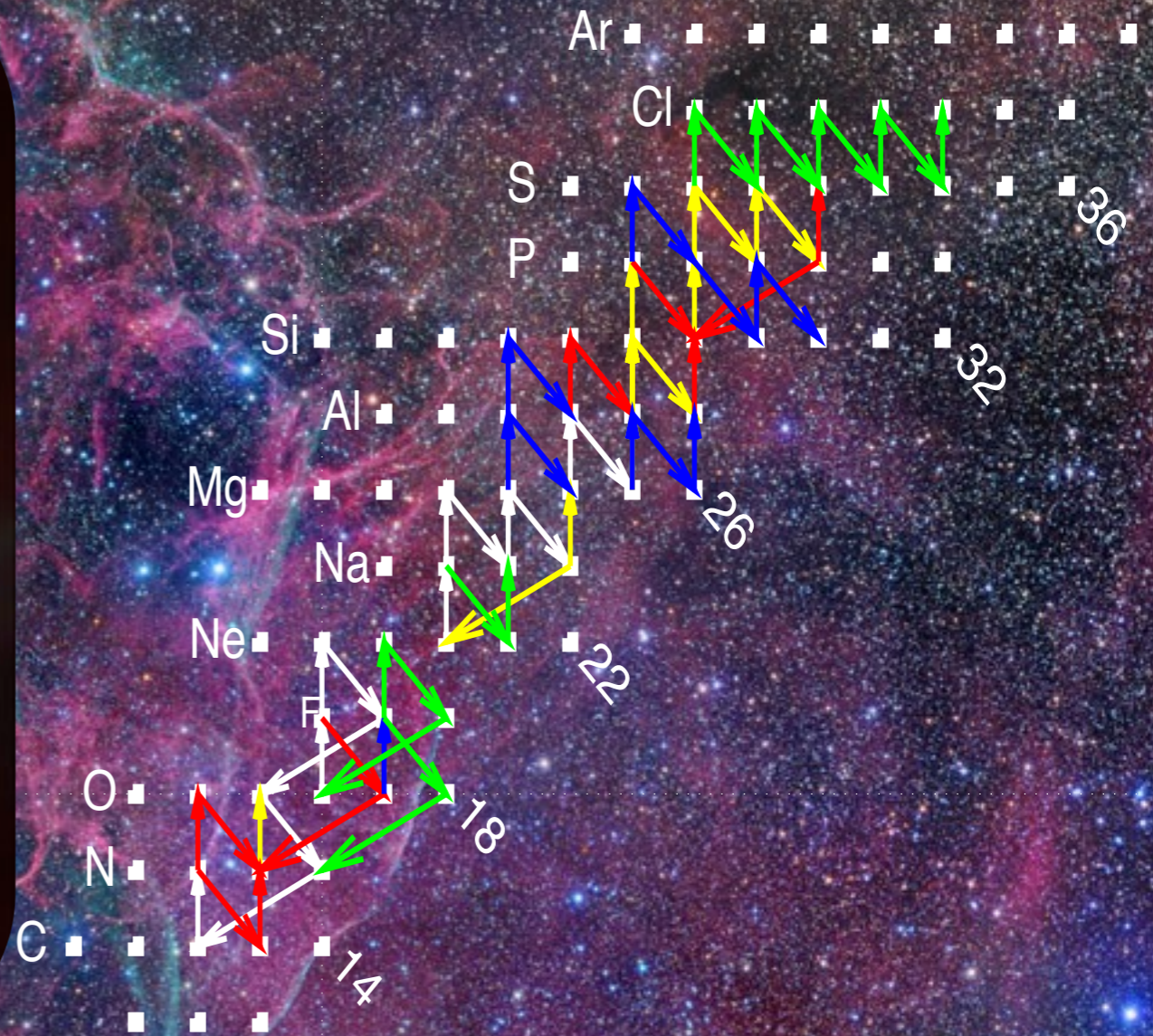


# THERMONUCLEAR REACTION NETWORKS FOR ASTROPHYSICS

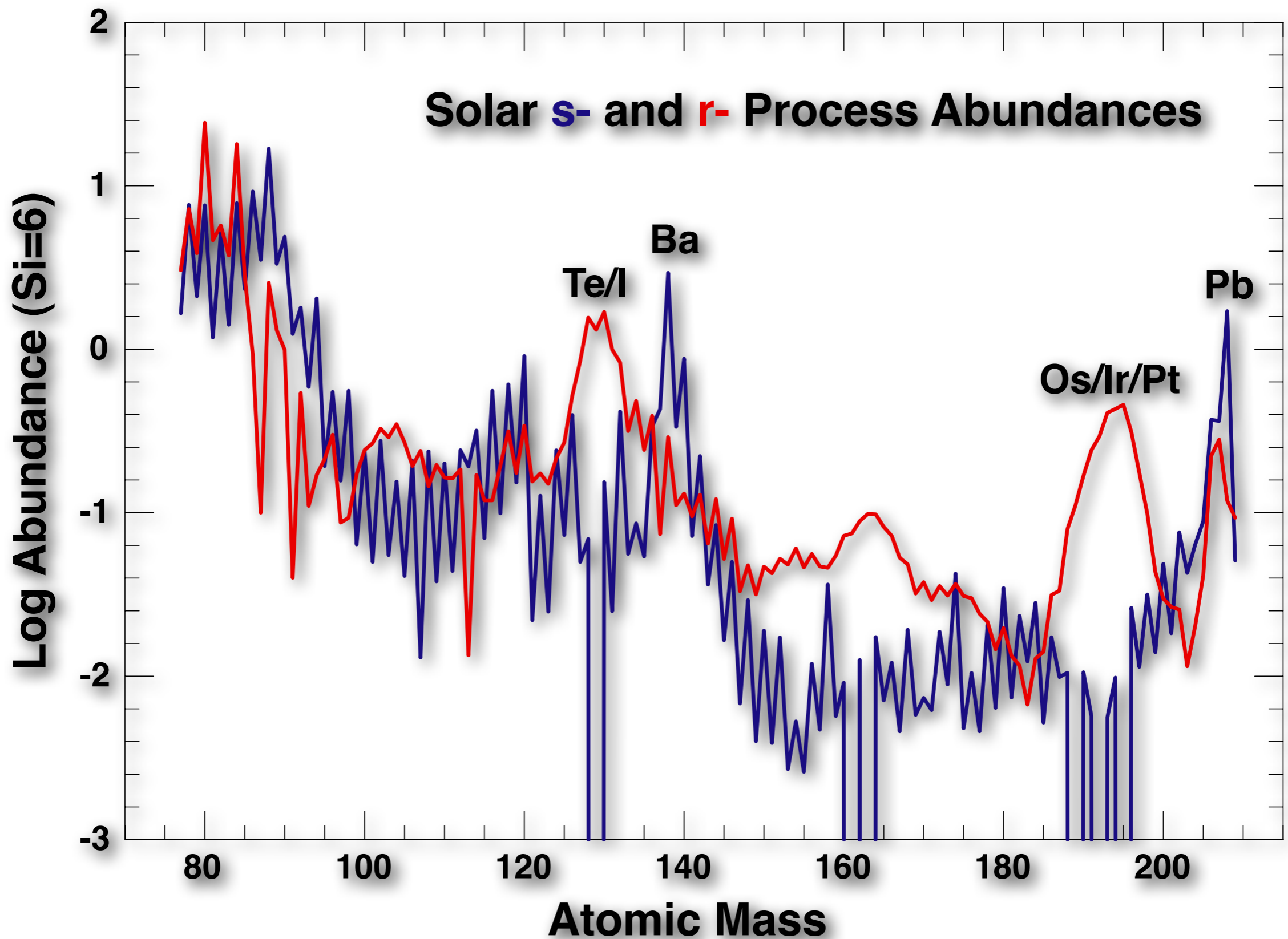
SNR Cassiopeia A (Hughes et al/Chandra/NASA)



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# OF WHAT ARE WE MADE?



# 2 ESSENTIAL QUESTIONS OF NUCLEAR ASTROPHYSICS



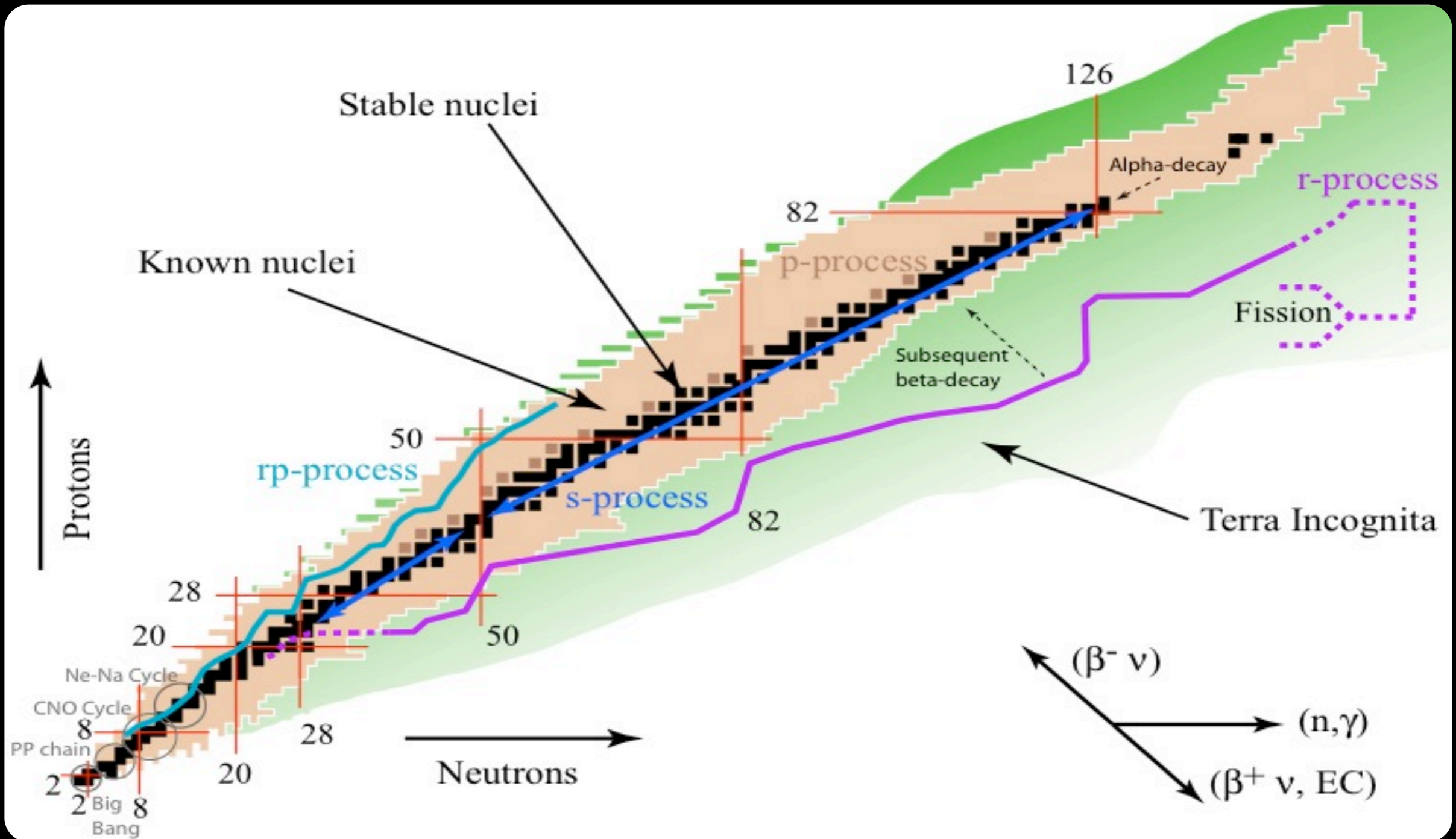
**1) How do nuclei get made?**

When? Where? Is it an ongoing process?

**2) How does making nuclei affect the stellar  
and galactic environment?**

Quiescent or Explosive? Exothermic or Endothermic?

# PROCESSES & SITES



Understanding Origins means understanding **processes** that transmute nuclei and the **sites** where these processes occur.

# NUCLEAR INPUT

## 1) Reaction Rates

For most astrophysical processes, a wide variety of **reaction rates** are needed.

## 2) Masses and Partition Function

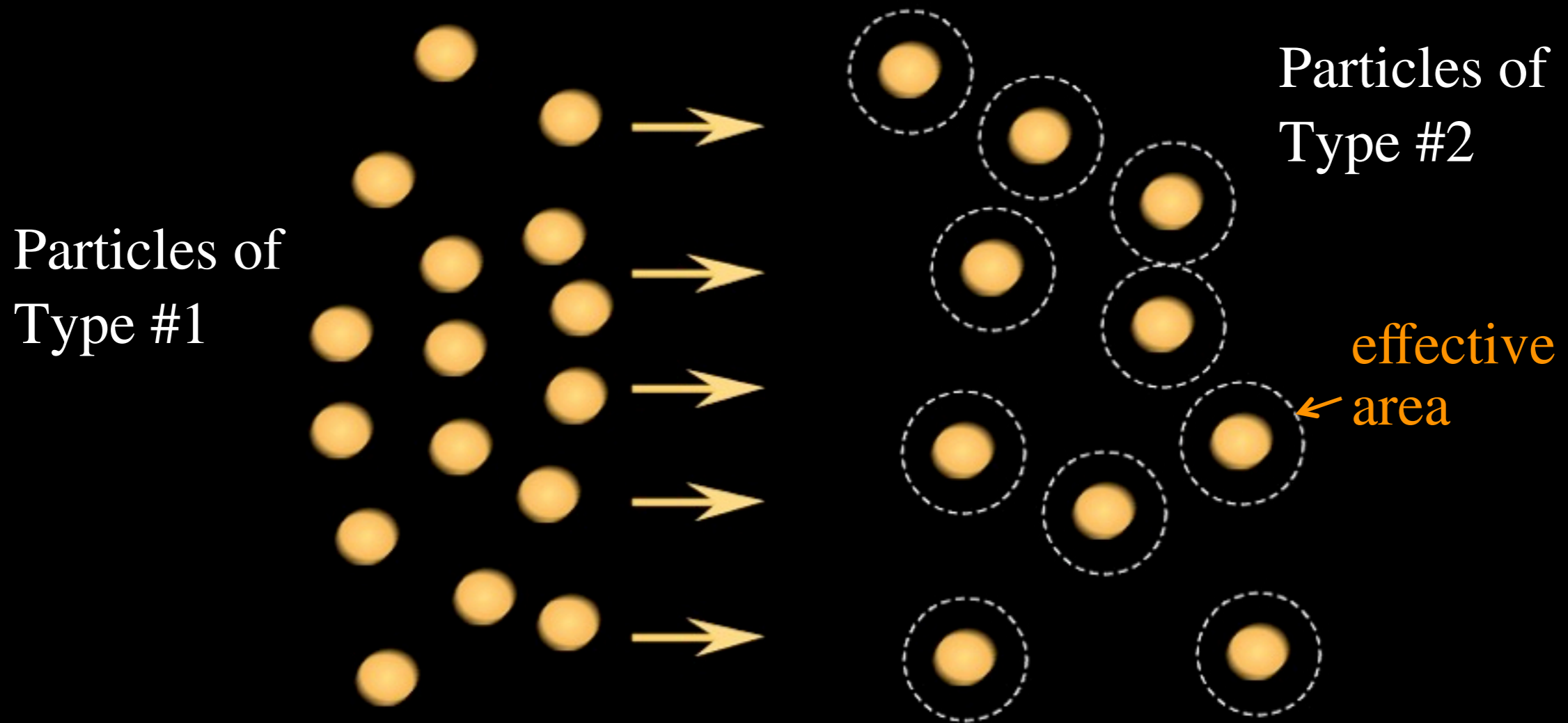
In equilibrium, rates are unimportant because of detailed balance.

Equilibrium populations depend on **relative masses** and **partition functions**, the sum of thermally populated levels.

## 3) Nuclear Matter

For Neutron Stars and their natal supernovae, significant fractions of a solar mass are at **densities similar to nucleons in a nucleus**. Consider a nucleus with  $A \sim 10^{57}$  held together by gravity.

# WHAT ARE REACTION RATES?



Reactions /  $\text{cm}^3 / \text{s} =$

relative flux particles #1 ( $\text{cm}^{-2} \text{s}^{-1}$ )

× number of target particles #2 ( $\text{cm}^{-3}$ )

× effective area of particle #2 in reaction ( $\text{cm}^2$ )

# RATES INTO DIFFERENTIAL EQN.

Define

$n_1$  = number of particles of type 1 per volume ( $\text{cm}^{-3}$ )

$n_2$  = number of particles of type 2 per volume ( $\text{cm}^{-3}$ )

$v$  = relative velocity ( $\text{cm s}^{-1}$ )

$\sigma(v)$  = effective cross sectional area for a reaction ( $\text{cm}^2$ )

Then

$n_1 \times v$  = relative flux of 1 relative to 2 (particles  $\text{cm}^{-2} \text{ s}^{-1}$ )

Reactions /  $\text{cm}^3 / \text{s} =$

relative flux particles 1 ( $\text{cm}^{-2} \text{ s}^{-1}$ )

$\times$  number of particles 2 ( $\text{cm}^{-3}$ )

$\times$  effective area of each particle 2 for a reaction ( $\text{cm}^2$ )

Reactions /  $\text{cm}^3 / \text{s} = (n_1 \times v) \times n_2 \times \sigma(v) = n_1 n_2 \sigma(v) v$

As a differential Equation,  $\frac{dn_1}{dt} = -n_1 n_2 \sigma(v) v$

# ABUNDANCE & MASS FRACTION

Number density,  $n_i$ , naturally depends on the **mass density**,  $\rho$  ( $\text{g cm}^{-3}$ ).

It is possible to separate this dependence by defining the abundance,  $Y_i = n_i / \rho N_A$ , where  $N_A$  is Avagadro's Number.

**Abundance** has units of mole  $\text{g}^{-1}$  and is the fraction of a mole of species  $i$  per gram of matter, so it also called Molar Fraction.

Multiplying the abundance by the molecular weight of species  $i$ ,  $A_i$ , which has units of  $\text{g mole}^{-1}$  gives the **mass fraction**,  $X_i = A_i Y_i$ .

Mass fraction is convenient for presentation as  $\sum_i X_i = 1$ .

This is in fact an expression of **nucleon number conservation**.



# LOCALIZING NUCLEAR EFFECTS

Nuclear reactions are not the only process capable of **altering** the mass density and **number densities**.

$$\frac{\partial n_1}{\partial t} + \frac{\partial n_1 u}{\partial x} = n_1 n_2 \langle \sigma v \rangle$$

Practically, it will be the responsibility of the **hydrodynamic solver** to follow the advection of nuclear species in space.

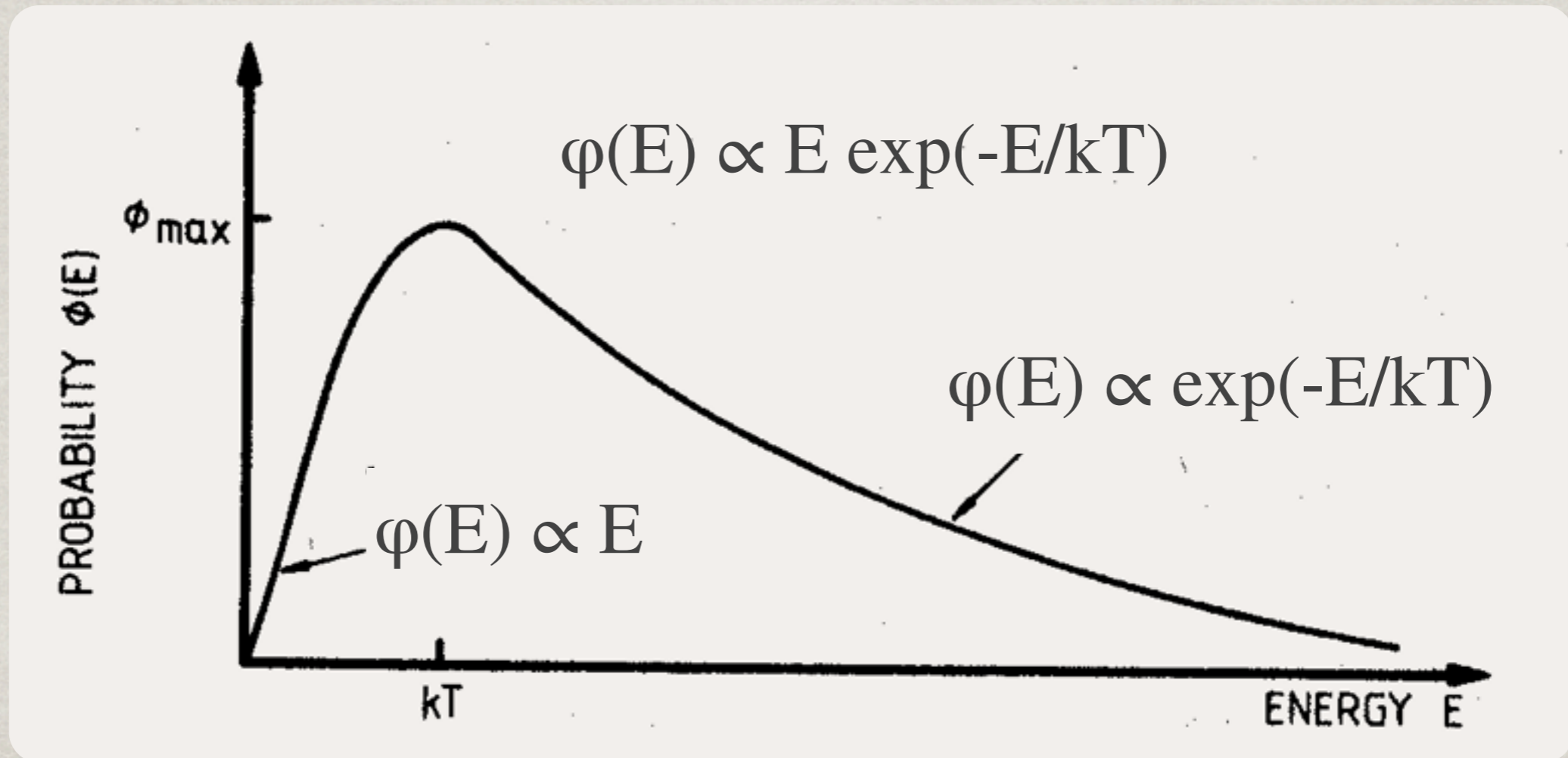
Splitting the hydrodynamic changes in density from the **local nuclear effects**, using  $n_i = \rho N_A Y_i$ , allows isolation of local changes.

$$\left. \frac{dn_i}{dt} \right|_{\rho} = \rho N_A \frac{dY_i}{dt} = -\rho^2 N_A^2 Y_i Y_j \sigma(v_{ij}) v_{ij}$$

This leaves an **ordinary differential equation** for just the thermonuclear reactions.

$$\frac{dY_i}{dt} = -\rho N_A Y_i Y_j \sigma(v_{ij}) v_{ij}$$

# MAXWELL-BOLTZMANN



Nuclei in the stellar plasma are **far from monoenergetic**.

For a given temperature, there is a **distribution of relative velocities** between any pair of particles in the star.

For most circumstances, a **Maxwell-Boltzmann Distribution** is sufficient.

# NUCLEAR REACTION RATES

**Integrating** over the MB velocity distribution gives the **thermal average cross section**, denoted  $\langle \sigma v \rangle$ .

$$\frac{dY_i}{dt} = -\rho N_A Y_i Y_j \langle \sigma v \rangle$$

Define  $N_A \langle \sigma v \rangle$  ( $\text{cm}^3 \text{ s}^{-1} \text{ mole}^{-1}$ ) as the “Reaction Rate”.

Important Distinction:

**Cross Section**: function of relative **velocity** (or energy)

**Reaction Rate**: function of **temperature** (not energy)

Thermal average of cross sections needed for rates!

But rate at any **temperature** depends on  $\sigma(E)$  over range of energies.

# M-B DETAILS

The Maxwell-Boltzmann distribution, for **velocity**,  $v$ , as a function of **temperature**,  $T$ , and **mass**,  $m_i$ , is

$$\phi_i(v, T) = 4\pi v^2 \left( \frac{m_i}{2\pi k_B T} \right)^{3/2} \exp \left( \frac{-m_i v^2}{2kT} \right)$$

With

$$\int_0^{\infty} \phi_i(v, T) dv = 1$$

Reaction Rate is

$$N_A \langle \sigma v \rangle (T) = \int_0^{\infty} \int_0^{\infty} N_A \phi_1(v_1, T) \phi_2(v_2, T) \sigma(v_1 - v_2) (v_1 - v_2) dv_1 dv_2$$

Change to **center of mass coordinates**: relative velocity,  $v = (v_1 - v_2)$ , reduced mass,  $\mu$ , Center of Mass velocity,  $V$ , and total mass,  $M$

$$\phi(v, T) = 4\pi v^2 \left( \frac{\mu}{2\pi kT} \right)^{3/2} \exp \left( \frac{-\mu v^2}{2kT} \right)$$

$$\phi(V, T) = 4\pi V^2 \left( \frac{\mu}{2\pi kT} \right)^{3/2} \exp \left( \frac{-\mu V^2}{2kT} \right)$$

# REACTION RATE IN DETAIL

Using **center of mass coordinates**

$$N_A \langle \sigma v \rangle (T) = \int_0^\infty \int_0^\infty N_A \phi(v, T) \phi(V, T) \sigma(v) v \, dv \, dV$$

Since  $\int_0^\infty \phi_i(V, T) dV = 1$

**integration over  $V$**  yields

$$N_A \langle \sigma v \rangle (T) = N_A 4\pi \left( \frac{\mu}{2\pi kT} \right)^{3/2} \int_0^\infty v^3 \sigma(v) \exp\left( \frac{-\mu v^2}{2kT} \right) dv$$

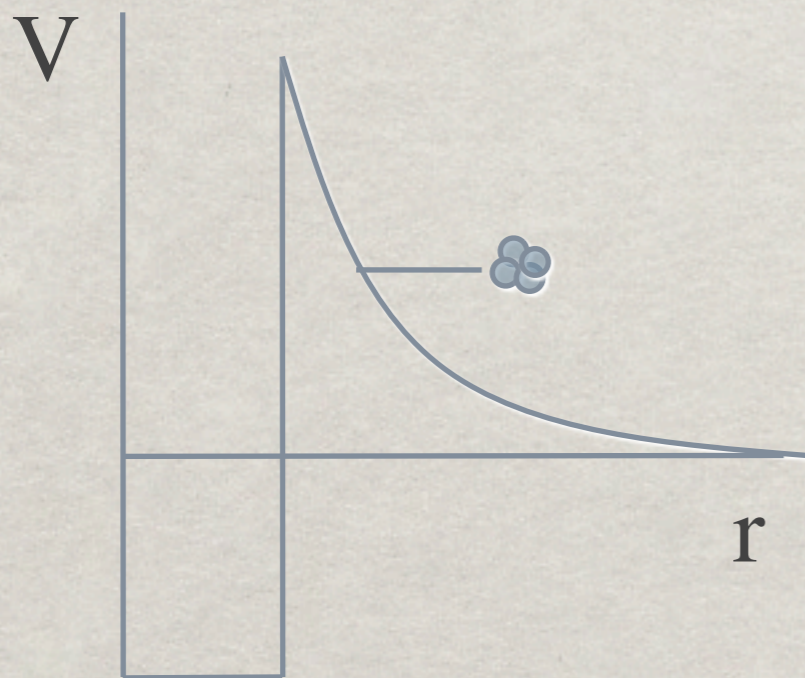
Change to **center of mass energy  $E = \frac{1}{2} \mu v^2$**

$$N_A \langle \sigma v \rangle (T) = N_A (8/\pi \mu)^{1/2} (kT)^{-3/2} \int_0^\infty \sigma(E) E \exp\left( \frac{-E}{kT} \right) dE$$

# CROSS SECTION & S-FACTOR

Helpful to simplify the rate expression for charged particle induced reactions by exploiting two well known energy dependences for  $\sigma(E)$

Charged particle Cross Sections  $\sigma(E)$



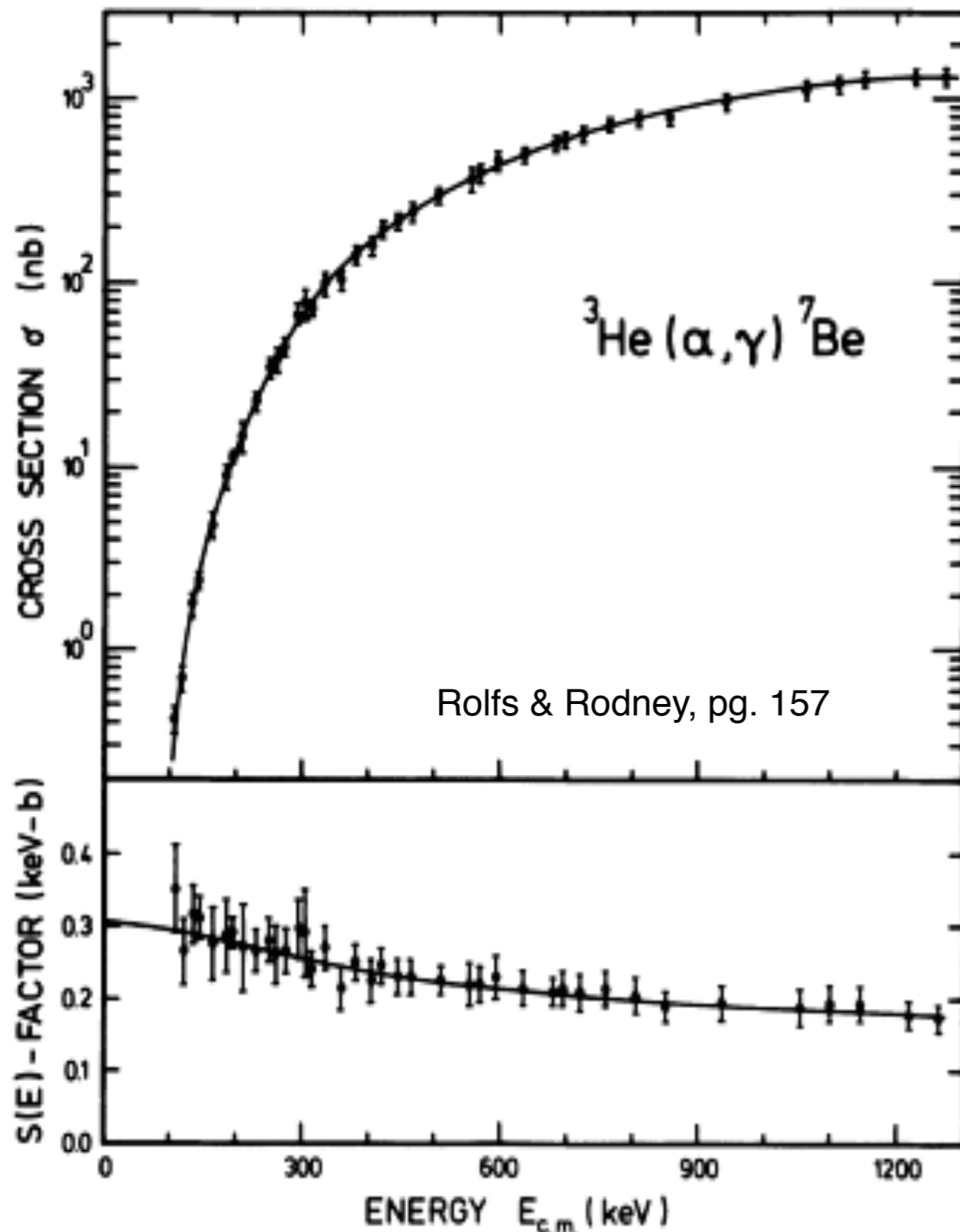
- 1) are proportional to probability for **coulomb barrier penetration**  $\exp[-(E_G/E)^{1/2}]$ , where the Gamow Energy,

$$E_G = 2\mu \left( \frac{\pi e^2 Z_1 Z_2}{h} \right)^2$$

- 2) are proportional to the **nuclear size**,  $\pi \lambda_{deBroglie}^2 \sim \frac{1}{E}$

The other energy dependencies are lumped together into  **$S(E)$  - the Astrophysical S-factor**

# NON-RESONANT REACTIONS



For many reactions, **MOST of the energy dependence** in  $\sigma(E)$  is described by the penetrability & nuclear size terms.

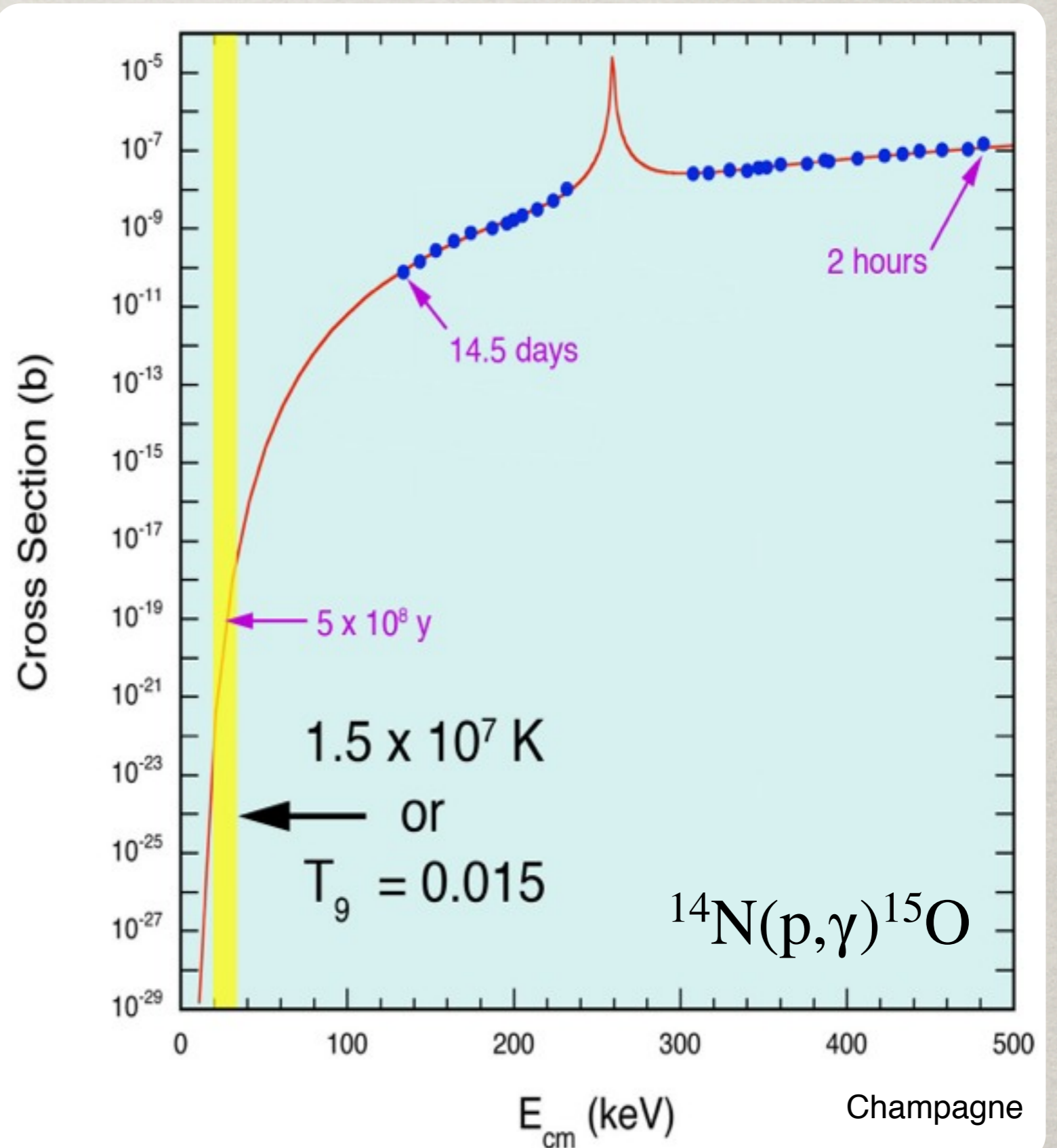
For non-resonant reactions,  $S(E)$  is **very slowly varying**.

Advantageous **to work with  $S(E)$**  rather than  $\sigma(E)$ .

# EXTRAPOLATING THE S FACTOR

For many reactions of astrophysical interest, the energies at which measurements are **feasible** are much larger than the energies at which the **reaction occurs in stars**.

**Extrapolating** the S factor is much more reliable.





# REACTION RATE & S FACTOR

By writing the cross section as

$$\sigma(E) = \left(\frac{1}{E}\right) \times \exp\left[-\left(\frac{E_G}{E}\right)^{\frac{1}{2}}\right] \times S(E)$$

the **Reaction Rate**

$$N_A \langle \sigma v \rangle (T) = N_A (8/\pi \mu)^{1/2} (kT)^{-3/2} \int_0^{\infty} \sigma(E) E \exp\left(\frac{-E}{kT}\right) dE$$

becomes

$$\begin{aligned} N_A \langle \sigma v \rangle (T) \\ = N_A (8/\pi \mu)^{1/2} (kT)^{-3/2} \int_0^{\infty} S(E) \exp\left[-\frac{E}{kT} - \left(\frac{E_G}{E}\right)^{\frac{1}{2}}\right] dE \end{aligned}$$

S-factor has units of **Energy × Area** ... typically keV-barn, MeV-barn where 1 barn =  $10^{-24}$  cm<sup>2</sup>.

# GAMOW PEAK

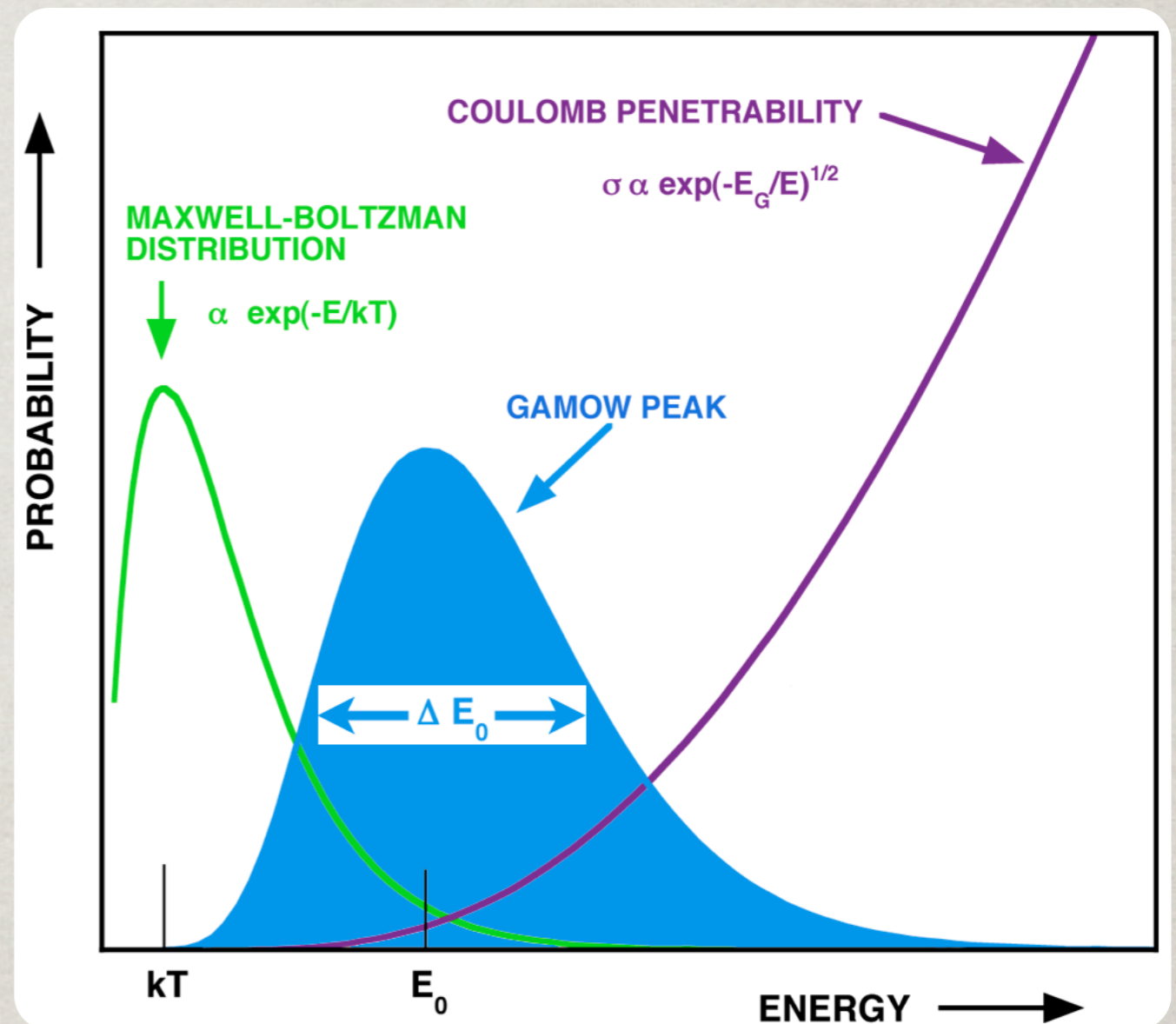
If  $S(E)$  is slowly varying, the integral is dominated by  $\exp[-E/kT - (E_G/E)^{1/2}]$ .

This **decreases at high energy** because of the left hand term.

This **decreases at low energy** because of the right hand term.

**Maximum at  $E_0$** , the *most effective stellar energy*

“Width” of  $\Delta E_0$ , the *Gamow Window*

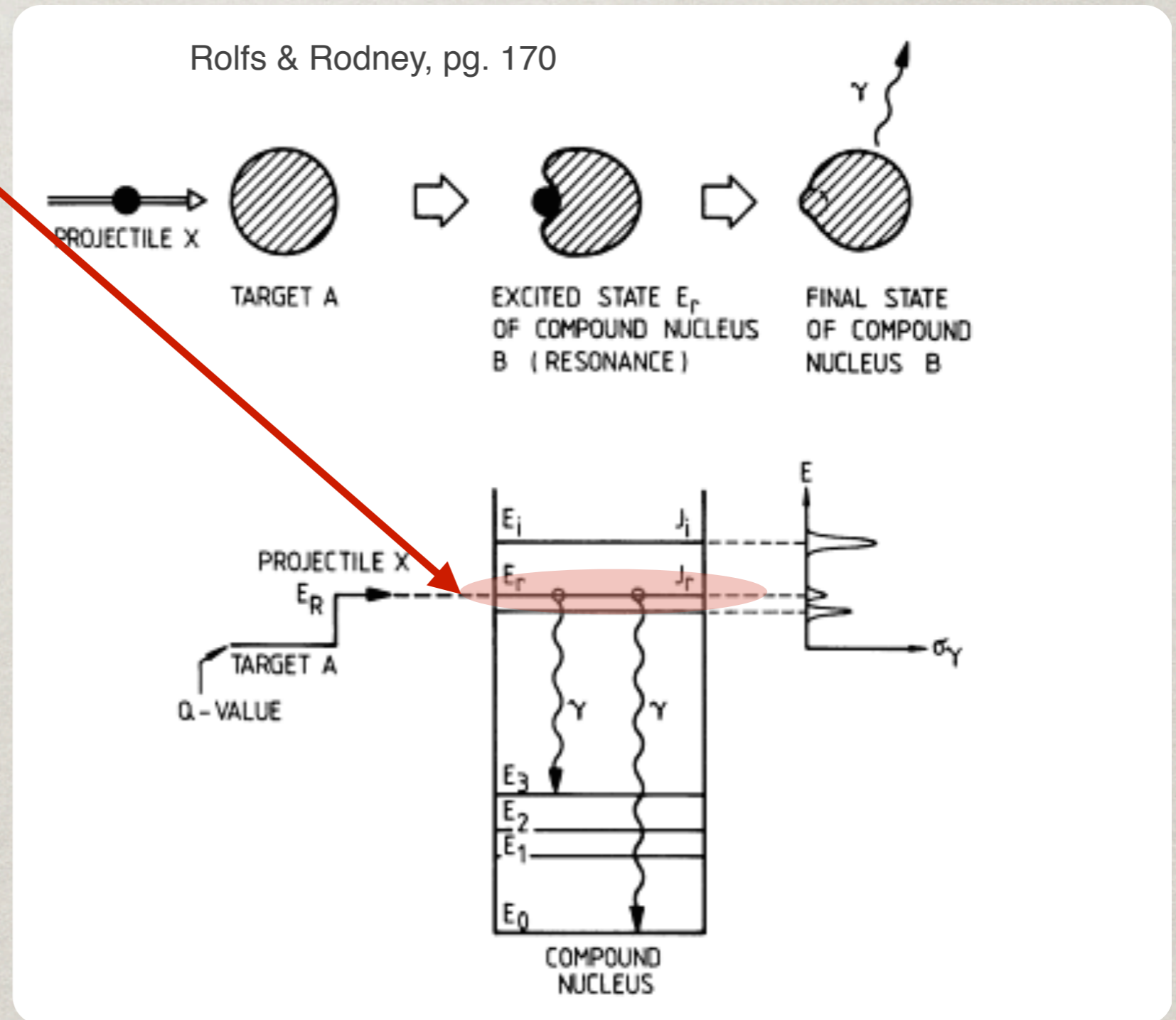


$$E_0 = E_G^{\frac{1}{3}} \left( \frac{KT}{2} \right)^{\frac{2}{3}}$$

$$\Delta E_0 = \frac{4}{\sqrt{3}} \left( \frac{E_0}{kT} \right)^{\frac{1}{2}}$$

# RESONANT REACTION RATES

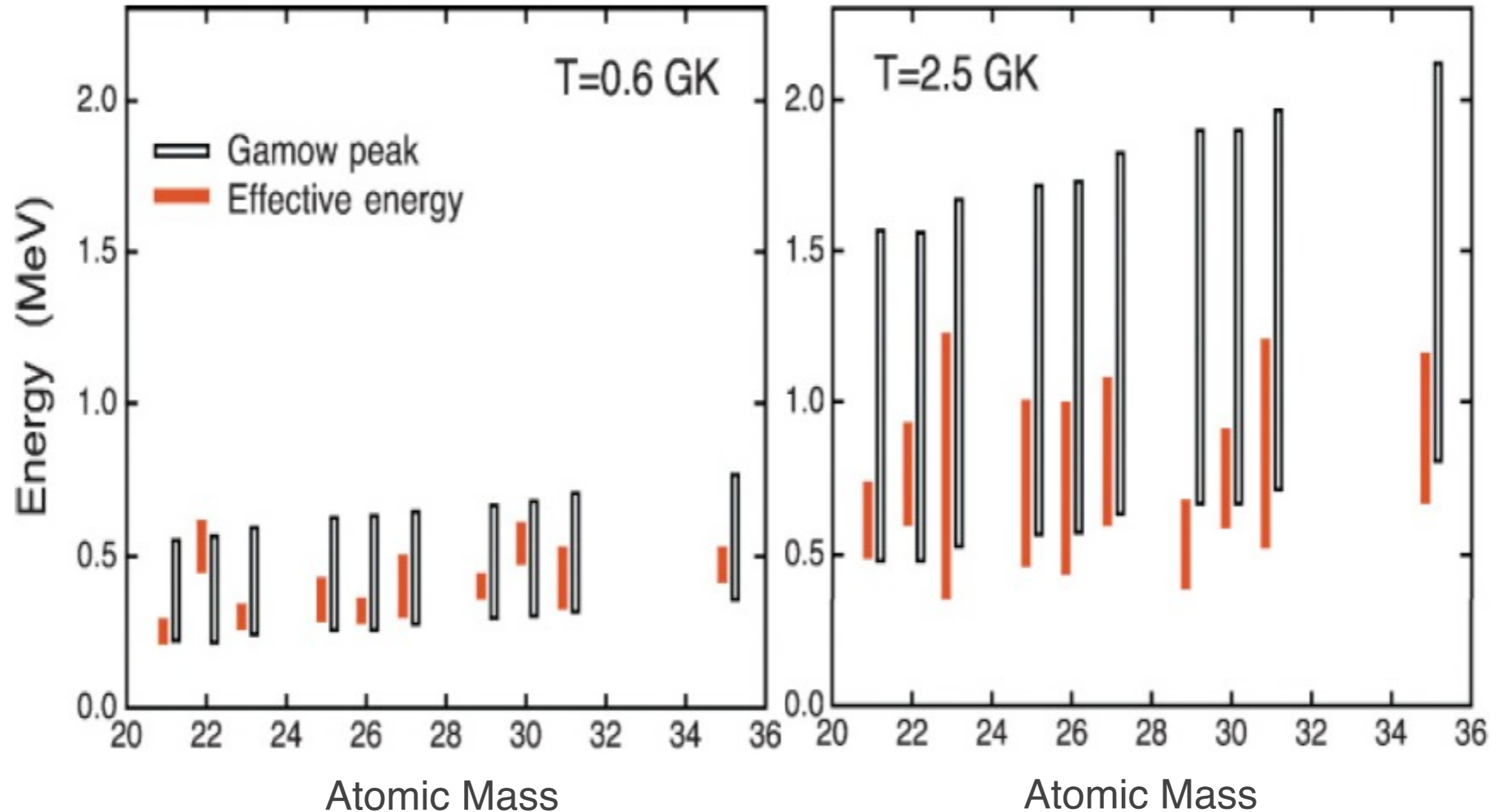
The presence of a **nuclear resonance** with an energy near the **Gamow Window** can dramatically increase the reaction rate by factors of **10 to  $10^7$**  in some cases.



The search for these resonances and **measurement of their properties** is extremely important.

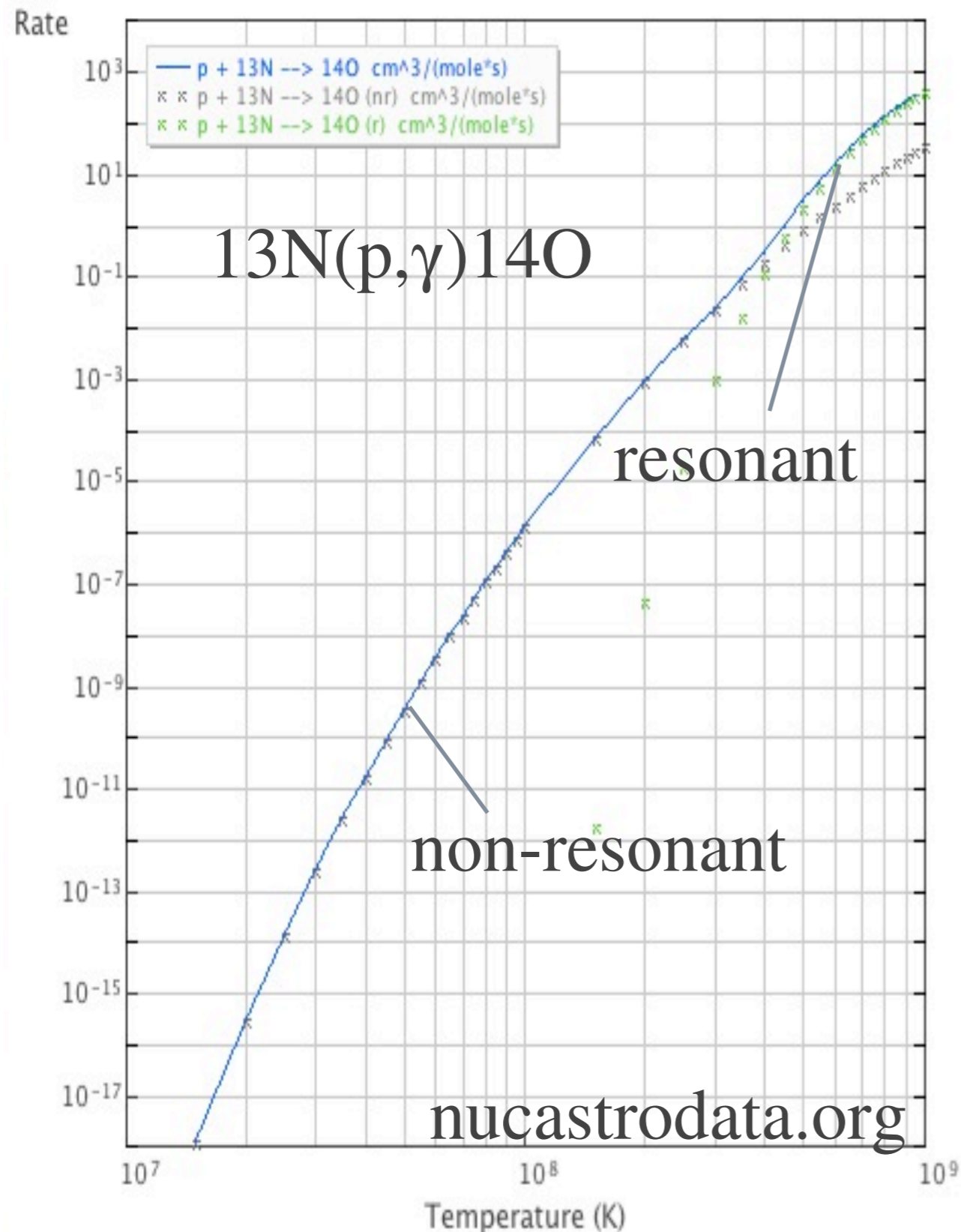
# GAMOW WINDOW EXAMPLES

Newton, Iliadis, Champagne, ... (2007)



Gamow Peak applies to direct capture, but **only 'back of the envelope'** estimate for resonances.

# REACTION RATE EXAMPLES



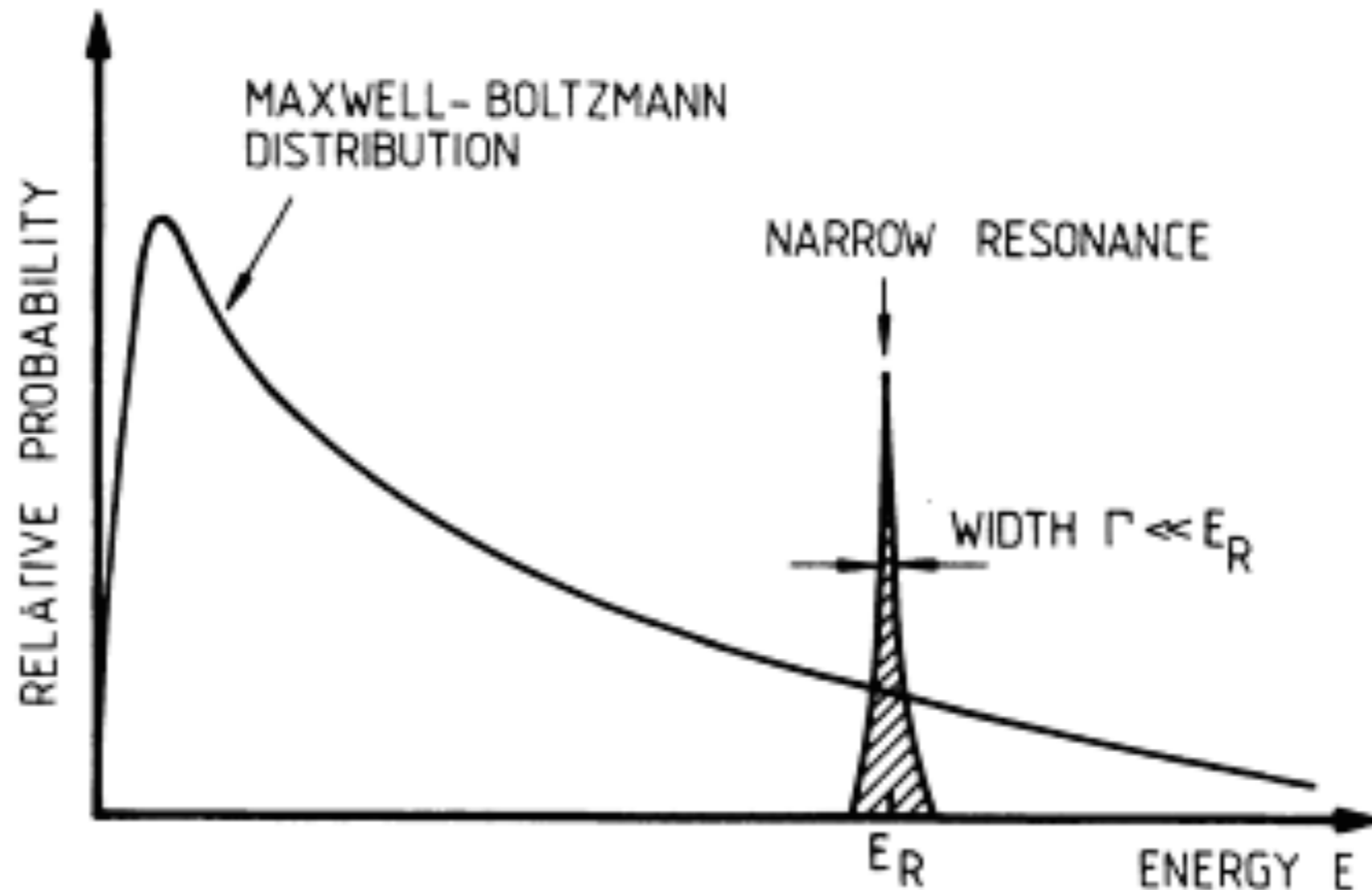
Non-resonant rates vary smoothly as function of temperature.

Rate changes by many orders of magnitude as temperature changes by 100.

Resonances add features, in this case an increase by a factor of 10 near 1 GK.

Plot from Computational Infrastructure for Nuclear Astrophysics.

# NARROW RESONANCES



For single resonances with a narrow total width, the resonance energy region effectively becomes the Gamow Peak

# BREIT-WIGNER FORMULA

For a Narrow (Lorentzian) resonance the cross sections  $\sigma(E)$

$$\sigma_{BW}(E) = \frac{\pi(\hbar c)^2}{2\mu E} \frac{(2J_r + 1)}{(2J_1 + 1)(2J_2 + 1)} \frac{\Gamma_{in}\Gamma_{out}}{[(E - E_r)^2 + (\Gamma_{tot}/2)^2]}$$

where

$J_r$  = spin of resonant state

$J_1, J_2$  = spin of reactant nuclei

$E_r$  = energy of resonant state

$\Gamma_{in}$  = energy width of reaction channel to form state  
(entrance channel) =  $\hbar / \tau_{in}$

$\Gamma_{out}$  = energy width of exit channel =  $\hbar / \tau_{out}$

$\Gamma_{tot}$  = total energy width of resonance =  $\hbar / \tau_{tot}$

# RESONANT REACTION RATES

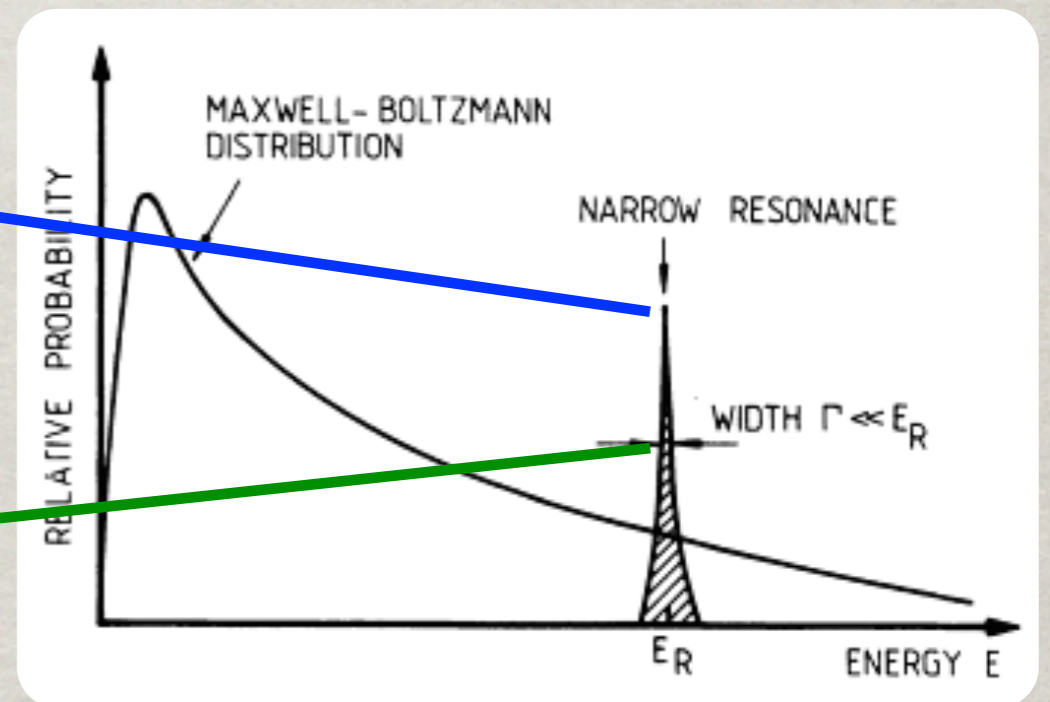
For narrow resonances

$$\begin{aligned}
 N_A \langle \sigma v \rangle (T) &= N_A (8/\pi \mu)^{1/2} (kT)^{-3/2} \int_0^\infty \sigma_{BW}(E) E \exp\left(\frac{-E}{kT}\right) dE \\
 &= N_A (8/\pi \mu)^{1/2} (kT)^{-3/2} E_r \exp\left(\frac{-E_r}{kT}\right) \int_0^\infty \sigma_{BW}(E) dE
 \end{aligned}$$

Integrating the cross section

$$\int_0^\infty \sigma_{BW}(E) dE = \frac{\pi}{2} \Gamma_{tot} \sigma_{BW}(E_r)$$

height points to  $\sigma_{BW}(E_r)$   
width points to  $\Gamma_{tot}$



where

$$\sigma_{BW}(E_r) = \frac{\pi(\hbar c)^2}{2\mu E_r} \frac{(2J_r + 1)}{(2J_1 + 1)(2J_2 + 1)} \frac{4\Gamma_{in}\Gamma_{out}}{\Gamma_{tot}^2}$$



# RESONANCE STRENGTH

Define

$$\omega = \frac{(2J_r + 1)}{(2J_1 + 1)(2J_2 + 1)} = \text{Statistical factor}$$

$$\gamma = \frac{\Gamma_{in}\Gamma_{out}}{\Gamma_{tot}}$$

$\omega\gamma$  is the **resonance strength** (units are in energy).

In terms of  $\omega\gamma$

$$\sigma_{BW}(E_r) = \frac{\pi(\hbar c)^2}{2\mu E_r} \frac{\omega\gamma}{\Gamma_{tot}} \quad \begin{array}{l} \text{Linear in strength} \\ \text{Exponential in} \\ \text{resonance energy} \end{array}$$

$$N_A \langle \sigma v \rangle (T) = N_A \left( \frac{2\pi}{\mu kT} \right)^{3/2} \hbar^2 \omega\gamma \exp\left(\frac{-E_r}{kT}\right)$$

For **multiple narrow resonances**

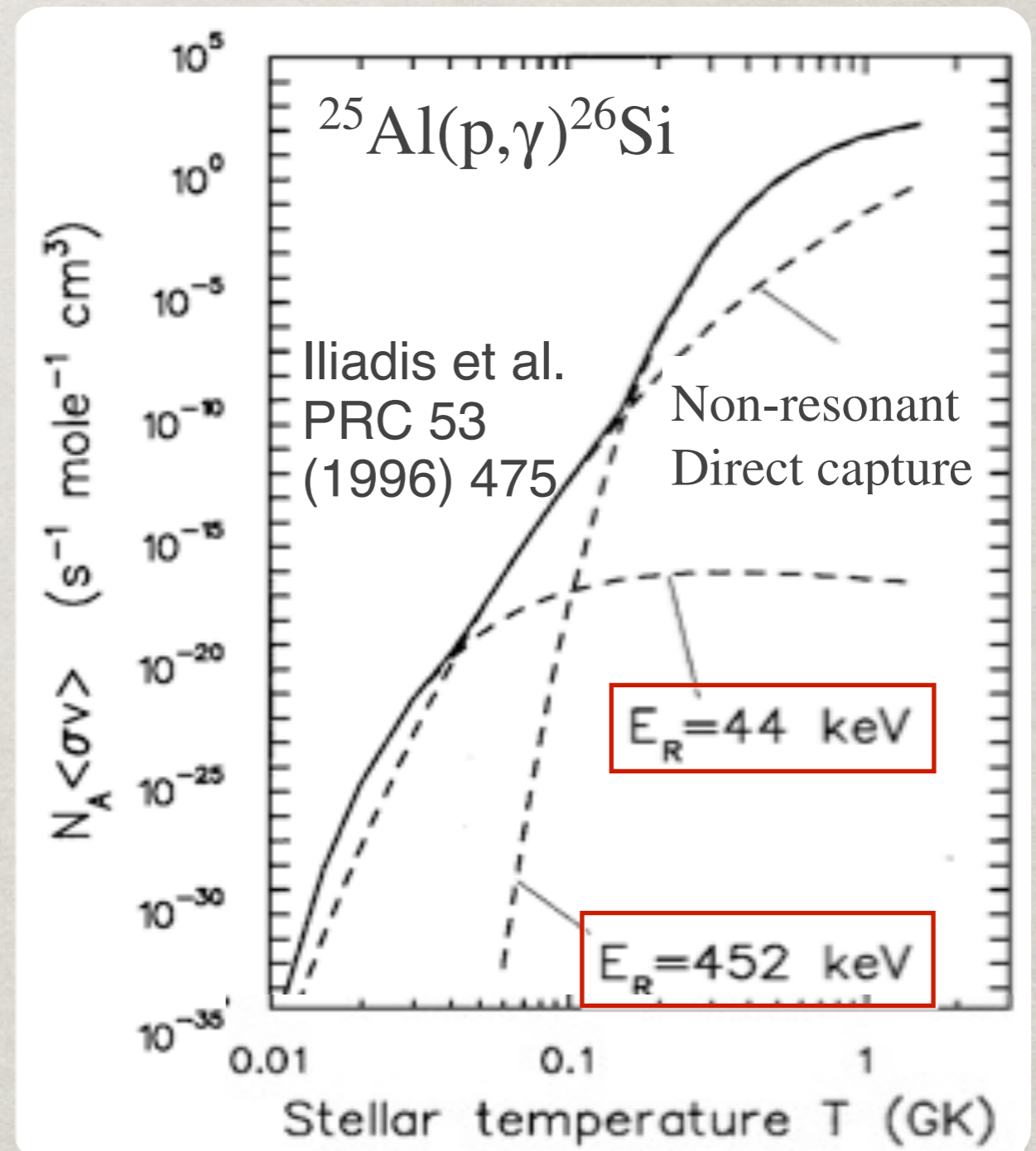
$$N_A \langle \sigma v \rangle (T) = N_A \left( \frac{2\pi}{\mu kT} \right)^{3/2} \hbar^2 \sum_i \omega_i \gamma_i \exp\left(\frac{-E_{r,i}}{kT}\right)$$

# WHICH RESONANCES?

The presence of resonances can make a **dramatic difference** (orders of magnitude) in reaction rates.

Resonances with **zero orbital angular momentum transfer** are important (strengths are often large).

Especially important are resonances with a **large strength** and a **low resonance energy**.



$$N_A \langle \sigma v \rangle (T) = N_A \left( \frac{2\pi}{\mu kT} \right)^{3/2} \hbar^2 \sum_i \omega_i \gamma_i \exp \left( \frac{-E_{r,i}}{kT} \right)$$

# REACTION VARIETY

While we have heretofore concentrated on reactions with two reactants, astrophysical circumstances include **reaction with only a single nuclear reactant**; for example, decays and interactions with photons and neutrinos.

Such reaction rates enter the differential equation in a form like

$$\frac{dY_i}{dt} = -\lambda_i Y_i$$

where  $\lambda_i$ , the **decay constant**, is related to the **half-life**,  $\tau_{1/2}$ , by  $\lambda_i = \ln 2 / \tau_{1/2}$ .

There are also instances where reactions, or effective reactions, including **three and four reactants** enter into the nuclear reaction network, taking the form,

$$\frac{dY_i}{dt} = \rho^2 N_A^2 \langle \sigma v \rangle_{j,k,l} Y_j Y_k Y_l,$$

# INVERSE REACTIONS

Many of these one nucleon reactions, especially the photo-disintegration reactions, are the **inverse of other reactions** in the network. Forward and inverse reactions are linked by **time reversal invariance**, thus their reaction rates are also linked.

For the reaction pair  $i + j \leftrightarrow l + m$ , this relation depends on the **energy difference** between products and reactants,  $Q_{lm}$ , and the partition functions,  $G = \sum_k (2J_k + 1) \exp(-E_k/kT)$ , the energy weighted density of states.

$$\langle \sigma v \rangle_{i,j} = \frac{G_l G_m}{G_i G_j} \left( \frac{A_l A_m}{A_i A_j} \right)^{3/2} \langle \sigma v \rangle_{l,m} \exp(-Q_{lm}/k_B T).$$

For the reaction pair  $j + \gamma \leftrightarrow l + m$ , the characteristics of the thermal **photon distribution** enter into the relation,

$$\lambda_{j,\gamma}(T) = \frac{G_l G_m}{G_j} \left( \frac{A_l A_m}{A_j} \right)^{3/2} \left( \frac{m_u k_B T}{2\pi \hbar^2} \right)^{3/2} \langle \sigma v \rangle_{l,m} \exp(-Q_{lm}/k_B T).$$

# TIMESCALES

Each reaction has a **characteristic timescale** which depends on the thermodynamic conditions and the current composition.

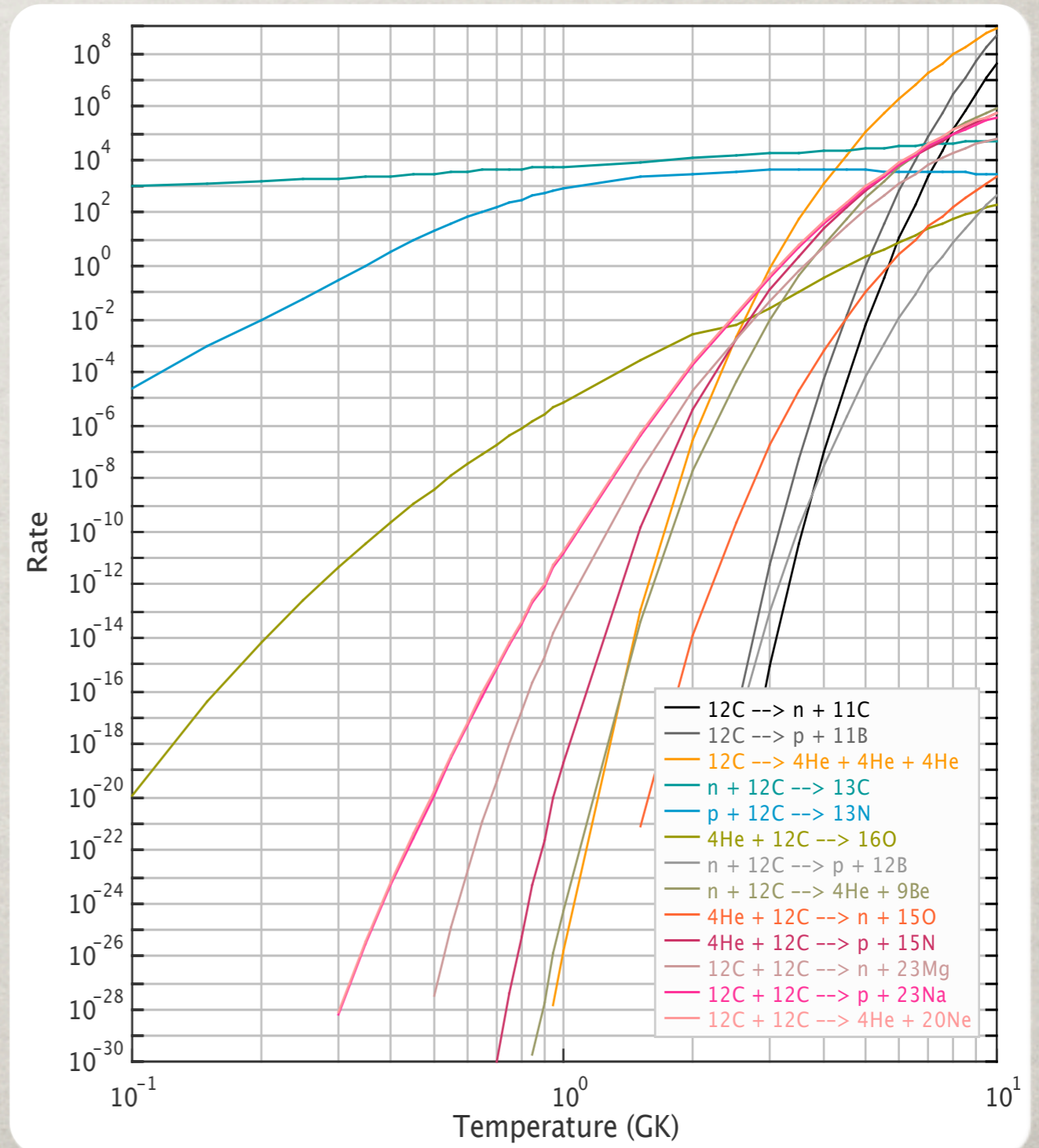
For example, for the single reactant case,

$$\tau_j(j) = \frac{1}{\lambda_j}$$

Reactions with multiple reactants have **timescales relative to each reactant**. For example, in the two reactant case,

$$\tau_k(j) = \frac{1}{\rho N_A \langle \sigma v \rangle_{j,k} Y_k}$$

These **timescales can vary by orders of magnitude**.



# NETWORK EQUATIONS

Bring all of the reaction rate terms together, we have a **system of ordinary differential equations** for the **temporal evolution** of the nuclear composition. For each species,  $i$ , this takes the form.

$$\begin{aligned}\dot{Y}_i = & \sum_j \mathcal{N}_j^i \lambda_j Y_j + \sum_{j,k} \mathcal{N}_{j,k}^i \rho N_A \langle \sigma v \rangle_{j,k} Y_j Y_k \\ & + \sum_{j,k,l} \mathcal{N}_{j,k,l}^i \rho^2 N_A^2 \langle \sigma v \rangle_{j,k,l} Y_j Y_k Y_l\end{aligned}$$

To specify the number of particles of species  $i$  that are **created or destroyed** in a reaction we introduce  $N_i$ .

To account for reactions involving the same **indistinguishable species**, we introduce  $\mathcal{N}$

$$\mathcal{N}_j^i = N_i \quad \mathcal{N}_{j,k}^i = \frac{N_i}{\prod_{m=1}^{n_{j,k}} |N_m|!} \quad \mathcal{N}_{j,k,l}^i = \frac{N_i}{\prod_{m=1}^{n_{j,k,l}} |N_m|!}$$

# EULER'S METHODS

The most straightforward discretization of this system of equations is

$$\frac{\vec{Y}(t + \Delta t) - \vec{Y}(t)}{\Delta t} = (1 - \Theta)\dot{\vec{Y}}(t + \Delta t) + \Theta\dot{\vec{Y}}(t)$$

For  $\Theta = 1$ , this is the explicit, **forward Euler method**.

For  $\Theta = 0$ , this is the implicit, **backward Euler method**.

Both Euler methods are first order accurate in time, the accuracy improves inversely proportional to the timestep.

For  $\Theta = 1/2$ , this is the semi-implicit **trapezoidal method**, which is second order accurate in time.

Both backward Euler and trapezoidal method are used in astrophysics. Forward Euler performs very poorly because of the **range in timescales**.

# STIFF EQUATIONS

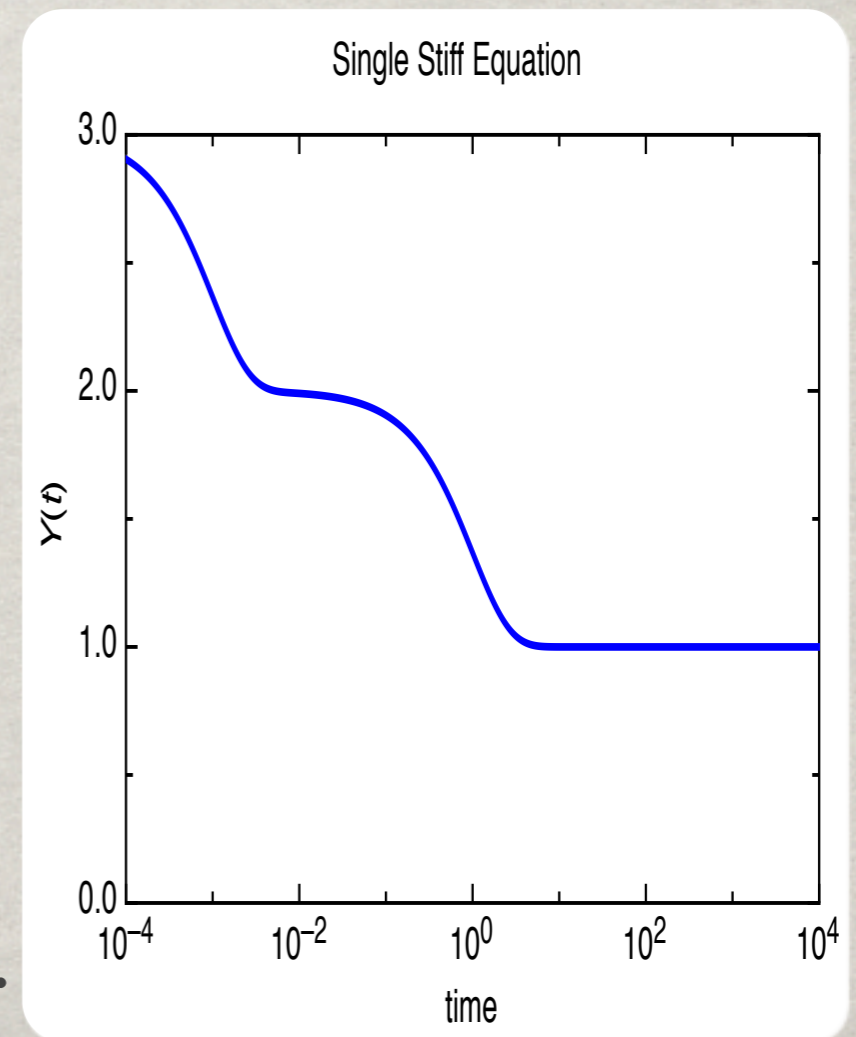
The wide range of timescales causes the reaction network system of equations to be *stiff*. Physically, this is a usable definition of stiffness.

Note that even a single equation can be stiff if it has **two very different timescales**, for example,  $Y(t) = e^{-1000t} + e^{-t} + 1$ .

The preferred behavior of the time step  $\Delta t$  is clear

- 1) For  $t < 0.01$  seconds,  $\Delta t \sim 1/10,000$  s
- 2)  $10^{-2} < t < 10$ ,  $\Delta t \sim 1/100$  s
- 3) for  $t > 10$ ,  $\Delta t \sim t$ .

However, **forward Euler** and many methods use  $\Delta t \sim 1/10,000$  s throughout.





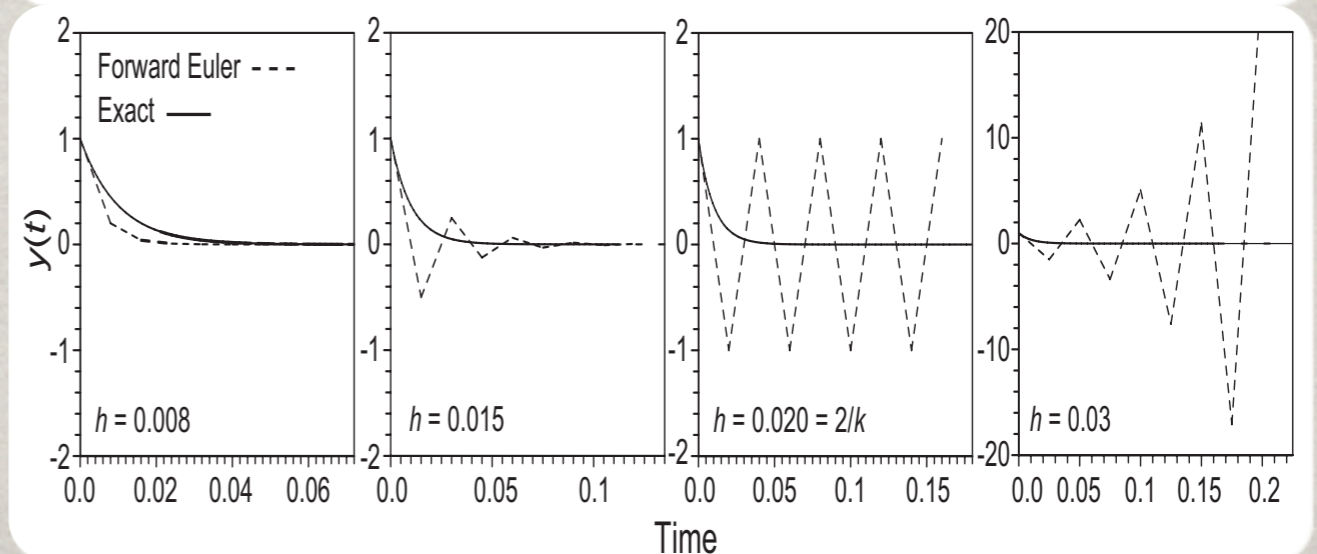
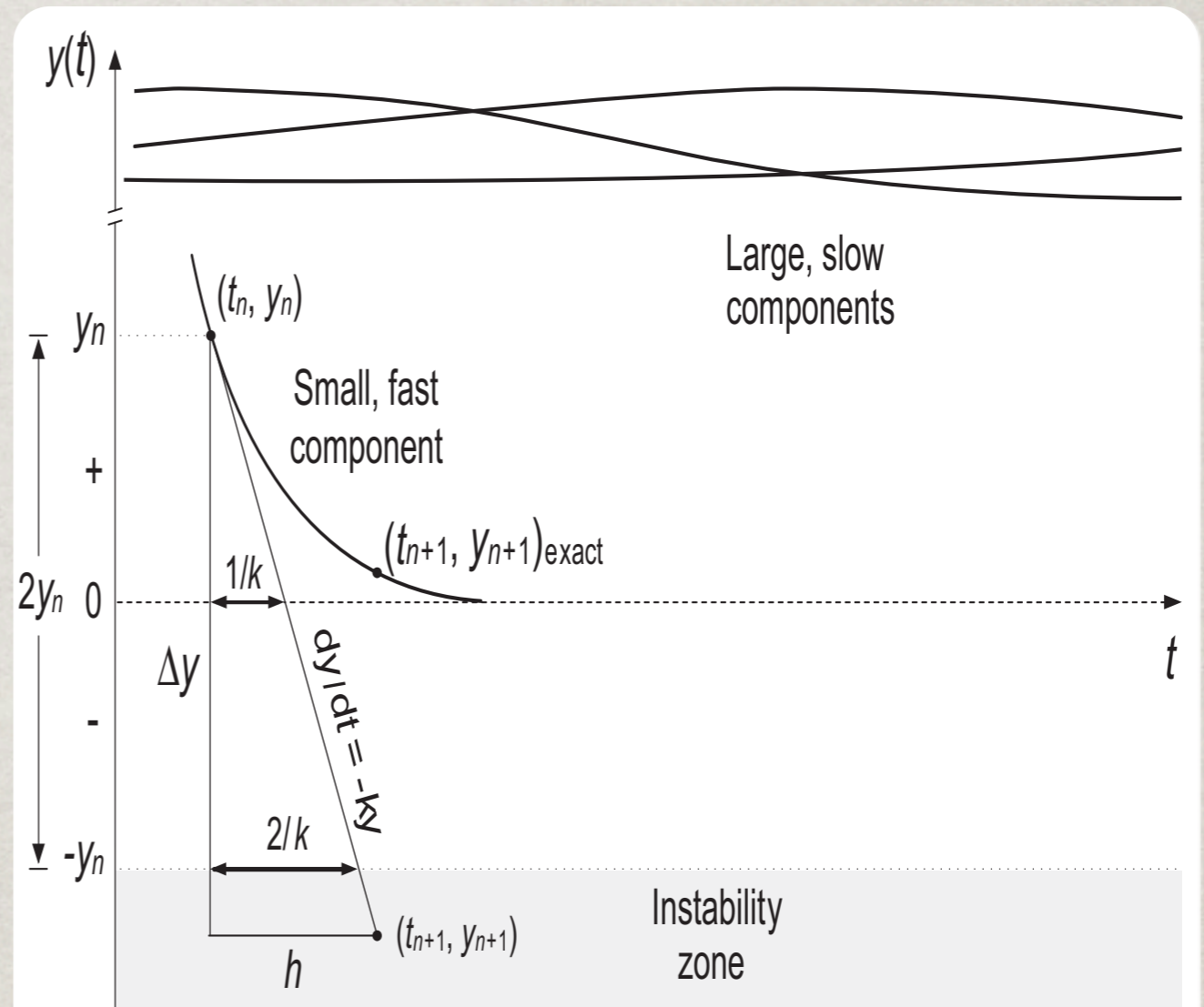
# EXPLICIT INSTABILITY

The challenge of stability is that even **inconsequential abundances can destroy the solution.**

Even in cases where the exact solution may asymptote to zero, the explicit update can produce **negative abundances** if

$$\Delta t > \frac{Y}{\dot{Y}} \text{ for any species.}$$

In contrast, implicit methods keep these **small abundances well behaved.**



# MEASURING STIFFNESS

From a mathematical perspective, a system of equations is stiff if the timestep must be chosen on the basis of the **stability of the system**, rather than the accuracy of the solution.

A more definition of stiffness can be stated for a system in the form

$$\dot{\vec{Y}} = \frac{\partial \dot{\vec{Y}}}{\partial \vec{Y}} \cdot \vec{Y}$$

which has **eigenvalues**  $\lambda_j$ . The system is stiff if real part of all  $\lambda_j < 0$  and

$$\mathcal{S} = \frac{\max|\Re(\lambda_j)|}{\min|\Re(\lambda_j)|} \gg 1$$

For many fields,  $\mathcal{S} \sim 10^4 - 10^6$ , but for astrophysical nuclear reaction networks,  $\mathcal{S} \sim 10^{15}$  is possible.

For example, in the Sun,  $p + p \rightarrow d + e^+ + \nu_e$  has a timescale of billions of years,  $p + d \rightarrow {}^3\text{He}$  has a timescale of seconds!

# BACKWARD EULER

While the explicit forward Euler method requires knowledge of the derivatives only at time  $t$ , the beginning of the timestep, the backward Euler method requires this information at the **future time**,  $t + \Delta t$ , making it an implicit method.

The solution of the Backward Euler method is equivalent to finding the zeros of the equation

$$\vec{\mathcal{F}}(t + \Delta t) \equiv \frac{\vec{Y}(t + \Delta t) - \vec{Y}(t)}{\Delta t} - \dot{\vec{Y}}(t + \Delta t) = 0 .$$

This is done via the **Newton-Raphson method**, producing a trial abundance change of

$$\Delta \vec{Y} = \left( \frac{\partial \vec{\mathcal{F}}(t + \Delta t)}{\partial \vec{Y}(t + \Delta t)} \right)^{-1} \vec{\mathcal{F}} = \left( \frac{\mathcal{J}}{\Delta t} - \frac{\partial \dot{\vec{Y}}(t + \Delta t)}{\partial \vec{Y}(t + \Delta t)} \right)^{-1} \vec{\mathcal{F}}$$

**Additional iterations** can be performed to refine the solution.

# SOLVER COSTS

Compared to forward Euler, backward Euler adds the computational cost of **building and solving the Jacobian matrix** for each of possibly several iterations for each timestep. This is a considerable cost, a factor of 10 or more.

Yet backward Euler is the more time efficient solver because the **larger timesteps** that can be taken more than ameliorate this added cost.

For any method of solving ordinary differential equations, including those we consider here,

$$\text{total numerical cost} = (\text{cost per timestep}) \times (\# \text{ of timesteps})$$

Methods with much larger costs per timestep **can be more efficient** if they allow larger timesteps.

# BADER-DEUFLHARD

Higher order methods attempt to take even larger timesteps than backward Euler and/or reduce the frequency of matrix solves. They also can provide **rigorous error estimates** by comparing solutions of differing orders.

One example is the variable order **Bader-Deuflhard** method.

This method divided the timestep into  $m$  substeps with  $\delta t = \Delta t/m$  and the matrix

$$\mathcal{A} = \mathcal{J} - \frac{\partial \dot{\vec{Y}}}{\partial \vec{Y}}$$

In the first substep, solving  $\mathcal{A} \cdot \Delta \vec{Y}_0 = \delta t \dot{\vec{Y}}_0$        $\vec{Y}_1 = \vec{Y}_0 + \delta \vec{Y}_0$

For  $k = 1$  to  $m-1$ ,  $\mathcal{A} \cdot x = \delta t \dot{\vec{Y}}_k - \Delta \vec{Y}_{k-1} \Rightarrow \delta \vec{Y}_k = \delta \vec{Y}_{k-1} + 2x$   
 $\Rightarrow \vec{Y}_{k+1} = \vec{Y}_k + \delta \vec{Y}_k$

For  $k = m$ ,  $\mathcal{A} \cdot \Delta \vec{Y}_m = \delta t(\dot{\vec{Y}}_m - \Delta \vec{Y}_{m-1}) \Rightarrow \vec{Y}(t + \Delta t) = \vec{Y}_m + \delta \vec{Y}_m$

BD is **twice as expensive as BE**, but may allow larger  $\Delta t$ .

# SPARSE MATRICES

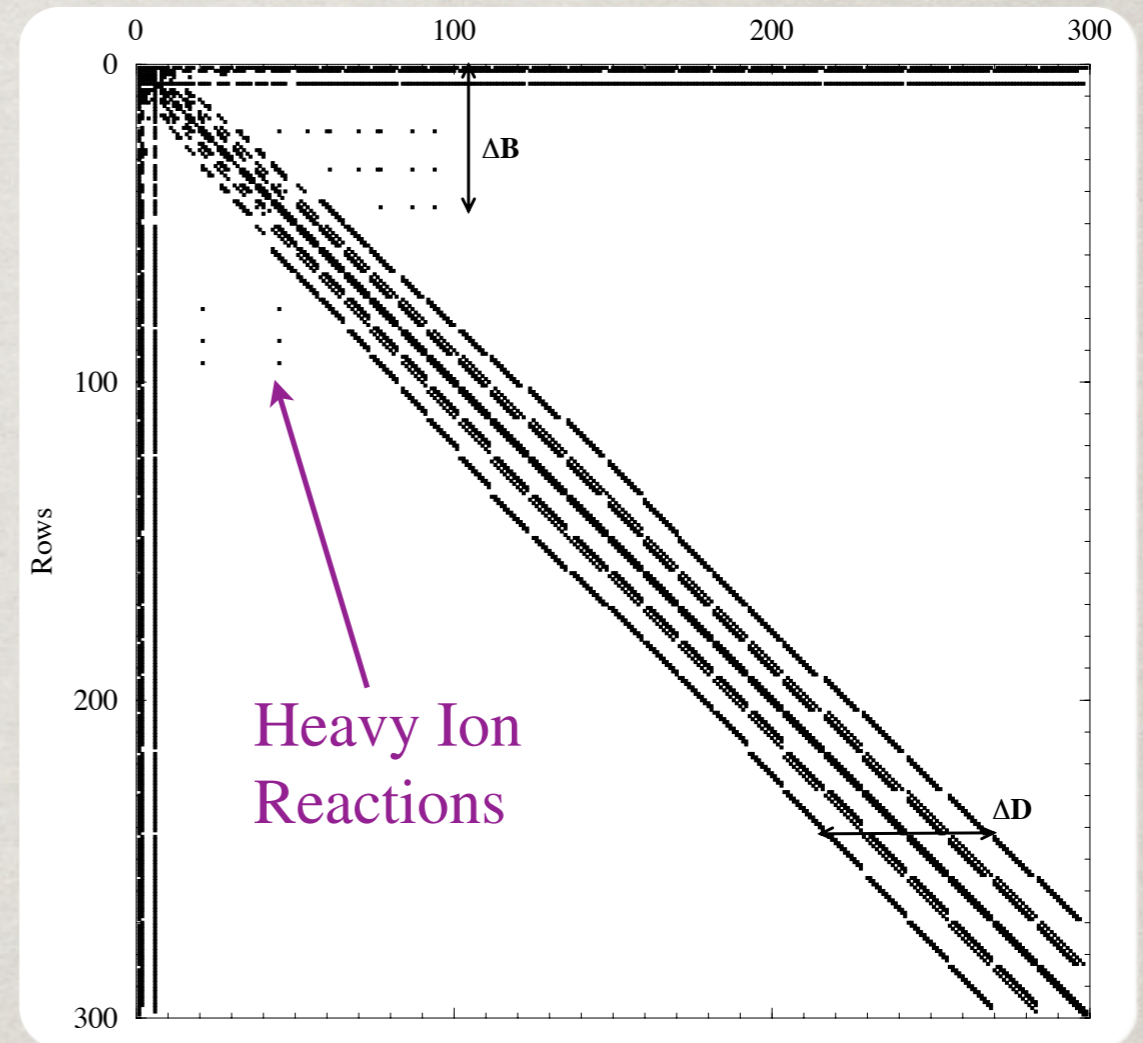
One way to speed up all implicit methods is to take advantage of the “emptiness” in the Jacobian matrix.

In principal, every species reacts with each of the hundreds of others, resulting in a dense matrix.

The **Coulomb term** in the nuclear potential ( $\propto Z_i Z_j$ ) causes captures of free neutrons and isotopes of H & He to occur much faster than fusions of heavier nuclei.

Likewise, **photodisintegrations** tend to eject nucleons or  $\alpha$  -particles.

Thus we **generally** need only consider **twelve reactions linking it to its nuclear neighbors** by the capture of an n, p,  $\alpha$  or  $\gamma$  and release a different one of these four.



# ASYMPTOTIC METHOD

Implicit methods succeed because they allow larger timesteps to be taken without the **less abundance species misbehaving**.

Finding an explicit method with this same behavior would save the cost of building and solving the Jacobian matrices. Some such methods have been used in other fields. One example is the **asymptotic method**.

We can write our network ODE in terms of reaction fluxes,

$$\dot{Y}_i = F_i(\vec{Y}, t) = \sum_j F_{ij}(t)$$

where  $F_{ij}$  is the **flux** between abundance  $i$  and abundance  $j$ .

If we divide  $F_i$  into fluxes which **add** to the abundance of  $i$  and those that **remove** abundance from  $i$

$$\dot{Y}_i = F_i^+(t) - F_i^-(t)$$

# ASYMPTOTIC METHOD 2

The flux out of  $i$  is proportional to  $Y_i$

$$F_i^-(t) = (k_1^i(t) + k_2^i(t) + \dots + k_m^i(t))Y_i(t) = k^i(t)Y_i(t)$$

where the  $k_n^i$  are rate parameters,  $\lambda_n$  or  $\langle \sigma v \rangle Y_n$ .

Rearranging this equation and substituting into the previous equations yields

$$Y_i(t) = \frac{F_i^+(t) - \dot{Y}_i}{k^i(t)}$$

In the asymptotic limit for species  $i$ ,  $F_i^+(t) \approx F_i^-(t)$  and  $\dot{Y} \Rightarrow 0$ , so a first approximation is

$$Y_i(t_n) = \frac{F_i^+(t_n)}{k^i(t_n)}$$

We can improve this by **approximating**

$$\dot{Y}_i = \frac{Y_i(t_n) - Y_i(t_{n-1})}{t_n - t_{n-1}} = \frac{1}{\Delta t} \left( \frac{F_i^+(t_n)}{k^i(t_n)} - \frac{F_i^+(t_{n-1})}{k^i(t_{n-1})} \right)$$



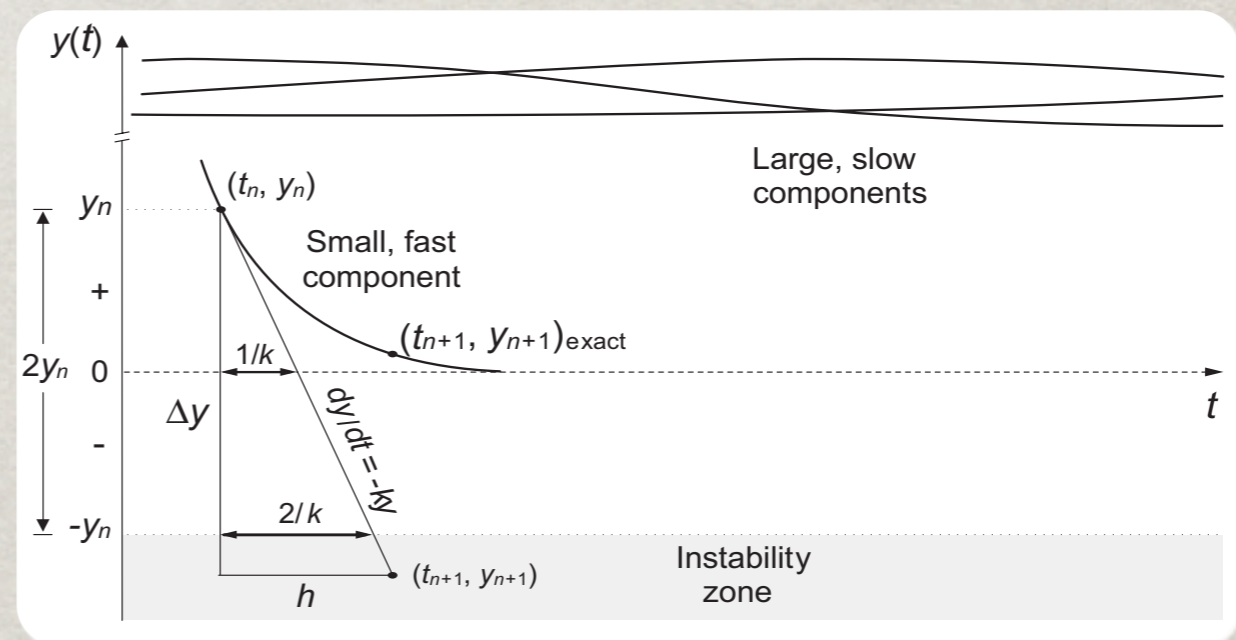
# ASYMPTOTIC METHOD 3

Using this expression for  $\dot{Y}$  yields

$$Y_i(t_n) \simeq \frac{F_i^+(t_n)}{k^i(t_n)} - \frac{1}{k^i(t_n)\Delta t} \left( \frac{F_i^+(t_n)}{k^i(t_n)} - \frac{F_i^+(t_{n-1})}{k^i(t_{n-1})} \right)$$

This approximation is most reliable when **the approximated derivative is small**, for example when  $k\Delta t$  is large.

The condition  $k\Delta t > 1$  is precisely the point at which forward Euler, and many other explicit methods, become unstable.



Thus **combining the Asymptotic method for  $k_i\Delta t > 1$**  with forward Euler allows an explicit update of all species, including those that would destabilize forward Euler alone.

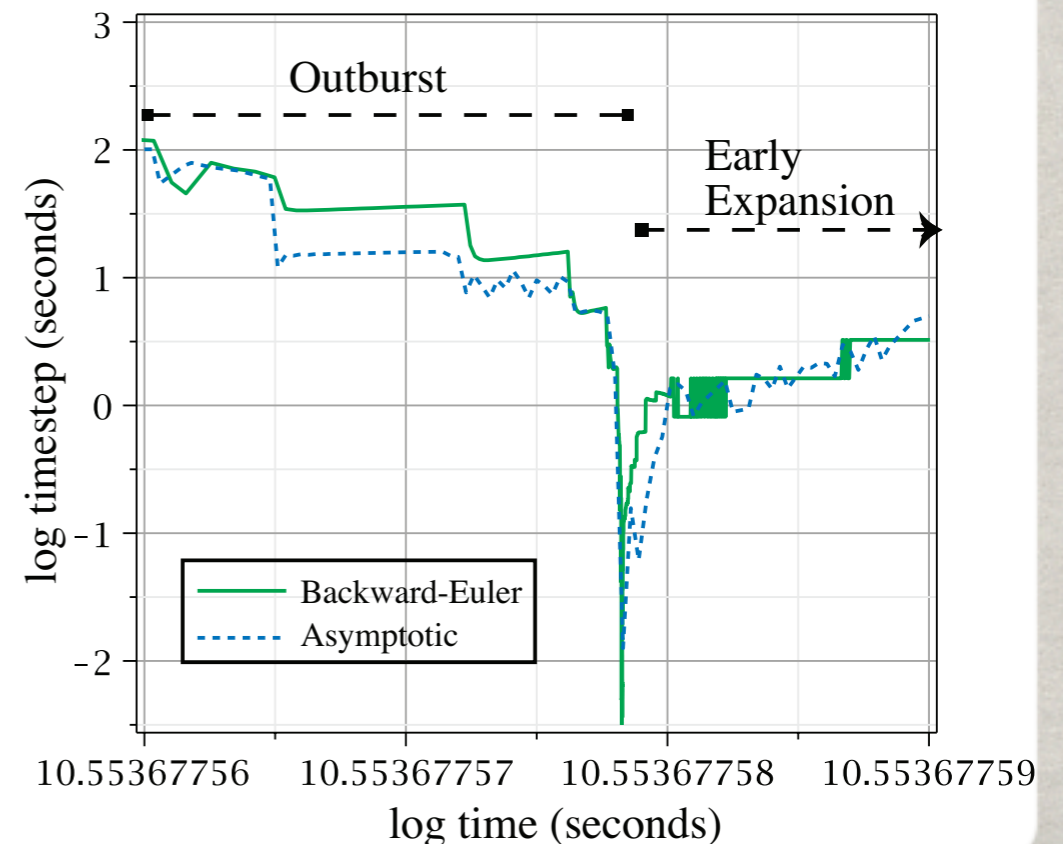
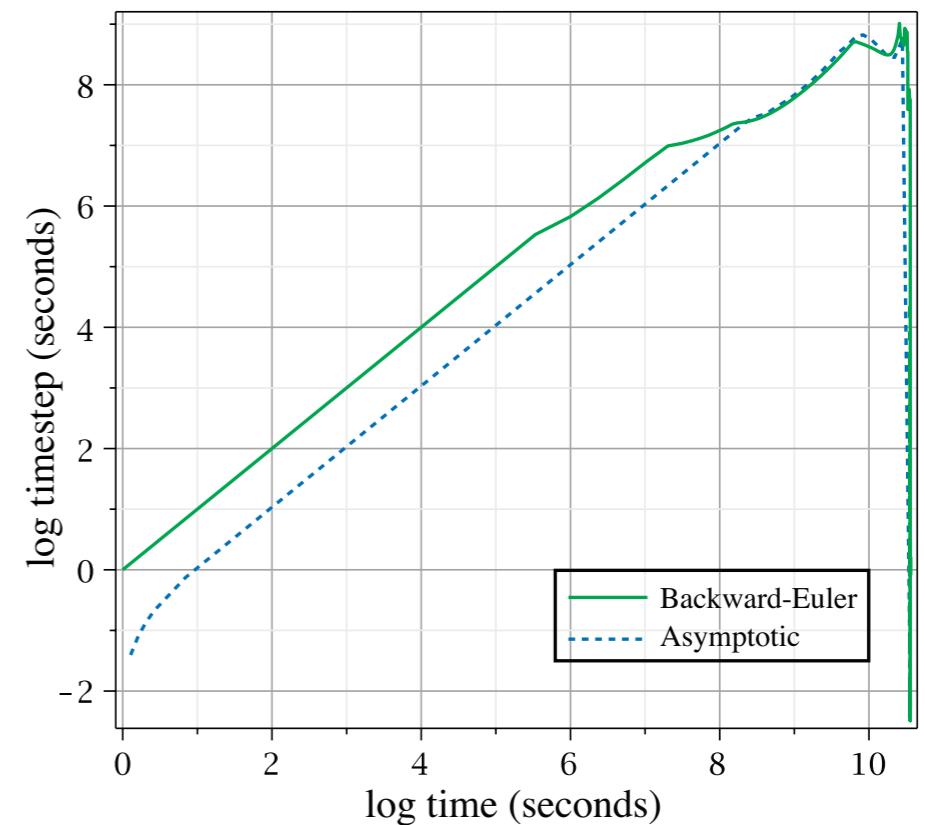
# NOVA SUCCESS

Feger et al showed an asymptotic method to be **competitive with BE** for a nova test problem.

The network used has 189 species. **Building and solving the matrix represented 87% of the network cost.**

All told, the asymptotic method needed  $\sim$  twice as many timesteps, but each timestep should be cheaper by  $\sim 1/(1-.87)$  or roughly a factor of 7.

This is **preliminary but promising.**



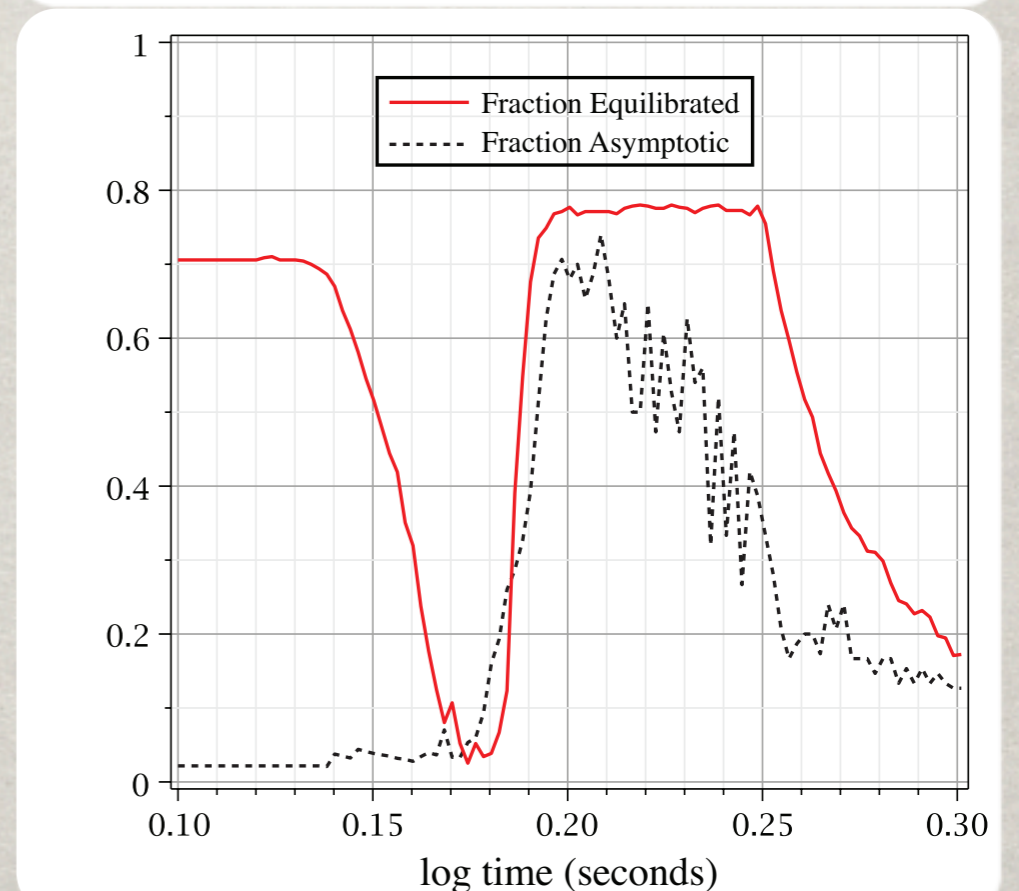
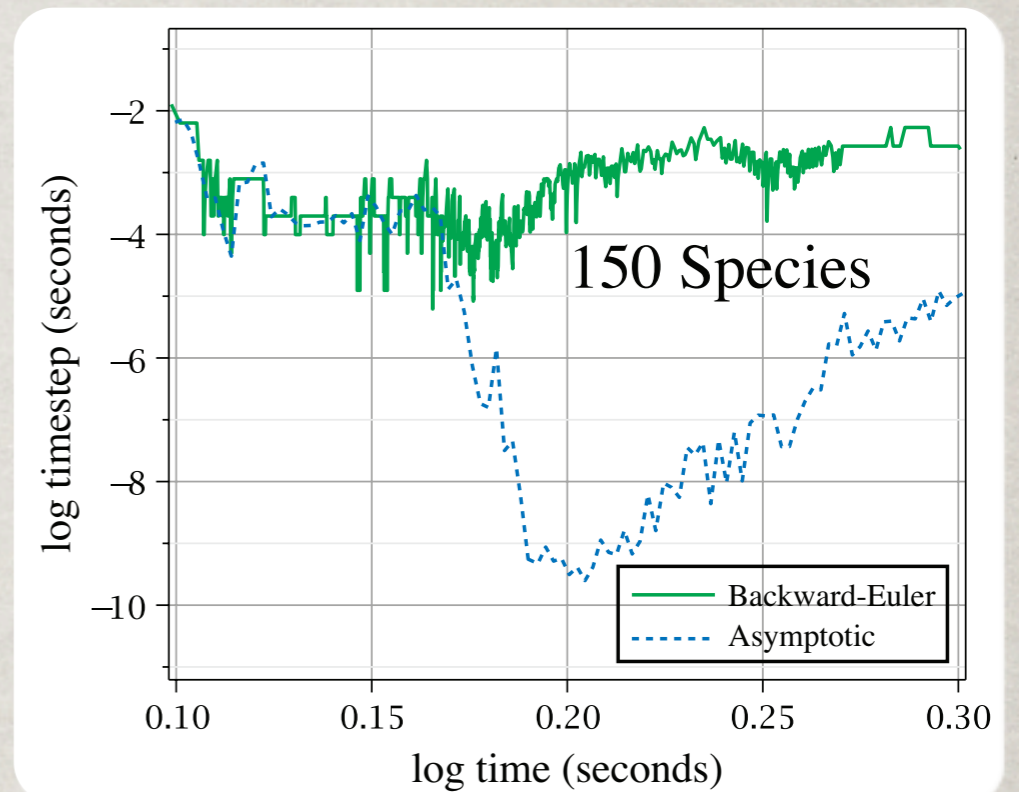
# TROUBLE WITH EQUILIBRIUM

The results are much less promising for this example of burning in a thermonuclear supernova.

For the first 1.5 seconds, the asymptotic method is competitive.

However, once the temperature exceeds 2 GK, the asymptotic timestep drops precipitously.

For temperatures in excess of 2 GK, many pairs of forward and inverse reaction reach equilibrium, which challenges the assumptions used to derive the method.

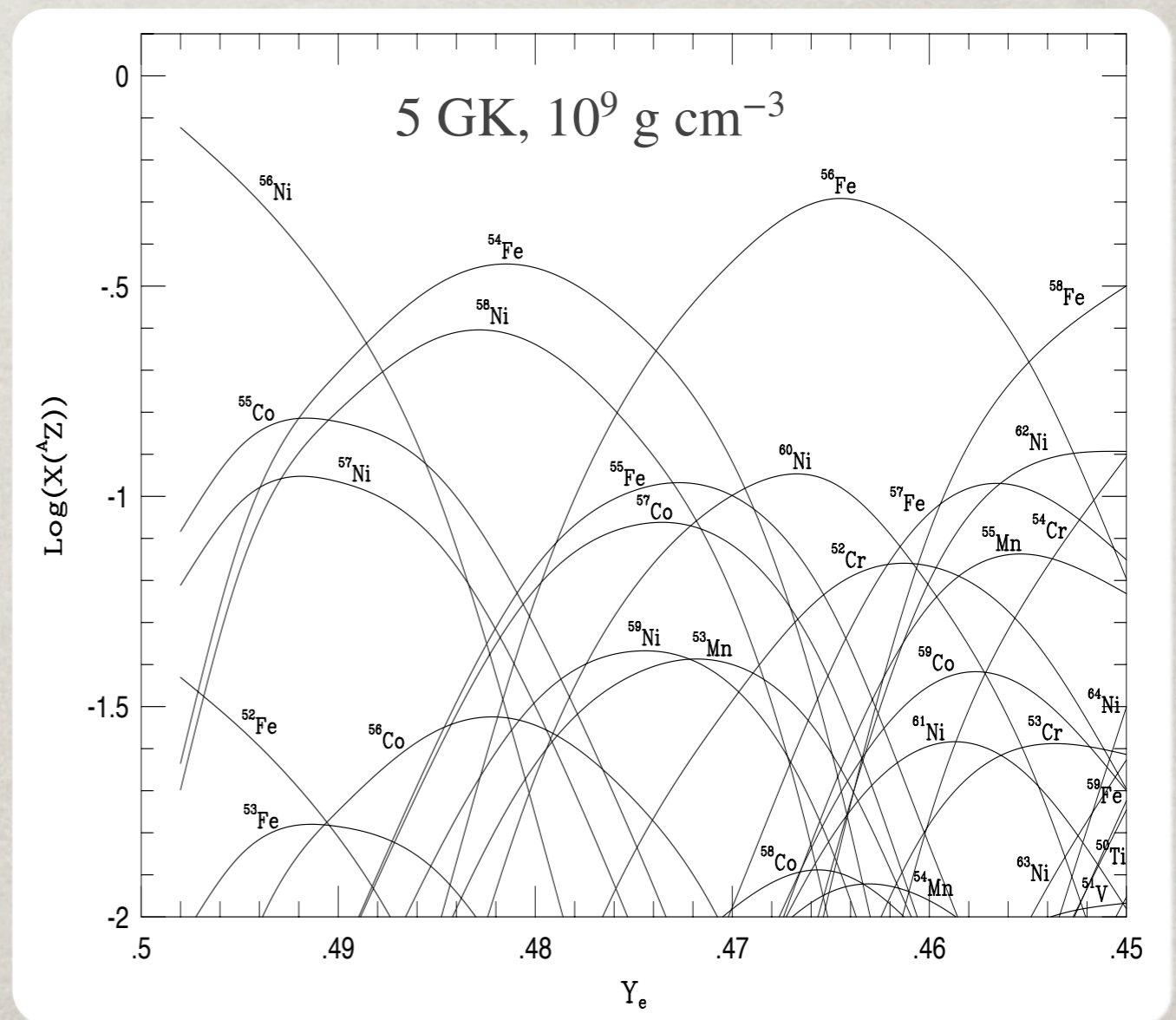


# THERMONUCLEAR EQUILIBRIA

At conditions of high temperature and density, thermonuclear reaction rates may be sufficiently rapid to achieve **Nuclear Statistical Equilibrium (NSE)** within the timescale set by the hydrodynamics of the astrophysical setting.

In most such cases, the strong and electromagnetic reactions equilibrate but **not the weak nuclear reactions**.

Thus the NSE composition depends on the neutron-richness, often represented by the **electron fraction**,  $Y_e = \sum Z_i Y_i$ .



# NUCLEAR STATISTICAL EQ.

The NSE abundance relation can be derived by extending detailed balance through proton and neutron captures, building nucleons into heavy nuclei. However, it is most easily computed via chemical potentials,  $Z \mu_p + N \mu_n = \mu(^AZ)$ .

For a Maxwell-Boltzmann gas, the **chemical potential** is

$$\mu_i = m_i c^2 + k_B T \ln \left[ \rho N_A \frac{Y_i}{G_i} \left( \frac{2\pi \hbar^2}{m_i k_B T} \right)^{\frac{3}{2}} \right]$$

where  $G(^AZ)$  and  $B(^AZ)$  are the partition function and **binding energy of the nucleus  $^AZ$** , and  $\theta = \left( \frac{m_u k_B T}{2\pi \hbar^2} \right)^{3/2}$

Solving for  $Y_i$  yields

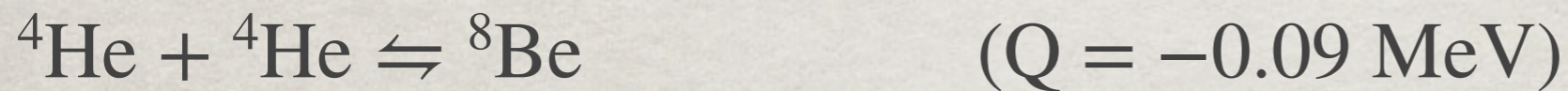
$$Y(^AZ) = \frac{G(^AZ)}{2^A} \left( \frac{\rho N_A}{\theta} \right)^{A-1} A^{\frac{3}{2}} \exp \left( \frac{B(^AZ)}{k_B T} \right) Y_n^N Y_p^Z \equiv C(^AZ) Y_n^N Y_p^Z$$

**2 unknowns**,  $Y_p$  &  $Y_n$  requires **2 constraints**,  $Y_e$  and  $\sum A_i Y_i = 1$ .

# EQUILIBRIA IN NETWORKS

**Local equilibrium** expressions are common in nuclear reaction networks, hidden in *three-particle processes*.

The most common example of this is the **triple  $\alpha$  process**,



With  $\tau({}^8\text{Be}) \sim 10^{-16}$  s, very rarely does a  ${}^8\text{Be}$  survive long enough for a third  $\alpha$  to capture.

$$Y({}^8\text{Be}) = \frac{\rho N_A}{\theta} \left(\frac{1}{2}\right)^{3/2} \exp\left(\frac{M({}^8\text{Be}) - 2M_\alpha}{k_B T}\right) Y_\alpha^2$$

For  $T > 0.1$  GK, the formation of the excited state of  ${}^{12}\text{C}$  is usually followed by a decay back to  ${}^8\text{Be}$

$$Y({}^{12}\text{C}^*) = \left(\frac{\rho N_A}{\theta}\right)^2 \left(\frac{3}{16}\right)^{3/2} \exp\left(\frac{M({}^{12}\text{C}^*) - 3M_\alpha}{k_B T}\right) Y_\alpha^3.$$

and the **reaction rate** is  $r_{3\alpha} = \rho N_A Y({}^{12}\text{C}^*) \Gamma_\gamma({}^{12}\text{C}^*) / \hbar$ .

# SUMMARY

The network of thermonuclear reactions linking a group of nuclear species creates a **system of ordinary differential equations** that can be solved for the temporal evolution of these species.

The presence of strong, electromagnetic and weak nuclear reactions within a nuclear reaction network produces an **extremely wide range of timescales** (as wide as  $10^{15}$ ), much wider than many other reactive systems.

This range of timescales causes the network ODEs to be **“stiff”** and require specialized techniques to integrate them.

These stiff system solution methods, though more expensive on a per timestep basis, allow the use of **much longer timesteps**, thus reducing the total integration time.