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

Terry Pratchett



SCHOOL OF EARTH

Nuclear Astrophysics: Reaction Networks

Frank Timmes



2009 NATIONAL NUCLEAR PHYSICS SUMMER SCHOOL

June 28-July 10, 2009 National Superconducting Cyclotron Laboratory (NSCL Michigan State University | East Lansing, Michigan

http://meetings.nscl.msu.edu/NNPSS09

U gell LLCLS , Heenis Battar Chail, Wolfgang Baue, Bater, Chail Chornesson TOOLS : Hotor Physics, Nacker Random, Nackel Bluchser, COL MIECE | ECULYPICS, Halder Random Lucher Buchser, CARL MIECE | ECULYPICS : Information Bluchser, Carlonna Bruchser, Carlonna Bruchser, Struc-Ramk Timese, University of Annual, Blill Zale, Caluttala University, Jahn Hardy, Tixona AM, University, Frank Timese, University of Annual, Blill Zale, Caluttala University, Jahn Hardy, Tixona AM, University, Strong Timese, University of Annual, Blill Zale, Caluttala University, Jahn Hardy, Tixona AM, University, Strong Timese, University, Machael Westerker, University, Handhards AM, University, Sponson, Vincelling, State University, Mattala Tange, Strathard of Nacker Theory, Sponson, National Blacker, Strathard Mattala Tange, Strathard Kola, Strathard, Steal, Jahner, Jahong Stat, Jahong Handring, State, University, Mattala Tange, Jahong Jahong Hand, Jahong Handhard, Jahong Hand, Jahong Hand, Jahong



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/



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,

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

 $W = mN_A$ 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 ¹²C atom at rest and in its ground state. For ¹²C, we define the molar mass to be W=12.0 g/mol. An amu then has W=1 g/mol. Hence,

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

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

$$m_k = Nm_n + Zm_p + Z(1-f)m_e - \Delta m$$

= $Nm_n + Zm_p + Z(1-f)m_e - \frac{B}{c^2}$

 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

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

where n_i is the number density of species *i*.

$$X_i = \frac{A_i n_i}{\rho N_A} = \frac{\rho_i}{\rho}$$

mass fraction, dimensionless

$$Y_i = \frac{X_i}{A_i} = \frac{n_i}{\rho N_A}$$

molar fraction.dimensionless

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

And finally (for today)

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



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.

tony lynch, 2002

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 $A + C \rightarrow D$ loses a unit of species A, while $2B \rightarrow A$, $B+E \rightarrow A+C$, $D \rightarrow A+C$ produces a unit of species A. So we write

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

A + C

2B

Volume Constant



 $Y_{A}, Y_{B}, Y_{C}, Y_{D}, Y_{E}$

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

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

 $Y_B = 2K_{A \to 2B} - 2K_{2B \to A} + K_{D \to B+E} - K_{B+E \to A+C}$

$$Y_C = -K_{A+C \to D} + K_{D \to A+C} + K_{B+E \to A+C}$$

 $Y_D = K_{A+C \to D} - \overline{K_{D \to A+C} - K_{D \to B+E}}$

 $Y_E = K_{D \to B+E} - K_{B+E \to A+C}$

B + E

A +

2B

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

For A+C→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 $Y_AY_C : K_{A+C \rightarrow D} = \gamma Y_A Y_C$.





Svante August Arrhenius Nobel Prize 1903 With mass action kinetics, our rate functions take the form



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

And our reaction network takes the form

 $A \xrightarrow{\alpha}{\beta} 2B$

 $C \xleftarrow{\gamma}{\delta} D$

3

A +

8

B

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

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

$$Y_C = -\gamma Y_A Y_C + \delta Y_D + \xi Y_B Y_E$$

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

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

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/cm²/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 cm².



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

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

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

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

where <σv>_{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

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

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.

$$\dot{Y}_{i} = -Y_{i}Y_{j}R_{ij}$$

 $\dot{Y}_{i} = -Y_{i}Y_{j}R_{ij}$
 $\dot{Y}_{k} = Y_{i}Y_{j}R_{ij}$
 $\dot{Y}_{k} = Y_{i}Y_{j}R_{ij}$

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.

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

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

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

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

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

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.

$$\dot{Y}_i = \sum_{\cdot} C_i R_j Y_j$$

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): -1.64E+13

Interlude

Nuclear Science

Expansion of the Universe

the Rig Yang, the column expended and readed. As down 12⁴ around, the uniteres constant of a ange of quarks, glarma, electrons, and a When the propagation of the Universe. The constraint in shore 10° K, this way reduced him presents, and decrement. As time of, some of the propagation propagation for the decrement. Software, and before a series and the series and the an multi to form neural metra. Due to gravity, clouds of avera constant line wass, when hydrogen and follows hand into zono manifer ind dynams. Signifizing man juggers and from the inter manim docume and iligous them into space. Our early we formul hore

٠	+						
11	100 H	Breadien Breadien H ²¹ E H ²¹ e	formation of formation and it to " its) to a	Annualiza of annual doma 4,000 X 400,000 yr	1111 Jan	Appendix of 	andry S.K. La to H ² W

Nuclear Science a durably of the anatom, properties, and increasions of the assess multi-Nuclear advertise telephone and research the masses, shapes, sizes, and decays of market at your and in collimons. They ask geometry, each as Why do anothers may to the medicar What conditionings of process and returned an proched What happens when stacked an improved as taptify summit What is the origin of the studie found as Earth?

Legend Calenna de 11 - gantel Z.max C promo (province (r*) (place field -terations (b) Labora Income antimatrice (1) places (1) North 1 8-2

Suble multido llinti i nanow white local on the Chart of



Nuclear career can relat in averal plane. When collisions rector marks, indeeded the state was seen by the set the sup has find its sufficiency light same name or dissisting a gas to machine the all farms. At must man fielt southerne man course time the usach plant plants that hadorenell, Cornet date seconds hive that allegating name affiniated the street it.





Nuclear Energy



II Beta plas così

-

-

Name of the state when the total scan of the perdown in loss than the most of the and the products of Allerton aler mulitum apil In Status, a real the recentage logismus the stands significant of them. ine Infedera, Ire man ein fei nombite to freit a man the plat and on a a state



man, Aphropen Dans in Rose Antonio Car Game of physics (Sight) and passes magin of Anthe products the shallow of two -

tras here a user grover days not



Magnetic Resonance Imaging

Animplifying pictures serving WARAWER shall not ACREWITH

@ Capyright 2019 Control protect Delawary Physics Delawar

of the digits eastern "gam to breas the do

and with the state sheet

Radioactivity



Chart of the Nuclides



-N-+

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.

600 million tons of hydrogen are converted into 596 million tons of helium every second 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 (¹H, ²H, ³He, ⁴He), and three binary reactions that couple these species; $p(p,e^+\nu)^2H$, $^2H(p,\gamma)^3He$, and $^3He(^3He,2p)^4He$.



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

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

 $Y_{3he} = Y_{p}Y_{d}R_{p,d} - Y_{he3}Y_{he3}R_{he3,he3}$

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



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

Holmgren & Johnston measured the ${}^{3}\text{He}(\alpha,\gamma){}^{7}\text{Be}$ cross section to be 2500 times larger than the previously accepted value, making this reaction compete with ${}^{3}\text{He}({}^{3}\text{He},2p){}^{4}\text{He}$ for ${}^{3}\text{He}$ 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 ⁷Be 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, $\varrho = 150$ g/cm³, 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



2009 NATIONAL NUCLEAR PHYSICS SUMMER SCHOOL

June 28-July 10, 2009 National Superconducting Cyclotron Laboratory (NSCL) Michigan State University | East Lansing, Michigan

meetings.nscl.msu.edu/NNPSS09 nnpss@nscl.msu.edu

NZERS Hendrik Schatz (Chair), Wolfgang Bauer, Shari Conroy, Michael Thoennessen Hadron Physics, Nuclear Reactions, Nuclear Structure, QCD,

Neutrinos, Nuclear Astrophysics, Fundamental Symmetries

Invited International Control of the State Control

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



