51 Sb
52 Te
53 I
54 Xe
83 Bi
84 Po
85 At
86 Rn
57 La
58 Ce
59 Pr
60 Nd
61 Pm
62 Sm
63 Eu
64 Gd
65 Tb
66 Dy
67 Ho
68 Er
69 Tm
70 Yb
89 Ac
90 Th
91 Pa
92 U
93 Np
94 Pu
95 Am
96 Cm
97 Bk
98 Cf
99 Es
100 Fm
101 Md
102 No

Some nomenclature

An isotope can be characterized by the dimensionless integers

Z = number of protons = atomic number

N = number of neutrons

A = Z + N = number of nucleons

The Avogadro number, from the 2006 CODATA values,

$$N_A = 6.02214179 \pm 0.00000030 \times 10^{23} \qquad 1/\text{mole}$$

is the number of ``entities'' in one mole. When an individual entity has a mass *m* in grams, the atomic weight or molar mass is

$$W = mN_A \qquad \text{g/mol.}$$

The mass of all entities is the number of moles times the molar mass.

The atomic mass unit (amu) is defined as 1/12 mass of an isolated ^{12}C atom at rest and in its ground state. For ^{12}C, we define the molar mass to be W=12.0 g/mol. An amu then has W=1 g/mol. Hence,

$$1\text{amu} = 1/N_A = 1.660538782 \pm 0.000000083 \times 10^{-24} \quad \text{g}.$$

Thus, one can say N_A has units of grams but care must be taken to apply the implicit mol/g conversion to other quantities of interest.

In this system of units, the molar mass W is dimensionless. Mixing the [1/mol] and [1/g] systems of units will cause confusion.

The rest mass of a single isotope k is

$$\begin{aligned} m_k &= \mathrm{N} m_n + \mathrm{Z} m_p + \mathrm{Z}(1-f) m_e - \Delta m \\ &= \mathrm{N} m_n + \mathrm{Z} m_p + \mathrm{Z}(1-f) m_e - \frac{\mathrm{B}}{c^2} \qquad \mathrm{g}, \end{aligned}$$

m_n is the neutron mass
m_p is the proton mass
m_e is the electron mass
f is the ionization fraction (0 for a neutral atom, 1 for full ionization),
Δm is the mass deficit
B is the nuclear binding energy in erg.

Sometimes terms like [15.7 $Z^{5/3}$ - 13.6 Z eV] are added to estimate the electronic binding energy. Such terms are usually negligible.
The molar mass of the isotope is $W_k = m_k N_A$.

For a mixture of isotopes, define

$$\rho = \frac{\sum n_i A_i}{N_A} \quad \mathrm{g\ cm^{-3}},\ \text{baryon mass density}$$

where n_i is the number density of species i.

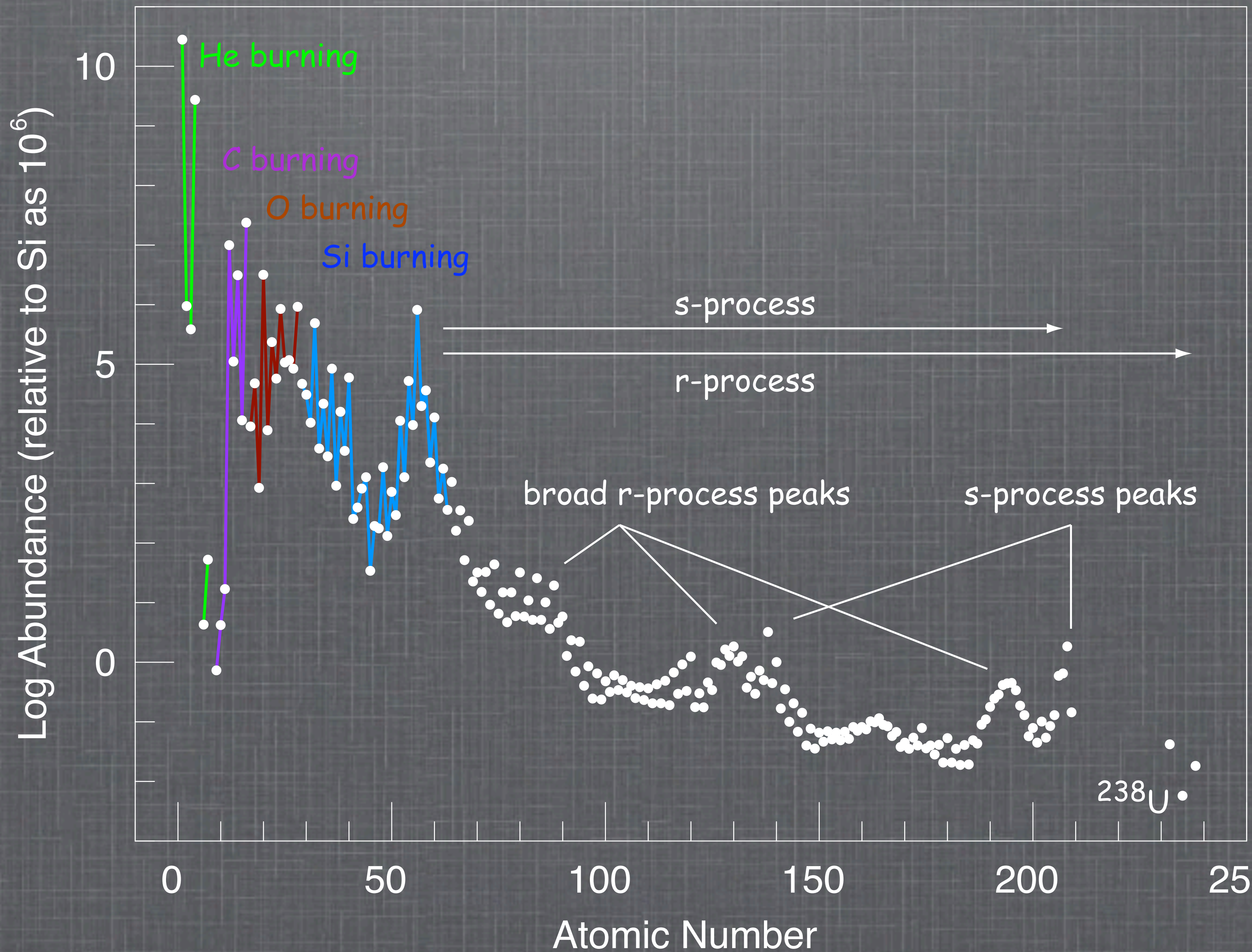
$$X_i = \frac{A_i n_i}{\rho N_A} = \frac{\rho_i}{\rho} \quad \text{mass fraction, dimensionless}$$

$$Y_i = \frac{X_i}{A_i} = \frac{n_i}{\rho N_A} \quad \text{molar fraction.dimensionless}$$

$$\sum_{i=1}^{k} X_i = 1 \quad \text{mass conservation}$$

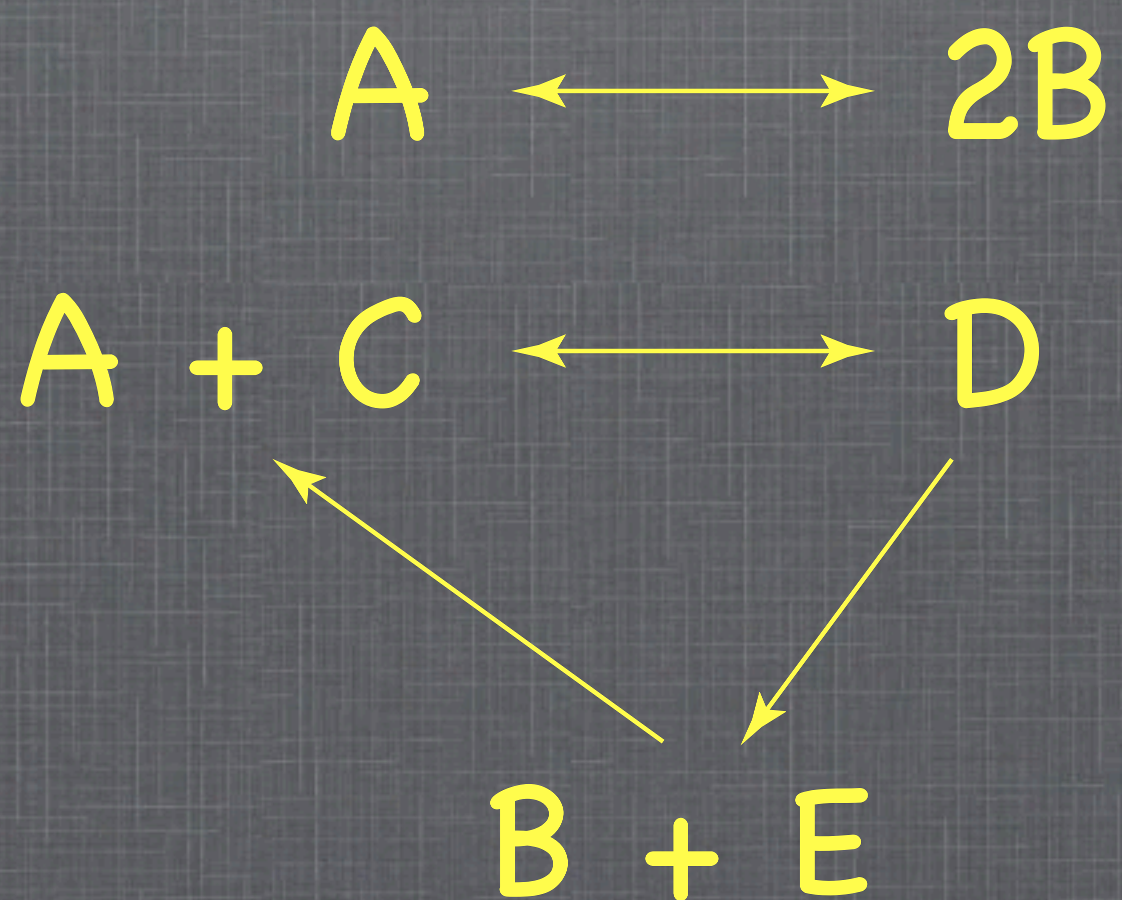
And finally (for today)

$$\overline{\mathrm{A}} = \frac{\sum n_i A_i}{\sum n_i} = \frac{1}{\sum Y_i} \qquad \overline{\mathrm{Z}} = \frac{\sum n_i Z_i}{\sum n_i} = \overline{\mathrm{A}} \sum Y_i Z_i$$



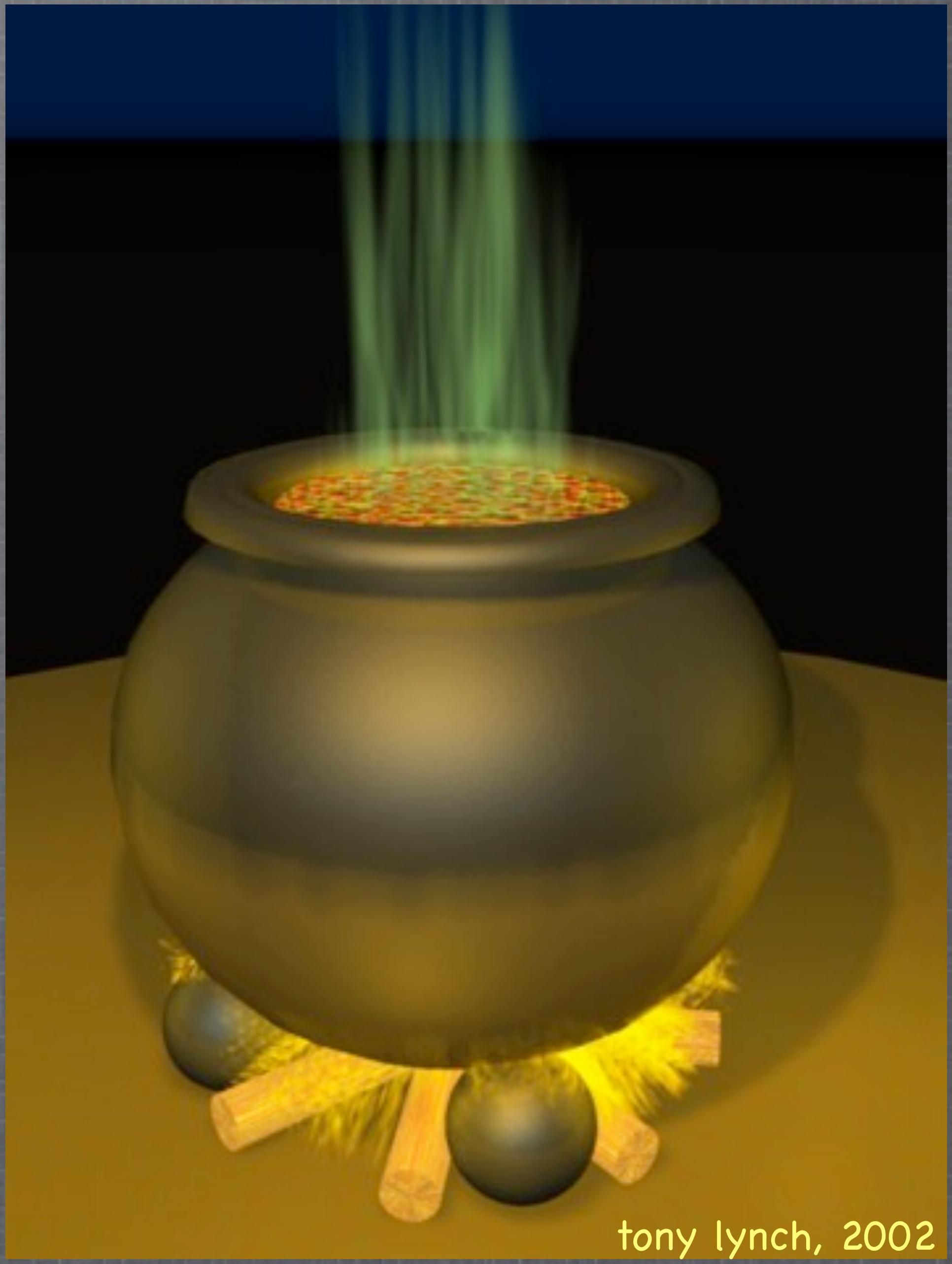
Let’s start talking about a special, but rather large class of ordinary differential equations (ODEs) - those that derive from nuclear/chemical/biological reaction networks.

Let’s walk through an example of a reaction network and indicate informally how it induces a system of ODEs.



Suppose we throw the various species in a pot that is constantly stirred so its contents remain spatially homogeneous for all time.

We'll also assume that the contents are kept at constant temperature and volume (constant density); hydrostatic burning.

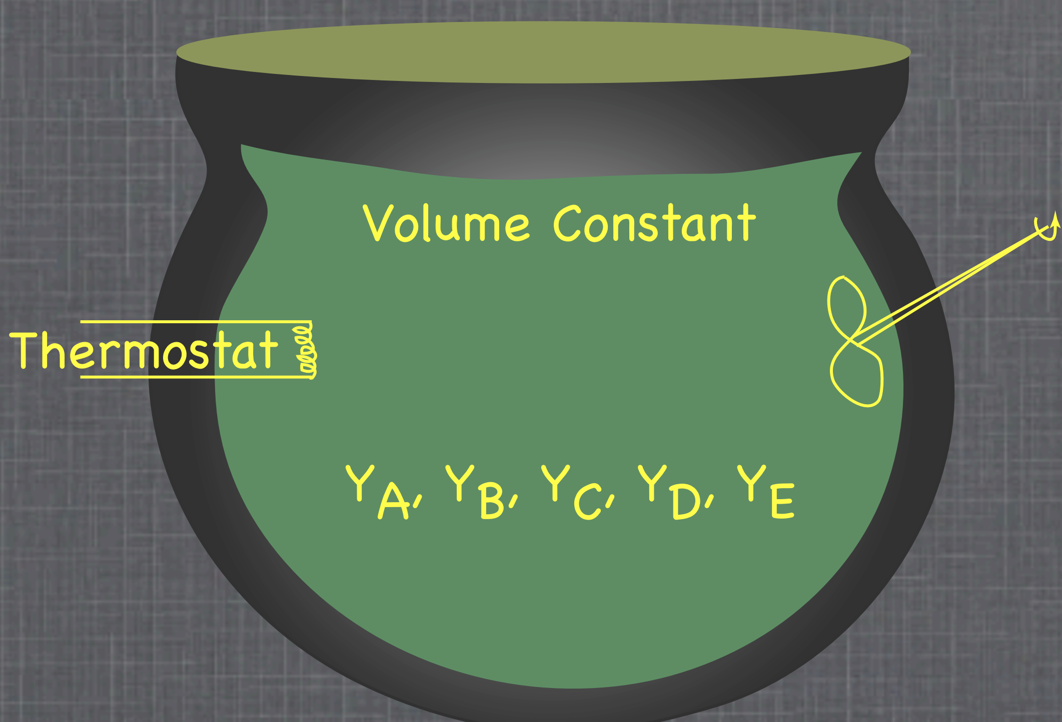


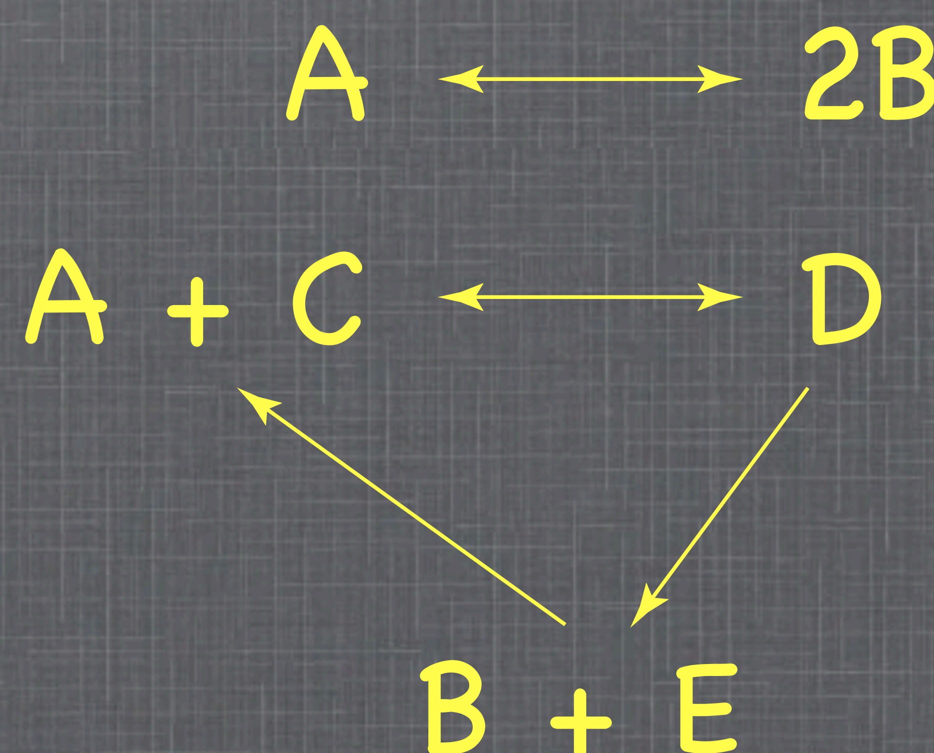
This is not to say the composition remains constant in time. Reactions will consume some species and generate others. In fact, it is the time evolution of the composition that we wish to investigate.

Denote the instantaneous values of the molar abundances by Y_A, Y_B, Y_C, Y_D, and Y_E. We want to write down five ODEs that describe the evolution of the five mole fractions.

Let's begin by considering the instantaneous rate of change of Y_A.

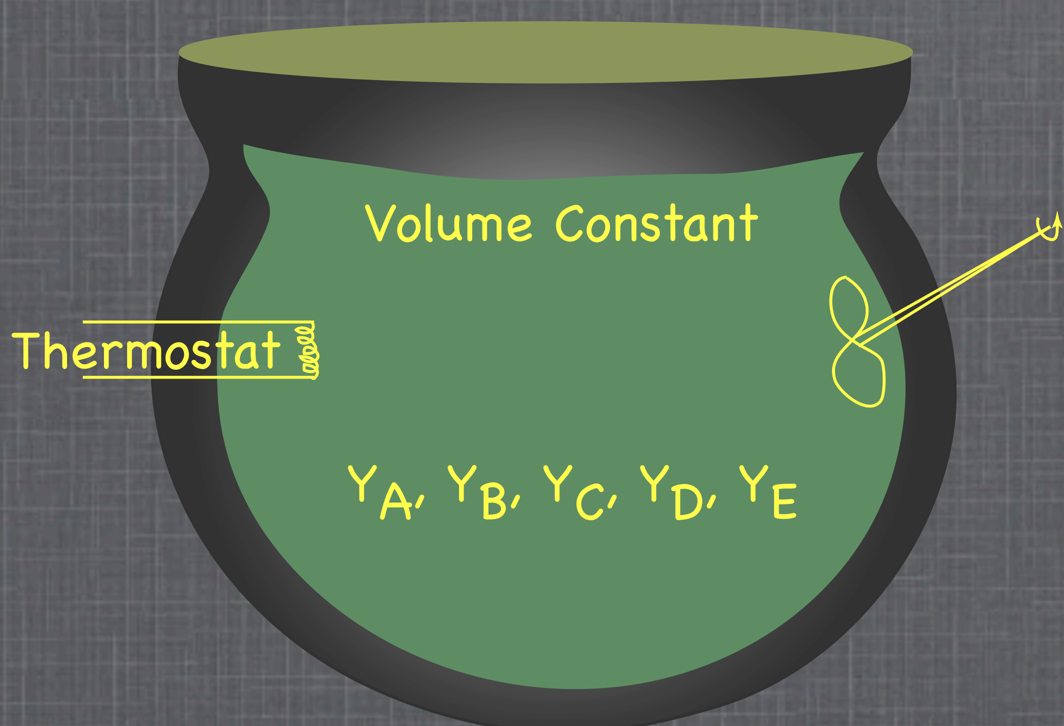
Every time $A \rightarrow 2B$ we lose one unit of A and this reaction occurs with an instantaneous, non-negative, real valued rate of $K_{A\rightarrow 2B}$.

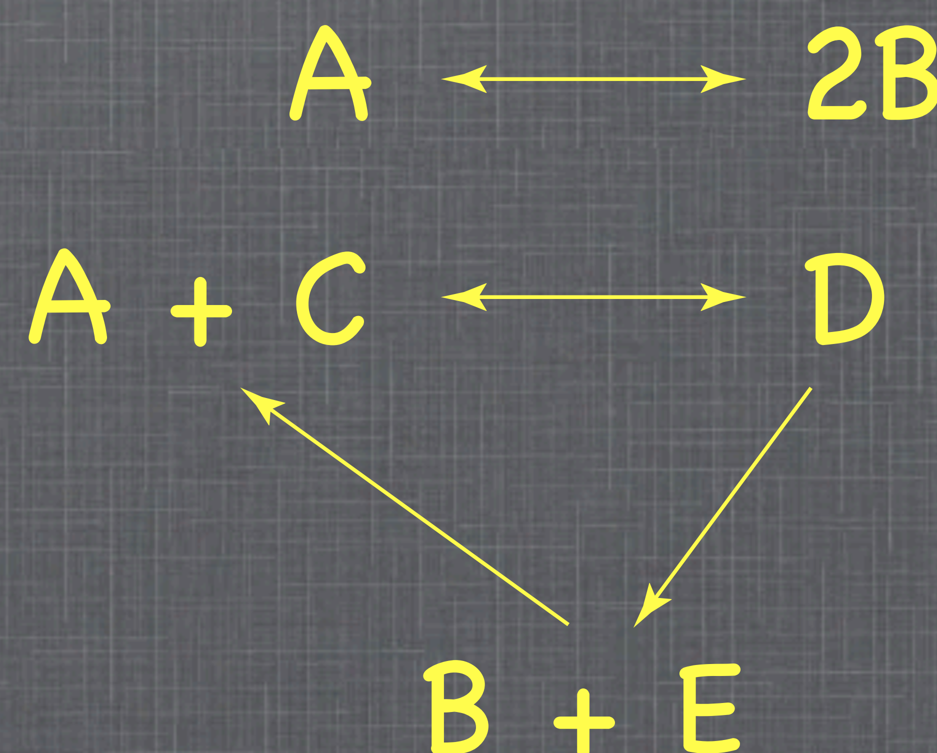




Similarly the reaction A + C→D loses a unit of species A, while 2B→A, B+E→A+C, D→A+C produces a unit of species A. So we write

$$\dot{Y}_A = -K_{A\to 2B} + K_{2B\to A} - K_{A+C\to D} + K_{D\to A+C} + K_{B+E\to A+C}$$





Continuing in this way, we can write down a system of ODEs that govern our reactor:

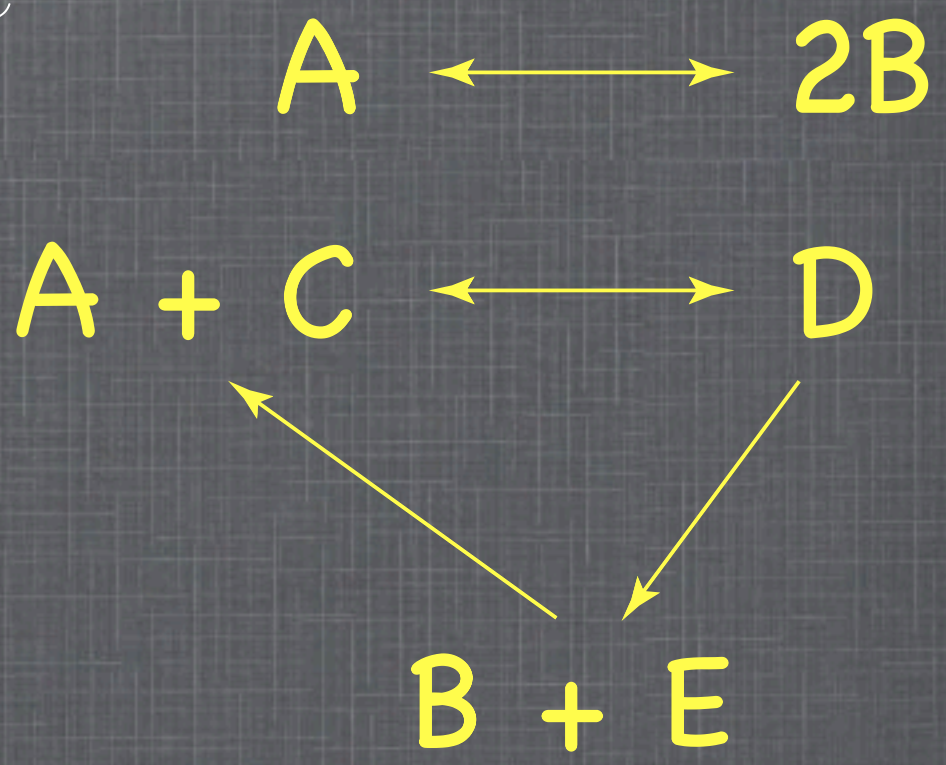
$$\dot{Y}_A = -K_{A\to 2B} + K_{2B\to A} - K_{A+C\to D} + K_{D\to A+C} + K_{B+E\to A+C}$$

$$\dot{Y}_B = 2K_{A\to 2B} - 2K_{2B\to A} + K_{D\to B+E} - K_{B+E\to A+C}$$

$$\dot{Y}_C = -K_{A+C\to D} + K_{D\to A+C} + K_{B+E\to A+C}$$

$$\dot{Y}_D = K_{A+C\to D} - K_{D\to A+C} - K_{D\to B+E}$$

$$\dot{Y}_E = K_{D\to B+E} - K_{B+E\to A+C}$$



We haven't said anything yet about the nature of the reaction rates.
For $A \rightarrow 2B$, the more A there is, the more reaction there will be.
We take the rate of $A \rightarrow 2B$ to be proportional to Y_A : $K_{A \rightarrow 2B} = \alpha Y_A$.

For $A+C \rightarrow D$, a unit of species A must meet a unit of species C.
We take the probability of such an encounter to be proportional to the product $Y_A Y_C$: $K_{A+C \rightarrow D} = \gamma Y_A Y_C$.

Svante August Arrhenius
Nobel Prize 1903

With mass action kinetics, our rate functions take the form

$$\mathcal{K}_{\mathrm{A}\to 2\mathrm{B}} = \alpha Y_A$$

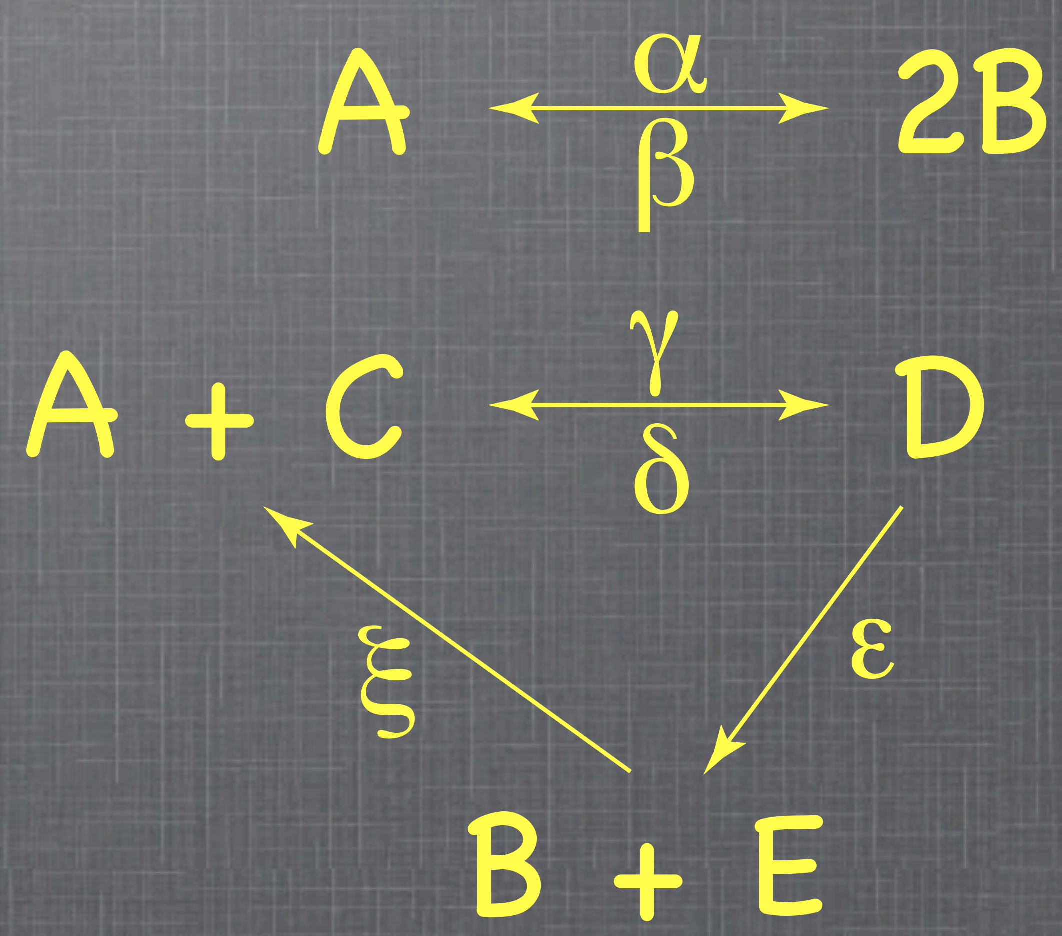
$$\mathcal{K}_{2\mathrm{B}\to \mathrm{A}} = \beta Y_B^2$$

$$\mathcal{K}_{\mathrm{A+C}\to \mathrm{D}} = \gamma Y_A Y_C$$

$$\mathcal{K}_{\mathrm{D}\to \mathrm{B+E}} = \varepsilon Y_D$$

$$\mathcal{K}_{\mathrm{D}\to \mathrm{A+C}} = \delta Y_D$$

$$\mathcal{K}_{\mathrm{B+E}\to \mathrm{A+C}} = \xi Y_B Y_E$$



The rate "constants" α, β, γ, δ, ε, and ξ may depend on temperature and density.

And our reaction network takes the form

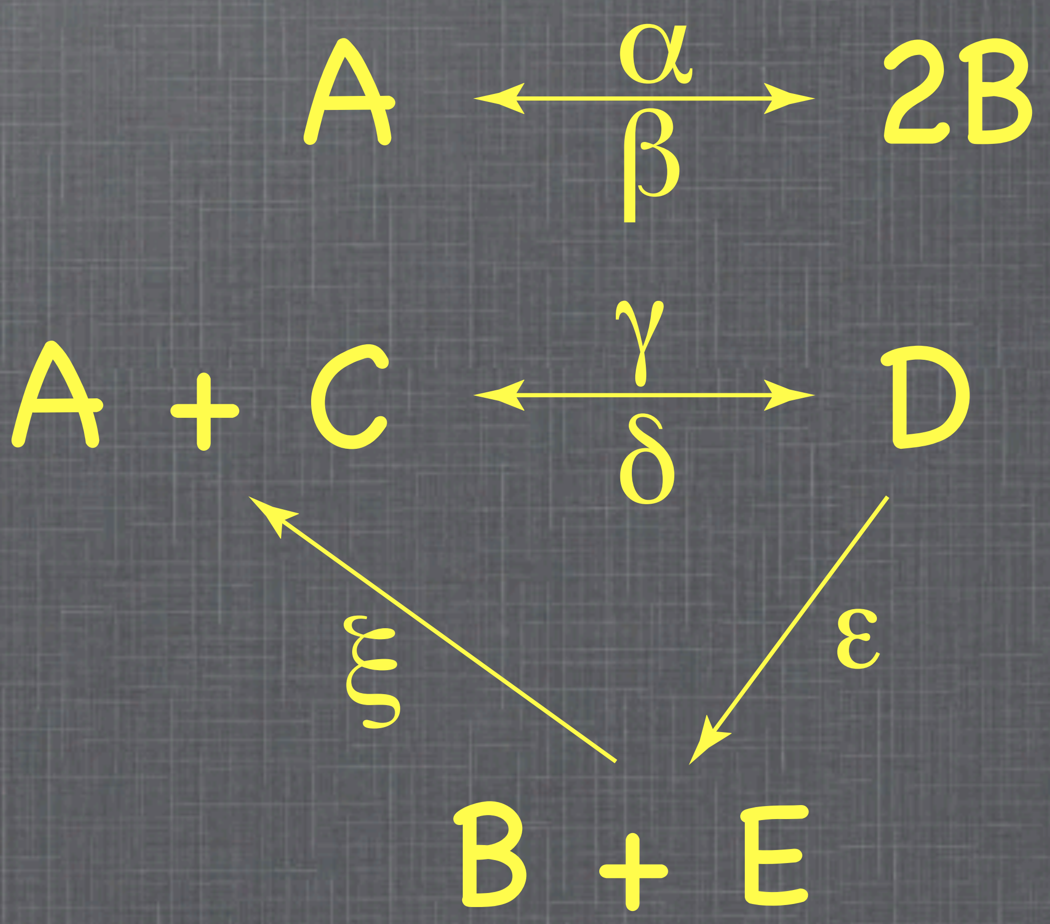
$$\dot{Y}_A = -\alpha Y_A + \beta Y_B^2 - \gamma Y_A Y_C + \delta Y_D + \xi Y_B Y_E$$

$$\dot{Y}_B = 2\alpha Y_A - 2\beta Y_B^2 + \epsilon Y_D - \xi Y_B Y_E$$

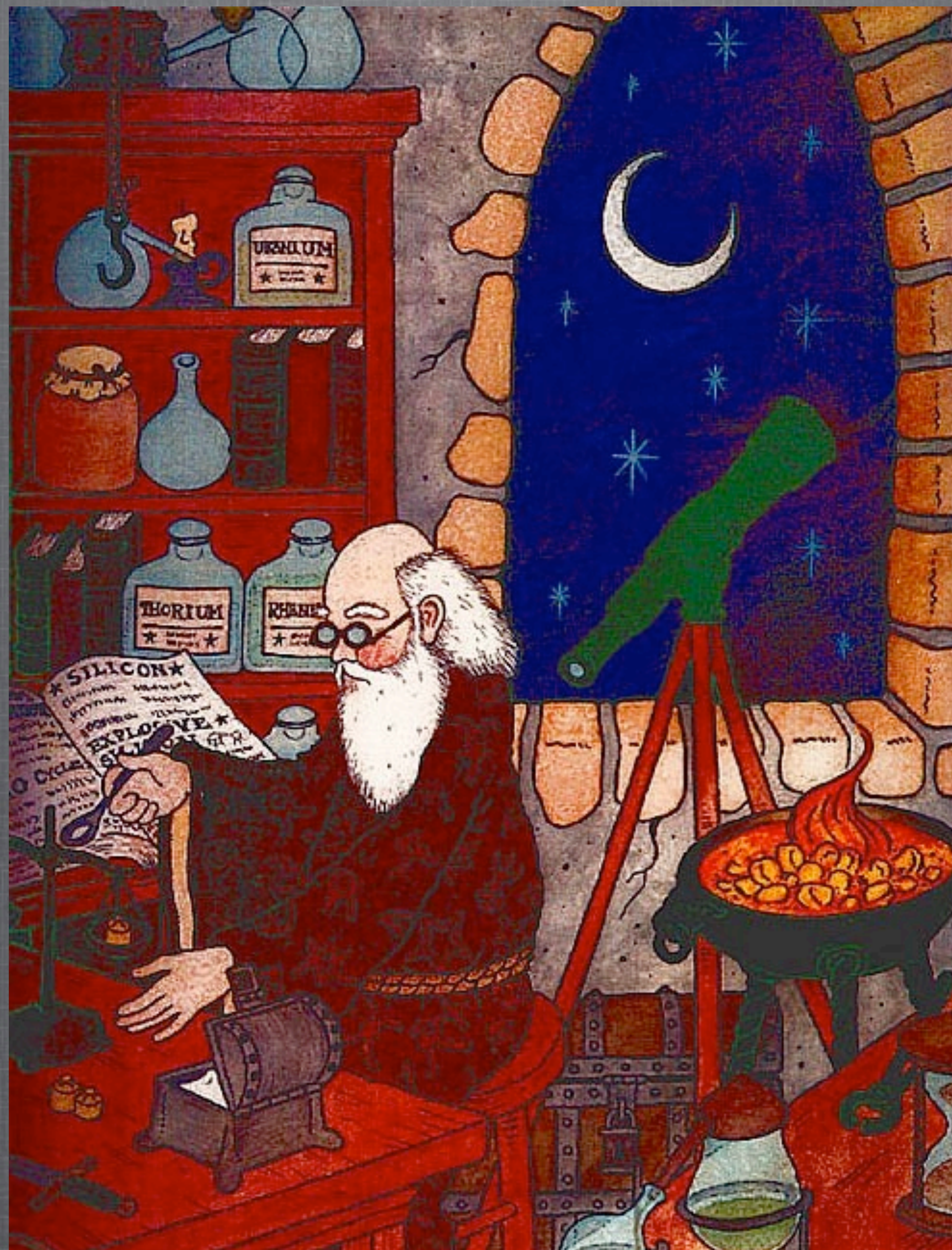
$$\dot{Y}_C = -\gamma Y_A Y_C + \delta Y_D + \xi Y_B Y_E$$

$$\dot{Y}_D = \gamma Y_A Y_C - \delta Y_D - \epsilon Y_D$$

$$\dot{Y}_E = \epsilon Y_D - \xi Y_B Y_E$$



Interlude

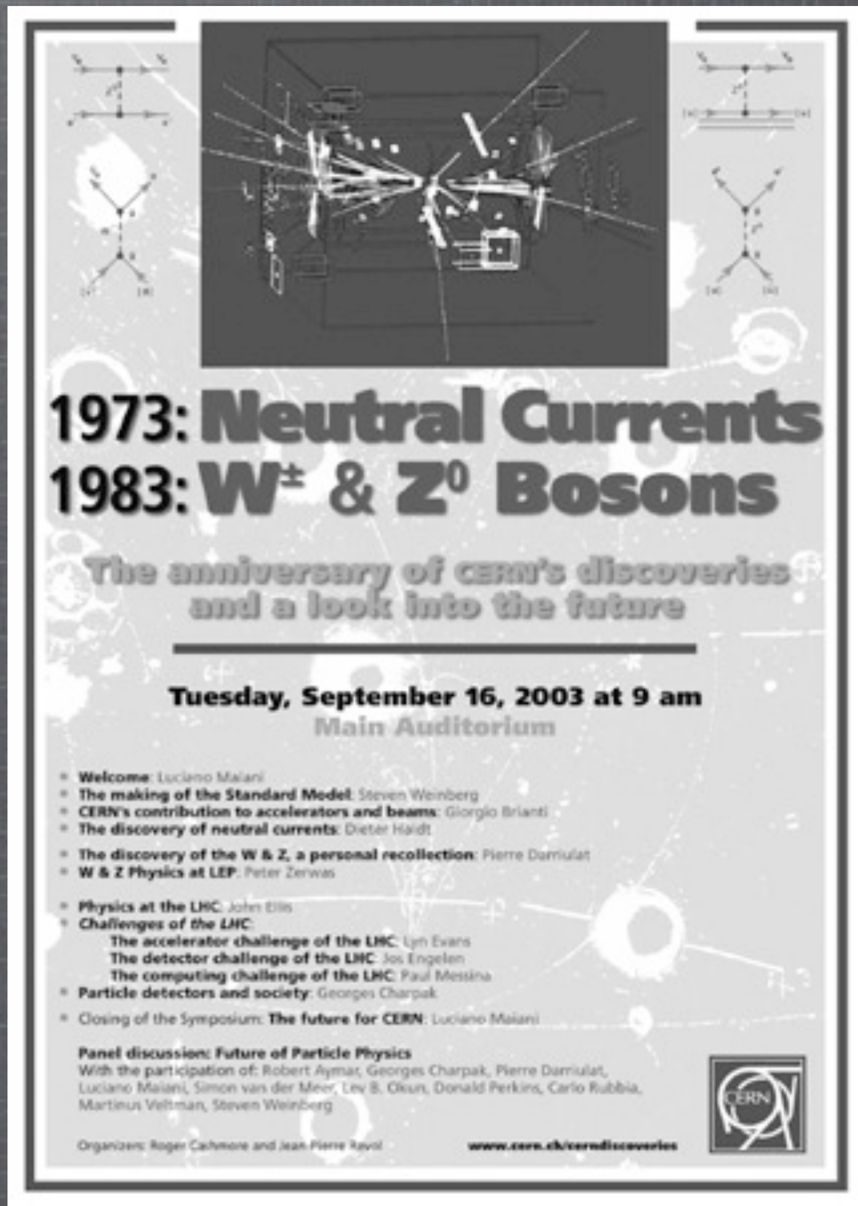


Gerry Wasserburg
1993

There are different of types of nuclear reactions: emission or absorption of nuclei and nucleons, photons (γ-rays) and leptons (electrons, neutrinos, and their anti-particles).

Nuclear reactions involve three of the four fundamental forces, the nuclear strong, electromagnetic and nuclear weak forces.

Weak interactions (those involving leptons) generally proceed more slowly than those involving nucleons and photons, but these are the only reactions that can change the global proton to neutron ratio.



A key quantity is the cross section σ for a nuclear reaction.

The cross section σ_{ij} for the reaction i(j,k)l is the number of reactions per target nucleus i per second divided by the flux of nuclei of type j (number/cm^2/s).

$$\sigma(v) = \frac{\text{number of reactions per sec}}{\text{flux of incoming projectiles}} = \frac{r_{ij}/n_i}{n_j v_{ij}}$$

Cross sections are usually reported in "barns", 10^{-24} cm^2.

The reaction rate per unit volume r_{ij} , in the simplest case, is then

$$r_{ij} = [\text{flux of } j] n_i \sigma_{ij}(v) = v_{ij} n_j n_i \sigma_{ij}(v) \quad \text{cm}^{-3}\text{s}^{-1}$$

More generally, the targets and projectiles have distributions of velocities, in which case r_{ij} is given by

$$r_{i,j} = \int \sigma(|\vec{v}_i - \vec{v}_j|)|\vec{v}_i - \vec{v}_j| d^3 n_i d^3 n_j \quad \text{cm}^{-3}\text{s}^{-1}$$

Evaluation of the integrals depends on the particle statistics. For nuclei i and j that obey Maxwell–Boltzmann statistics

$$d^3 n = n \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp\left(-\frac{mv^2}{2k_B T} \right) d^3 v$$

allowing n_i and n_j to be moved outside of the integral.

Then

$$r_{ij} < \sigma v >_{ij} n_i n_j = (N_A\rho)^2 < \sigma v >_{ij} Y_i Y_j \quad \mathrm{cm}^{-3}\mathrm{s}^{-1}$$

where $<\sigma v>_{ij}$ is the velocity integrated cross section.
The rate of change in the number density of species i with time is

$$\dot{n}_i = \sum_{j,k} r_{jk} \quad \mathrm{cm}^{-3}\mathrm{s}^{-1}$$

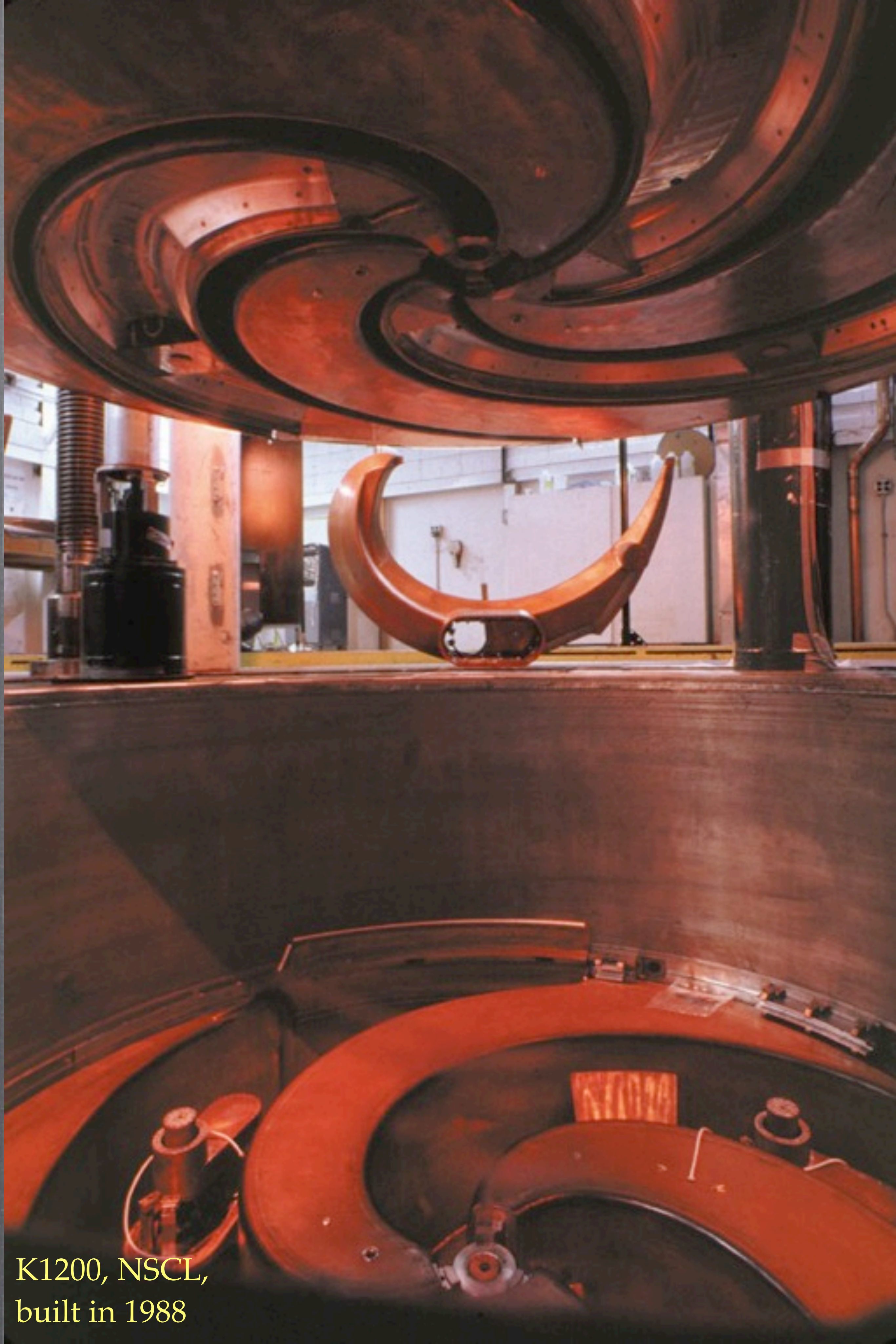
or

$$\dot{Y}_i = \sum_{j,k} N_A\rho < \sigma v >_{ij} Y_j Y_k = \sum_{j,k} \lambda_{ij}\rho Y_j Y_k = \sum_{j,k} R_{ij} Y_j Y_k \quad \mathrm{s}^{-1}$$

where λ_{ij} is what common reaction rate compilations list, and R_{ij} is "the reaction rate" used in our codes.

Michael Wiescher will say more about measuring cross sections and Q-values later in this school.

For now, we've established what we need to continue forming a nuclear reaction network.



K1200, NSCL, built in 1988

Consider a unidirectional binary reaction with unity coefficients.

$$i + j \rightarrow k + l$$

$$\dot{Y}_i = -Y_i Y_j R_{ij}$$

$$\dot{Y}_j = -Y_i Y_j R_{ij}$$

$$\dot{Y}_k = Y_i Y_j R_{ij}$$

$$\dot{Y}_l = Y_i Y_j R_{ij}$$

Where the reaction rate R_{ij} absorbs the density, Avogado number, and $\langle \sigma v \rangle_{ij}$ terms.

Now consider the case when the coefficients are not unity.

$$c_i i + c_j j \rightarrow c_k k + c_l l$$

$$\dot{Y}_i = -\frac{c_i}{c_i! c_j!} Y_i^{c_i} Y_j^{c_j} R_{ij}$$

$$\dot{Y}_j = -\frac{c_j}{c_i! c_j!} Y_i^{c_i} Y_j^{c_j} R_{ij}$$

$$\dot{Y}_k = \frac{c_k}{c_i! c_j!} Y_i^{c_i} Y_j^{c_j} R_{ij}$$

$$\dot{Y}_l = \frac{c_l}{c_i! c_j!} Y_i^{c_i} Y_j^{c_j} R_{ij}$$

If there are identical reactants, i=j, set $c_i = 2c_i$ and $c_j = 0$.

For a general bidirectional binary reaction

$$c_i i + c_j j \leftrightarrow c_k k + c_l l$$

$$\dot{Y}_p = \sum_{r,s} \frac{c_p}{c_r! c_s!} Y_r^{c_r} Y_s^{c_s} R_{rs} - \sum_q \frac{c_p}{c_p! c_q!} Y_p^{c_p} Y_q^{c_q} R_{pq}$$

If there are identical reactants, i=j, set $c_i = 2c_i$ and $c_q = c_s = 0$.

Reactions can be divided into three categories based on the number of reactants which are nuclei.

Reactions involving a single nucleus - decays, electron and positron captures, photodisintegrations, and neutrino induced reactions - depend on the number density of only the target species.

$$\dot{Y}_i = \sum_j C_i R_j Y_j$$

For a binary reaction,

$$\dot{Y}_i = \sum_{jk} \frac{C_i}{C_j! C_k!} R_{jk} Y_j Y_k$$

The C_i's can be positive or negative numbers that specify how many particles of species i are created or destroyed.

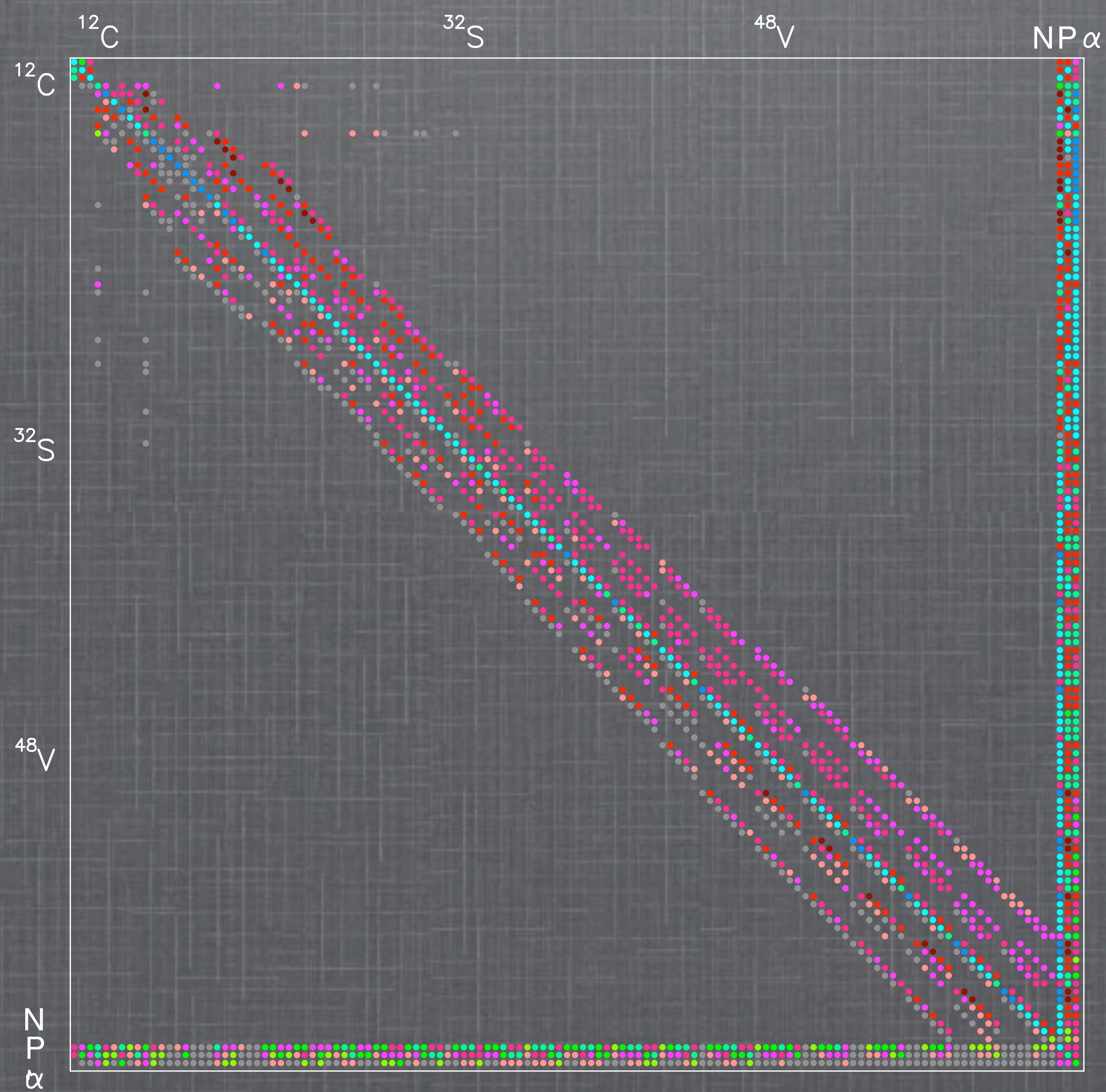
There are also a few important three-particle processes (like the triple-α process) which are commonly successive captures with an intermediate unstable target.

Using an equilibrium abundance for the unstable intermediate, the contributions of these reactions are commonly written in the form of a three-particle processes, depending on a trio of number densities.

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

A reaction network may described by the following set of ODEs

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



127 Isotopes

1270 Rates

87.6% Sparse

Flows (#/sec):

3.05E+13

3.30E+10

3.56E+07

3.84E+04

4.15E+01

-2.23E+01

-2.07E+04

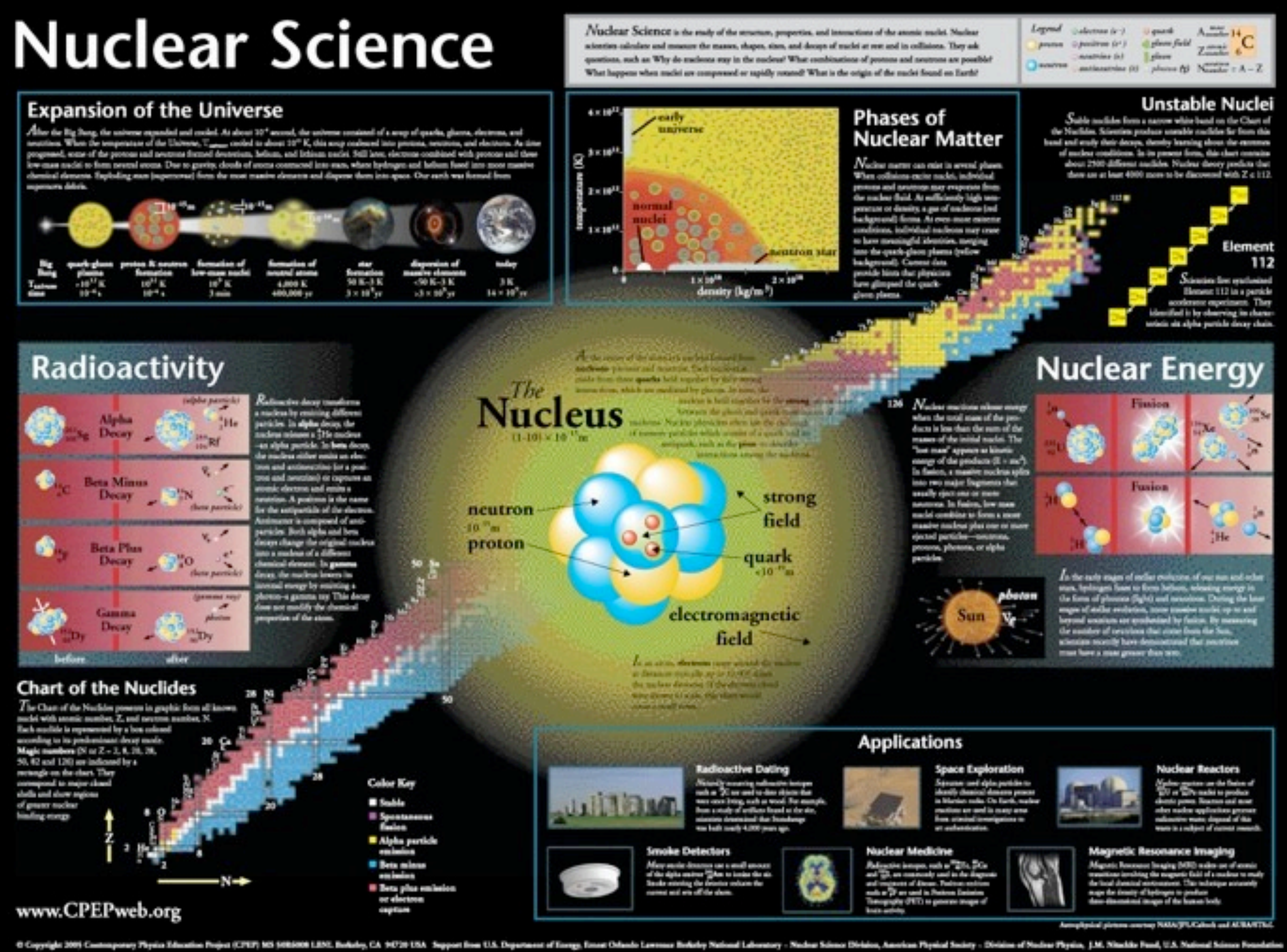
-1.91E+07

-1.77E+10

-1.64E+13

-1.52E+16

Interlude


Nuclear Science
Expansion of the Universe
Phases of Nuclear Matter
early universe
normal nuclei
neutron star
temperature (K)
density (kg/m³)
Unstable Nuclei
Element 112
Radioactivity
Alpha Decay
Beta Minus Decay
Beta Plus Decay
Gamma Decay
before
after
The Nucleus
neutron
proton
strong field
quark
electromagnetic field
Nuclear Energy
Fission
Fusion
Sun
photon
Chart of the Nuclides
Color Key
Stable
Spontaneous fission
Alpha particle emission
Beta minus emission
Beta plus emission or electron capture
Applications
Radioactive Dating
Space Exploration
Nuclear Reactors
Smoke Detectors
Nuclear Medicine
Magnetic Resonance Imaging
www.CPEPweb.org

How does the Sun shine?

Wood - Ancient Greeks
lasts 2000 years

Coal - Middle Ages
lasts 4000 years

Gravitational - 1800's
lasts 4 million years

Nuclear reactions - 1940's
lasts 10 billion years

Four hydrogen nuclei get transformed into one helium nucleus. The limiting step is a rare reaction; hence a long lived Sun.

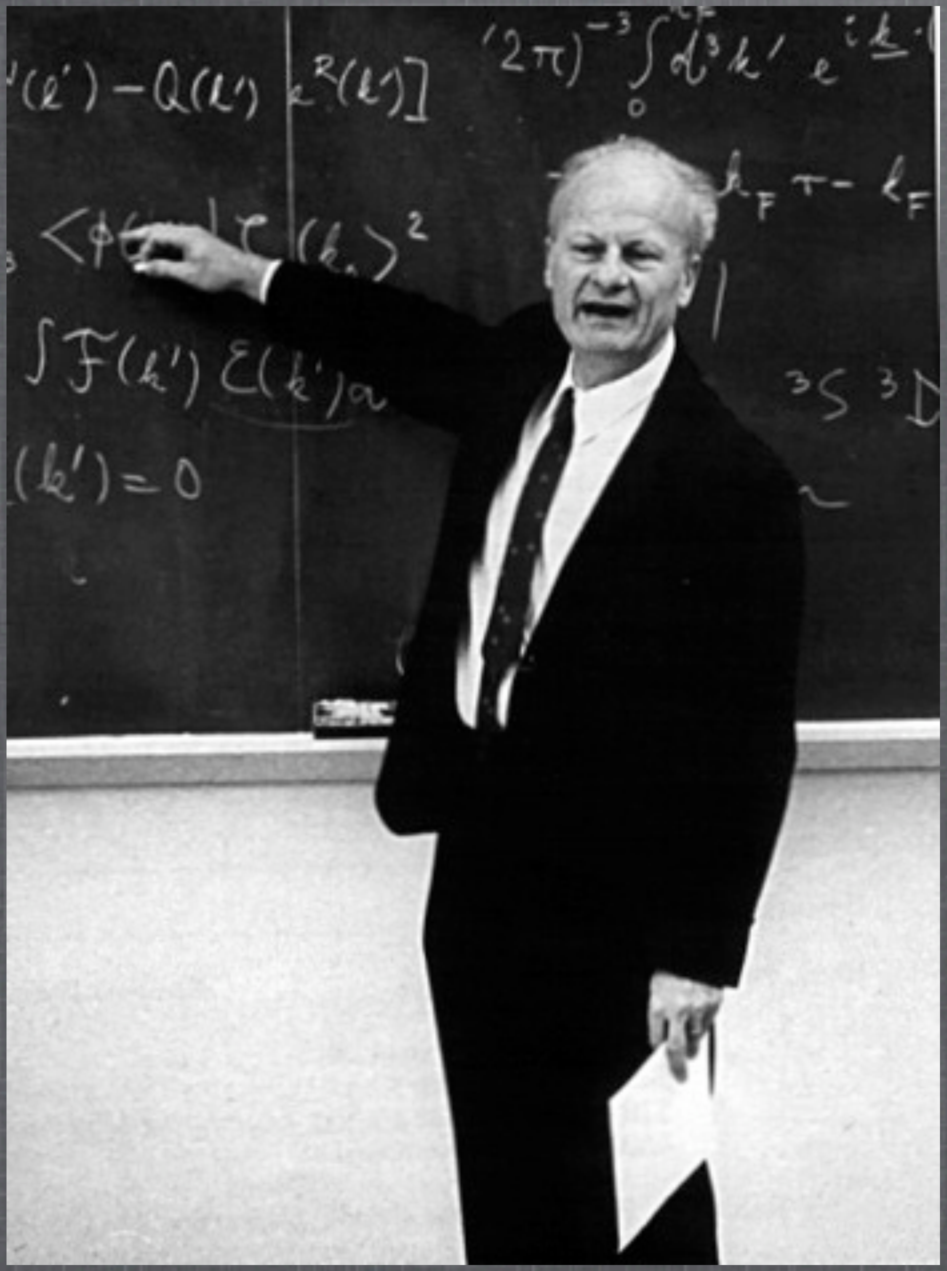
But the mass of 4 hydrogen nuclei is larger than the mass of 1 helium nucleus. Where did the missing mass go?

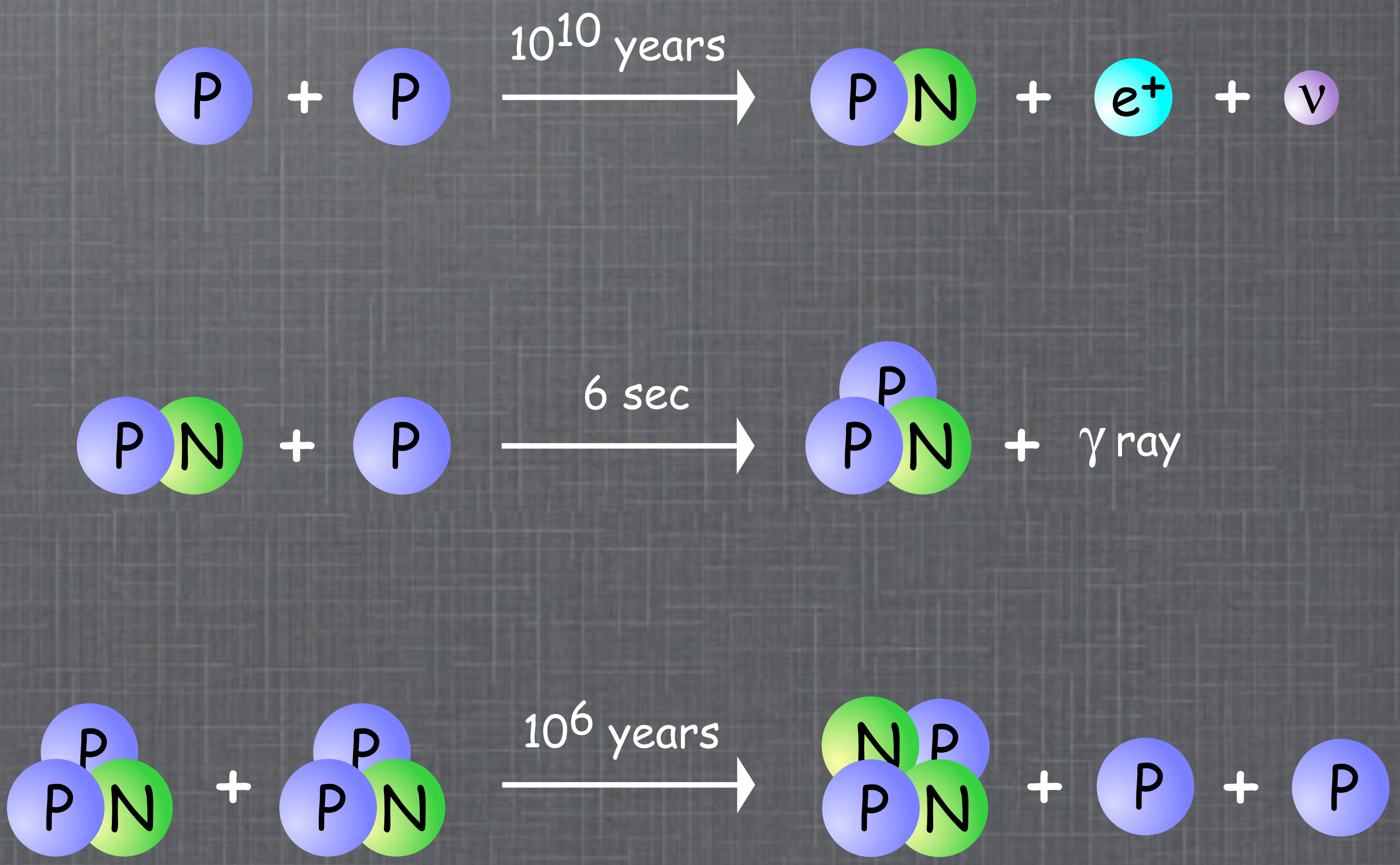
$E = mc^2$

The sun presently shines by burning hydrogen (fuel) into helium (ash) in its core.

proton-proton chains

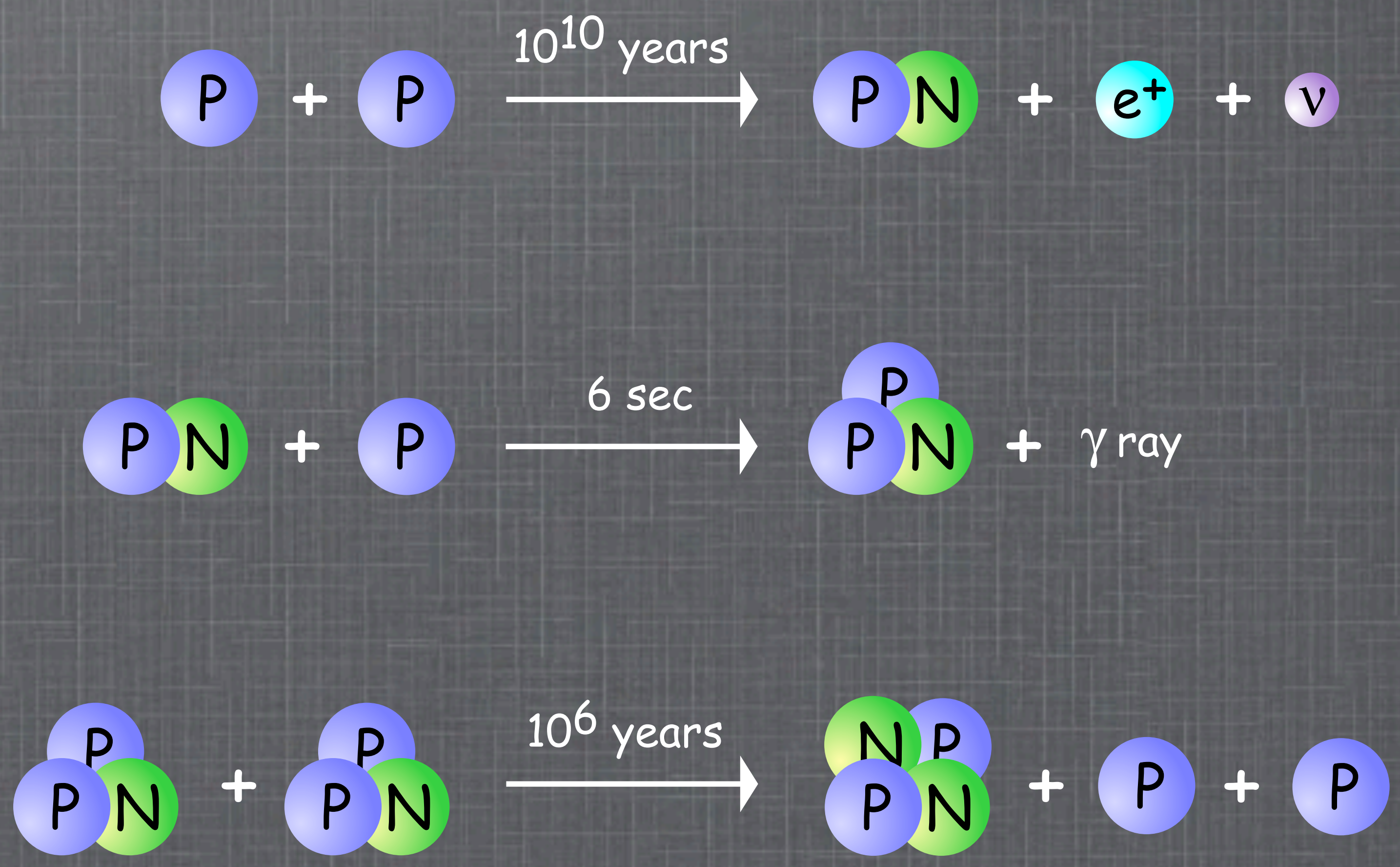
Hans Bethe realized in 1939 that a weak interaction could convert a proton into neutron during the brief encounter of a scattering event.



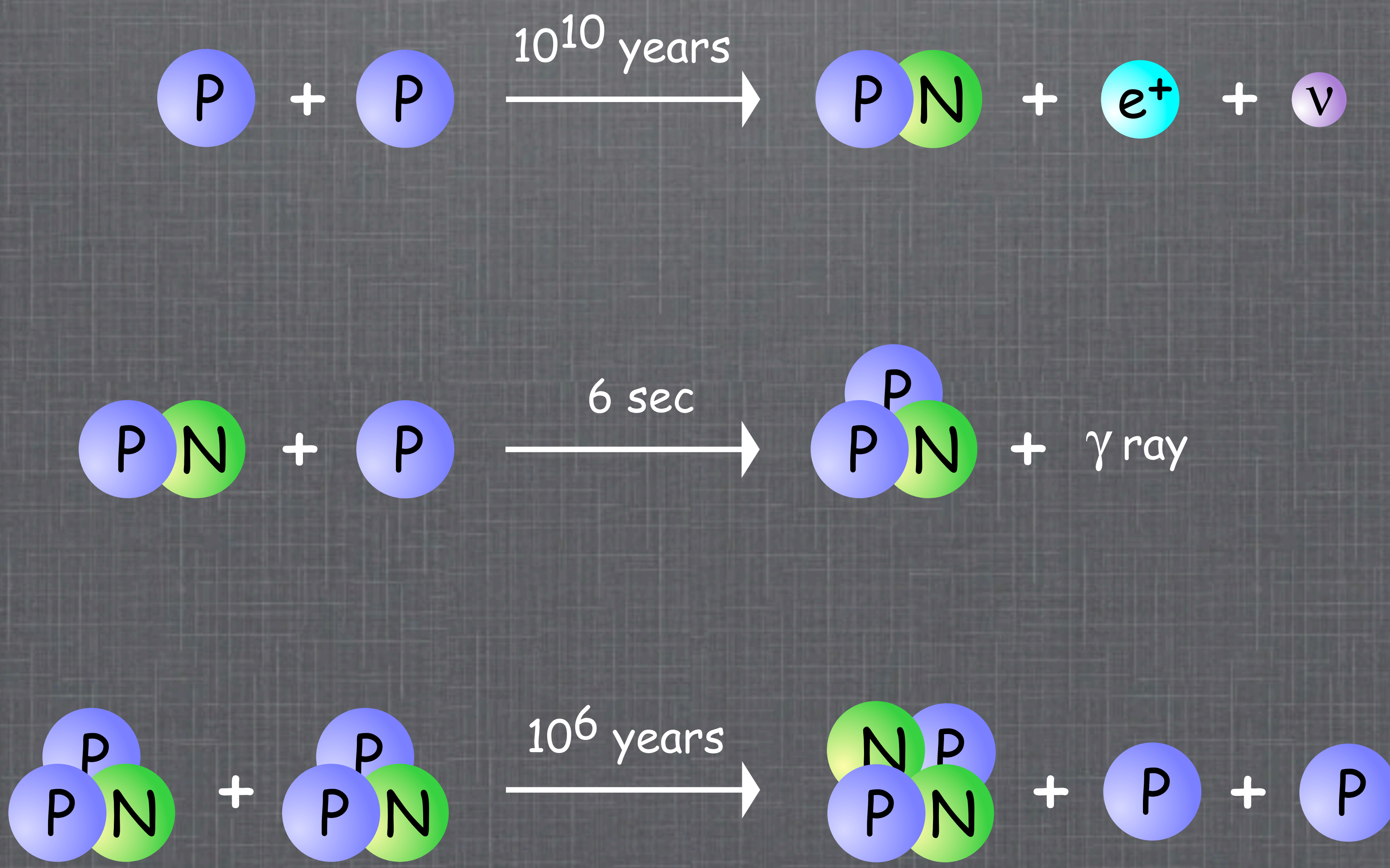


Since the neutron is more massive than a proton, such a decay would require energy (endothermic) except that the neutron can appear in a bound state with the proton in the form of deuterium.

The binding energy is sufficient (2.2245 MeV) to make the reaction exothermic.



We have four species to track (^{1}H, ^{2}H, ^{3}He, ^{4}He), and three binary reactions that couple these species; p(p,$e^+\nu$)^{2}H, ^{2}H(p,γ)^{3}He, and ^{3}He(^{3}He,2p)^{4}He.

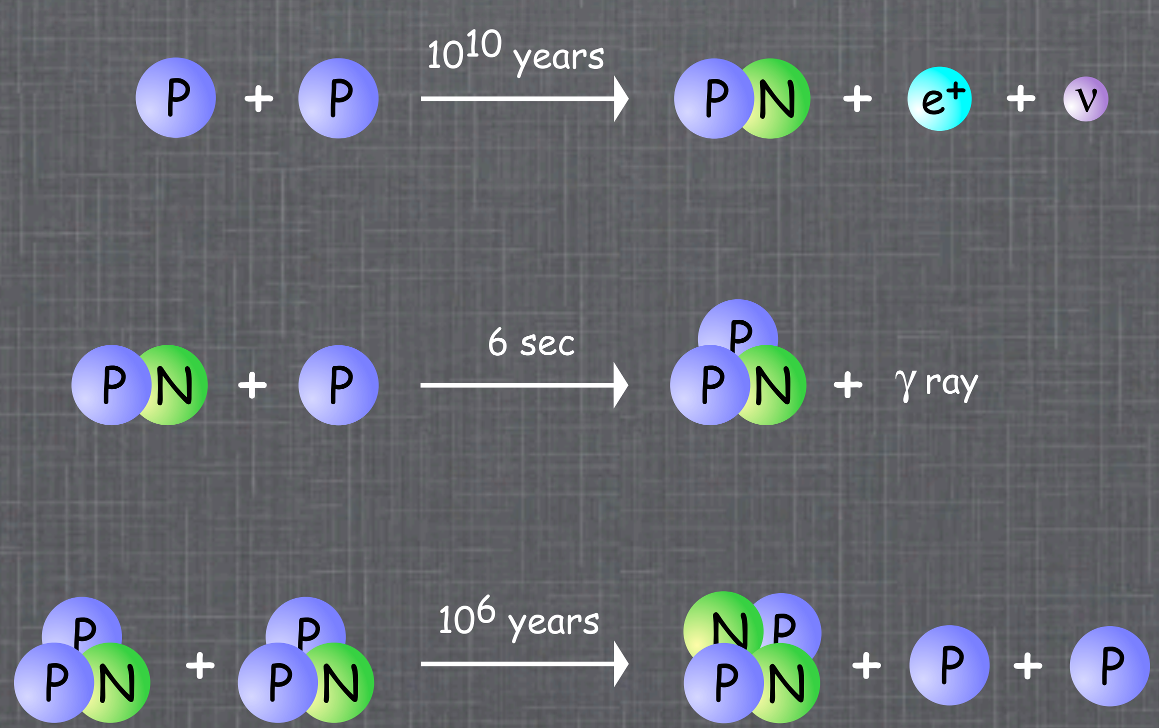


$$\dot{Y}_{\rm p} = -Y_{\rm p}Y_{\rm p}R_{\rm p,p} - Y_{\rm p}Y_{\rm d}R_{\rm p,d} + Y_{\rm 3he}Y_{\rm 3he}R_{\rm 3he,3he}$$

$$\dot{Y}_{\rm d} = 0.5Y_{\rm p}Y_{\rm p}R_{\rm p,p} - Y_{\rm p}Y_{\rm d}R_{\rm p,d}$$

$$\dot{Y}_{\rm 3he} = Y_{\rm p}Y_{\rm d}R_{\rm p,d} - Y_{\rm he3}Y_{\rm he3}R_{\rm he3,he3}$$

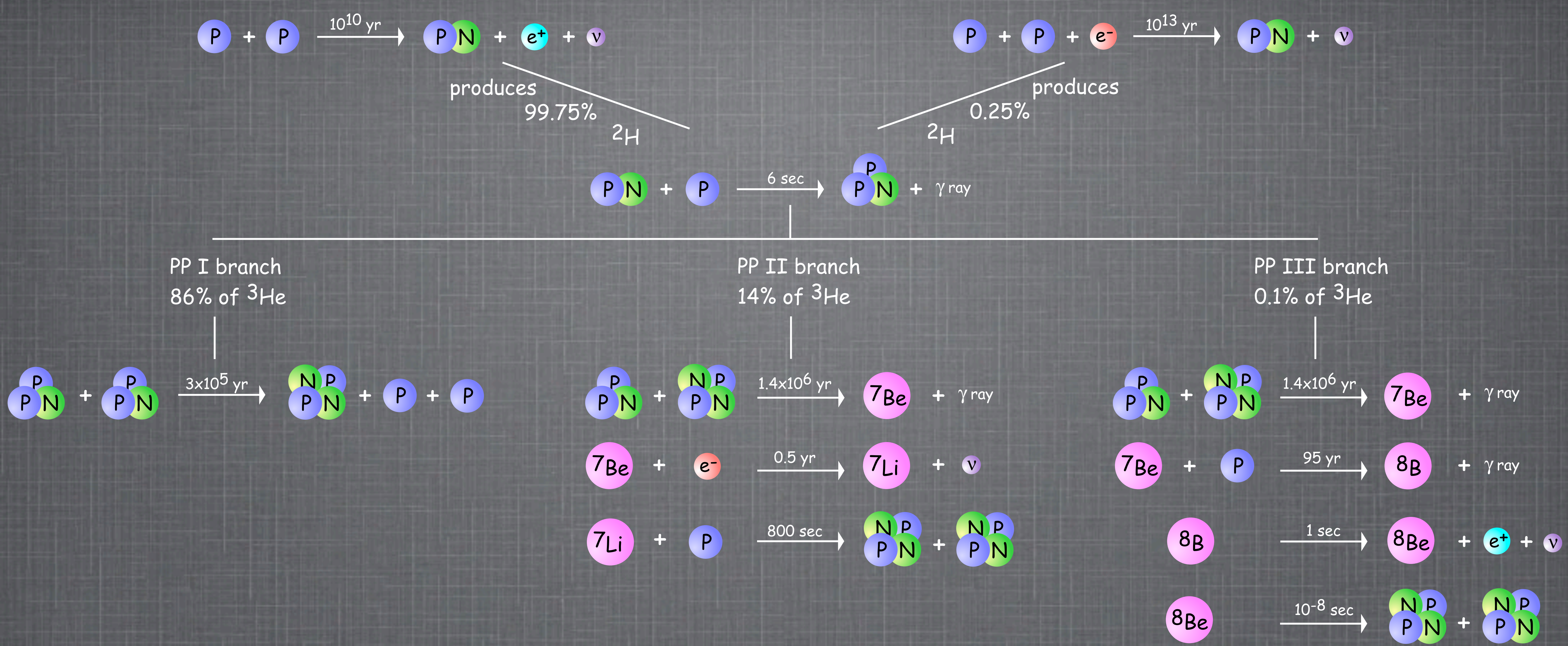
$$\dot{Y}_{\rm 4he} = 0.5Y_{\rm he3}Y_{\rm he3}R_{\rm he3,he3}$$



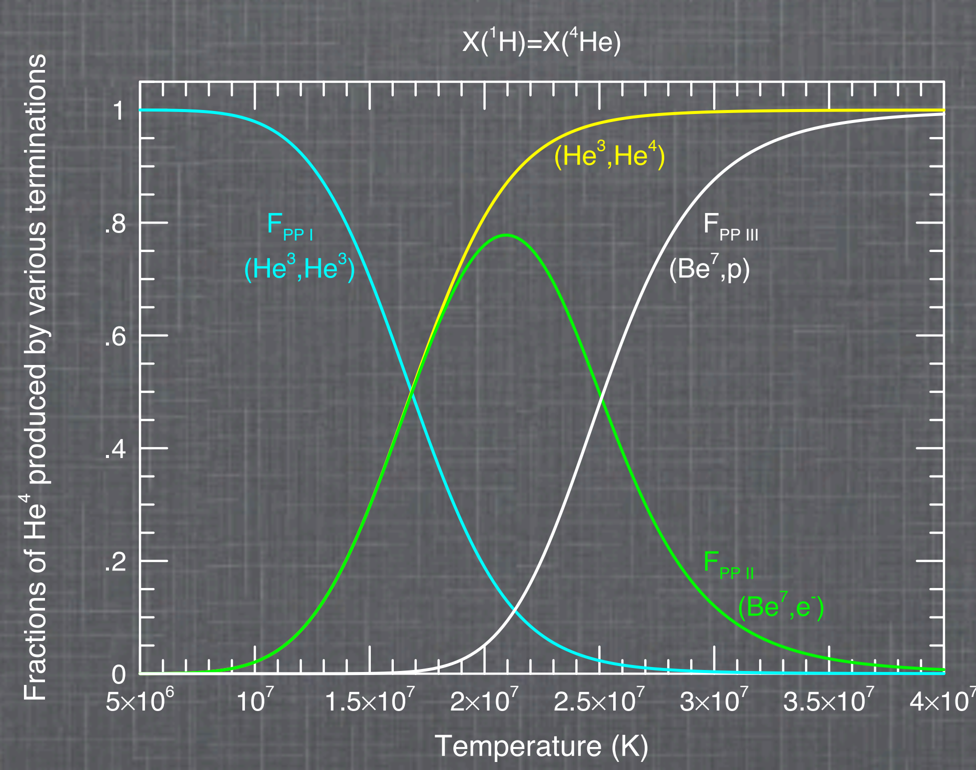
Prior to 1958 it was believed the PPI chain would proceed under most conditions, even if lots of ^{4}He were present.

Holmgren & Johnston measured the $^{3}He(\alpha,\gamma)^{7}Be$ cross section to be 2500 times larger than the previously accepted value, making this reaction compete with $^{3}He(^{3}He,2p)^{4}He$ for ^{3}He nuclei, particularly at higher temperatures.

This leads to two new chains for converting H to He, PPII and PPIII, corresponding to the two possible fates of the ^{7}Be nucleus.



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}.



After Parker, Bahcall & Fowler ApJ 139, 602, 1964. Also see Clayton figure 5-10.

Tasks for the day

Derive the ODE equations for the PPI chain.

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

Run the code in hydrostatic mode for $T = 1.5 \times 10^7$ K, $\rho = 150$ g/cm^3,
and an initial composition of 75% H and 25% He by mass.
Plot the abundance evolution.
How much hydrogen is currently left in the center of the Sun?
How long will the Sun live?

Questions and Discussion