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

Terry Pratchett

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

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

Sites of the week

- nobelprize.org/physics/articles/fusion/index.html
- hyperphysics.phy-astr.gsu.edu/hbase/astro/procyc.html
- www.che.eng.ohio-state.edu/~FEINBERG/LecturesOnReactionNetworks/
- www.cococubed.com/papers/hix_meyer_2004.pdf

Purpose

- The Joint Institute for Nuclear Astrophysics (JINA), a National Foundation for Science Physics Frontier Center, is organizing its second school on "Tools and Toys for Nuclear Astrophysics".

- The school will focus on "Nuclear Reaction Network Techniques" and will take place at Notre Dame, IN between June 20 - July 1, 2005.

- Reaction network techniques have been developed as an important tool for applications in nuclear astrophysics and many other physics areas.

JINA

Purpose

- This technique is particularly important for simulating nucleosynthesis processes and for predicting element production as well as energy generation in both stellar evolution and stellar explosion processes.

- The increasing need for using computational networking techniques requires special training in the development and application of network programs.

- This school will provide an overview about the mathematical background as well as the computational network techniques.

Purpose

- Different applications for stellar nucleosynthesis simulations will be presented and discussed.

- In addition to the lectures, the participants will have time to work with the various network codes under the guidance of the lecturers.

- Codes will be shared freely and will be available to participants after the workshop.

STELLAR INTERIORS
SINS
& NUCLEOSYNTHESIS

Abundance Variables

$$N_A = 6.022 \times 10^{23} \text{ number/mole} = \text{Avogadro's number}$$

$$\text{number} = \text{moles} \cdot N_A$$

$$N = M \cdot N_A$$

$$n = m \cdot N_A$$

A_i = number of protons + neutrons in species i
= atomic mass number
= molar mass [g/mole]

Z_i = number of protons in species i
= charge
= atomic number

Abundance Variables

$$\text{mass} = \text{moles} \cdot \text{molar mass}$$

$$\text{mass} = M \cdot A$$

1 mole of ^{12}C has a mass of 12 g

$$\rho = m \cdot A$$

Number density, mass density, mole fraction for a pure composition

$$n = \frac{\rho\ N_A}{A} \quad \text{cm}^{-3} \qquad\qquad \rho = \frac{n\ A}{N_A} \quad \text{g cm}^{-3}$$

$$Y = \frac{1}{A} = \frac{n}{\rho N_A} \quad \text{mole/g , molar fraction}$$

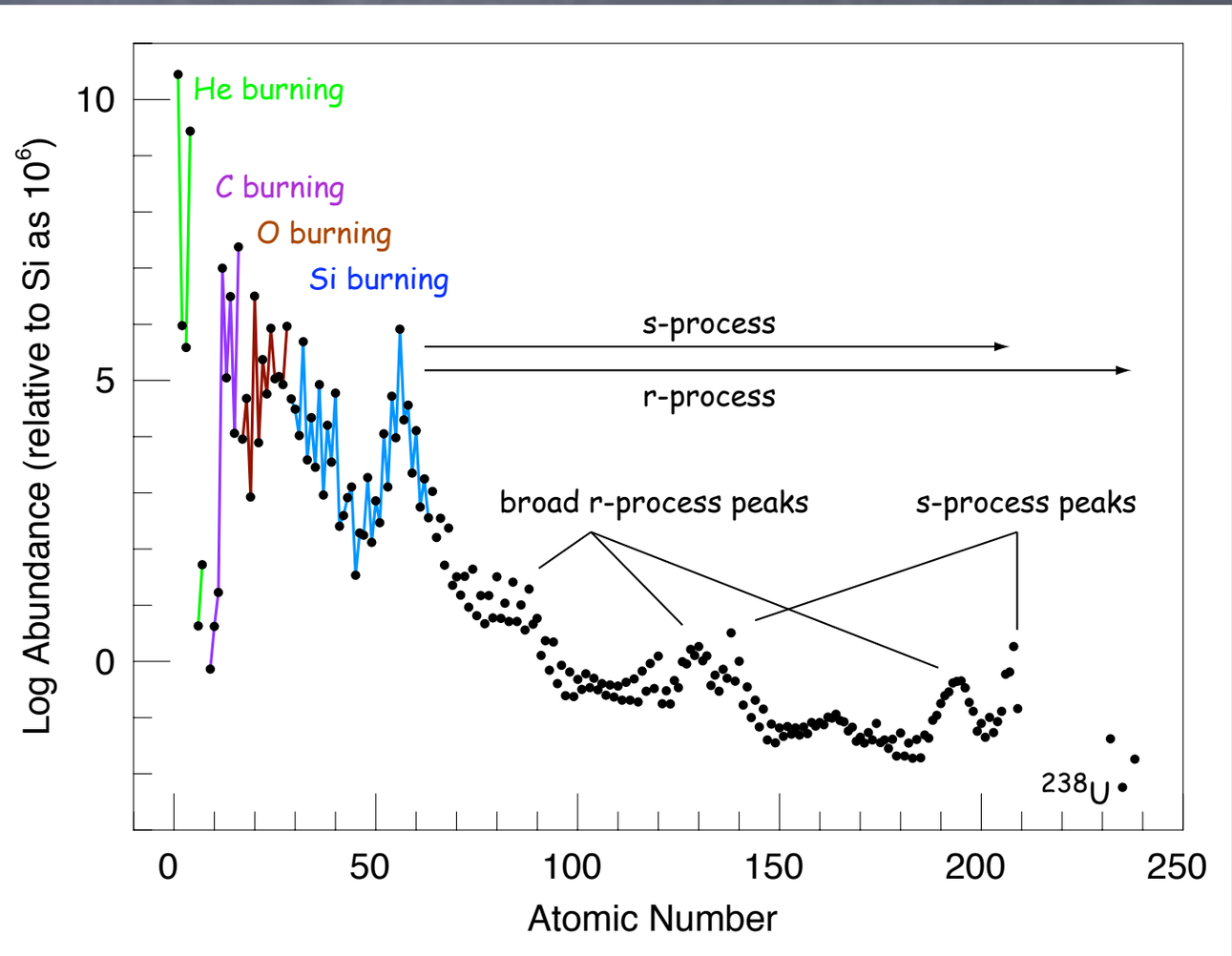
Abundance Variables

For a mixture of isotopes,

$$Y_i = \frac{n_i}{\rho N_A} \quad \text{mole/g , molar fraction}$$

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

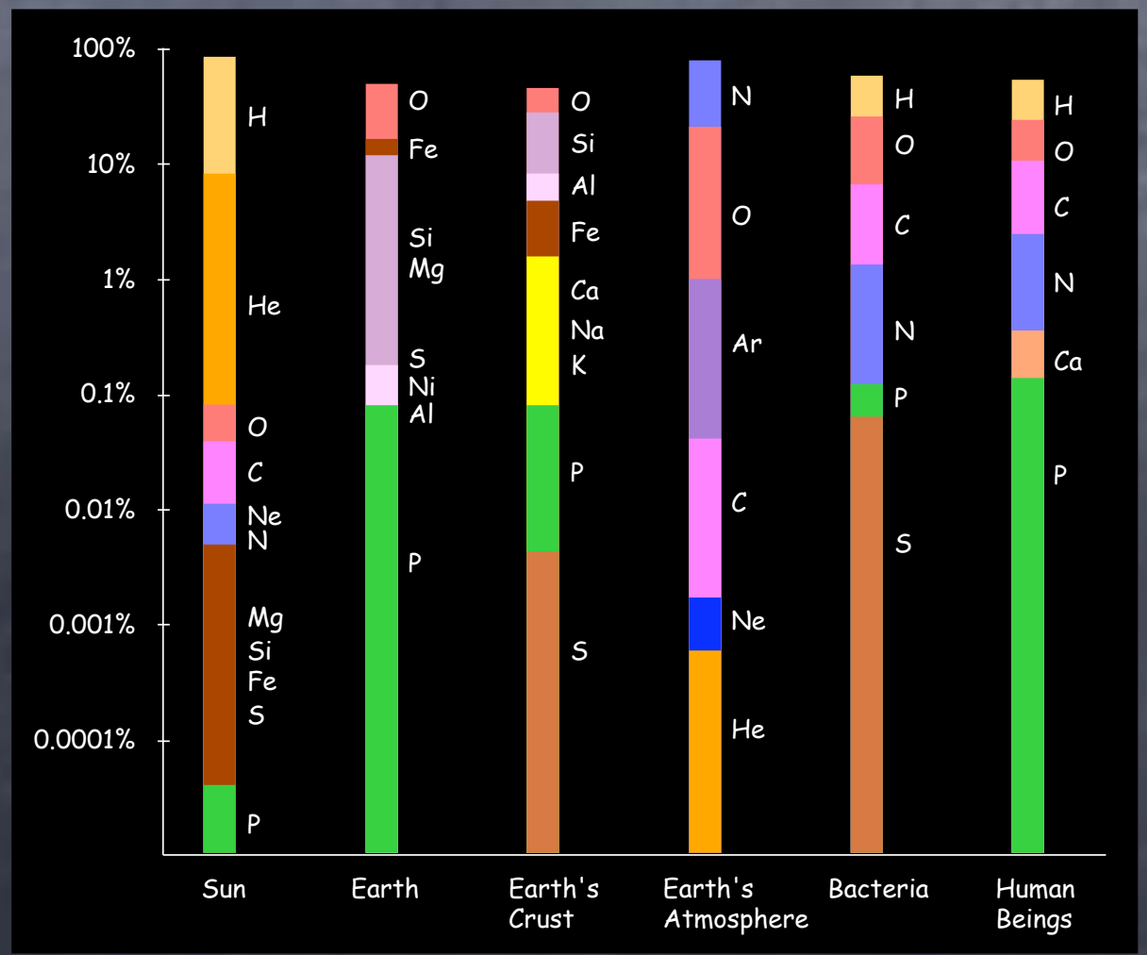
$$\sum_{i=1}^{k} X_i = 1$$



Abundance Variables

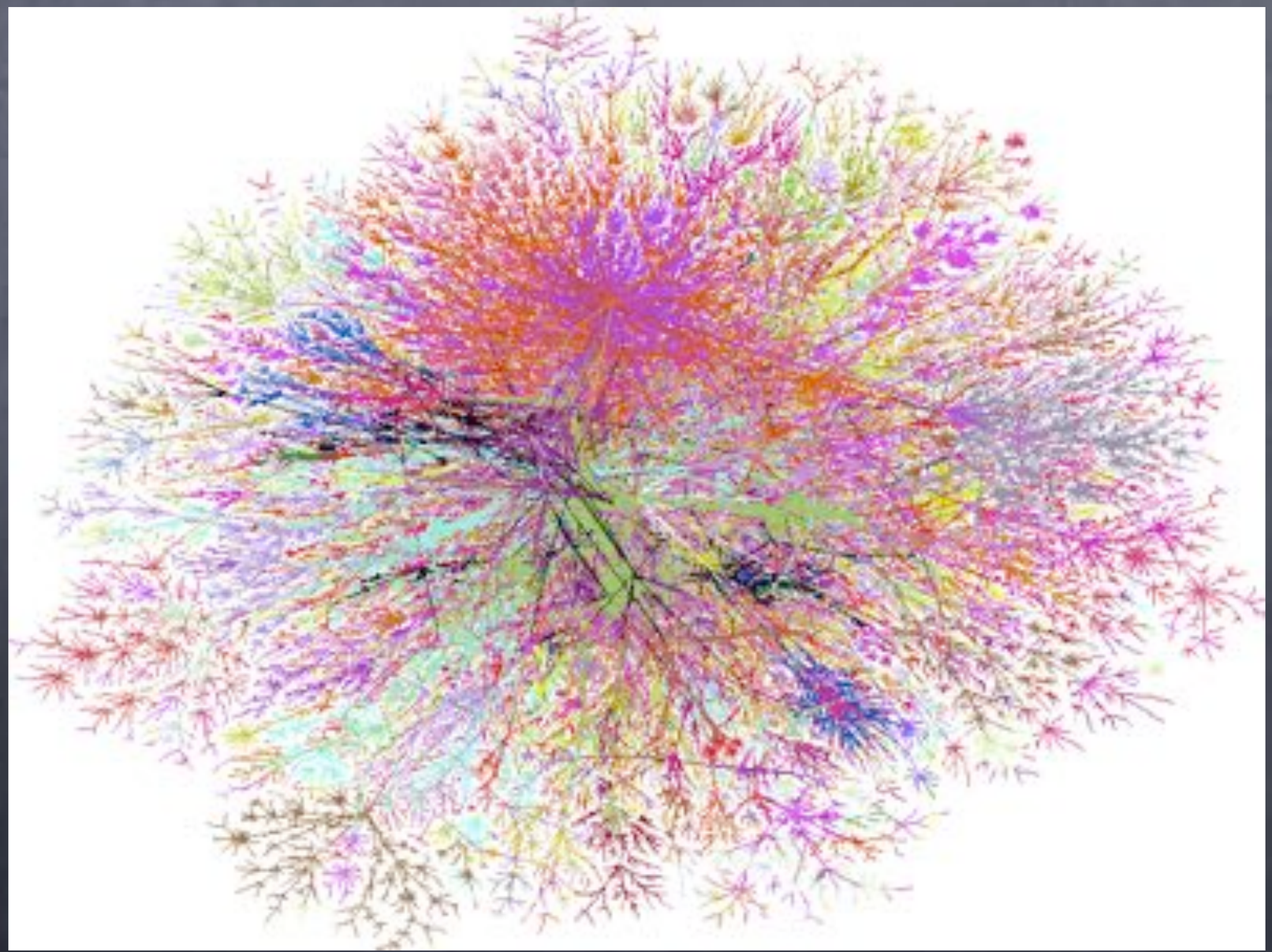
$$\overline{A} = \frac{\sum n_i A_i}{\sum n_i} = \frac{1}{\sum Y_i} \quad \text{g mole}^{-1} \qquad \overline{Z} = \frac{\sum n_i Z_i}{\sum n_i} = \overline{A} \sum Y_i Z_i$$

$$n = \frac{\rho}{\overline{A}} N_A \quad \text{cm}^{-3} \qquad \rho = \frac{n}{N_A} \overline{A} \quad \text{g cm}^{-3}$$



Overview

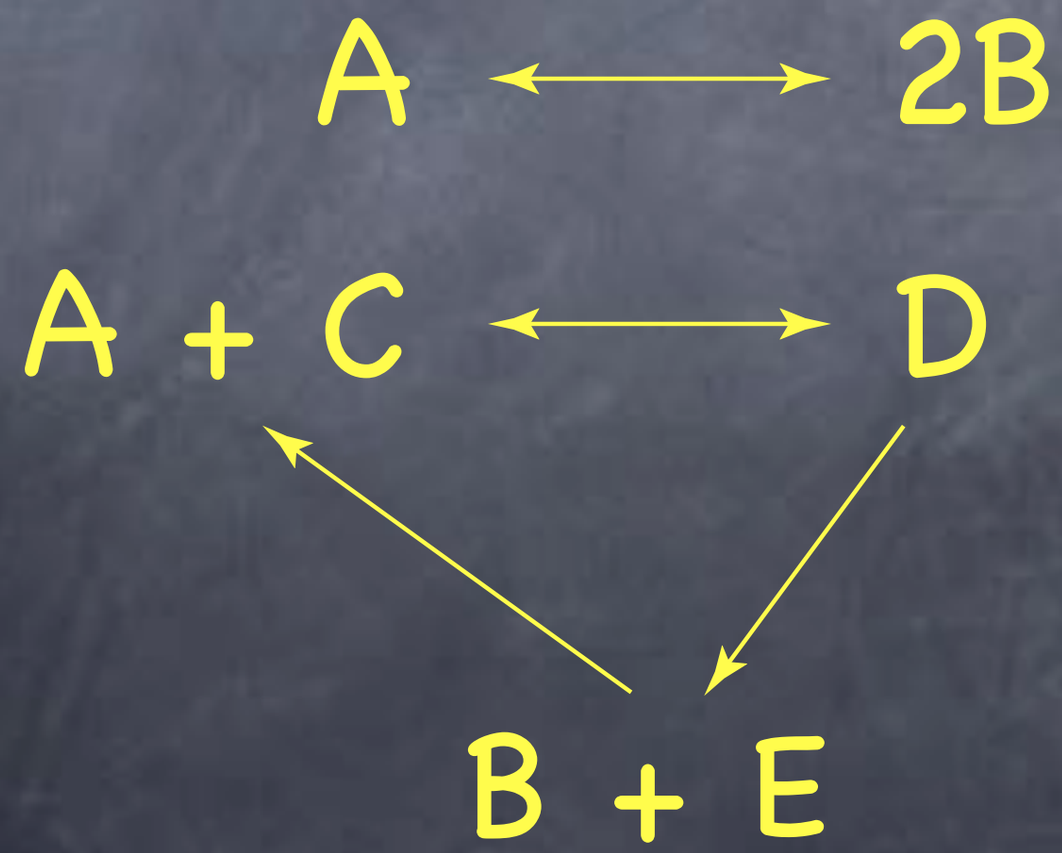
- These lectures will be about a special, but rather large class of ordinary differential equations (ODEs) - those that derive from nuclear/chemical/ionization/biological reaction networks.



the internet,
sept3, 2004 9:22am UTC

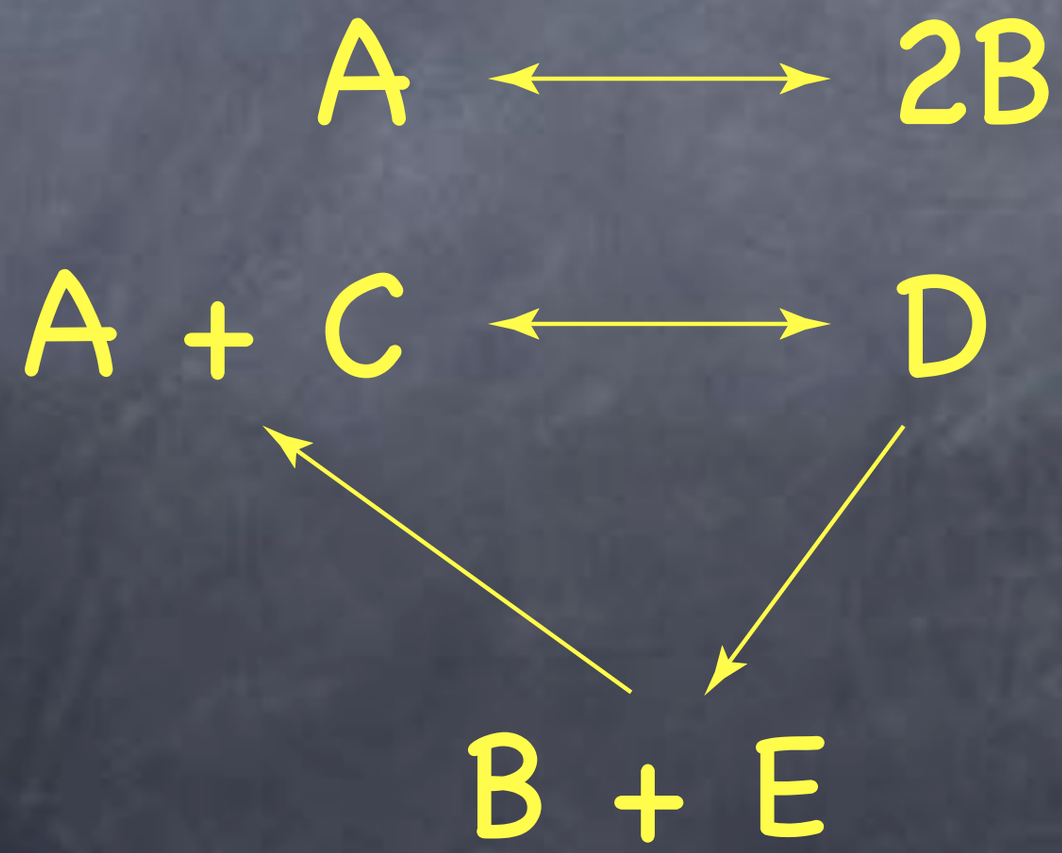
Motivation

- In order to provide a sense of how these equations come about, it is useful to write down an example of reaction network and indicate informally how it induces a system of ODEs.



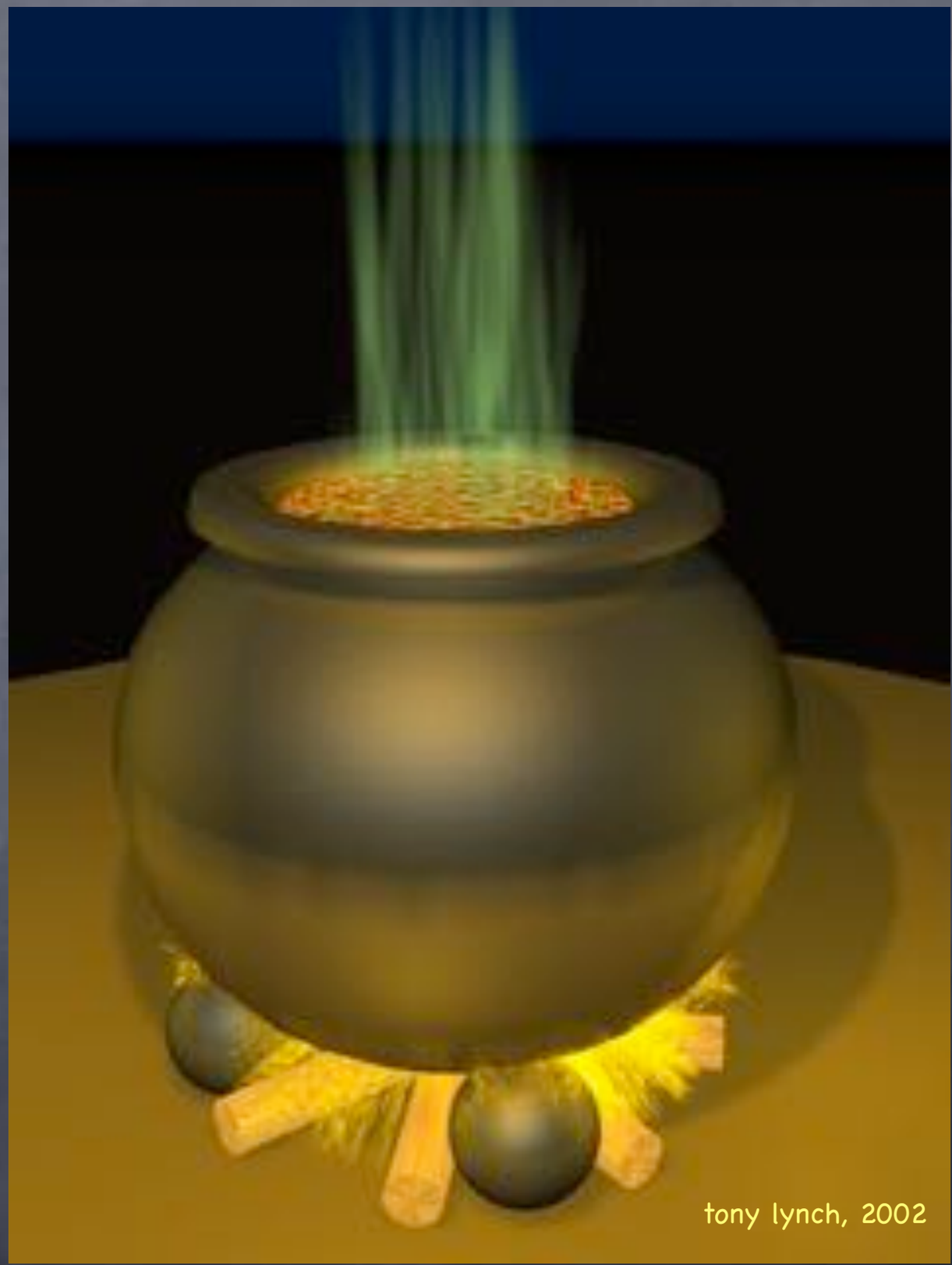
Motivation

- This is a diagram for a reaction network. It indicates that species A can decompose into two units of species B, that two units of B can combine to form one unit of A, that a unit of species A can react with a unit of species C to form a unit of species D, and so on.



Motivation

- Suppose we throw the various species in a pot.
- The pot is stirred constantly so that its contents remain spatially homogeneous for all time.
- We'll also assume that the contents of the pot are forever maintained at constant temperature and total volume.



Motivation

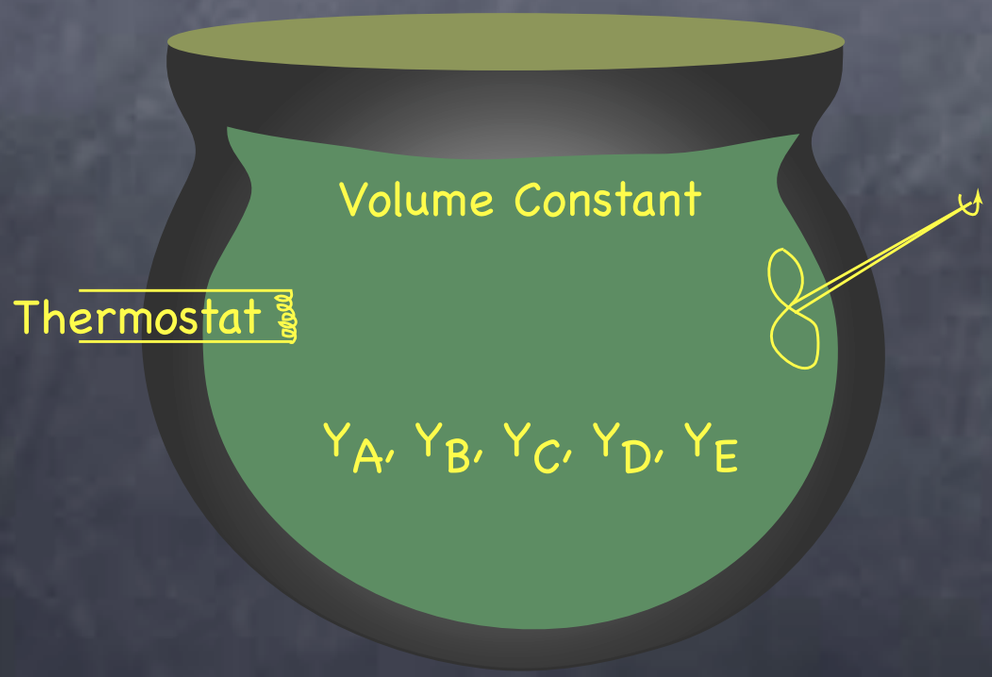
- This is not to say the composition within the pot will remain constant in time, for the occurrence of reactions will consume some species and generate others. In fact, it is the temporal evolution of the composition that we wish to investigate.

Cosmic Cauldon
Marilynn Flynn,
1995

Motivation

- 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 differential equations that describe the evolution of the five mole fractions.

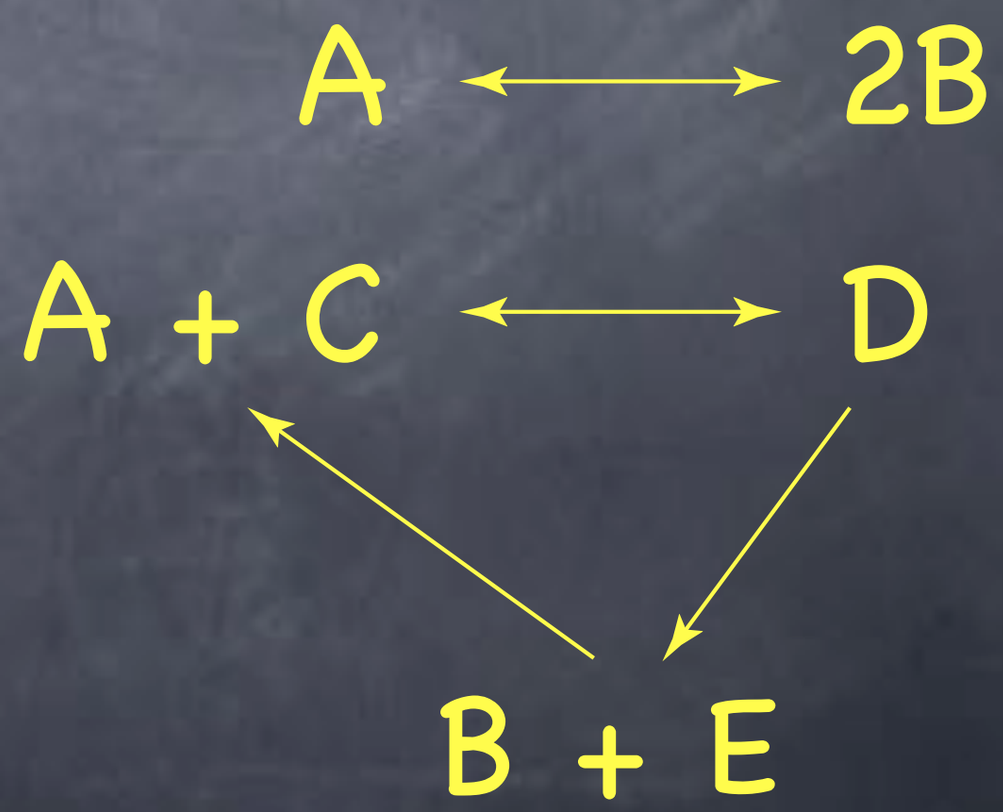
- The key to writing down the ODEs lies in knowing how rapidly each of the several reactions occurs. We assume the instantaneous rate of each reaction depends (in its own way) on the instantaneous composition vector Y.



Motivation

- That is, we assume there exists non-negative, real valued rate function $\mathcal{K}_{\mathrm{A}\to 2\mathrm{B}}$ that gives the instantaneous rate of the reaction A -> 2B. Similarily we assume a rate function $\mathcal{K}_{2\mathrm{B}\to\mathrm{A}}$ for the reaction 2B -> A, a rate function $\mathcal{K}_{\mathrm{A}+\mathrm{C}\to\mathrm{D}}$ for the reaction A+C -> D, and so on.

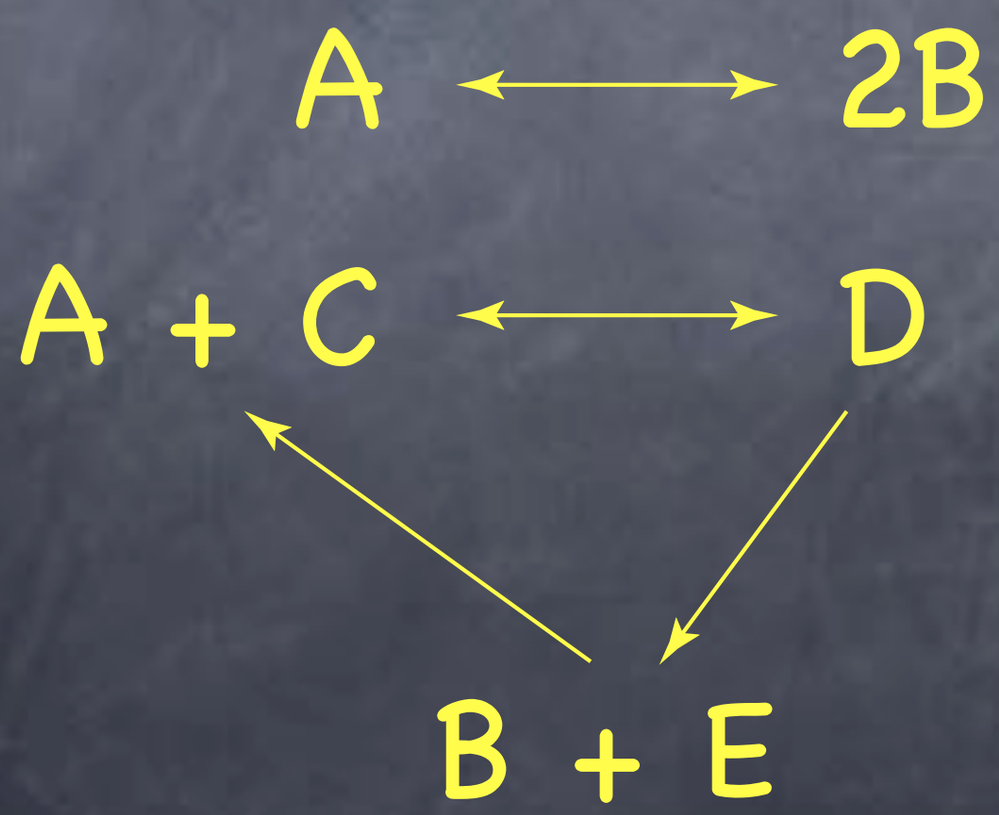
The kinetics for a reaction network is an assignment of a rate function for each reaction in the network.



Motivation

- Let's begin by considering the instantaneous rate of change of Y_A. Every time the reaction A -> 2B occurs we lose a unit of species A, and that reaction has an occurrence rate of $\mathcal{K}_{\mathrm{A}\rightarrow 2\mathrm{B}}$

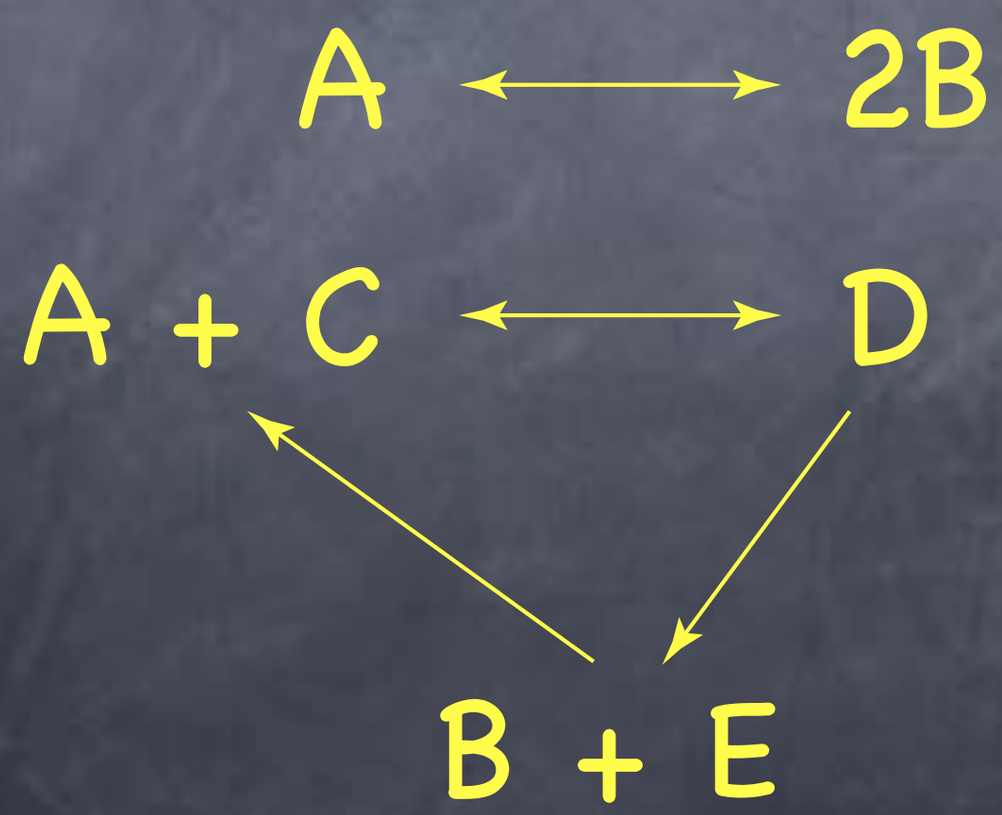
- On the other hand, every time 2B -> A occurs, we gain a unit of species A, and that reaction occurs at rate $\mathcal{K}_{2\mathrm{B}\rightarrow \mathrm{A}}$



Motivation

- Similarly the reactions B+E -> A+C and D -> A+C produce a unit of species A with each occurrence, while the occurrence of A+C -> D results in a loss of a unit of species A. So we write

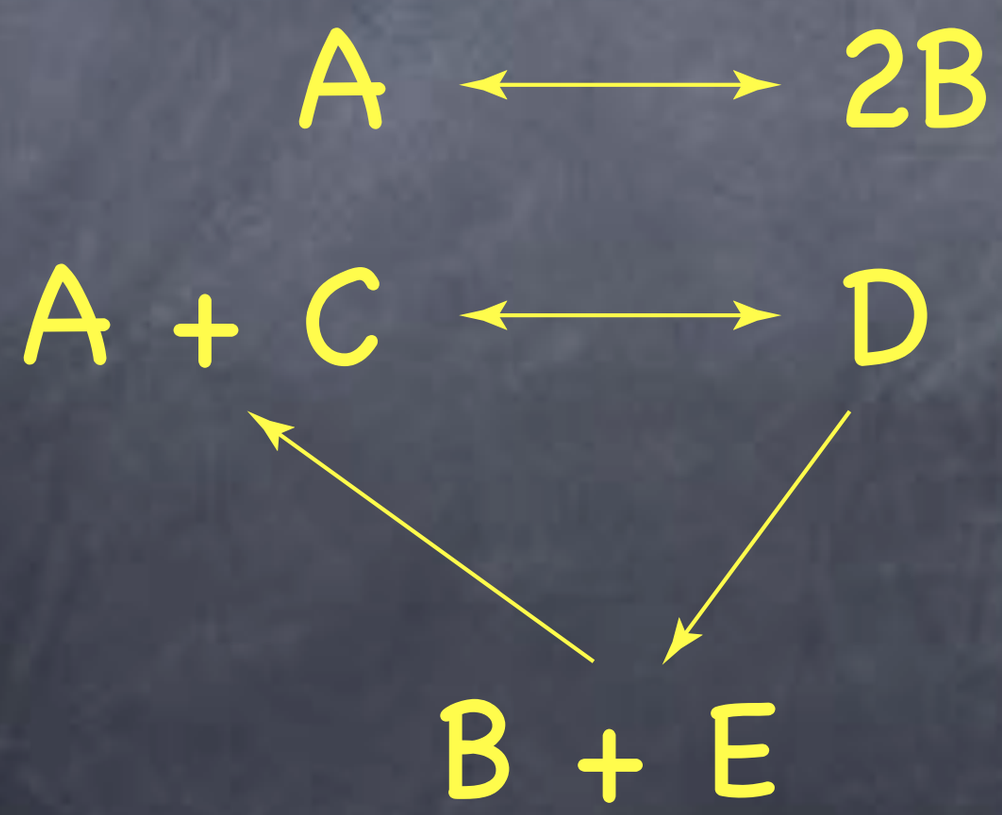
$$\dot{Y}_{\mathrm{A}} = -\mathcal{K}_{\mathrm{A}\to 2\mathrm{B}} + \mathcal{K}_{2\mathrm{B}\to\mathrm{A}} - \mathcal{K}_{\mathrm{A}+\mathrm{C}\to\mathrm{D}} + \mathcal{K}_{\mathrm{D}\to\mathrm{A}+\mathrm{C}} + \mathcal{K}_{\mathrm{B}+\mathrm{E}\to\mathrm{A}+\mathrm{C}}$$



Motivation

- For species B, whenever A -> 2B occurs we gain two units of B, and whenever 2B -> A occurs we lose two units of B. When D -> B+E occurs we gain a unit of B, and we lose a unit of B when B+E -> A+C occurs. Thus,

$$\dot{Y}_{\mathrm{B}} = 2\mathcal{K}_{\mathrm{A}\to 2\mathrm{B}} - 2\mathcal{K}_{2\mathrm{B}\to\mathrm{A}} + \mathcal{K}_{\mathrm{D}\to\mathrm{B}+\mathrm{E}} - \mathcal{K}_{\mathrm{B}+\mathrm{E}\to\mathrm{A}+\mathrm{C}}$$



Motivation

- Continuing in this way we can write down equations for the other three species to generate the full system of ODEs that govern our reactor:

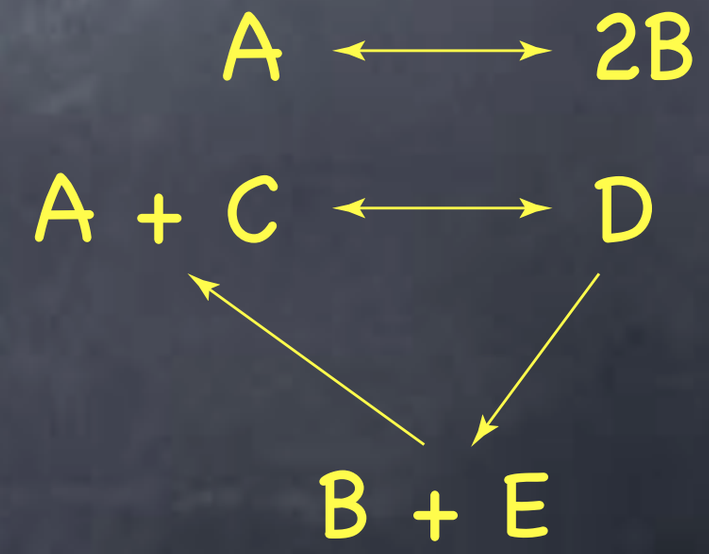
$$\dot{Y}_{\mathrm{A}} = -\mathcal{K}_{\mathrm{A}\to 2\mathrm{B}} + \mathcal{K}_{2\mathrm{B}\to\mathrm{A}} - \mathcal{K}_{\mathrm{A}+\mathrm{C}\to\mathrm{D}} + \mathcal{K}_{\mathrm{D}\to\mathrm{A}+\mathrm{C}} + \mathcal{K}_{\mathrm{B}+\mathrm{E}\to\mathrm{A}+\mathrm{C}}$$

$$\dot{Y}_{\mathrm{B}} = 2\mathcal{K}_{\mathrm{A}\to 2\mathrm{B}} - 2\mathcal{K}_{2\mathrm{B}\to\mathrm{A}} + \mathcal{K}_{\mathrm{D}\to\mathrm{B}+\mathrm{E}} - \mathcal{K}_{\mathrm{B}+\mathrm{E}\to\mathrm{A}+\mathrm{C}}$$

$$\dot{Y}_{\mathrm{C}} = -\mathcal{K}_{\mathrm{A}+\mathrm{C}\to\mathrm{D}} + \mathcal{K}_{\mathrm{D}\to\mathrm{A}+\mathrm{C}} + \mathcal{K}_{\mathrm{B}+\mathrm{E}\to\mathrm{A}+\mathrm{C}}$$

$$\dot{Y}_{\mathrm{D}} = \mathcal{K}_{\mathrm{A}+\mathrm{C}\to\mathrm{D}} - \mathcal{K}_{\mathrm{D}\to\mathrm{A}+\mathrm{C}} - \mathcal{K}_{\mathrm{D}\to\mathrm{B}+\mathrm{E}}$$

$$\dot{Y}_{\mathrm{E}} = \mathcal{K}_{\mathrm{D}\to\mathrm{B}+\mathrm{E}} - \mathcal{K}_{\mathrm{B}+\mathrm{E}\to\mathrm{A}+\mathrm{C}}$$



Motivation

- So far we haven't said anything about the nature of the rate functions. For nuclear reaction networks, the kinetics is taken to be of a mass action type.

- For A -> 2B we assume the more A there is, the more occurrences of the reaction there will be. Thus, we take the instantaneous rate of A -> 2B to be proportional to Y_A :

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

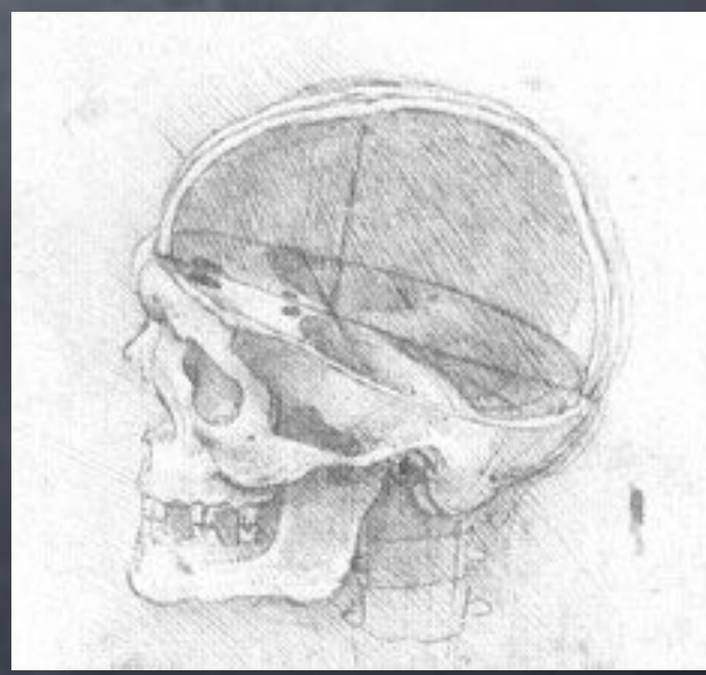
Svante August Arrhenius
Nobel Prize 1903

Motivation

- For A+C -> D, an occurrence requires a unit of species A meet a unit of species C in the reactor, and we take the probability of such an encounter to be proportional to the product $Y_A Y_C$.

- Although we don't presume that every encounter yields a unit of species D, we still take the occurrence rate to be given by

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



Skull cross section
Leonardo da Vinci

Motivation

- With mass action kinetics, our rate functions take the form

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

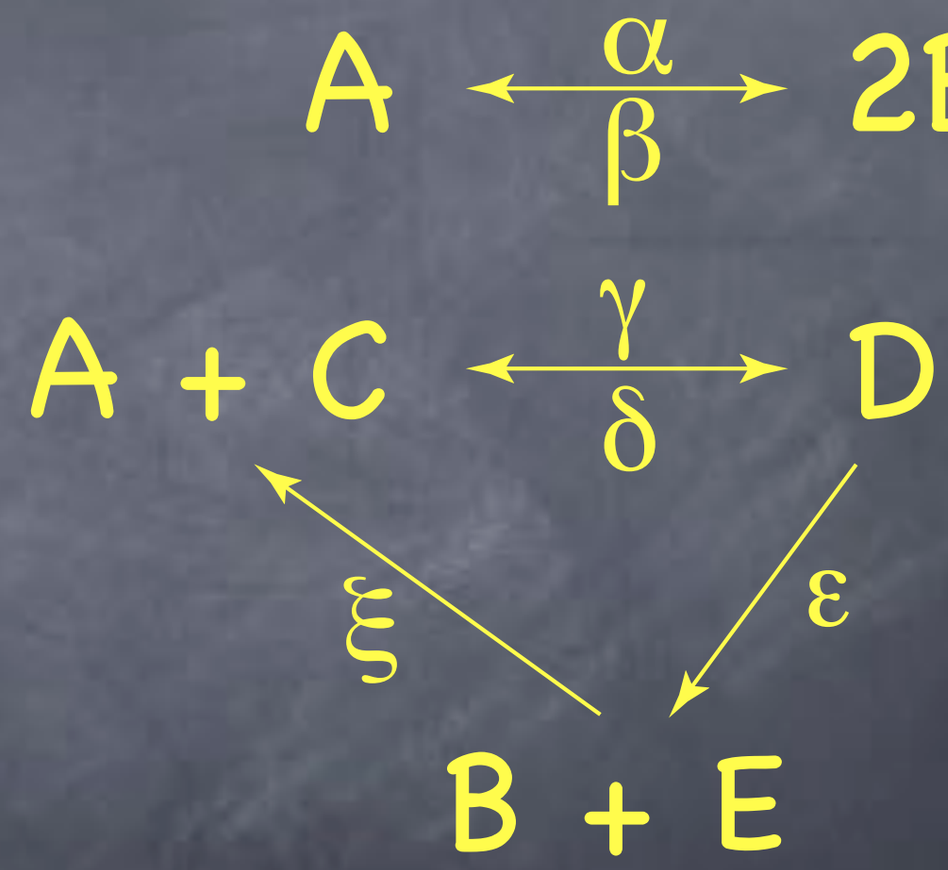
$$\mathcal{K}_{2\mathrm{B}\to \mathrm{A}} = \beta Y_B^2$$

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

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

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

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



The rate constants may depend on temperature and density

Motivation

- And our reaction network takes the form

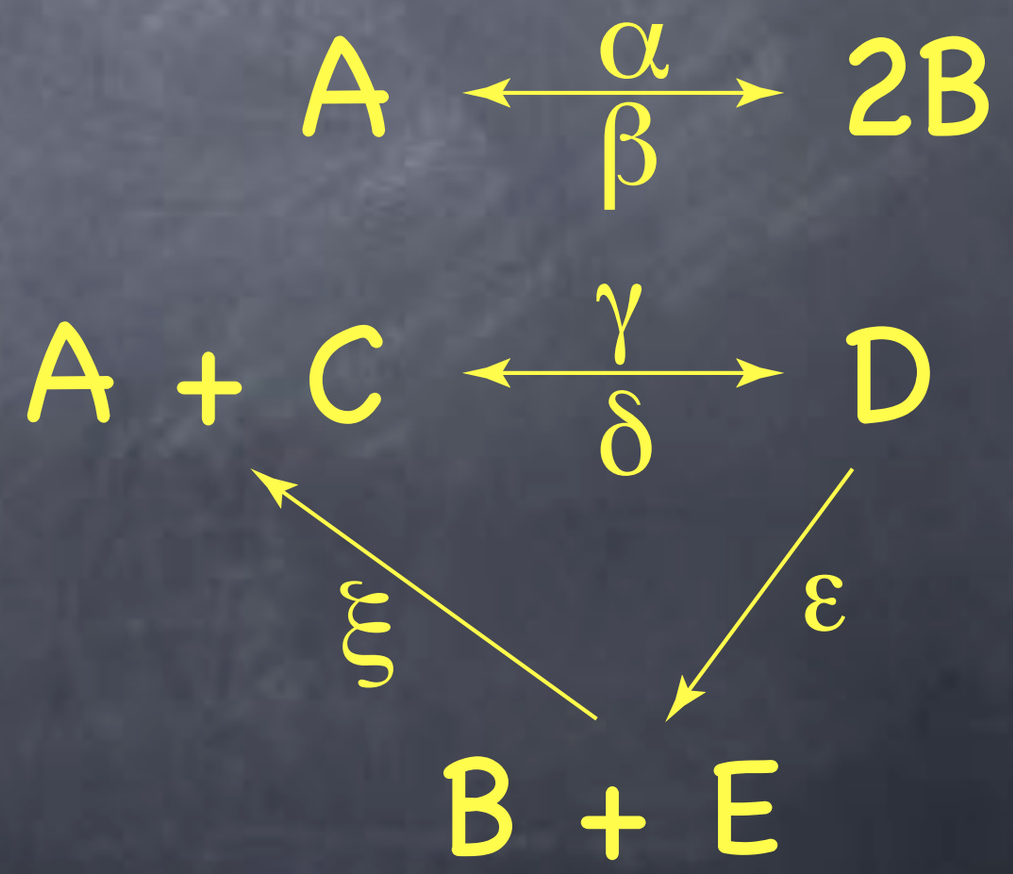
$$\dot{Y}_{\rm A} = -\alpha Y_A + \beta Y_B^2 - \gamma Y_A Y_C + \delta Y_D + \xi Y_B Y_E$$

$$\dot{Y}_{\rm B} = 2\alpha Y_A - 2\beta Y_B^2 + \varepsilon Y_D - \xi Y_B Y_E$$

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

$$\dot{Y}_{\rm D} = \gamma Y_A Y_C - \delta Y_D - \varepsilon Y_D$$

$$\dot{Y}_{\rm E} = \varepsilon Y_D - \xi Y_B Y_E$$



Interlude

Gerry Wasserburg
1993

Nuclear reaction networks

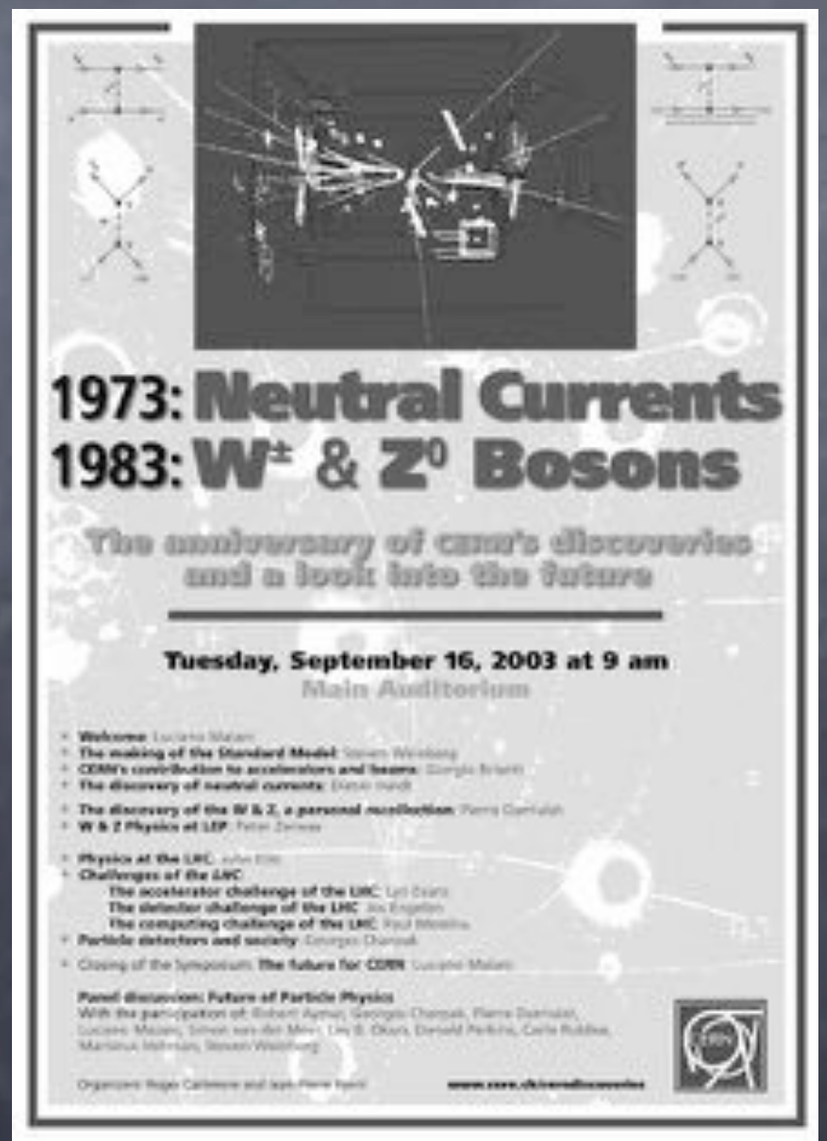
- There are a number of types of nuclear reactions which are of astrophysical interest.

- In addition to the emission or absorption of nuclei and nucleons, nuclear reactions can involve the emission or absorption of photons (γ-rays) and leptons (electrons, neutrinos, and their anti-particles).

- As a result, nuclear reactions involve three of the four fundamental forces, the nuclear strong, electromagnetic and nuclear weak forces.

Forming a reaction network

- Weak interactions (those involving leptons) proceed much more slowly than those involving only nucleons and photons; however, these reactions are important because only weak interactions can change the global ratio of protons to neutrons.



Forming a reaction network

- The key quantity that describes the nuclear properties of a species important to nucleosynthesis or stellar energy generation is the cross section σ for interaction.

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

$$\sigma = \frac{\text{number of reactions target}^{-1}\text{sec}^{-1}}{\text{flux of incoming projectiles}} \quad \text{cm}^2$$

- A representative unit is a barn, or 10^{-24} cm^2.

Forming a reaction network

- The reaction rate per unit volume, R_{ij} , in the simplest case is given by the flux of particles i times the number density of j times σ_{ij}.

$$R_{ij} = [\text{flux of } j]\ n_i\ \sigma_{ij} = v_{ij} n_j\ n_i\ \sigma_{ij} = n_i n_j \sigma_{ij} v_{ij}$$

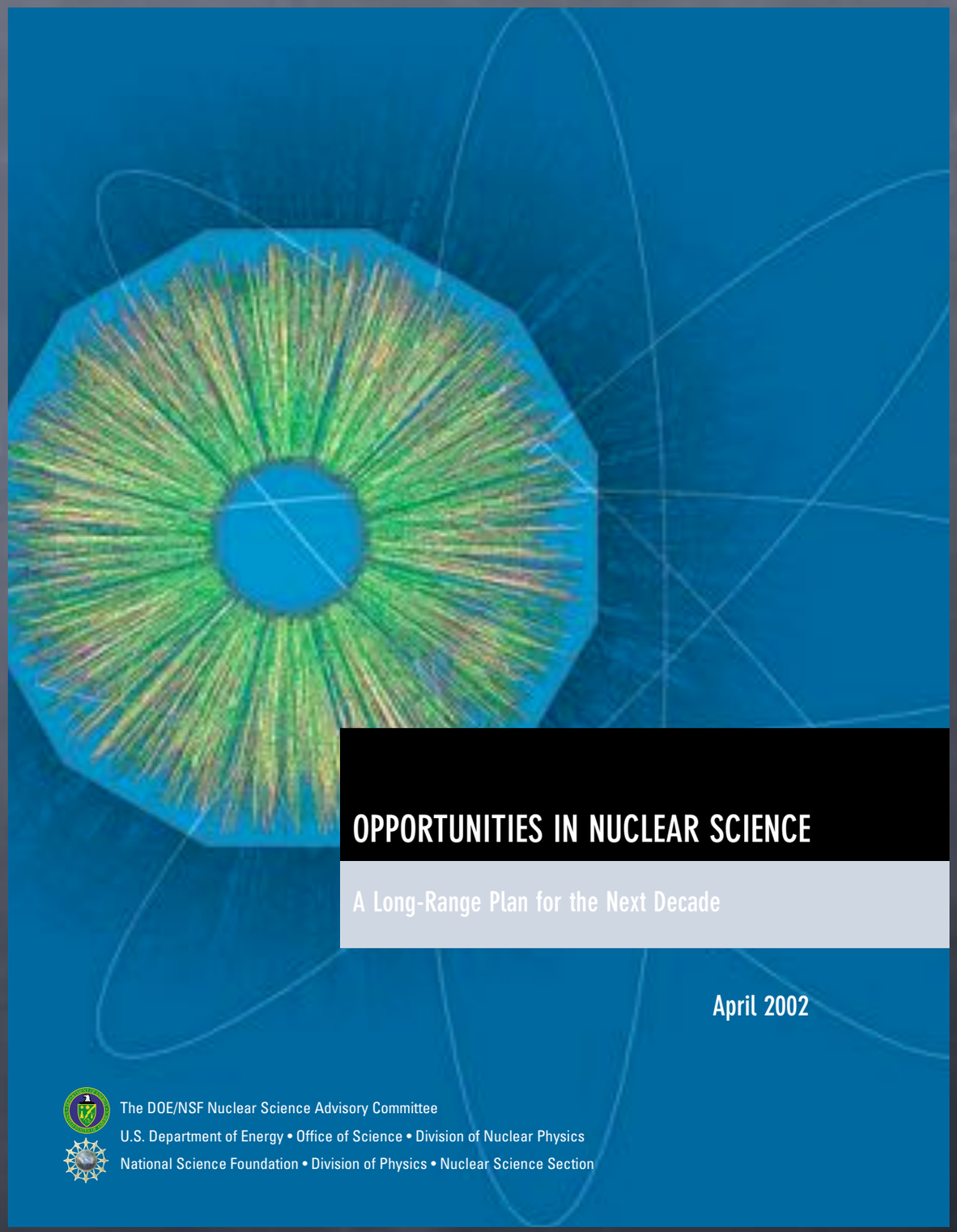
- As the astrophysicist is concerned, nuclear physics boils down to the determination of the relevant cross sections (and the energy released by the reaction) which are usually averaged over a distribution of particle fluxes.

$$R_{i,j} = \int \sigma(|\vec{v}_i - \vec{v}_j|)|\vec{v}_i - \vec{v}_j| d^3 n_i d^3 n_j$$

Forming a reaction network

- We'll have more to say about the nature of cross sections and Q-values later on in this lecture series.

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



Forming a reaction network

- Let's start with a unidirectional binary reaction with unity coefficients.

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

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

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

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

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

Forming a reaction network

- Now consider the case when the coefficients are not unity.

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

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

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

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

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

- The factorial denominators avoid double counting. If identical reactants i=j (for example p + p) simply set c_j =0.

Forming a reaction network

- A general formula for a general 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 identical reactants i=j, simply set the c_q=c_s=0.

Forming a reaction network

- The reaction types can be divided into three categories based on the number of reactants which are nuclei.

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

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

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

Forming a reaction network

- For binary reactions, another general formula is

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

Binary sea exchange
2003

Forming a reaction network

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

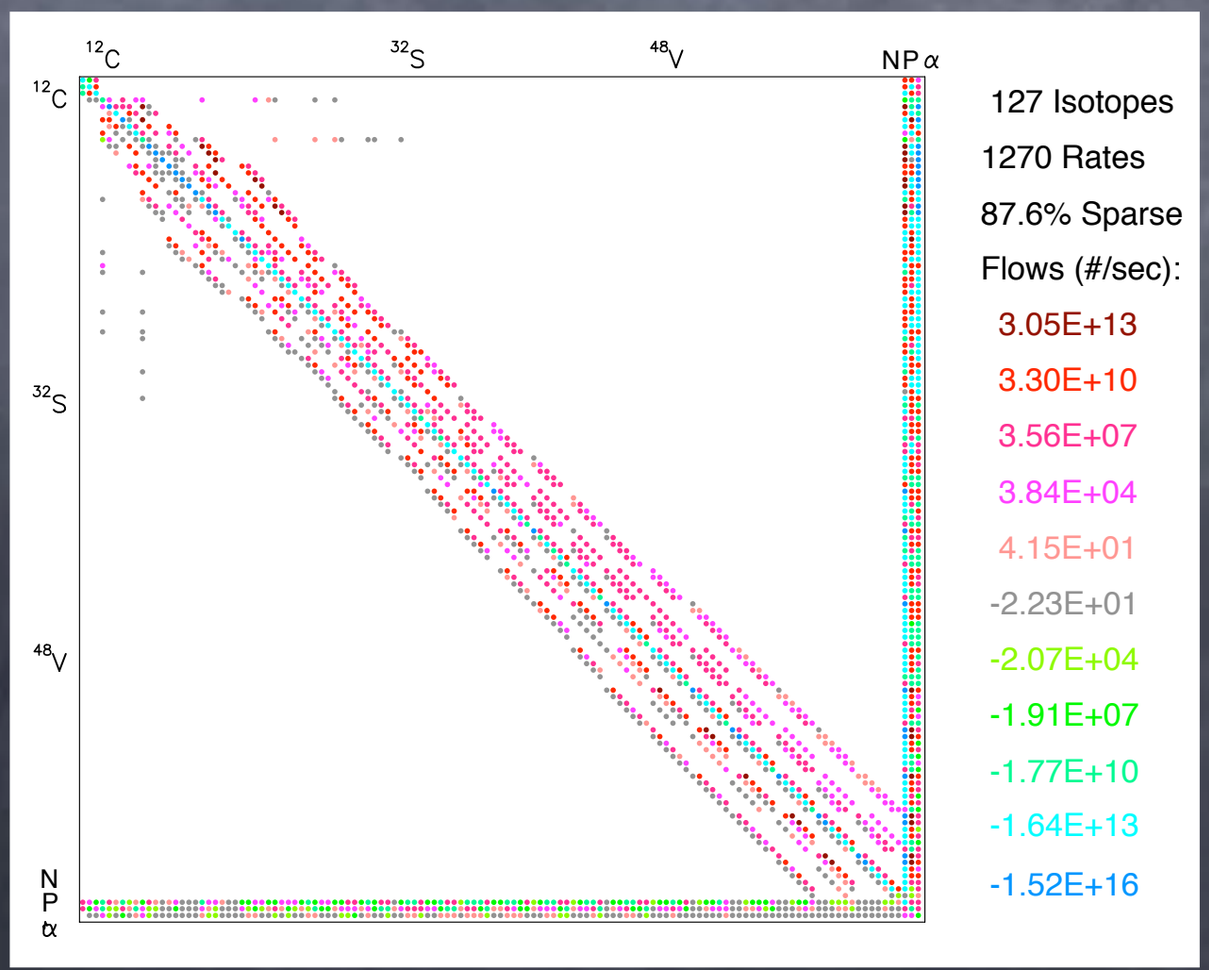
- Using an equilibrium abundance for the unstable intermediate, the contributions of these reactions are commonly written in the form of a three-particle processes, depending on a trio of number densities.

$$\dot{Y}_i = \sum_{jkl} \frac{C_i}{C_j!C_k!C_l!}\ \rho^2 N_A^2\ R_{jkl}\ Y_j\ Y_k Y_l$$

Forming a reaction network

- In terms of the reaction cross sections and molar abundances, a reaction network may described by the following set of ODEs

$$\dot{Y}_i = \sum_j C_i R_j Y_j + \sum_{jk} \frac{C_i}{C_j! C_k!} \rho N_A \, R_{jk} \, Y_j \, Y_k + \sum_{jkl} \frac{C_i}{C_j! C_k! C_l!} \rho^2 N_A^2 \, R_{jkl} \, Y_j \, Y_k Y_l$$



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

How does the Sun shine?

- 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?

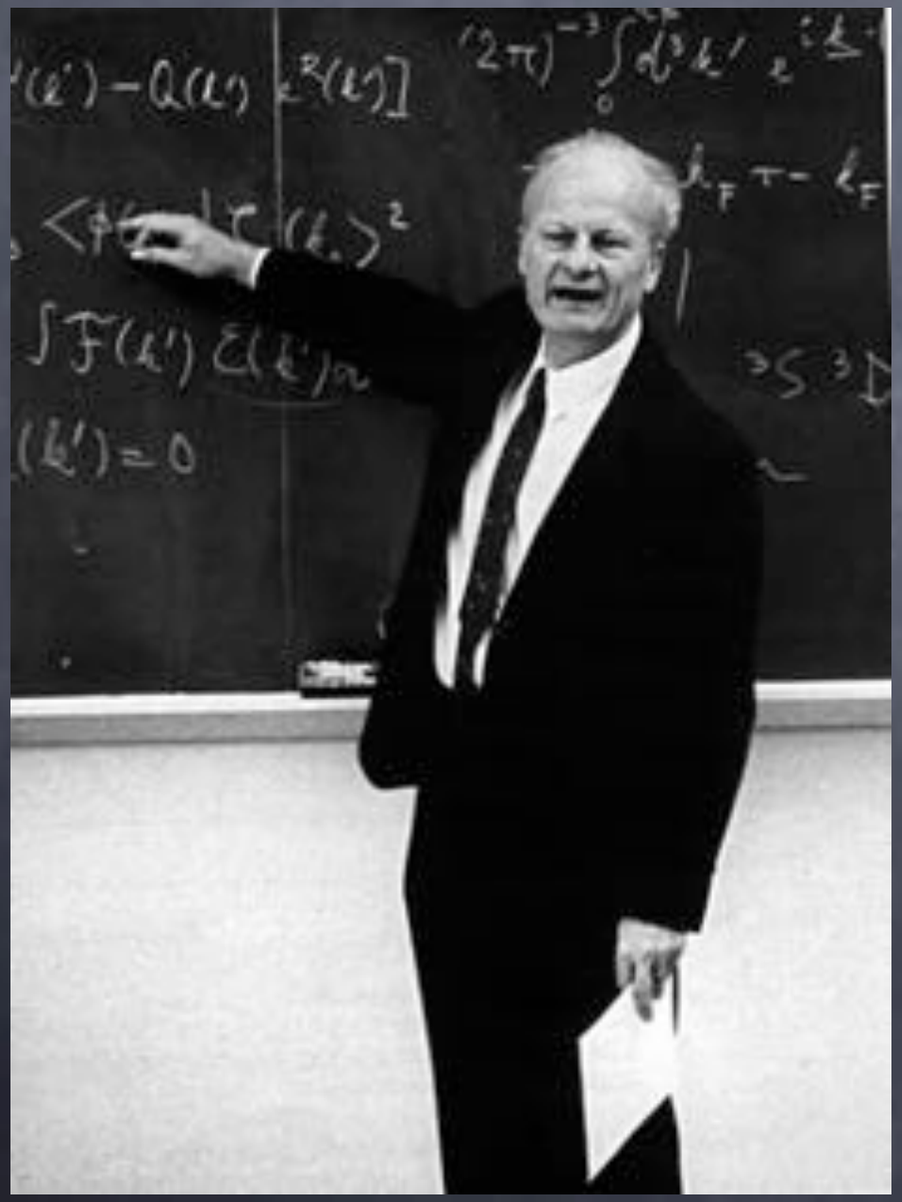
- $E = mc^2$

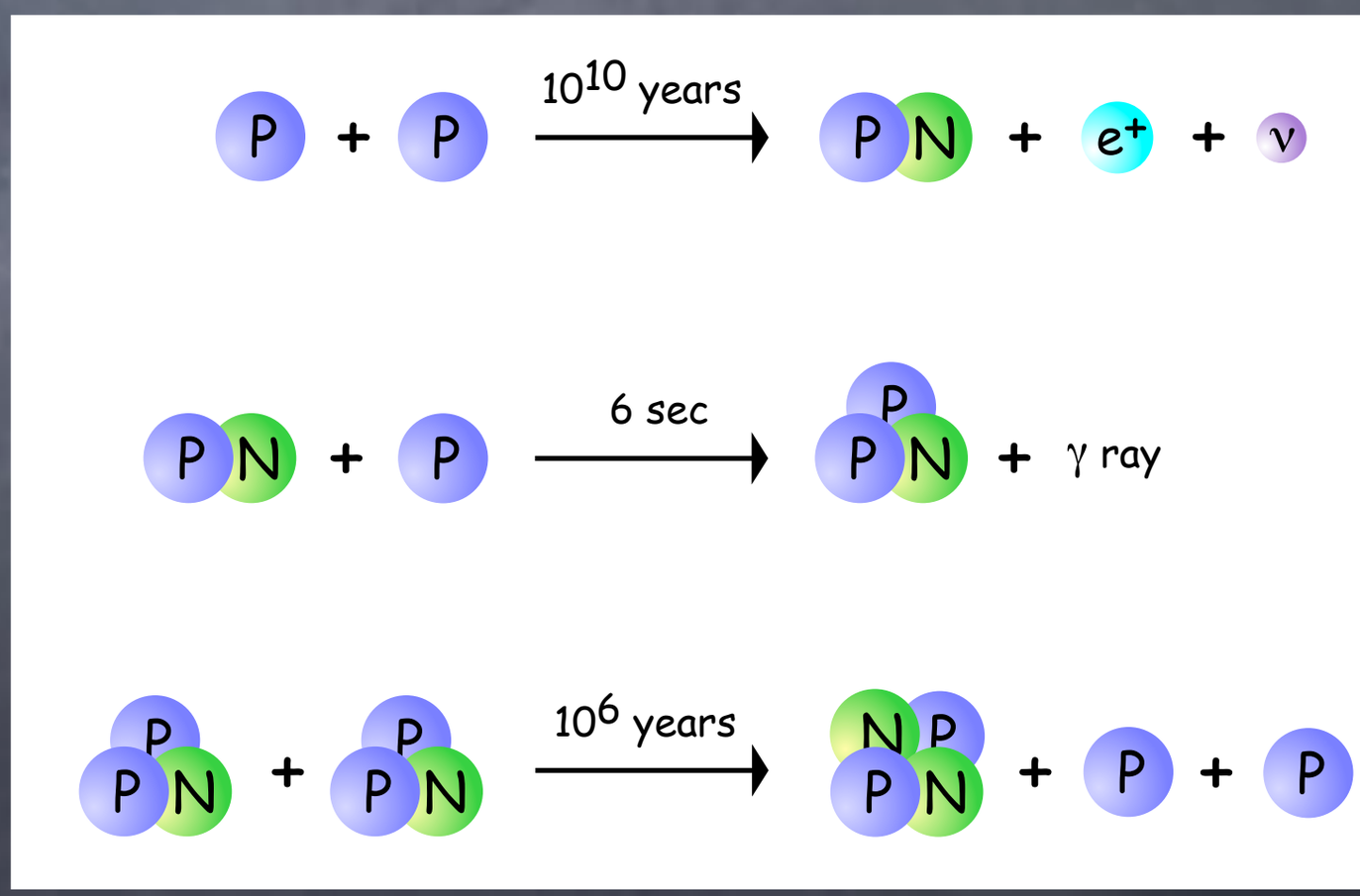
- The sun presently shines by burning hydrogen (fuel) into helium (ash) in its core.

600 million tons of hydrogen are converted into 596 million tons of helium every second

proton-proton chains

- Hans Bethe realized in 1939 that the weak interaction was capable of converting a proton into neutron during the brief encounter of a scattering event.

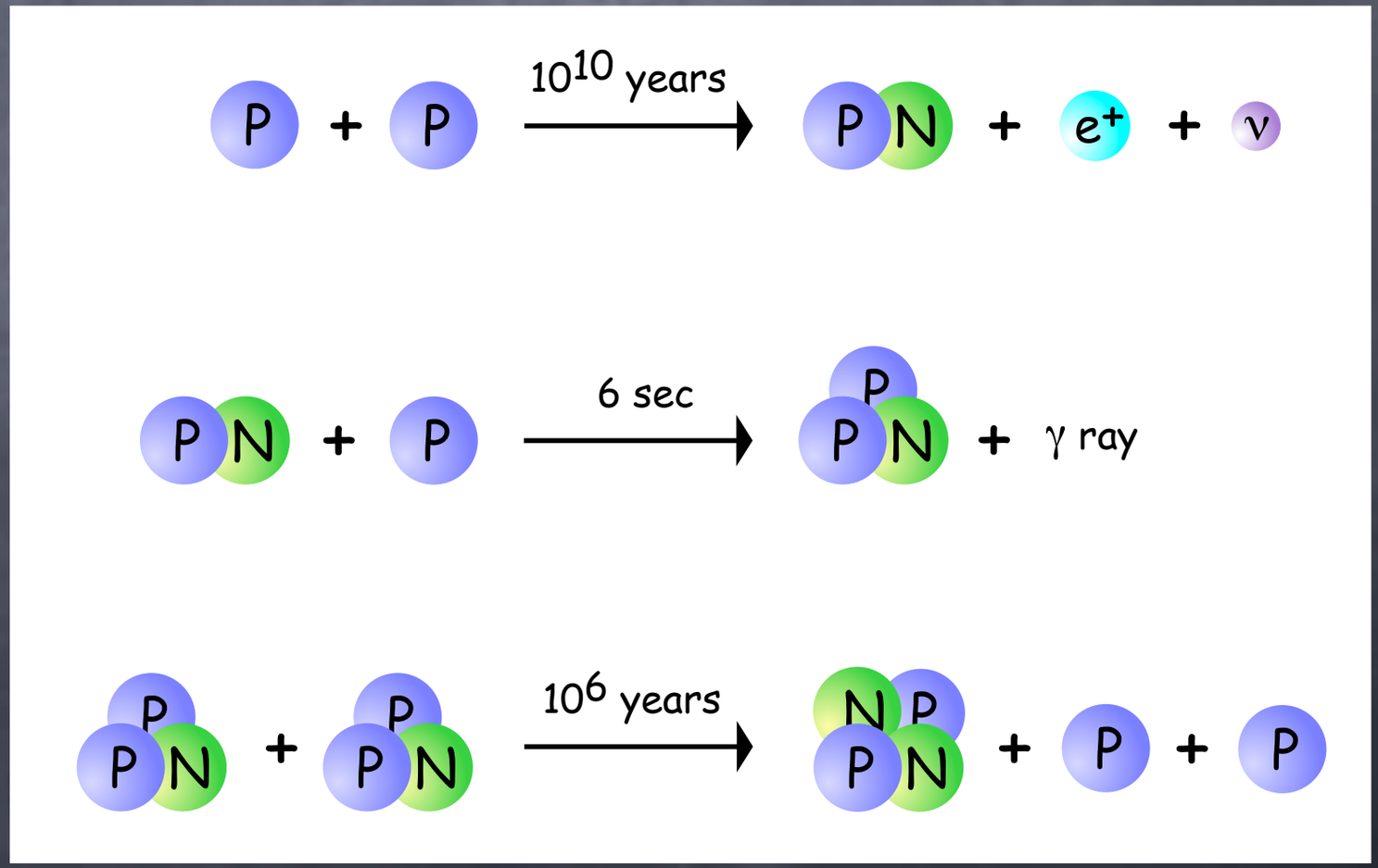




proton-proton chains

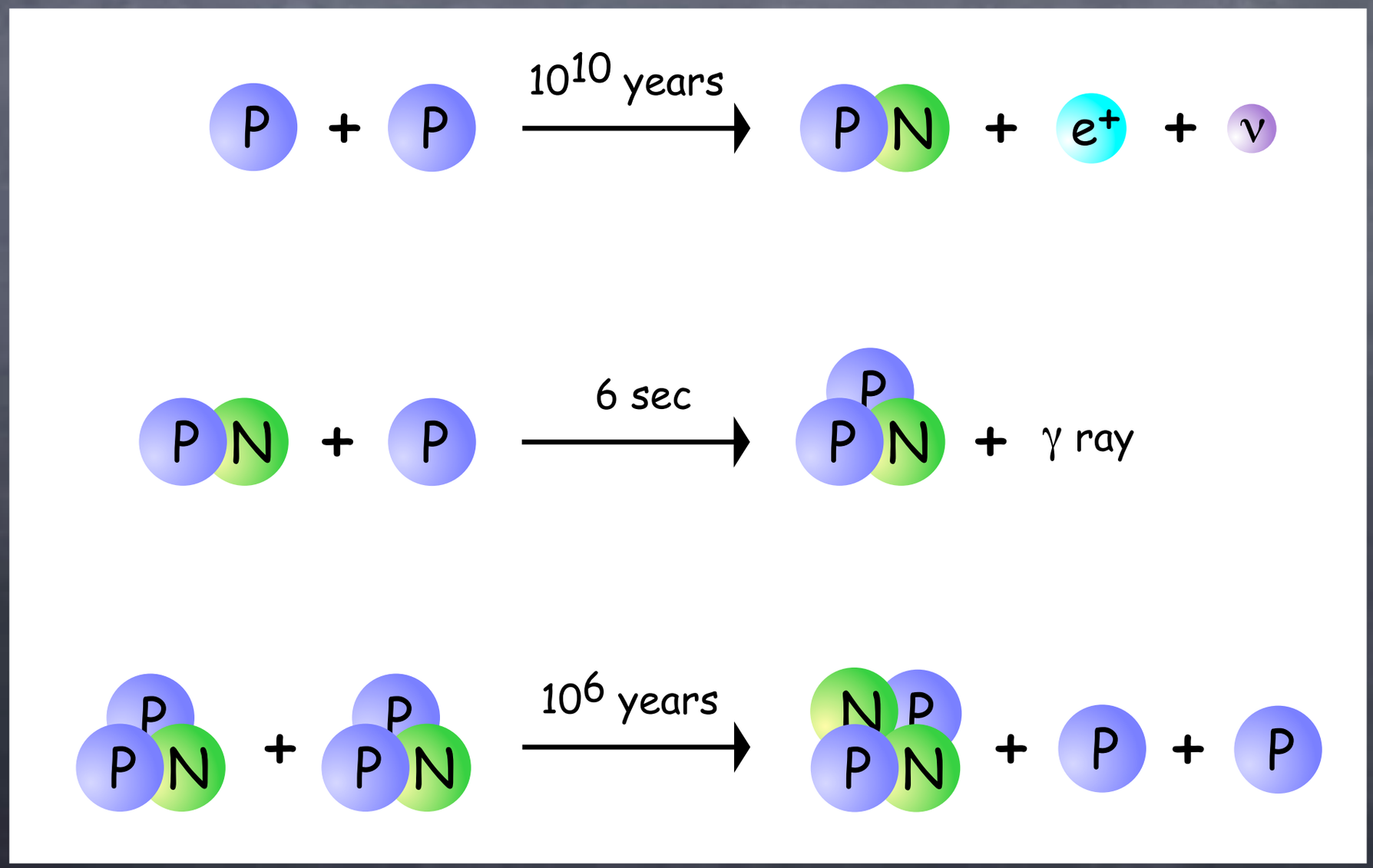
- Since the neutron is more massive than a hydrogen nuclei, such a decay would require energy (endothermic) except for the fact that the neutron can appear in a bound state with proton in the form a deuterium nucleus.

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



proton-proton chains

- 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.



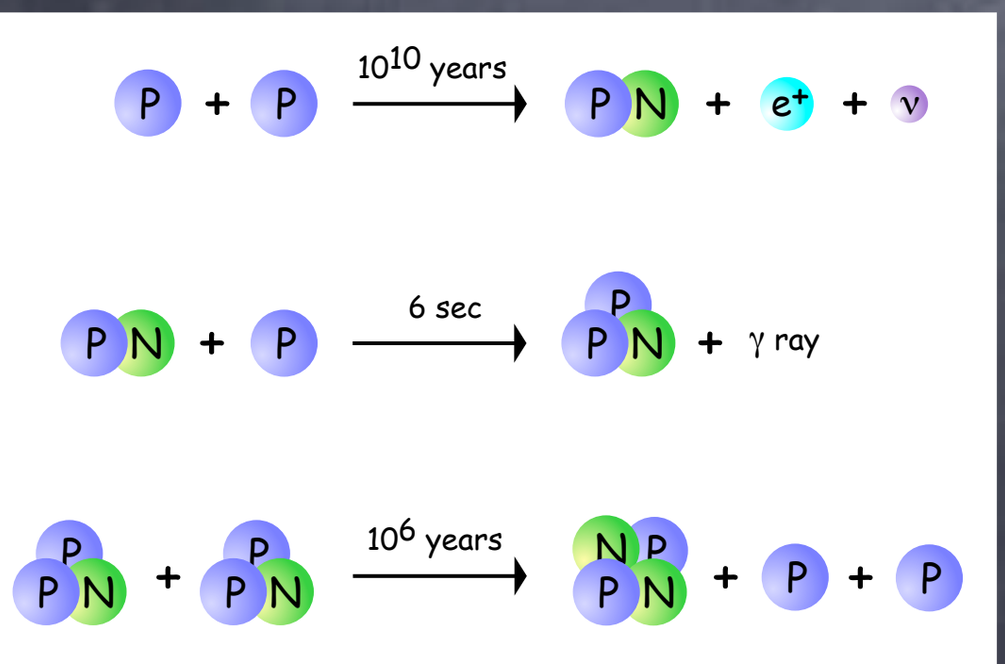
proton-proton chains

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

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

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

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



Where the density and Avogadro number dependence has been folded into the reaction rates

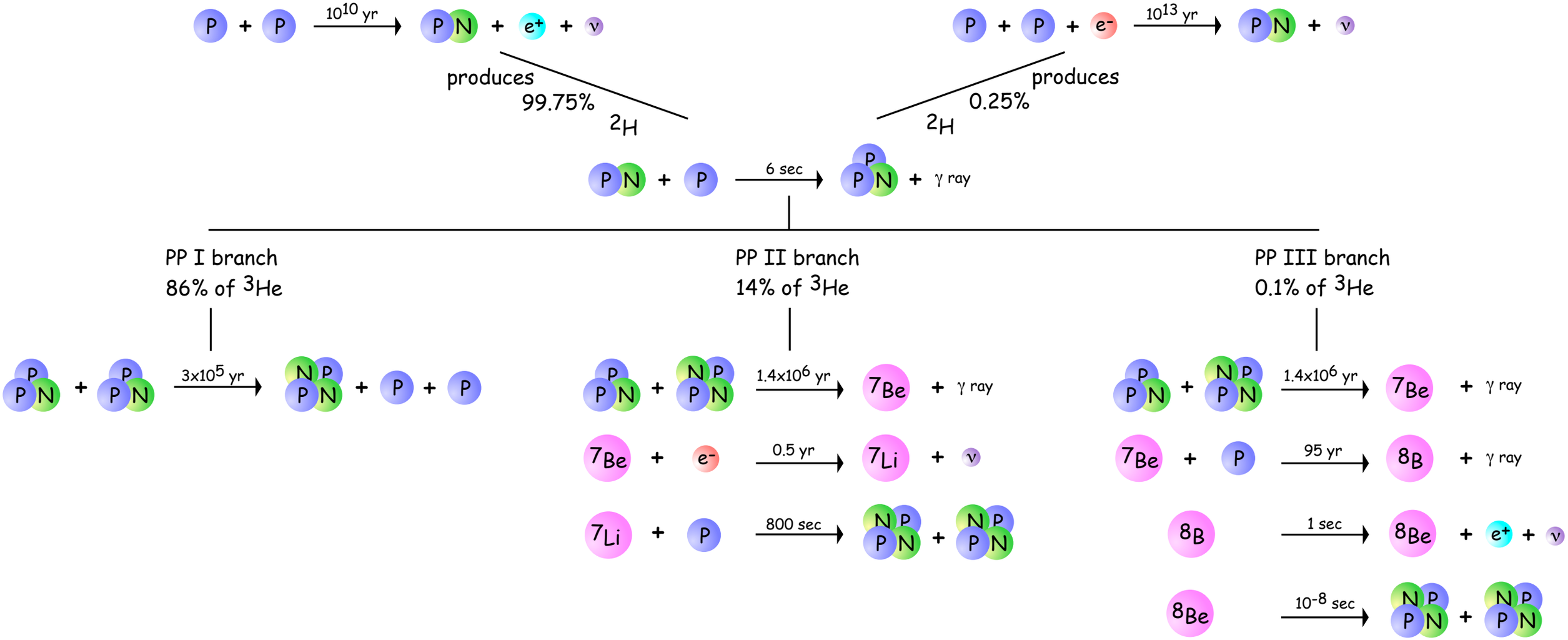
proton-proton chains

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

- Holmgren & Johnston measured the ^{3}He(α,γ)^{7}Be cross section to be 2500 times larger than the previously accepted value, so that this reaction competes with ^{3}He(^{3}He,2p)^{4}He for ^{3}He nuclei, particularly at elevated temperatures.

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

proton-proton chains



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}.

Tasks for the day

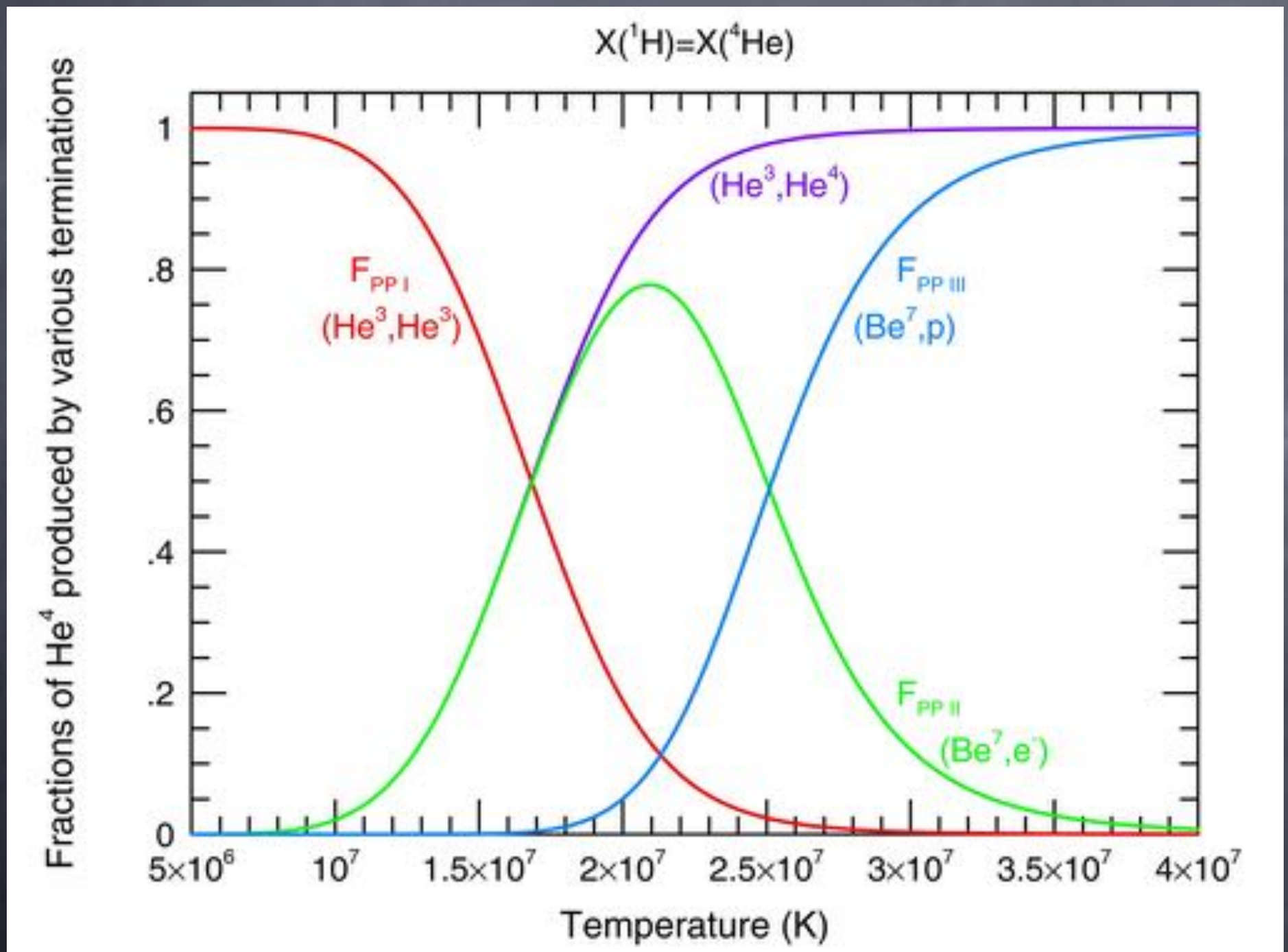
- Derive the ODE equations for the PPI chain.

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

- Plot the abundances for temperatures of 1.0×10^7 K, 2.0×10^7 K, and 3.0×10^7 K for a density of 150 g/cm^3 and an initial composition of 75% H and 25% He by mass. Based on your calculations: How much hydrogen is left in the center of the Sun? How long will the Sun live? What do you conclude from the runs with different temperatures?

Tasks for the day

- For those who enjoy a challenge, reproduce the following plot.



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

Tools and Toys in Nuclear Astrophysics

Copper Cauldron with Three Eggs,
1734, oil on panel,
Jean-Baptiste-Siméon Chardin