# Neutrino Interactions and Nucleosynthesis: Lecture 2

## Thermonuclear reaction networks

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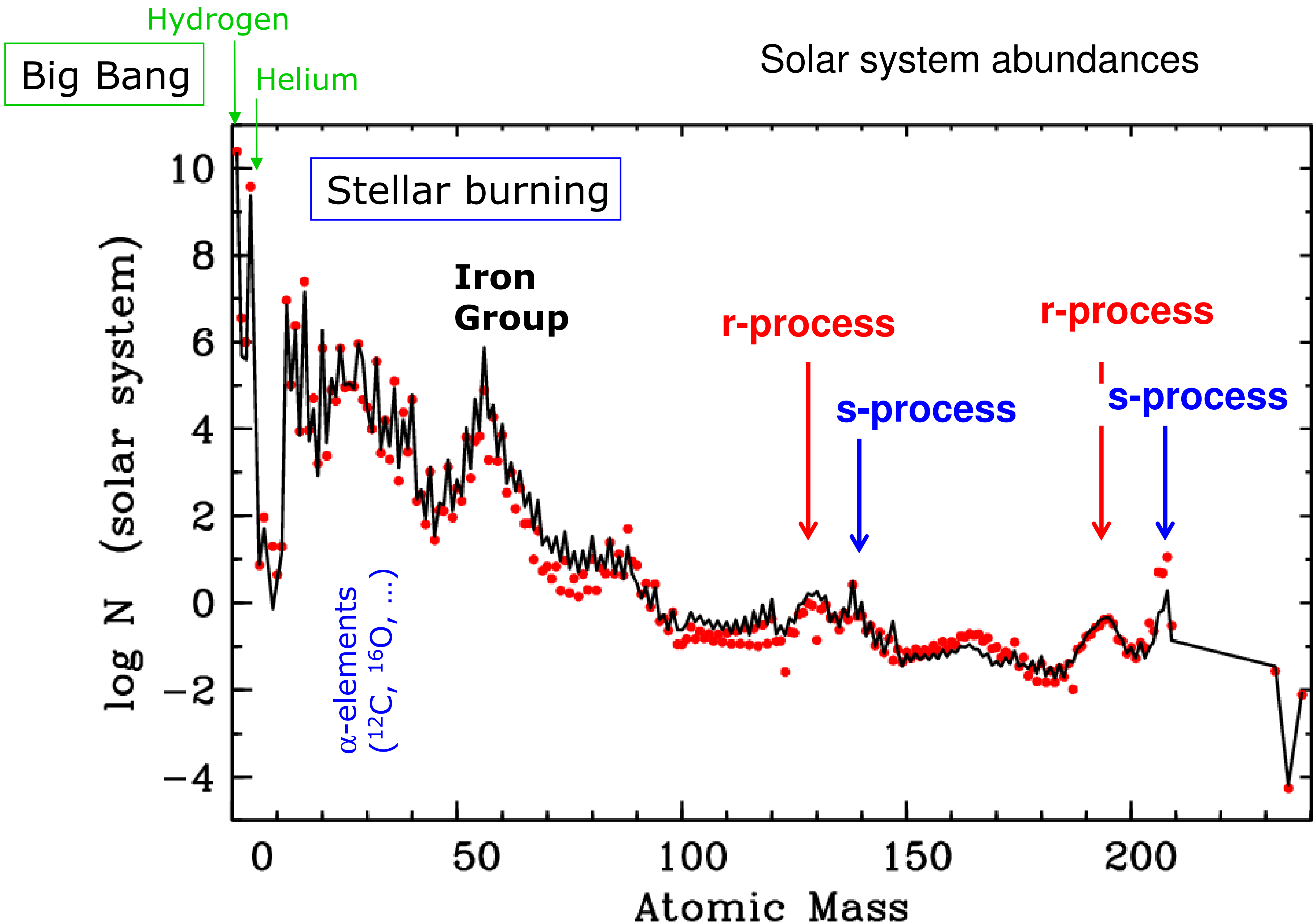
# Lecture plan

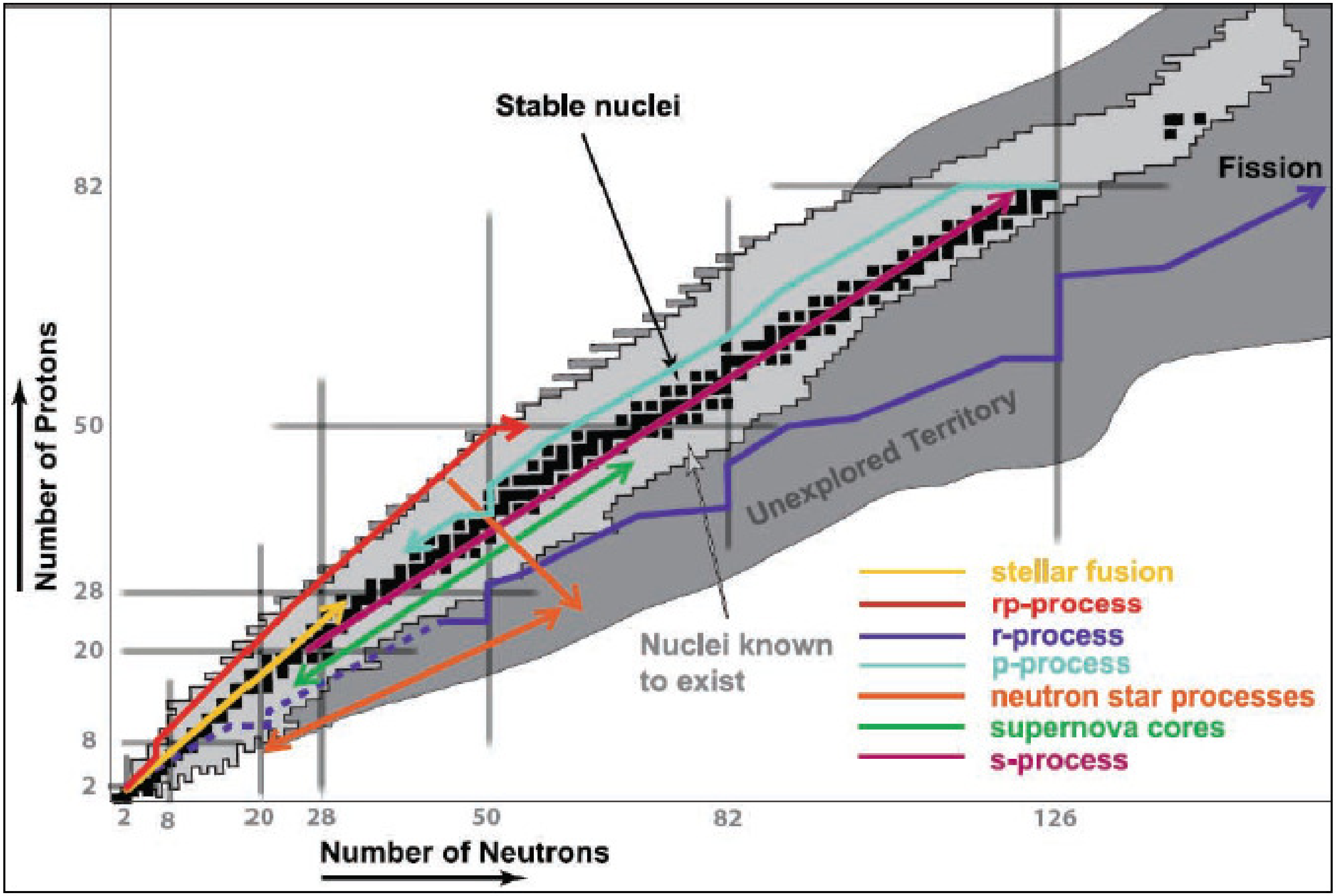
- Lecture 1
  - How to make heavy elements
  - Neutrinos set the conditions
  - Neutron-rich nucleosynthesis
  - Proton-rich nucleosynthesis

- Lecture 2
  - Thermonuclear reaction networks
  - Nuclear inputs

# Origin of elements



# Origin of elements




How are nuclei made? Where? Through what processes?

# Nuclear physics

- Need to know the relevant nuclear physics:
  - Properties of nuclei (mass, half-life, spin, levels, etc)
  - Properties of reactions between nuclei (and leptons, photons)

# Reaction rates

Consider:

- $n_i$: number density of particles of type i   $cm^{-3}$
- $n_j$: number density of particles of type j   $cm^{-3}$
- $\sigma$: cross section (effective area for reaction)   $cm^2$


- Reactions per time per volume
  = relative flux of particles i   $cm^{-3}$ cm $s^{-1}$
  × number of particles j   $cm^{-3}$
  × cross section   $cm^2$

  $r = n_i \, v \, n_j \, \sigma(v)$   $cm^{-3} \, s^{-1}$

# Reaction rates

- Previously: particles i move at constant v
- For constant relative velocity between particles i and j

→ reacts / vol / time: $r_{i;j} = \int \sigma \cdot |\vec{v}_i - \vec{v}_j| dn_i dn_j$

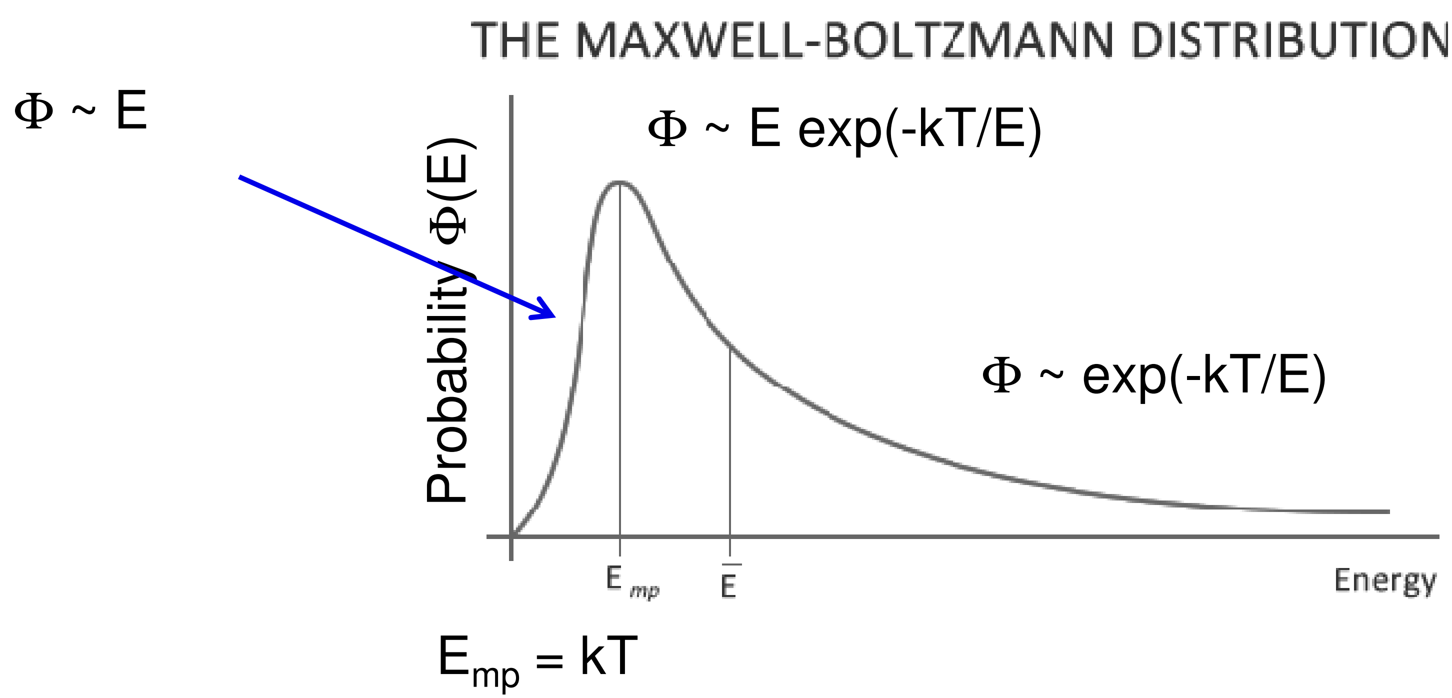
- General: projectiles and targets follow velocity distribution

$$r_{i;j} = n_i n_j \int \sigma(|\vec{v}_i - \vec{v}_j|)|\vec{v}_i - \vec{v}_j|\phi(\vec{v}_i)\phi(\vec{v}_j)d^3v_i d^3v_j$$

Integral depends on type of particles and distribution

# Maxwell-Boltzmann distribution

- Nuclei in astrophysical plasma are not mono-energetic
- They obey MB distribution



# Reaction rates

- Use center-of-mass coordinates, carry out integration, and remember that $\int \phi(\vec{V}) d^3V = 1$

  reaction rate becomes $r_{i;j} = n_i n_j \langle \sigma v \rangle_{i;j}$

  with the thermonuclear cross section <σv>

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

  - Only depends on temperature
  - If we know σ (E), we can get <σv>

# Astrophysical S-factor

- Use known energy dependence of $\sigma(E)$

- For charged particles: $\sigma(E)$ is proportional to:
  - Coulomb barrier penetration ~exp(-E $^{½}$ )
  - Nuclear size ~1/E

- All other energy dependencies are lumped together into astrophysical S-factor S(E)

- Why?
  - For non-resonant reactions: S(E) is slowly varying

  → better to work with S(E) if extrapolations are needed

# Astrophysical S-factor

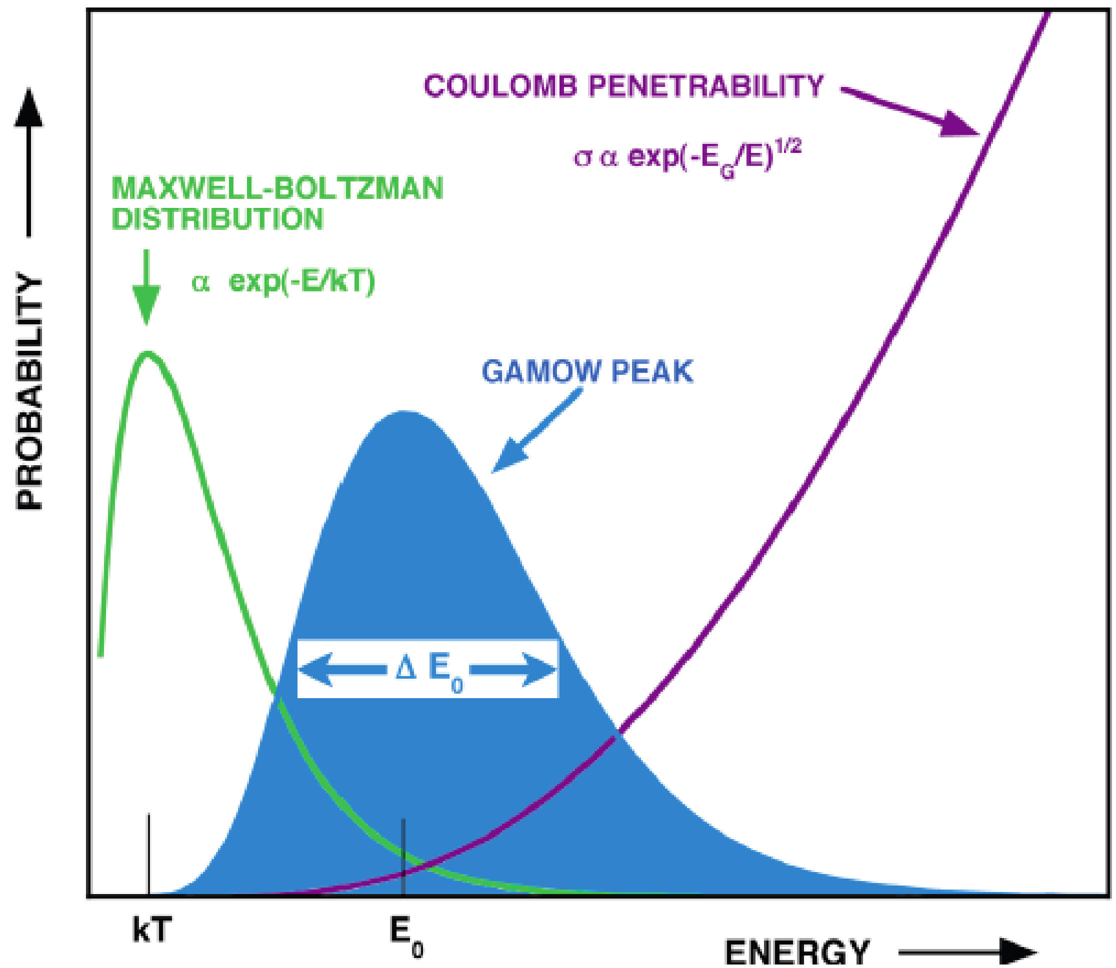
- Cross section $\sigma = E^{-1} \times \exp(-E^{½}) \times S(E)$

- Reaction rate becomes

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

  - S(E) is slowly varying with E, so integral is dominated by the two exponentials

# Gamow peak




Most effective stellar energy

# Nuclear reaction networks

- Turn number of reactions per volume and time into differential equation, for a reaction $i(j,o)m$

$$r_{i;j} = \frac{1}{1+\delta_{ij}} n_i n_j \langle \sigma v \rangle \longrightarrow \begin{array}{l} (\frac{\partial n_i}{\partial t})_\rho = (\frac{\partial n_j}{\partial t})_\rho = -r_{i;j} \\ (\frac{\partial n_o}{\partial t})_\rho = (\frac{\partial n_m}{\partial t})_\rho = +r_{i;j}. \end{array}$$

- Total rate of change of number density:

$$\dot{n}_i = (\frac{\partial n_i}{\partial t})_\rho + n_i \frac{\dot{\rho}}{\rho}$$

  - Includes changes due to density change (we are not interested in those)

# Abundances, mass fractions

- Matter density $\rho$ (g $cm^{-3}$)
- Number density n depends on matter density

- Can we separate dependence on matter density?

→ Define abundance $Y = n / \rho N_A$

- Units of abundance: mole $g^{-1}$

- Mass fraction $X_i = A_i Y_i$ with normalized sum

# Nuclear reaction networks

- Use abundance $Y_i = \frac{n_i}{\rho N_A}$ $\dot{Y}_i = \frac{\dot{n}_i}{\rho N_A} - \frac{n_i}{\rho N_A}\frac{\dot{\rho}}{\rho}$
- Derivative becomes:

$$\dot{Y}_i = \frac{1}{\rho N_A}(\frac{\partial n_i}{\partial t})_\rho = -\frac{r_{i;j}}{\rho N_A} = -\frac{1}{1+\delta_{ij}}\rho N_A \left\langle \sigma v \right\rangle_{i;j} Y_i Y_j$$

- For decays (and reactions with photons and leptons):
  - "decay rate" λ
  - Derivate becomes $\dot{Y}_i = -\lambda_i Y_i$

# Inverse reactions

- Many reactions are the inverse of an other reaction
- Forward and inverse reactions are linked by time reversal invariance

- For reaction i(j,o)m the thermonuclear cross section depends on
  - Q-value (energy difference between products and reactants)
  - Partition functions (Energy weighted density of states)

$$\langle \sigma v \rangle_{i;j,o} = \frac{1+\delta_{ij}}{1+\delta_{om}} \frac{G_m g_o}{G_i g_j} \left(\frac{\mu_{om}}{\mu_{ij}}\right)^{3/2} \exp(-Q_{o,j}/kT) \langle \sigma v \rangle_{m;o,j}$$

# Nuclear reaction networks

- Set of coupled differential equations

$$\dot{Y}_i = \sum_j N^i_j \lambda_j Y_j + \sum_{j,k} N^i_{jk} \rho N_A \langle \sigma v \rangle_{jk} Y_j Y_k + \sum_{j,k,l} N^i_{jkl} \rho^2 N_A^2 \langle \sigma v \rangle_{jkl} Y_j Y_k Y_l$$

Specify number of particles created or destroyed; take into account reactions between the same (indistinguishable species)

Thermonuclear cross section

Y .. Abundance
$\lambda$ …decay rate

# Nuclear reaction networks

- Set of coupled differential equations

$$\dot{Y}_i = \sum_j N^i_j \lambda_j Y_j + \sum_{j,k} N^i_{jk} \rho N_A \langle \sigma v \rangle_{jk} Y_j Y_k + \sum_{j,k,l} N^i_{jkl} \rho^2 N_A^2 \langle \sigma v \rangle_{jkl} Y_j Y_k Y_l$$

- Decays, photodisintegrations, reactions with leptons ($e^-$,$e^+$, $\nu$)
- Two-particle reactions
- Three-particle reactions (e.g. triple-$\alpha$ reaction)

# Discretization and Euler's method

- Discretization of system of DEs:

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

  - Explicit, forward Euler method for $\Theta=1$
  - Implicit, backward Euler method for $\Theta=0$

- Accuracy:
  - to first order in time
  - Improves inversely with timestep size

- Forward Euler gives poor performance in astrophysics due to range of timescales
  → stiff system

# Backward Euler method

- Backward Euler method requires knowledge of derivative at future time t+Δt

- Solving backward Euler method is equivalent to finding zeros of

$$\mathscr{L}(t+\Delta t) \equiv \frac{\boldsymbol{Y}(t+\Delta t)-\boldsymbol{Y}(t)}{\Delta t} - \dot{\boldsymbol{Y}}(t+\Delta t) = 0.$$

- Use Newton-Raphson method with trial abundance

$$\Delta \boldsymbol{Y} = \left(\frac{\partial \mathscr{L}(t+\Delta t)}{\partial \boldsymbol{Y}(t+\Delta t)}\right)^{-1} \mathscr{L},$$

# Computational aspects

- Backward Euler method costs:
  - Build Jacobian matrix
  - Solve Jacobian matrix

- But can make use of sparseness of matrix
  - General: every species reacts with every species (dense matrix)
  - Reality: Coulomb terms suppresses captures of heavy nuclei; photodisintegrations emit nucleons or alphas → only need to consider ~ a dozen reactions linking each species to each nuclear neighbors

# Computational aspects

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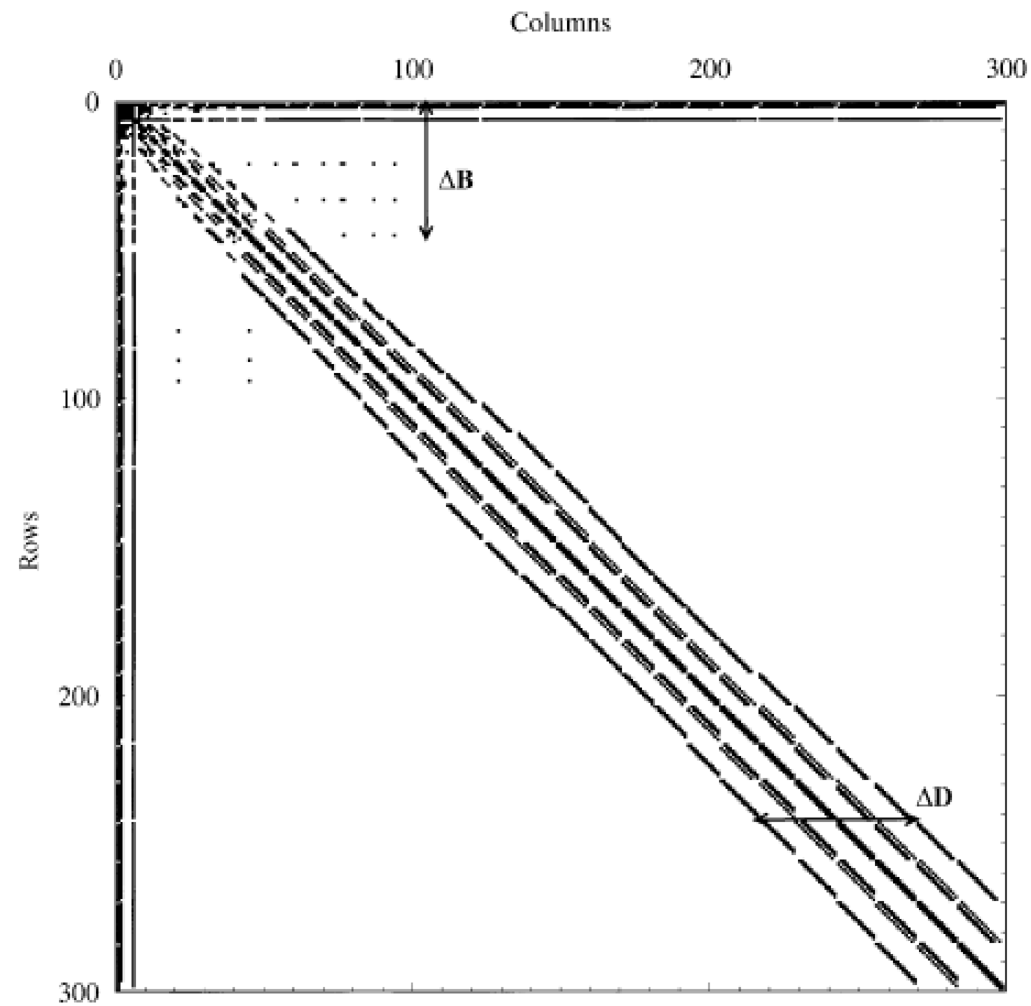


# How to Model Nucleosynthesis

In principle: need 3D hydro in order to follow convection, mixing, explosion

Problems:

- Coupling of hydro to reaction networks (nucleosynthesis, energy generation)
- Explosions

Compromise:

- (1D) hydro with reduced energy generation network
- Mixing length theory, convection criteria
- Parameterized explosions (mass cut and/or explosion energy as free parameters)

Nevertheless: mostly reliable nucleosynthesis expected (except for nuclides dependent on explosion mechanism)

# Implementation of Networks

- Fully coupled
  - Energy feedback + abundances
- Operator splitting
  - Reduced network for energy generation
  - Abundances in full network (mixing, convection)
- Post-processing
  - Reduced network for energy generation
  - Other abundances from post-processing

# Nuclear reaction networks

- Set of coupled differential equations

$$\dot{Y}_i = \underbrace{\sum_j N^i_j \lambda_j Y_j}_{} + \underbrace{\sum_{j,k} N^i_{jk} \rho N_A \langle \sigma v \rangle_{jk} Y_j Y_k}_{} + \underbrace{\sum_{j,k,l} N^i_{jkl} \rho^2 N_A^2 \langle \sigma v \rangle_{jkl} Y_j Y_k Y_l}_{}$$

  - Decays, photodisintegrations, reactions with leptons ($e^-$,$e^+$, $\nu$)
  - Two-particle reactions
  - Three-particle reactions (e.g. triple-$\alpha$ reaction)

# Nuclear physics

- Need to know the relevant nuclear physics:
  - Properties of nuclei (mass, half-life, spin, levels, etc)
  - Properties of reactions between nuclei (and leptons, photons)

- Can measure (if stable or long-lived):
  - mass, half-life, spin, levels
  - Some cross sections

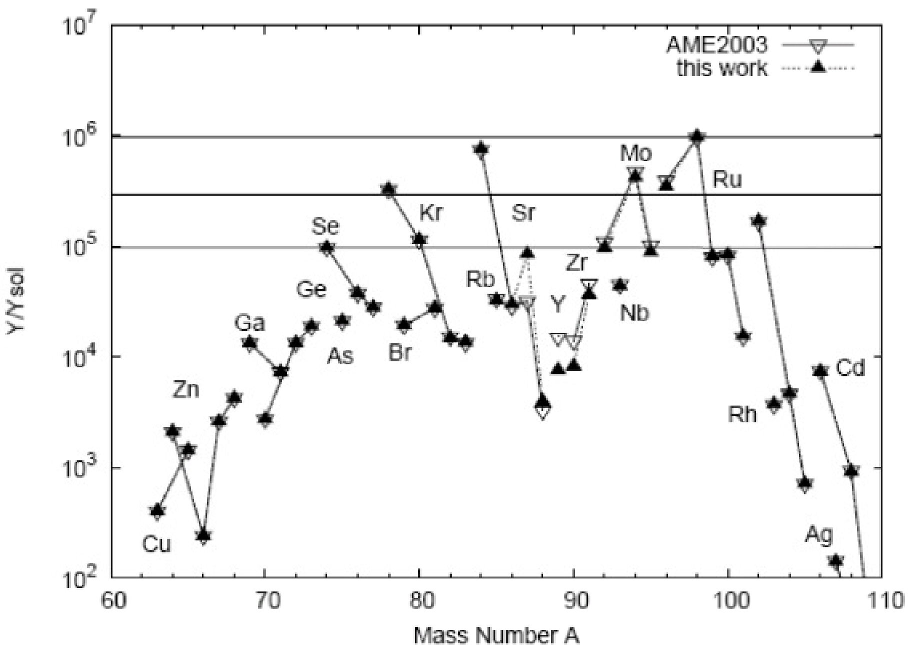
- But need also very short-lived nuclei and their reactions
  - → theoretical predictions

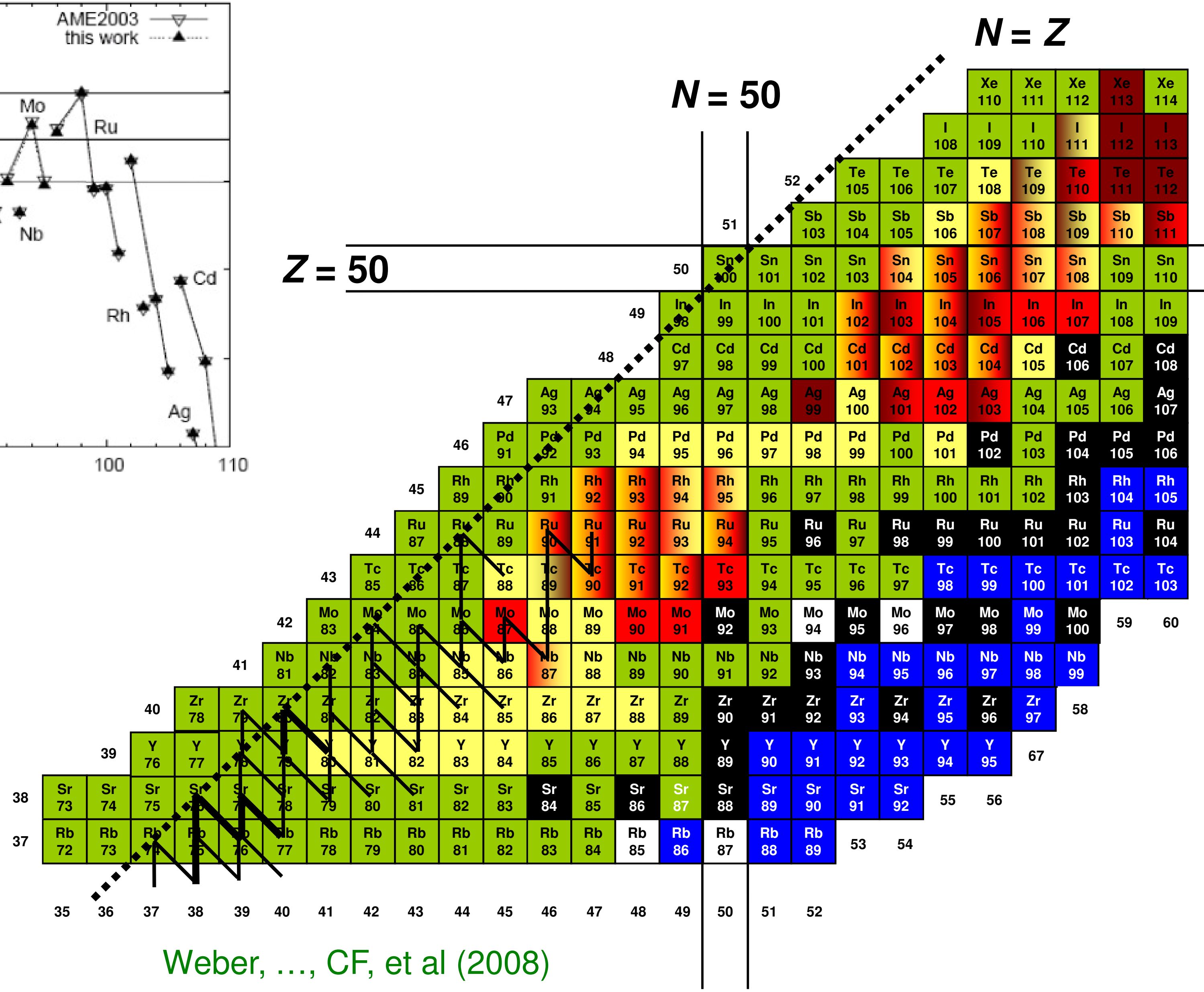
# Example: $\nu$p-process

# Nuclear Physics

- All involved reaction rates from theory predictions (Hauser-Feshbach calculations)
- Nuclear masses: increasing number measured at Penning traps (SHIPTRAP, JYFLTRAP, CPT, etc)
- Upgrades to current facilities and future facilities hold promise to gain more experimental information in the relevant region

# Penning Trap Mass Measurements




CANADIAN TRAP
at Argonne NL

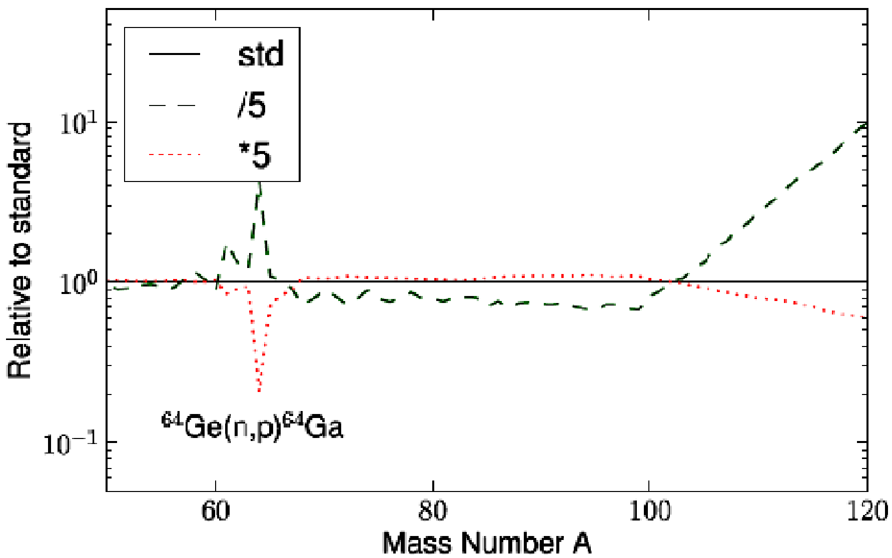
SHIPTRAP

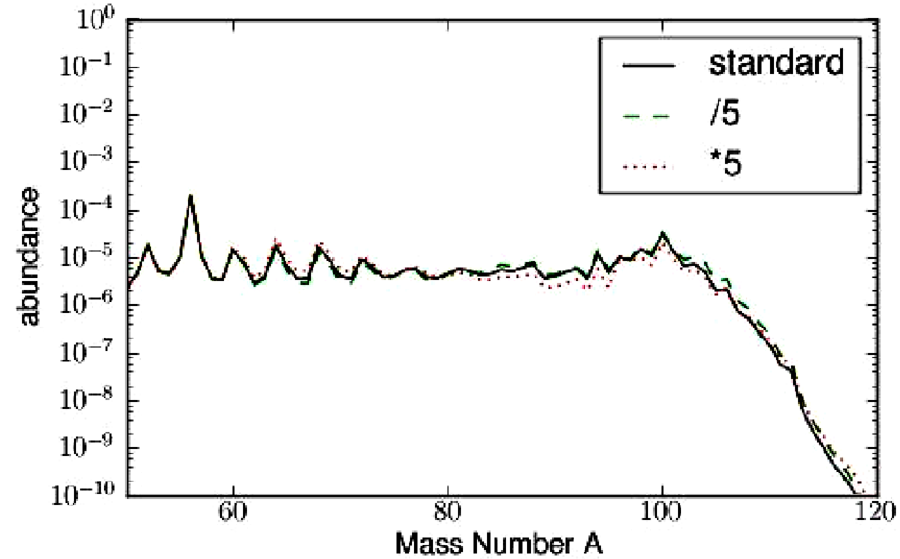
JYFLTRAP

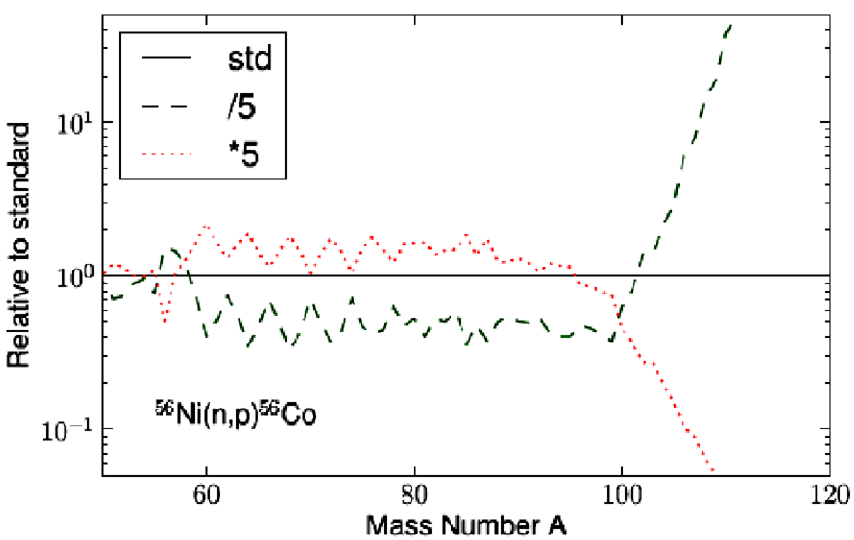
Weber, …, CF, et al (2008)

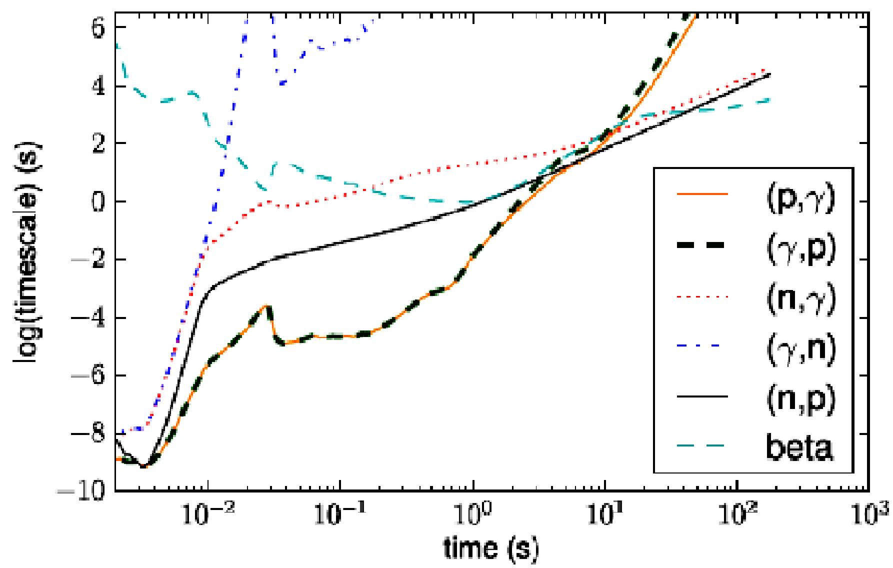
# Critical (and not so critical) reactions

Frohlich et al (2012)

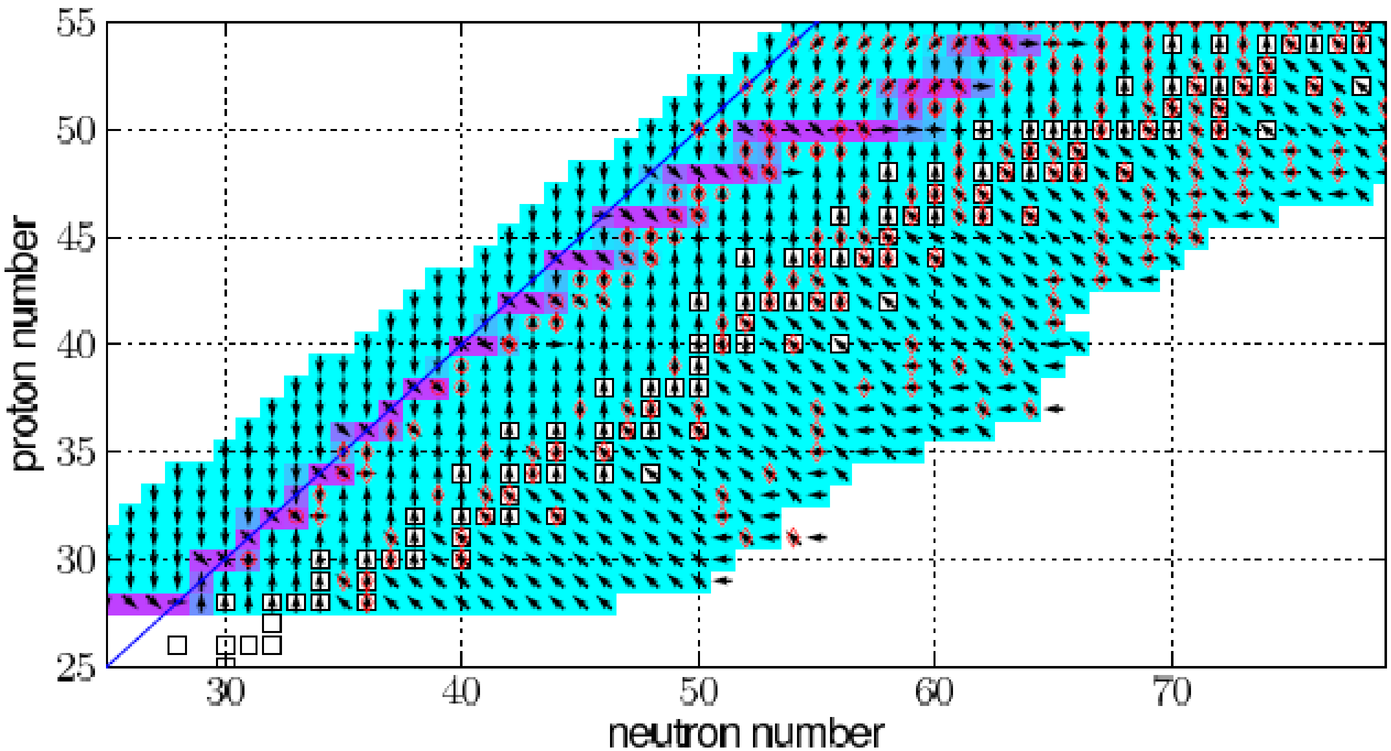


# Trajectory independence



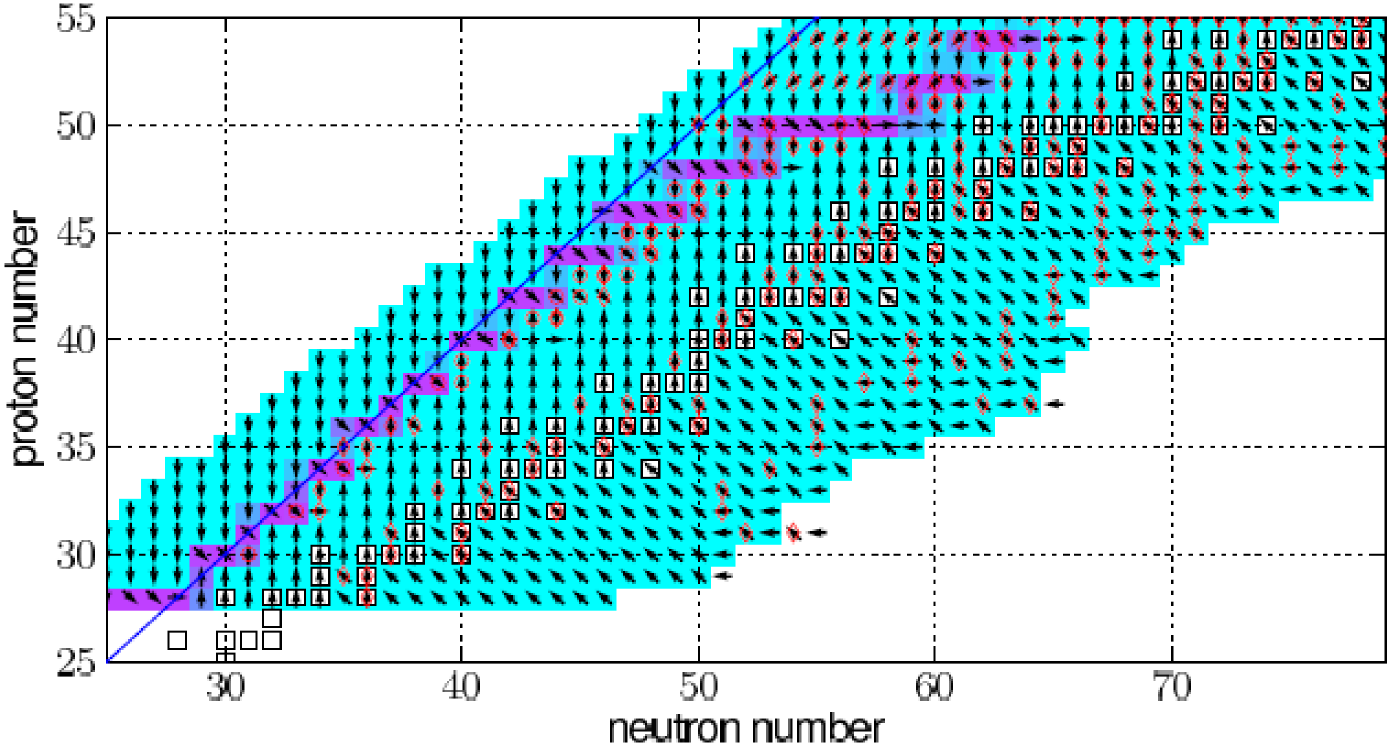

Frohlich et al (2012)

(p,g)-(g,p) equilibrium abundances shown

(n,p) reactions on nuclei with highest abundances determine upward flow

Mass uncertainties may impact equilibrium

# Trajectory independence




Frohlich et al (2012)

Nuclear properties (Q-values, lifetimes, reaction rates) determine location of path; nucleosynthesis possible only within well constrained values of $Y_n$, $Y_p$, $T$, $r$

Also set the timescale required to reach heavier nuclei

Trajectory variations only determine how long “effective” conditions prevail how much of the path upwards can be covered

“Trajectory-independent” determination of nuclear uncertainties

# Implications for Experiments

Frohlich et al (2012)

TABLE VII: List of important reactions with additional information: target half-life, references to the section in which a reaction is discussed, a prioritization, and whether an experimental investigation constrains the rate. For each reaction, also the following is shown for the two plasma temperatures 1.5 and 3.0 GK: the astrophysical energy window [52], the predicted laboratory cross section $\sigma^{\rm lab}$ at the upper end of the window, and the ground state contribution $\mathcal{X}$.

| Reaction | Half-life of target | $T = 1.5$ GK Energy window (MeV) | $\sigma^{\rm lab}$ (mbarn) | $\mathcal{X}$ | $T = 3.0$ GK Energy window (MeV) | $\sigma^{\rm lab}$ (mbarn) | $\mathcal{X}$ | Section | Constraint |
|---|---|---|---|---|---|---|---|---|---|
| $^{56}$Ni(n,$\gamma$)$^{57}$Ni | 6.1 d | 0.00 – 0.43 | 8.1 | 1.00 | 0.00 – 0.84 | 6.6 | 1.00 | IV, V B, V D | ok |
| $^{56}$Ni(n,p)$^{56}$Co | | 0.00 – 0.62 | 256 | 1.00 | 0.05 – 1.34 | 493 | 1.00 | IV, V B, V D | ok |
| $^{56}$Ni(n,$\alpha$)$^{53}$Fe | | 0.12 – 1.45 | 0.005 | 1.00 | 0.87 – 3.36 | 1.6 | 0.76 | V D | ok |
| $^{56}$Ni(p,$\alpha$)$^{53}$Co | | 9.00 – 10.73 | 0.0002 | 0.05 | 10.24 – 13.13 | 0.3 | 0.02 | V D | Q |
| $^{57}$Ni(n,$\gamma$)$^{58}$Ni | 35.6 h | 0.00 – 0.39 | 8.1 | 1.00 | 0.00 – 0.77 | 5.9 | 0.92 | IV, V B, V D | ok |
| $^{57}$Ni(n,p)$^{57}$Co | | 0.00 – 0.48 | 598 | 0.99 | 0.00 – 1.02 | 643 | 0.84 | IV, V B, V D | ok |
| $^{57}$Ni(n,$\alpha$)$^{54}$Fe | | 0.00 – 0.50 | 8.9 | 1.00 | 0.00 – 1.14 | 12.7 | 0.85 | V D | ok |
| $^{57}$Ni(p,$\gamma$)$^{58}$Cu | | 0.70 – 1.47 | 0.0005 | 1.00 | 0.82 – 2.13 | 0.001 | 0.98 | V D | ok |
| $^{57}$Ni(p,$\alpha$)$^{54}$Co | | 5.82 – 7.55 | 0.0002 | 0.12 | 7.06 – 9.93 | 0.13 | 0.03 | V D | Q |
| $^{58}$Ni(n,$\gamma$)$^{59}$Ni | stable | 0.00 – 0.43 | 17.5 | 1.00 | 0.00 – 0.90 | 15.0 | 0.98 | IV, V B, V D | ok |
| $^{58}$Ni(n,p)$^{58}$Co | | 0.59 – 1.60 | 8.9 | 0.79 | 0.95 – 2.72 | 114.0 | 0.24 | IV, V B, V D | low |
| $^{58}$Ni(n,$\alpha$)$^{55}$Fe | | 0.04 – 1.27 | 0.05 | 0.97 | 0.69 – 3.02 | 4.5 | 0.42 | V D | low |
| $^{58}$Ni(p,$\gamma$)$^{59}$Cu | | 0.86 – 1.75 | 0.02 | 1.00 | 1.06 – 2.59 | 0.1 | 0.99 | V D | ok |
| $^{58}$Ni(p,$\alpha$)$^{55}$Co | | 4.00 – 5.71 | 0.003 | 0.24 | 5.21 – 8.07 | 1.3 | 0.07 | V D | Q |
| $^{59}$Ni(n,$\gamma$)$^{60}$Ni | $7.6 \times 10^4$ yr | 0.00 – 0.34 | 21.8 | 0.93 | 0.00 – 0.66 | 8.6 | 0.73 | IV, V B, V D | ok |
| $^{59}$Ni(n,p)$^{59}$Co | | 0.01 – 0.58 | 25.5 | 0.73 | 0.05 – 1.31 | 55.5 | 0.42 | IV, V B, V D | low |
| $^{59}$Ni(n,$\alpha$)$^{56}$Fe | | 0.00 – 0.46 | 2.4 | 0.89 | 0.00 – 1.28 | 4.9 | 0.55 | V D | low |
| $^{59}$Ni(p,$\gamma$)$^{60}$Cu | | 0.92 – 1.86 | 0.12 | 0.91 | 1.18 – 2.60 | 0.3 | 0.72 | V D | ok |

(continued on next page)