Challenges in nucleosynthesis of nuclei beyond Fe

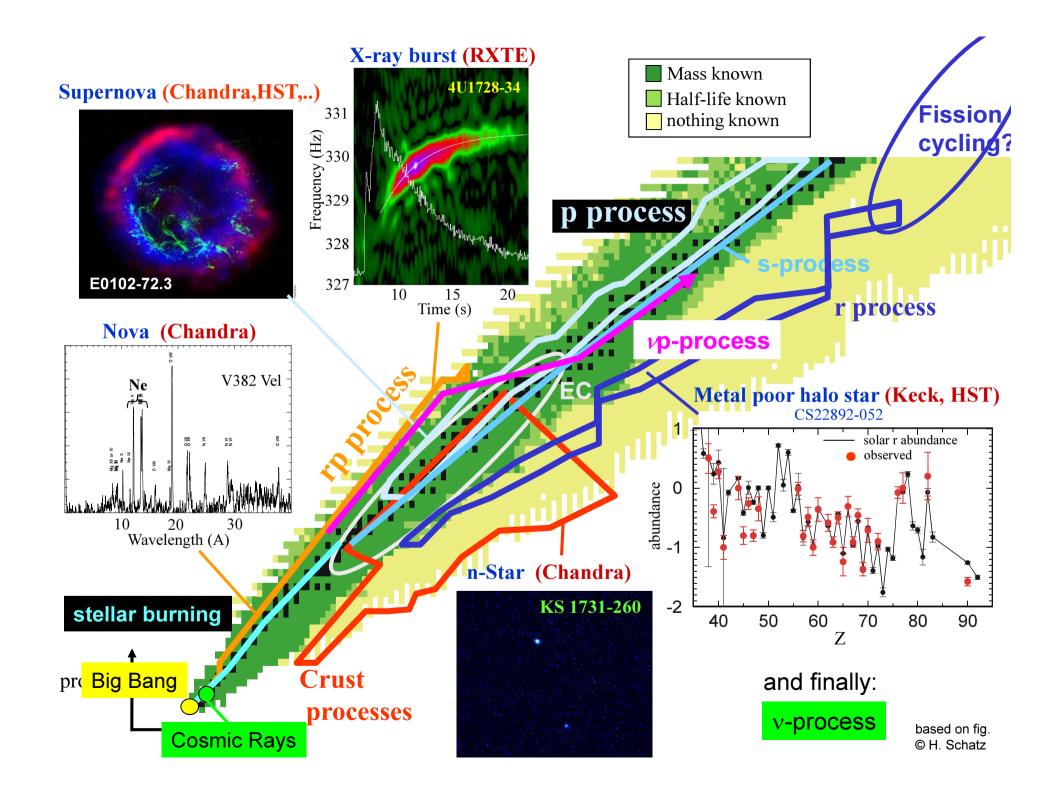
T. Rauscher

Centre for Astrophysics Research University of Hertfordshire, UK

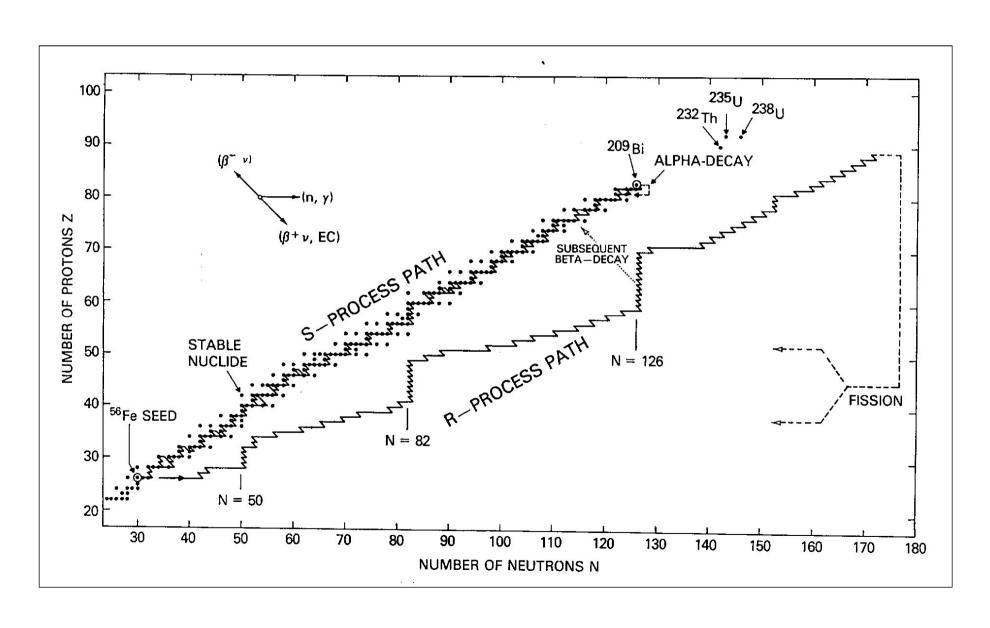
TOC

- Intro: Origin of elements beyond Fe
- <u>Differences between light and heavy element nucleosynthesis</u>
- Reaction Mechanisms
 - Reaction Models
 - Nuclear Properties
- Uncertainties + Sensitivities
- Stellar Rates and the problem of inclusion of experimental data
- Possible further complications far off stability
 - α+nucleus optical potential
 - E1 strength
 - Direct neutron capture
- Conclusion

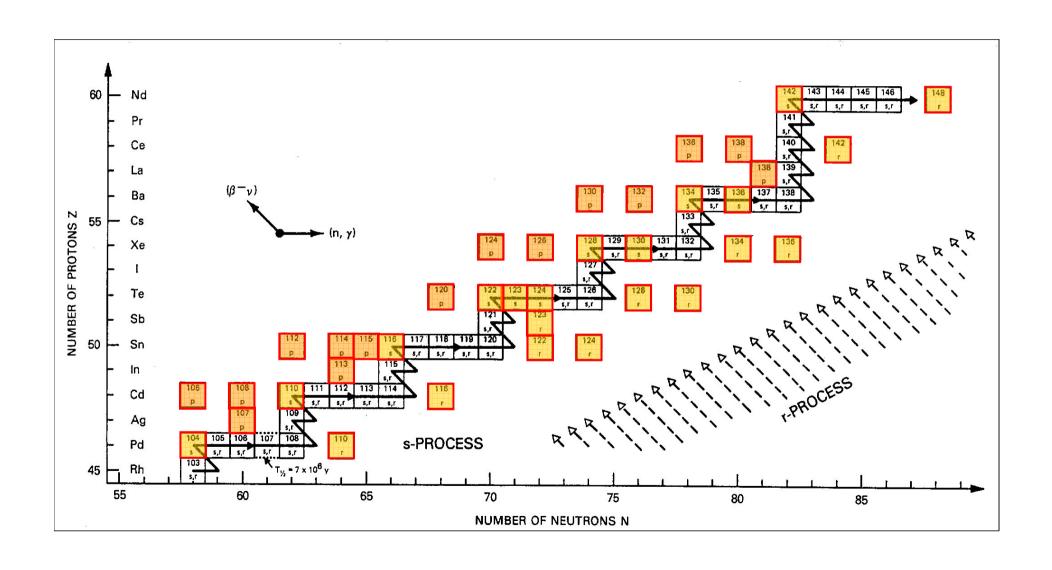
Astro Intro



s- and r-Process Paths



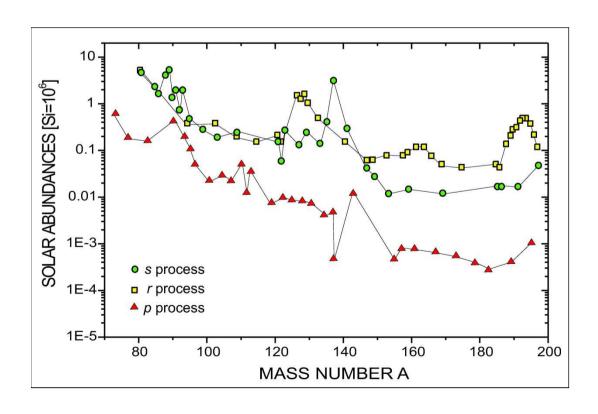
r-, s- and p-Nuclides



p-Nuclei

Def.: "What is not made by s- and r-process"

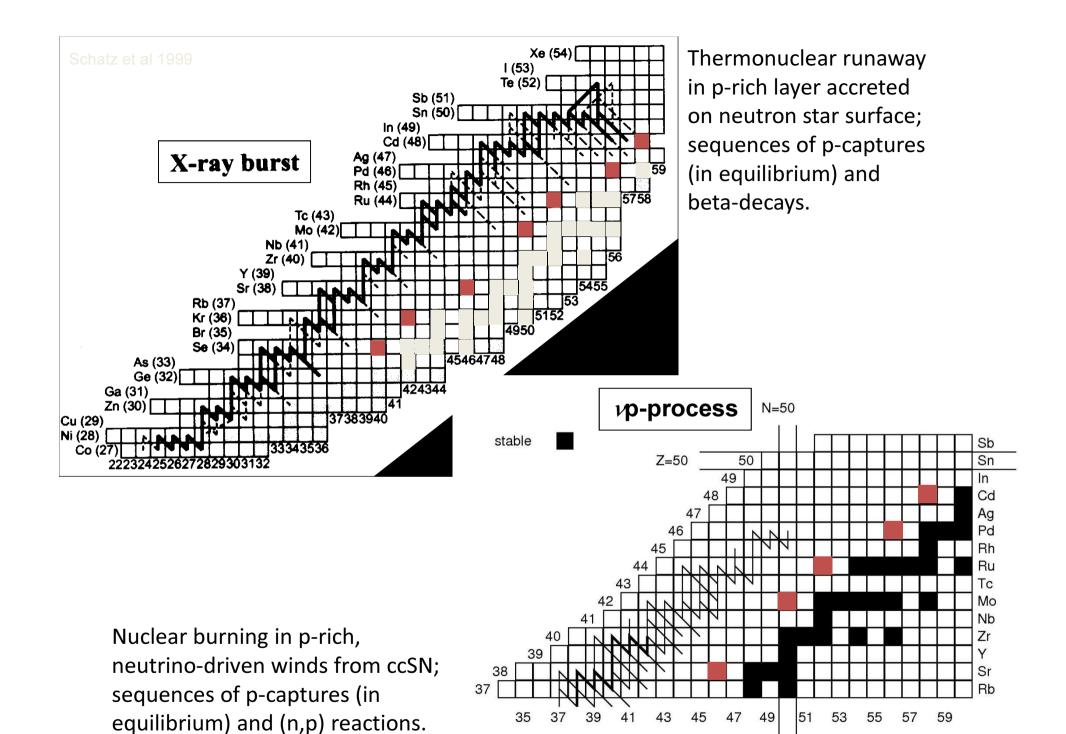
- Originally 35 proton-rich nuclei assigned but:
 - "time-dependent" definition
 - perhaps fewer (s: ¹¹³In, ¹¹⁵Sn?, ¹⁵²Gd, ¹⁶⁴Er, ...)



- Tiny abundances but details complicated
- Production process not yet fully understood
- "Few" nuclei involved, but also only few simulations and measurements (astro, nuclear) available

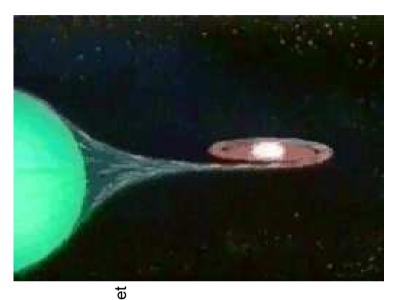
Popular Scenarios

- Currently "best" studied: <u>γ-process</u> in O/Ne shell of massive stars
 - consistent p-production across large range of nuclei
 - deficiencies for A<100 and 150<A<165
 - additional ν -process for 138 La and 180 Ta
- Explosion of <u>mass-accreting white dwarf</u>
 - "regular" SN Ia and/or sub-Chandrasekhar WD
 - combination of p-captures and γ -process (and np-process)
 - Problems: requires seed enhancement, sensitive to details of the hydrodynamics
- Extremely p-rich scenarios: <u>rp-process</u>, <u>vp-process</u>
 - decay of p-rich progenitors
 - problem: detailed modelling, ejection, ⁹²Nb in meteorites puts tight constraint



Pruet et all 2006; Fröhlich et al 2006, Weber et al 2009

p-Synthesis in "canonical" SN la and sub-Chandrasekhar WD explosions



Type I (a) Supernova

*O+IC III #He

Companion star

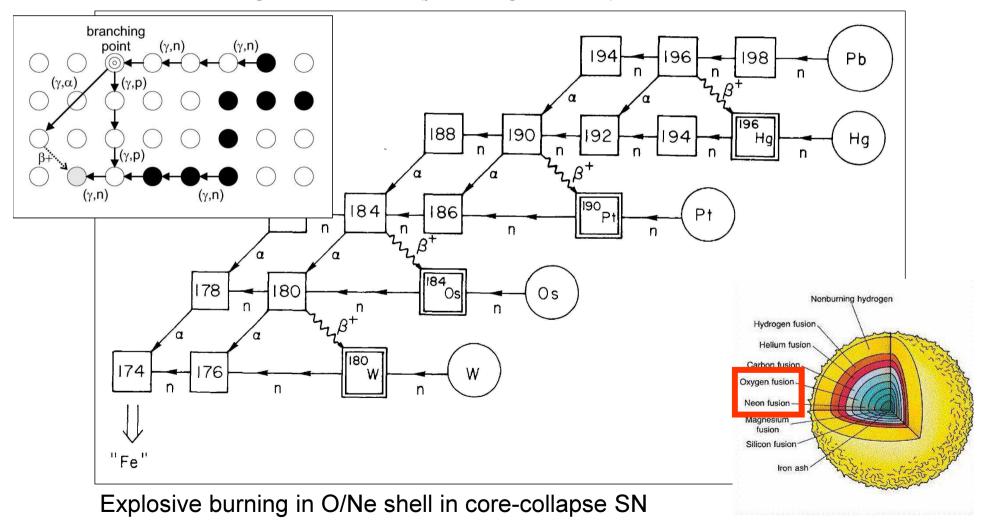
white dwarf

1) binary system 2 compression 3) central ignition

4) complete disruption

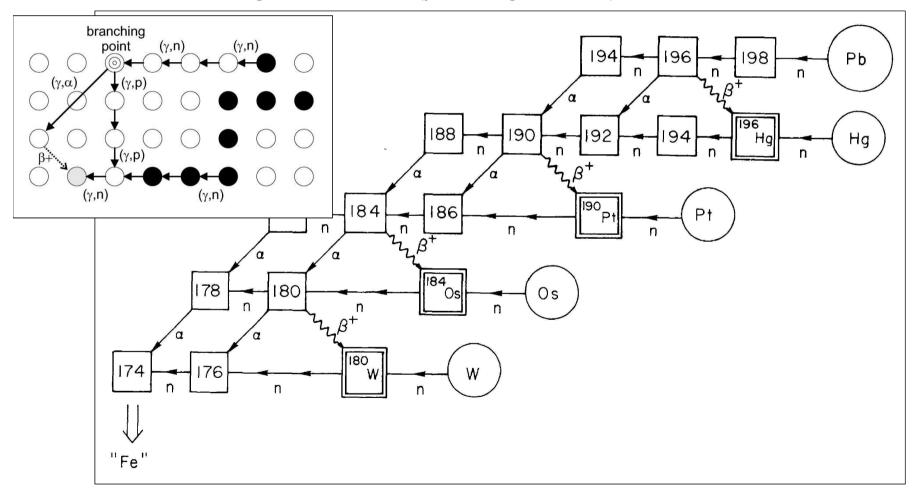
The \gamma-Process

Photodisintegration of seed nuclei (produced in situ or inherited from prestellar cloud). NOT total disintegration, of course! (just the right amount)



The *y*-Process

Photodisintegration of seed nuclei (produced in situ or inherited from prestellar cloud). NOT total disintegration, of course! (just the right amount)



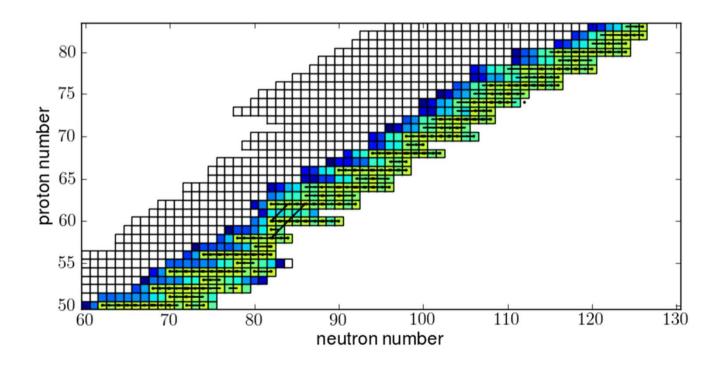
Type Ia SN

Photodisintegration of stable seed nuclei

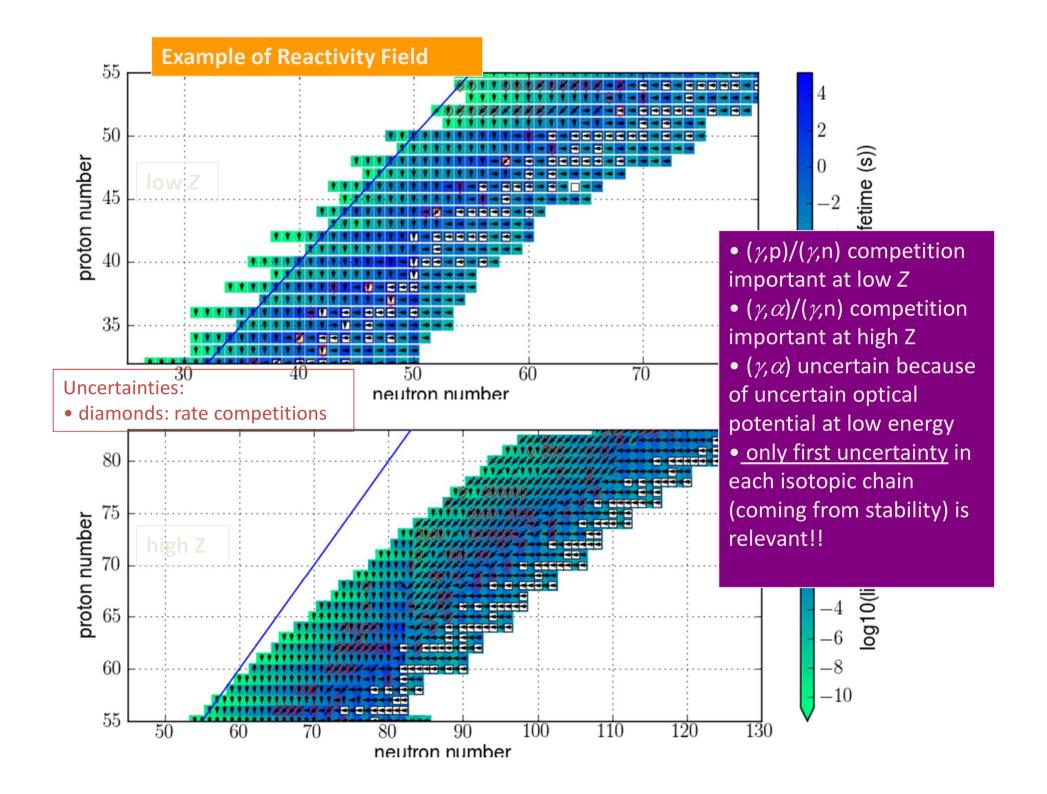
- Not an equilibrium process!
- Competition of (γ,n) , (γ,p) , (γ,α) rates determine path and destruction speed at each temperature.
- Strong nuclear constraints on required astrophysical conditions for each group of nuclei,

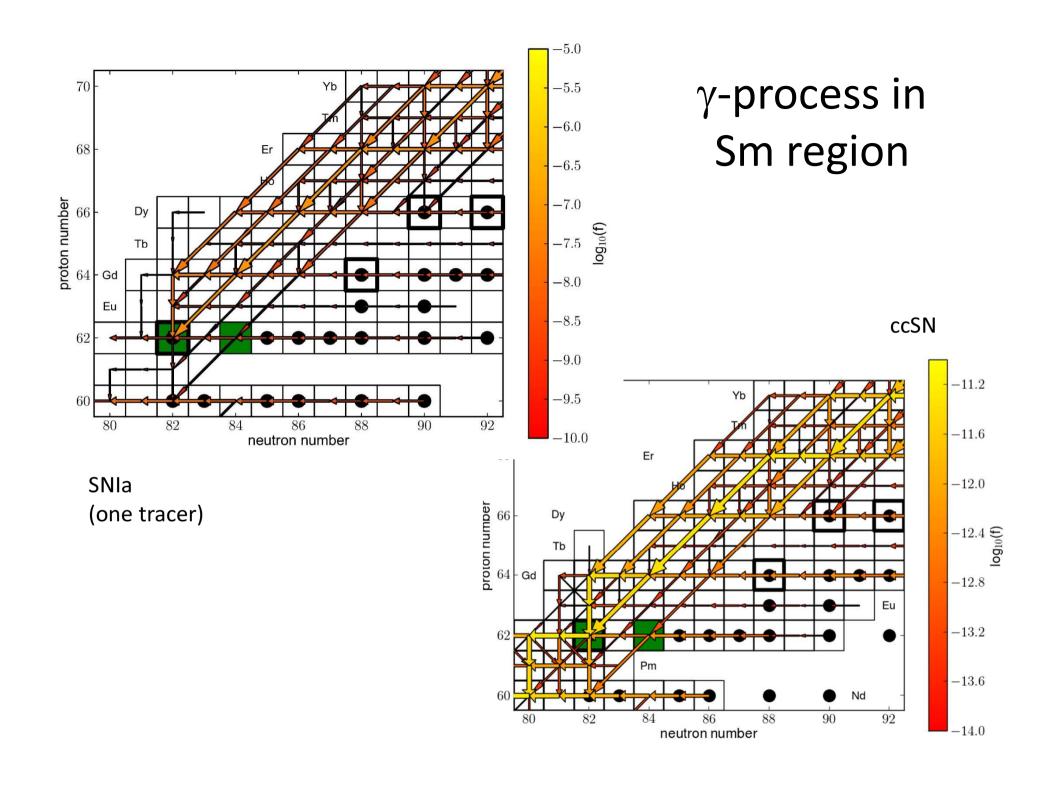
$$T_9 = 2.250 \ \rho = 2.747e + 05$$

e.g., at high *T* all heavier nuclei are destroyed.



(animation)





Photodisintegration and the process

- The γ -process derives its name from the importance of (γ,n) , (γ,p) , (γ,α) reactions
- But stellar photodisintegration rates are different from laboratory photodisintegration
- Not just because of thermal photon distribution but more so due to thermal excitation: the Q-value rule!
- Can be calculated from capture with reciprocity formula!

Connection to capture rate by <u>detailed balance</u>:

$$\lambda_{m\gamma} = \left(\frac{A_i A_j}{A_m}\right)^{\frac{3}{2}} \frac{(2J_i + 1)(2J_j + 1)}{2J_m + 1} \frac{G_i^{\text{norm}}(T)}{G_m^{\text{norm}}(T)} \left(\frac{\mu kT}{2\pi\hbar^2}\right)^{\frac{3}{2}} e^{-\frac{Q_{ij}}{kT}} \left\langle \sigma^* v \right\rangle_{ij}$$

Reaction Mechanisms

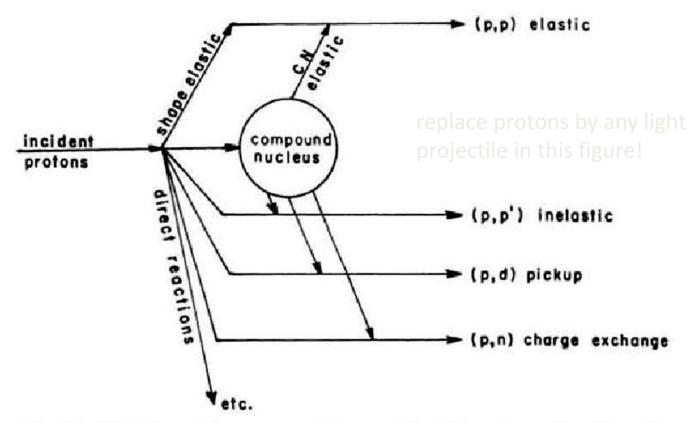
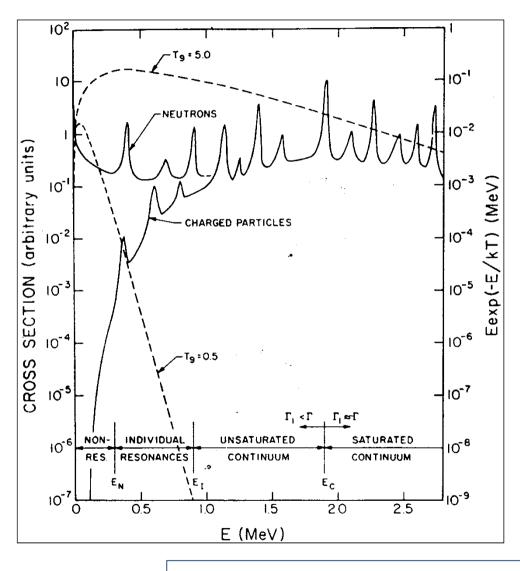


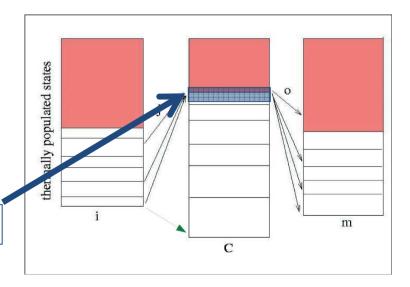
Fig. 1.2. Depiction of the processes that are typical of proton-nucleus interactions. (Adapted from P. E. Hodgson, 1971.)

Reaction Mechanisms



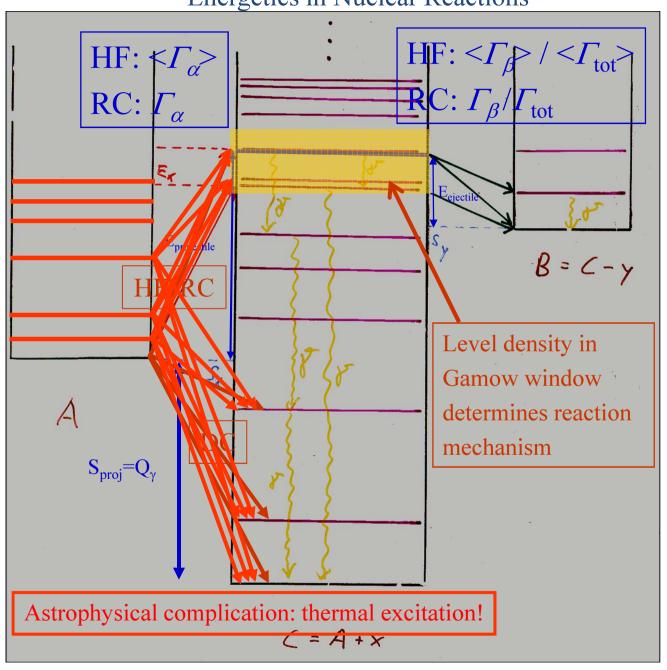
Regimes:

- 1. Overlapping resonances: statistical model (Hauser-Feshbach)
- 2. Single resonances: Breit-Wigner, R-matrix
- 3. Without or in between resonances: Direct reactions



Determined by nucl. level density

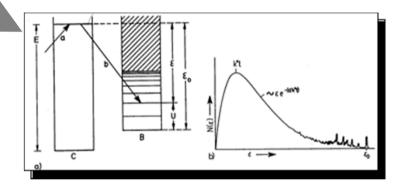
Energetics in Nuclear Reactions



Reaction Mechanisms II

Statistical Model (Hauser-Feshbach): $\sigma_{\alpha \to \beta}^{\text{CN}} = \sigma_{\alpha}^{\text{form}} b_{\beta} = \sigma_{\alpha}^{\text{form}} \frac{\left\langle \Gamma_{\beta} \right\rangle}{\left\langle \Gamma_{\text{tot}} \right\rangle} \propto \frac{\left\langle \Gamma_{\alpha} \right\rangle \left\langle \Gamma_{\beta} \right\rangle}{\left\langle \Gamma_{\text{tot}} \right\rangle}$

Compound Reaction



Direct Reaction



$$\Rightarrow B \xrightarrow{a} \gamma$$

$$A + a \rightarrow B + \gamma$$

A ... target nucleus

a ... projectile

 $B = A \oplus a$... residual nucleus

$$\frac{d\sigma}{d\Omega} = \left| \left\langle \Phi_{\beta} \middle| O_{EM} \middle| \chi_{\alpha} \Phi_{\alpha} \right\rangle \right|^{2} \propto S \left| \int d\vec{R} \, \Phi_{Aa} O_{EM} \chi_{\alpha} \right|^{2}$$

Hauser-Feshbach (statistical model) cross section is averaged Breit-Wigner cross section

$$\sigma_i(j,o)_{HF}$$

$$= \frac{\pi}{k_j^2} \sum_{J} (2J+1) \frac{(1+\delta_{ij})}{(2I_i+1)(2I_j+1)} W(j,o,J,\pi) \frac{T_j(E,J,\pi)T_o(E,J,\pi)}{T_{tot}(E,J,\pi)} \quad \text{stat. model}$$

$$= \langle \sigma_i(j, o)_{BW} \rangle$$
 with

$$\sigma_i(j,o)_{BW} = \frac{\pi}{k_j^2} \sum_n (2J_n + 1) \frac{(1 + \delta_{ij})}{(2I_i + 1)(2I_j + 1)} \frac{\Gamma_{j,n} \Gamma_{o,n}}{(E - E_n)^2 + (\Gamma_n/2)^2}$$

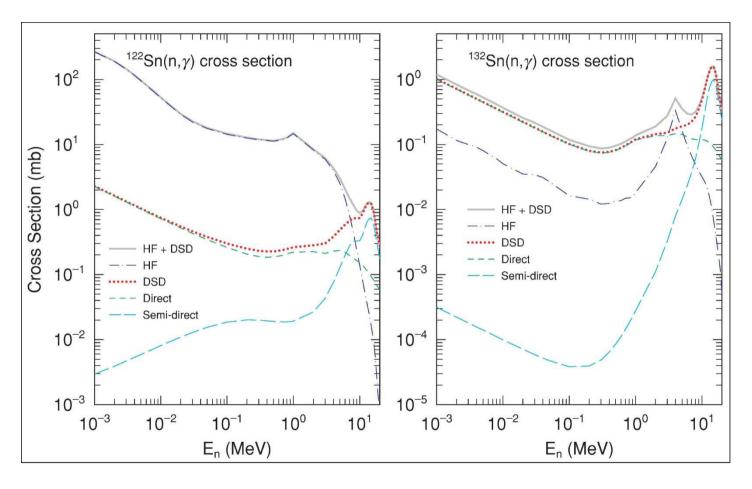
Breit-Wigner

$$T_j(E, J, \pi) = \frac{2\pi}{D(E, J, \pi)} \langle \Gamma_j(E, J, \pi) \rangle$$

Transmission coeffs.

$$W(j,o,E,J,\pi) = \left\langle \frac{\Gamma_j(E,J,\pi)\Gamma_o(E,J,\pi)}{\Gamma_n(E,J,\pi)} \right\rangle \cdot \frac{\langle \Gamma(E,J,\pi) \rangle}{\langle \Gamma_j(E,J,\pi) \rangle \langle \Gamma_o(E,J,\pi) \rangle}$$
width fluctuation corrections

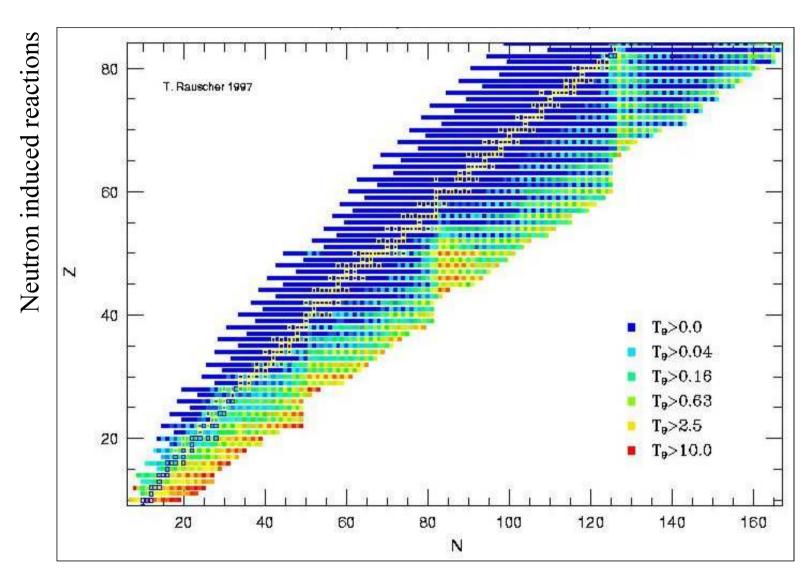
What about Direct-Semidirect Capture?



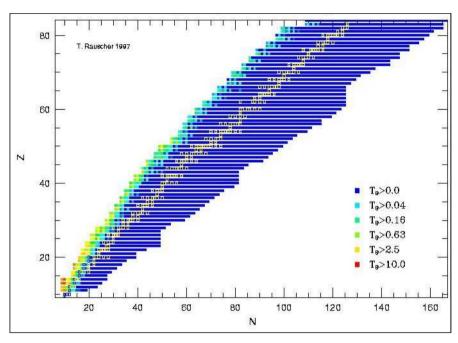
Chiba et al, PRC 77 (2008) 015809

- ➤ Pre-equilibrium effect
- > at energies higher than astrophysically relevant

Applicability of the Statistical Model

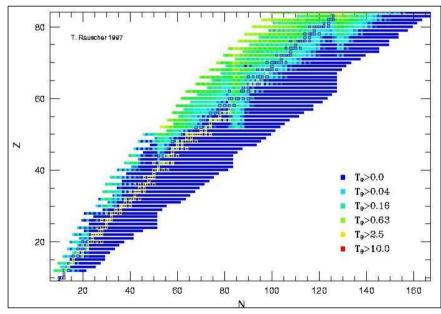


Applicability of Statistical Model



Proton induced reactions

α-induced reactions



Nuclear Properties

See review: Rauscher, Int. J. Mod. Phys. E 20, 1071 (2011)

Relevant Nuclear Properties

(in no particular order!)

- Masses (Q-values, sep. energies, equilibria path location)
 - Shell quenching?
- Optical Potentials (stat. mod. inp., DC (different?))
- Nuclear level density (stat. mod. input, for applicab. + T_{γ})
 - Also single <u>low-lying states important</u> (DC+stat. mod.)
 - Systematics
 - Shell quenching?
- Spectroscopic factors, scattering lengths (DC input)
- EM resonances (stat. mod. inp.)
 - Low energy behavior
 - Pygmy Resonances?
- Nucleon density distribution (deformation, neutron skin; also needed for *potentials*)
- Fission barriers
- β -decay (time scales), weak rates (collapse and explosion)

Prediction of Nuclear Properties Near To And Far From Stability

- Global models advantageous for large-scale calculations
 - Microscopic, macroscopic-microscopic
 - Parameterized
- Parameterized models should be derived from basic understanding and/or microscop. models → then often better suited for large-scale calculations
- Real understanding of nuclear structure far off stability still lacking
 - Competing microscop. models yield different results

Input for different (averaged) widths

- Neutron widths:
 - Spin, parity of ground state and low-lying excited states in target or final nucleus
 - Optical neutron+(target) nucleus potential
 - Nuclear mass density distributions for certain optical potentials
 - Neutron separation energy (from mass differences)
- Proton widths:
 - Spin, parity of ground state and low-lying excited states in target or final nucleus
 - Optical proton+(target) nucleus potential
 - Nuclear mass density distributions for certain optical potentials
 - Proton separation energy (from mass differences)
- Alpha widths:
 - Spin, parity of ground state and low-lying excited states in target or final nucleus
 - Optical alpha+(target) nucleus potential
 - Nuclear mass density distributions for certain optical potentials
 - Alpha separation energy (from mass differences)
- Photon (Gamma) Width:
 - E1 strength function at about $S_{proj}+E_{proj}-3$ MeV
 - Nuclear level density (or levels) at same energy
 - M1 strength functions

Input for Resonance Widths

- Separation energies (from mass differences)
- Close to and within astrophysical energy window:
 - Resonance energy
 - Resonance partial widths
- If widths have to be calculated:
 - Ground state and excited states in target and final nucleus (energies, spins, parities)
 - Depending on type of calculated width, similar input as already listed for averaged widths
 - Spectroscopic factors

Remark 1: Uncertainty propagation from MC input variation provided already by STARLIB for lighter nuclei

Remark 2: Usually simple Breit-Wigner formula used or R-Matrix

Input for Direct Capture

- Separation energies (from nuclear mass differences)
- Spins, Parities, Energies of ground state and low-lying excited states in target and final nucleus
- Spectroscopic factors
 - ATTENTION: Spectroscopic factors have also to be known for excited states in TARGET nucleus (usual spectroscopic factors are measured/calculated relative to target ground state)!
- Effective interaction potential between projectile and target
 - perhaps calculated from nuclear mass density distribution
 - This is not necessarily the same as the optical potential used in Hauser-Feshbach theory.

Sensitivities

Uncertainties in Nucleosynthesis Calculations

- 1. Impact of uncertainties in:
 - Nuclear properties required for cross section calculations
 - model, model input
 - Reaction cross sections
 - model, model input
 - Astrophysical reaction rates
 - cross section input
- 2. Experimental constraint of rates through a measurement
 - Inclusion of experimental error in rate uncertainty
- 3. Impact of rate uncertainties on predicted abundances
 - Identification of major flows, Monte Carlo variation

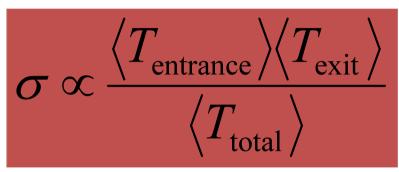
here: focus on trans-Fe nuclei (high NLD, high Coulomb barrier) but many conclusions apply similarly to lighter nuclei + resonant reactions

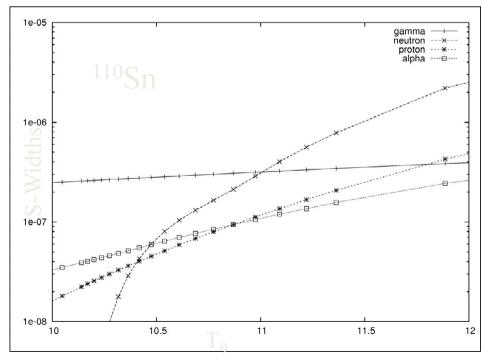
Detailed discussion in: ApJL 755, L10 (2012); ApJS 201 (2012) 26; AIP Advances 4 (2014) 041012.

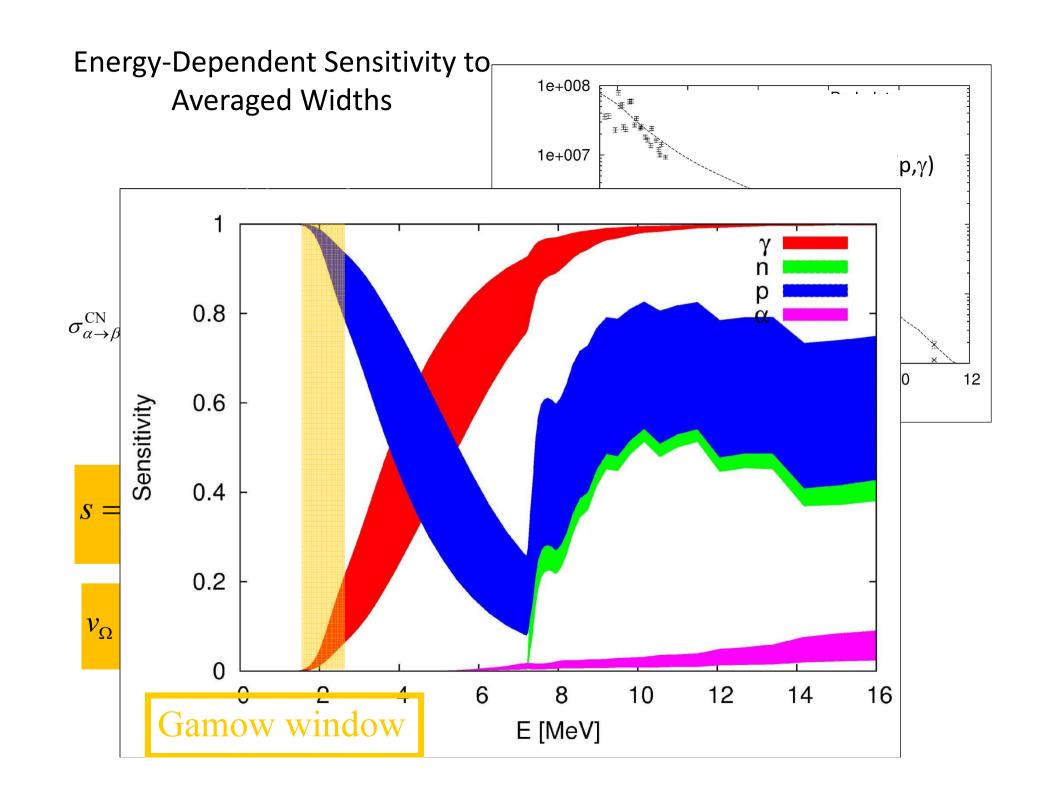
Relative importance of widths

Average widths
 (=transmission
 coefficients)
 determine the Hauser Feshbach cross
 section

 γ-widths not necessarily the smallest ones at astrophysical energies!







Energy-Dependent Sensitivity to (Averaged) Widths

$$\sigma_{\alpha \to \beta}^{\text{CN}} = \sigma_{\alpha}^{\text{form}} b_{\beta} = \sigma_{\alpha}^{\text{form}} \frac{\left\langle \Gamma_{\beta} \right\rangle}{\left\langle \Gamma_{\text{tot}} \right\rangle} \propto \frac{\left\langle \Gamma_{\alpha} \right\rangle \left\langle \Gamma_{\beta} \right\rangle}{\left\langle \Gamma_{\text{tot}} \right\rangle}$$

$$s = \frac{v_{\Omega} - 1}{v_{q} - 1} = \frac{q_{\text{old}}}{\Omega_{\text{old}}} \frac{d\Omega}{dq}$$

$$v_{\Omega} = \frac{\Omega_{\mathrm{new}}}{\Omega_{\mathrm{old}}}, \quad v_{q} = \frac{q_{\mathrm{new}}}{q_{\mathrm{old}}}$$

- Cross sections and rates have different sensitivities due to contribution of excited states (addt'l reactions with smaller relative energy)
- Data outside the astrophysical energy range may not provide constraint on reaction rate
- Applies similarly to resonant rates (Breit-Wigner widths)

Sensitivity

Variation factors

 Ω ...cross sections, rates

q...input (widths: NLD, opt. pot., GDR, spectroscopy)

Energy-Dependent Sensitivities

- ALL sensitivities between Ne and Bi from p-drip to n-drip tabulated in ApJS 201, 26.
- Allows to disentangle uncertainty treatment of nuclear input determining widths from calculation of cross sections and rates: impact of variation can immediately be seen without need of further cross section calculation!
 - Just determine by how much a property changes in your new model and use sensitivity to determine impact.
- <u>Disentangles comparison of predictions to measurements and theory discussion of width calculations!</u>
 - Experimentalists can make a *first estimate* of what has to be changed in models to fit predictions to measurements without need for new calculations, use:

$$s = \frac{v_{\Omega} - 1}{v_{q} - 1} = \frac{q_{\text{old}}}{\Omega_{\text{old}}} \frac{d\Omega}{dq}$$

$$\Omega_{\text{new}} = \Omega_{\text{old}} \left(s \left(v_q - 1 \right) + 1 \right)$$

Sensitivity

$$v_{\Omega} = \frac{\Omega_{\mathrm{new}}}{\Omega_{\mathrm{old}}}, \quad v_{q} = \frac{q_{\mathrm{new}}}{q_{\mathrm{old}}}$$

Variation factors

 Ω ...cross sections, rates

q...input (widths: NLD, opt. pot., GDR, spectroscopy)

It is better to look at the rates than at the cross sections:

• Rates are the relevant quantities

cross section sensitivity

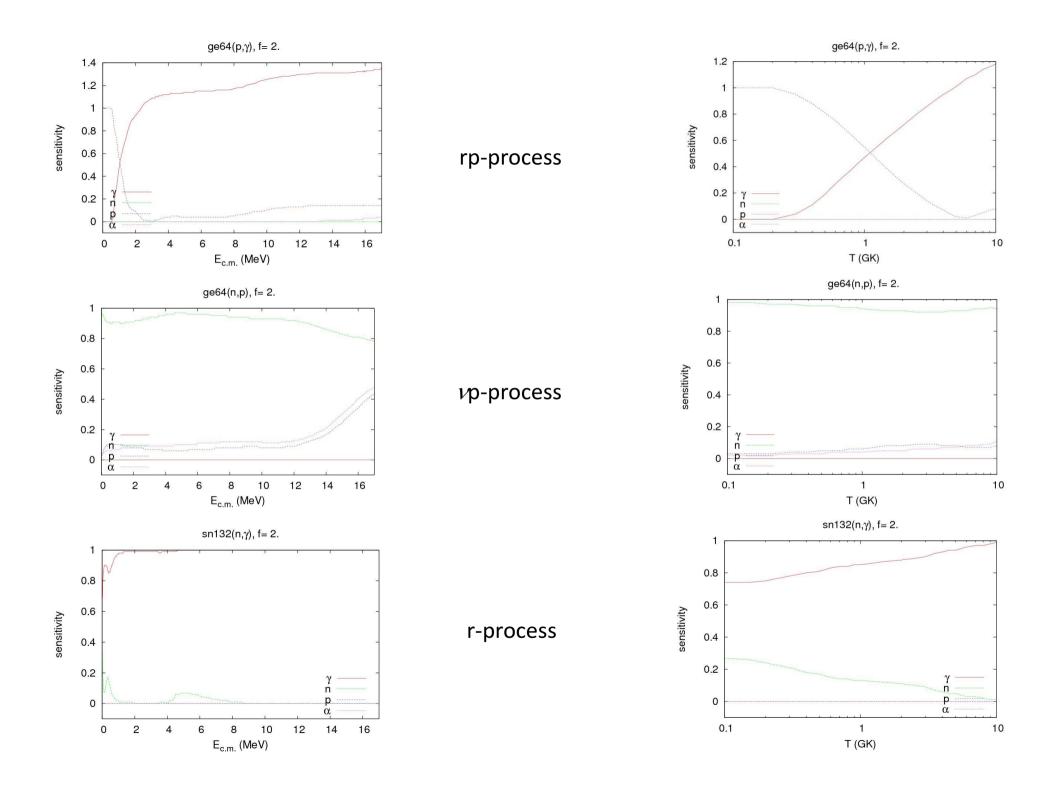
• No need to separately compute the Gamow window

Examples relevant to the γ -process

rate sensitivity

mo92(p, γ), f= 2. mo92(p, γ), f= 2. 1.2 2.5 2 0.8 1.5 sensitivity sensitivity 0.6 0.4 0.5 0.2 0 0 2 8 10 12 14 16 0.1 10 E_{c.m.} (MeV) T (GK)

calculations performed with SMARAGD v0.8.1s



Stellar Rates and g.s. Contributions

Stellar rate and stellar cross section

$$r^* = \frac{n_a n_A}{1 + \delta_{aA}} \int_0^\infty \sigma^*(E) \Phi(E, T) \ dE = \frac{n_a n_A}{1 + \delta_{aA}} R^*$$

Stellar rate

$$R^*(T) = w_0 R_0 + w_1 R_1 + w_2 R_2 + \dots$$

$$R_i(T) = \int_0^\infty \sigma_i(E_i) \, \Phi(E_i, T) \, dE_i \quad w_i = (2J_i + 1)e^{-E_i/(kT)}$$

Boltzmann weights

The measured cross section σ_0 determines R_0

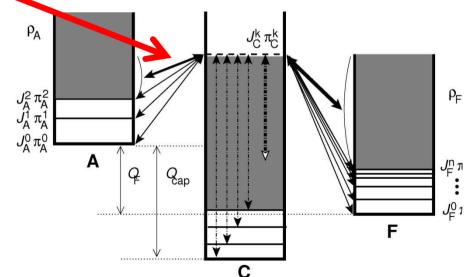
$$\sigma^{*}(E,T) = \frac{\sigma^{\text{eff}}(E)}{G_{0}(T)} = \frac{1}{\sum_{i} P_{i}} \sum_{i} \sum_{j} \frac{2J_{i} + 1}{2J_{0} + 1} \frac{E - E_{i}}{E} \sigma^{i \to j} (E - E_{i})$$

$$= \frac{1}{\sum_{i} P_{i}} \sum_{i} \sum_{j} \frac{2J_{i} + 1}{2J_{0} + 1} W_{i} \sigma^{i \to j} (E - E_{i}) ,$$

Stellar cross section

$$P_i = \frac{2J_i + 1}{2J_0 + 1} \exp\left(-\frac{E_i}{kT}\right)$$
 Population factor

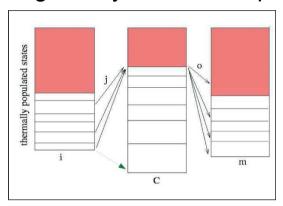
$$W_i = rac{E-E_i}{E} = 1 - rac{E_i}{E}$$
 Weight of excited state



Thermally excited target nuclei

Ratio of nuclei in a thermally populated excited state to nuclei in the ground state

is given by the Saha Equation:



$$\frac{n_{\rm ex}}{n_{\rm gs}} = \frac{g_{\rm ex}}{g_{\rm gs}} e^{-\frac{E_x}{kT}}$$

$$g = (2J + 1)$$

Ratios of order 1 for E_x~kT

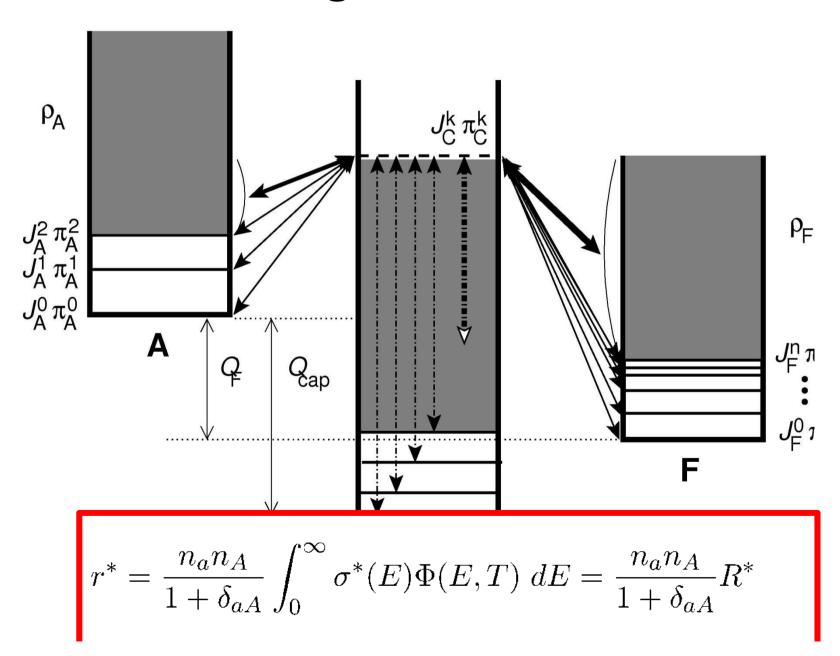
For nuclear astrophysics, location of Gamow window has to be compared to average level spacing in nuclei.

Only small correction for:

- light nuclei (level spacing several MeV)
- Gamow window at low energy: at low T
- LARGE correction, when
 - low lying (~100 keV) excited state(s) exist(s) in the target nucleus
 - temperatures are high (explosive nucleosynthesis)
 - the populated state has a very different rate

The correction for this effect has to be calculated.

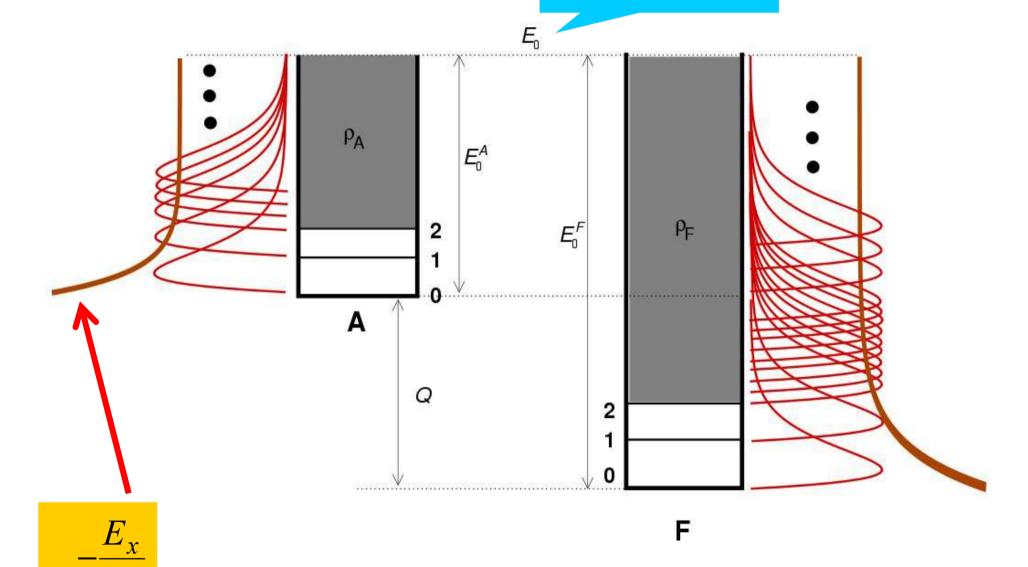
Effective weights of excited states



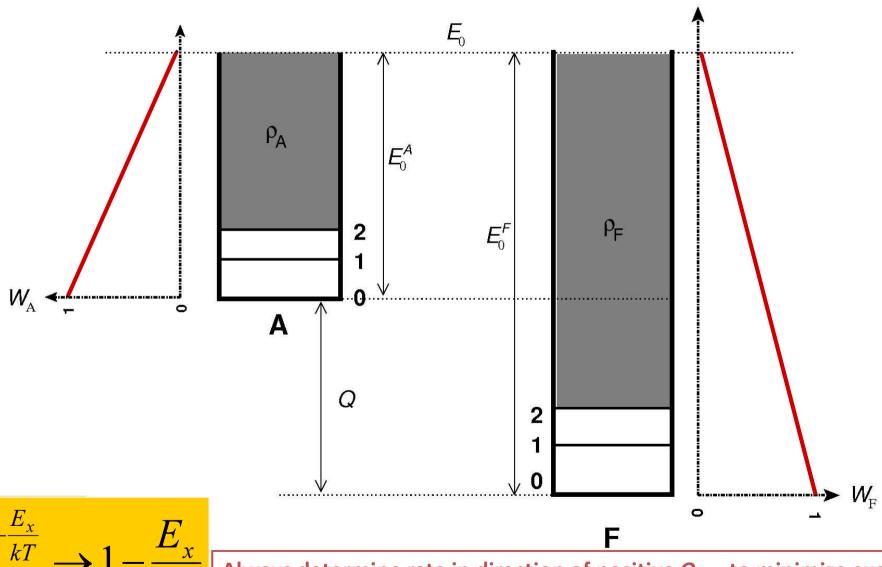
Effective weights

Gamow energy

tates



Effective weights of excited states



 $e^{-\frac{E_x}{kT}} \to 1 - \frac{E_x}{E_0}$

Always determine rate in direction of positive Q_{Aa} , to minimize exc. state contribution and numerical errors.

Ground state contribution to stellar rate

$$X = \frac{R_0}{R^* G_0} = \frac{\int \sigma^{\text{lab}}(E) \Phi_{\text{MB}}(E, T) dE}{\int \sigma^{\text{eff}}(E) \Phi_{\text{MB}}(E, T) dE}$$

$$fractional Stellar Entropy for the following fraction of the stellar Entropy for the following formula and the following formula for the following for the following formula for the following for the following formula for the following formula for the following for the followin$$

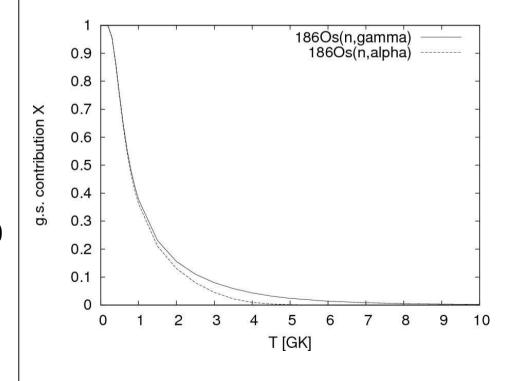
Traditional Stellar Enhancement

$$f_{ ext{SEF}} = rac{R^*}{R_0} \, { ext{(SEF does not give} top exc. state contribution!)}}$$

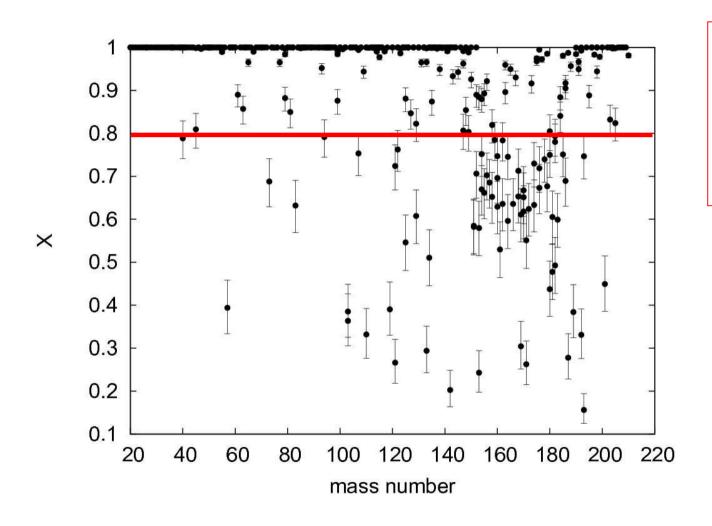
•g.s. contribution (X)

- gives g.s. contribution to stellar rate
- =1 at *T*=0
- confined to 0<=X<=1
- monotonically decreasing to 0
- Uncertainty scales with G₀ and is related to X:

•
$$u = (1 - X)u'$$



Ground-state contributions to s-process neutron capture?

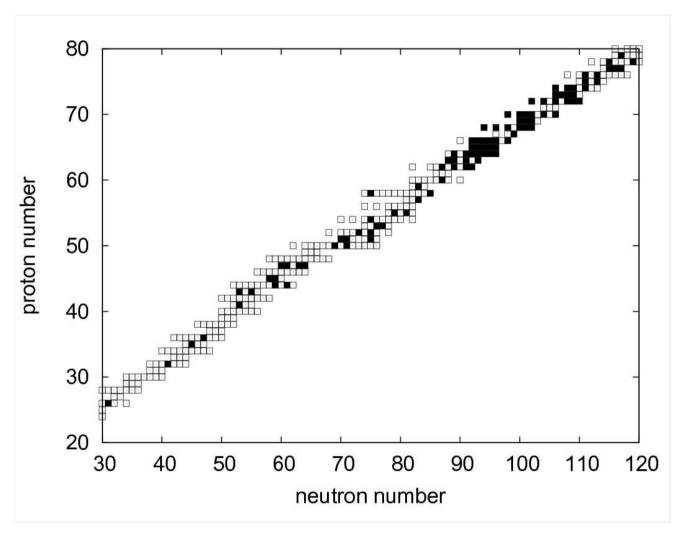


X directly also gives the maximally possible reduction in (theory) uncertainty by experiments!

- Nuclides from KADoNiS
- (n, γ) at kT=30 keV

Rauscher P. Mohr, I. Dillmann, R. Plag; Ap. J. 738 (2011) 143.

Ground-state contributions to s-process neutron capture?

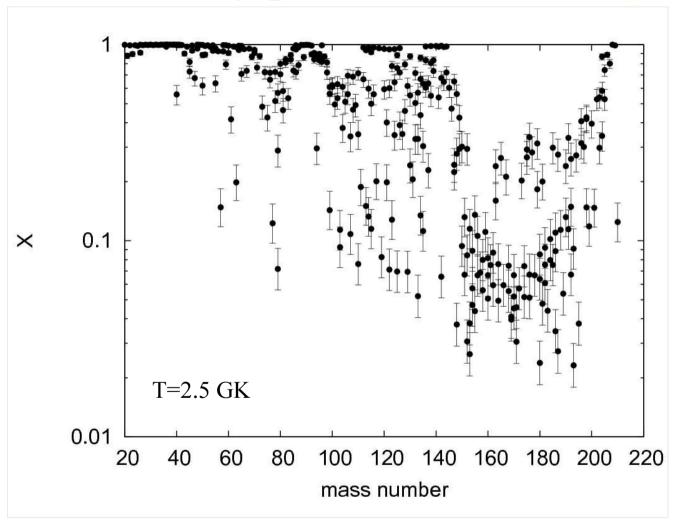


X directly also gives the maximally possible reduction in (theory) uncertainty by experiments!

- Nuclides from KADoNiS
- (n, γ) at kT=30 keV

Black squares are nuclei for which error cannot be reduced by more than 80%

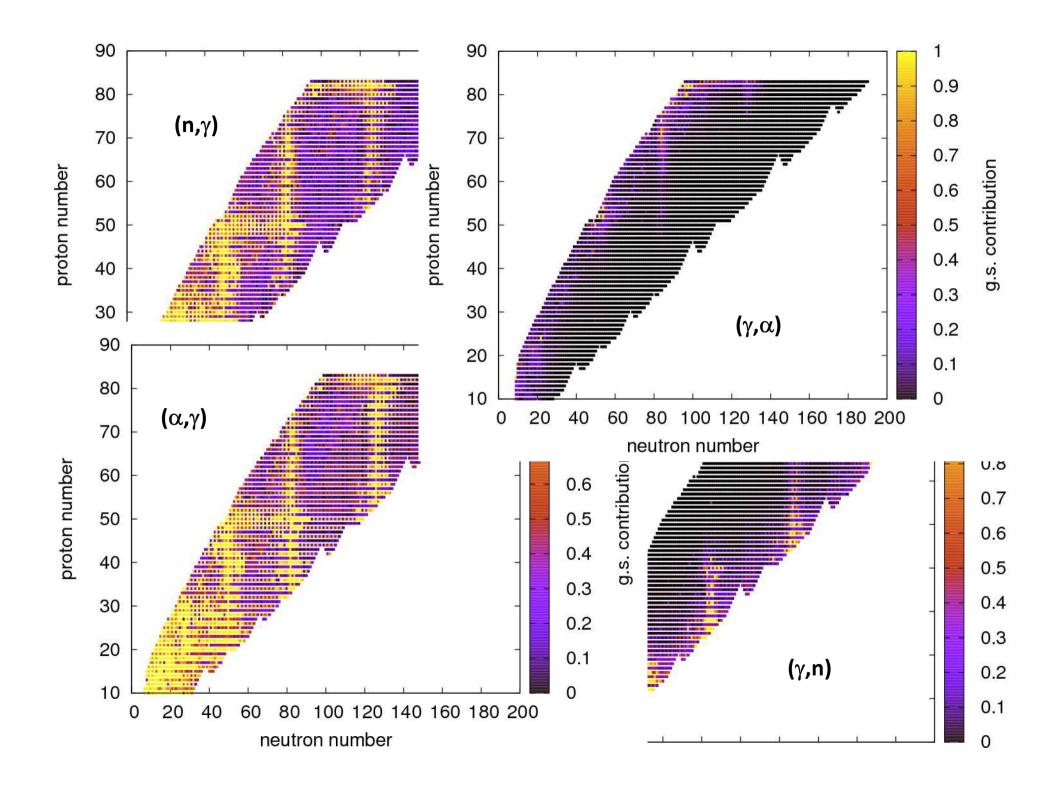
Rauscher P. Mohr, I. Dillmann, R. Plag; Ap. J. 738 (2011) 143.



X directly also gives the maximally possible reduction in (theory) uncertainty by experiments!

Nuclides from KADoNiS

Rauscher P. Mohr, I. Dillmann, R. Plag; Ap. J. 738 (2011) 143.



g.s. Contributions in Stellar Photodisintegration Rates

Target	(γ,n) g.s contribution $(T_9=2.5)$
$^{86}\mathrm{Sr}$	0.00059
$^{90}{ m Zr}$	0.00034
$^{96}{ m Zr}$	0.0061
⁹⁴ Mo	0.0043
$^{-142}\mathrm{Nd}$	0.0028
$^{155}\mathrm{Gd}$	0.0012
$^{186}\mathrm{W}$	0.00049
$^{185}\mathrm{Re}$	0.00021
$^{187}\mathrm{Re}$	0.00024

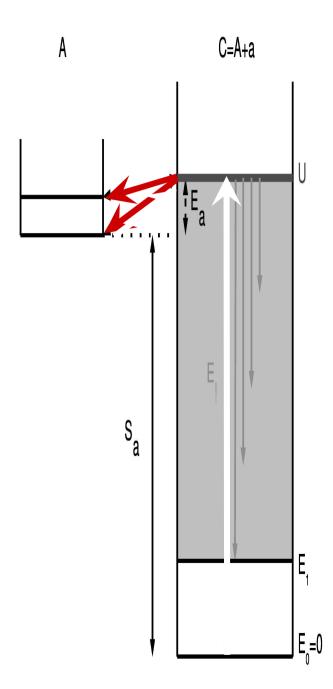
Target	(γ,n) g.s contribution $(T_9=2.5)$
$^{186}\mathrm{Os}$	0.00016
$^{190}\mathrm{Pt}$	0.000069
$^{192}\mathrm{Pt}$	0.00011
$^{198}\mathrm{Pt}$	0.0018
$^{197}\mathrm{Au}$	0.00035
$^{196}\mathrm{Hg}$	0.00043
$^{198}\mathrm{Hg}$	0.00084
$^{204}\mathrm{Hg}$	0.0088
$^{204}\mathrm{Pb}$	0.0059

Always determine rate in direction of CAPTURE, to maximize g.s. contribution and numerical errors. (For numerical stability in reaction networks, forward and backward rates have to be computed from ONE source!)

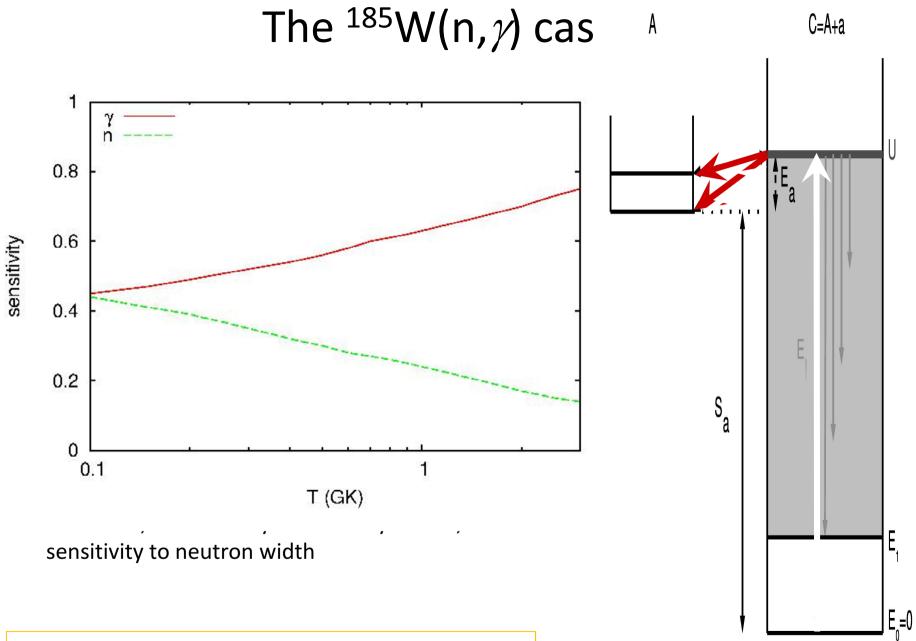
EXCEPTION: Coulomb suppression effect of excited state contributions (PRL 101, 191101; PRC 80 (2009) 035801) when larger Coulomb barrier in entrance channel of reaction with negative Q-value.

The 185 W(n, γ) case

- 185 W(n, γ) is important in s-process branching, 185 W unstable
- 9% exp. uncertainty quoted in KaDoNiS database
- This is from rescaled prediction compared to (γ,n) data!
 - For $(n, \gamma) X_0 = 0.98 0.75$, for kT = 8 30 keV
 - Therefore rate error would be strongly constrained by experiment
 - For $(\gamma, n) X_0 = 0.007 0.005$, no constraint!
 - Only helpful, if same error applies to all γ -transitions
 - Unlikely, because main contribution comes from <u>lower</u>
 <u>y-energies</u> further away from GDR
 - Moreover, not the only uncertainty in rate, also sensitivity to neutron width

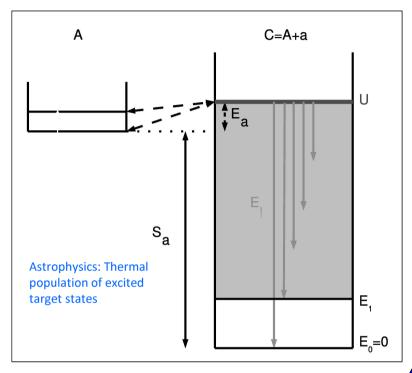


Uncertainty in this rate not yet constrained!



Uncertainty in this rate not yet constrained!

Relevant γ -transition energies for capture



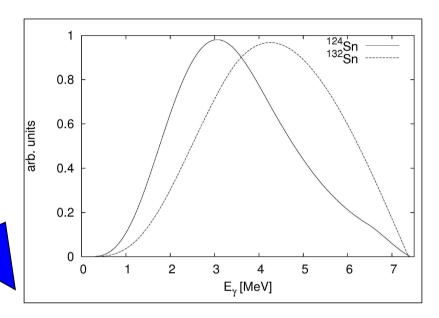
Competition between level density increase and decrease of transition strength:

$$\rho \propto \frac{\mathrm{e}^{2\sqrt{aU}}}{U^{5/3}}$$

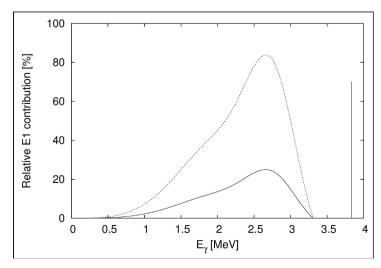
$$T_{\rm E1} \propto \frac{\Gamma_{\rm GDR} {E_{\gamma}}^4}{\left({E_{\gamma}}^2 - {E_{
m GDR}}^2\right)^2 + {\Gamma_{
m GDR}}^2 {E_{\gamma}}^2}$$

$$T_{\rm M1} \propto {E_{\gamma}}^3$$

Rauscher, PRC 78 (2008) 032801(R)



Transition to g.s. or isolated excited states often suppressed by selection rules:



Combination of theory and measurement for stellar rate

How to combine theory and measurement in a revised stellar rate

$$X_i(T) = \frac{2J_i + 1}{2J_0 + 1} e^{-E_i/(kT)} \frac{\int \sigma_i(E)\Phi(E, T)dE}{\int \sigma^{\text{eff}}(E)\Phi(E, T)dE}$$

Contribution of i-th excited state

Here, we use measured g.s. reactivity as example:

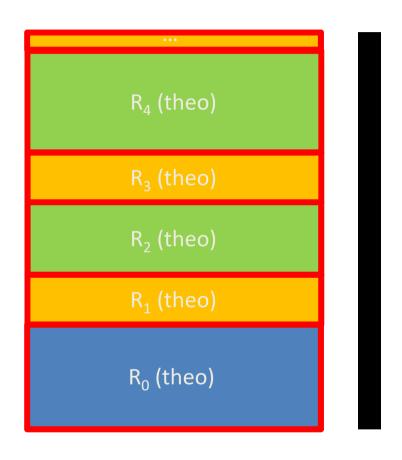
$$X_0(T) = \frac{\int \sigma_0(E)\Phi(E,T)dE}{\int \sigma^{\text{eff}}(E)\Phi(E,T)dE}$$

Contribution of g.s. state

One of two assumptions can be made, either:

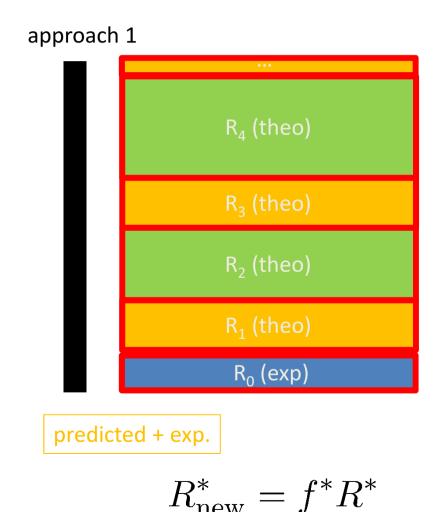
- 1. adopt only what has been measured, or
- 2. include some <u>theoretical</u> considerations (correlations between g.s. and exc. states)

Derivation of *stellar* reactivity using *experimental* g.s. contribution

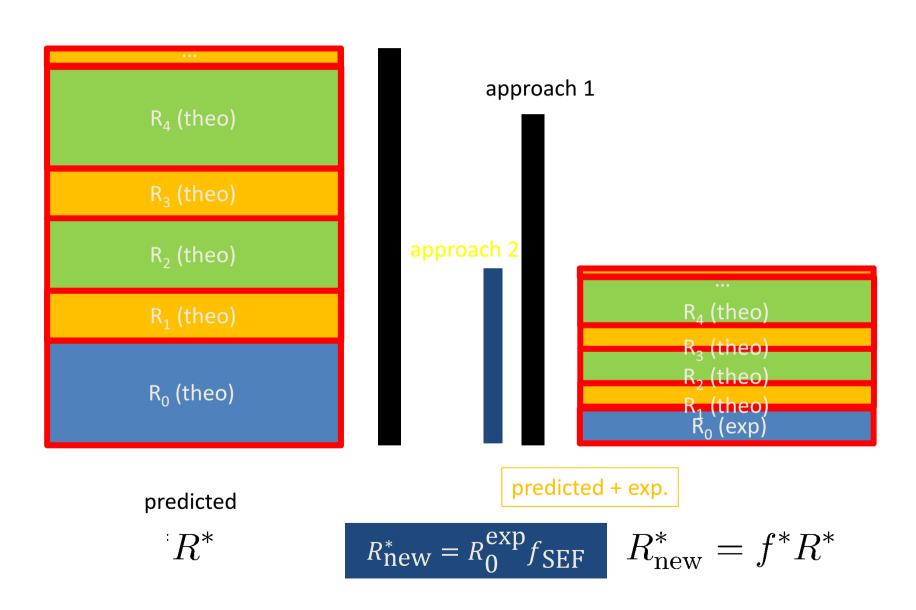


predicted

 R^*



Derivation of *stellar* reactivity using *experimental* g.s. contribution



How to combine theory and measurement in a revised stellar rate

Approach 1: Use experimental information without further assumptions

$$X_0(T) = \frac{\int \sigma_0(E)\Phi(E,T)dE}{\int \sigma^{\text{eff}}(E)\Phi(E,T)dE}$$

Contribution of g.s. state

$$R_{\text{new}}^* = f^* R^*$$

Multiply the *theoretical* stellar reactivity by a factor *f**

$$f^* = 1 + X_0 \left(\frac{R_0^{\text{exp}}}{R_0} - 1 \right)$$

 $f^*=1+X_0\left(rac{R_0^{
m exp}}{R_0}-1
ight)$ The factor contains the *theoretical* and experimental g.s. reactivity and the g.s. The factor contains the theoretical and the contribution.

$$U_{\text{new}}^* = U_{\text{exp}} + (U^* - U_{\text{exp}})(1 - X_0)$$

The uncertainty factor of the revised reactivity is calculated from a combination of theoretical and experimental uncertainty.

How to combine theory and measurement in a revised stellar rate

Approach 2: Include additional theory assumptions

Can excited state contributions be renormalized by the same factor as theory R_0 ?

$$X_0(T) = \frac{\int \sigma_0(E)\Phi(E,T)dE}{\int \sigma^{\text{eff}}(E)\Phi(E,T)dE}$$

Contribution of g.s. state

$$R_{\text{new}}^* = f^* R^*$$

Multiply the *theoretical* stellar reactivity by a factor *f**

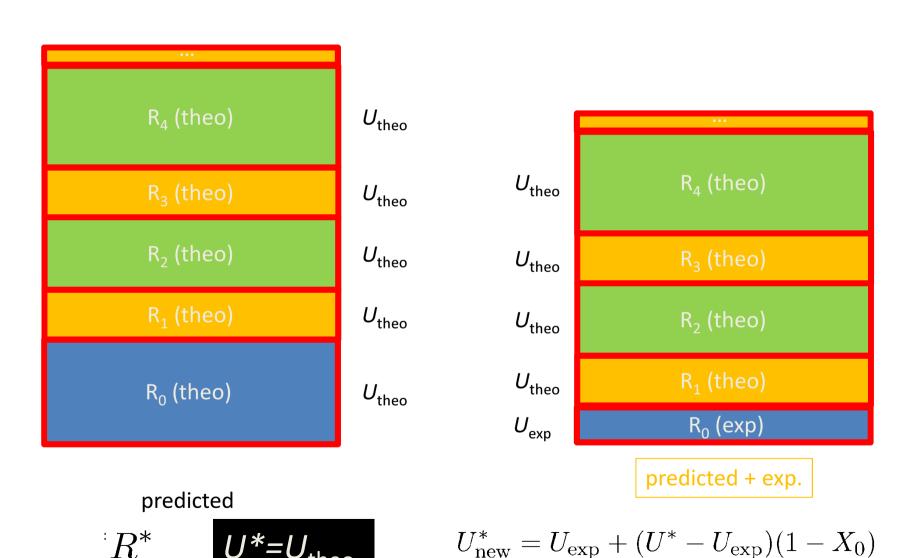
$$f^* = \frac{R_0^{\text{exp}}}{R_0} = f_{SEF}$$

$$U_{\text{new}}^* =$$
?

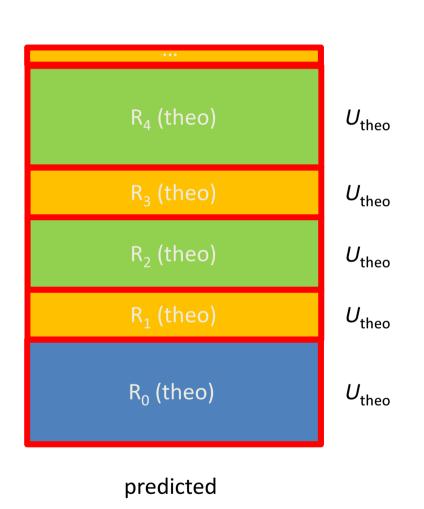
The uncertainty factor of the revised reactivity is calculated from a combination of theoretical and experimental uncertainty., if $X_0 < 1$

What about uncertainties? (aka "error bars")

Stellar rate uncertainty in approach 1 (only experimental information)



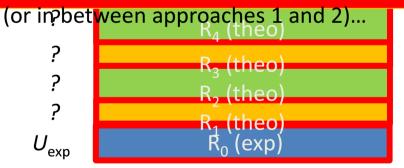
Stellar rate uncertainties in approach 2 (renormalize all excited state contributions)



Are uncertainties in all excited state contributions from same source (correlated) and show same relative impact on exc. state transitions??

- If so, then $U^*_{\text{new}} = U_{\text{exp}}$
- If there are different sources of uncertainty, then scaling may remove theory uncertainty only partially or not at all!

Then we are back to approach 1



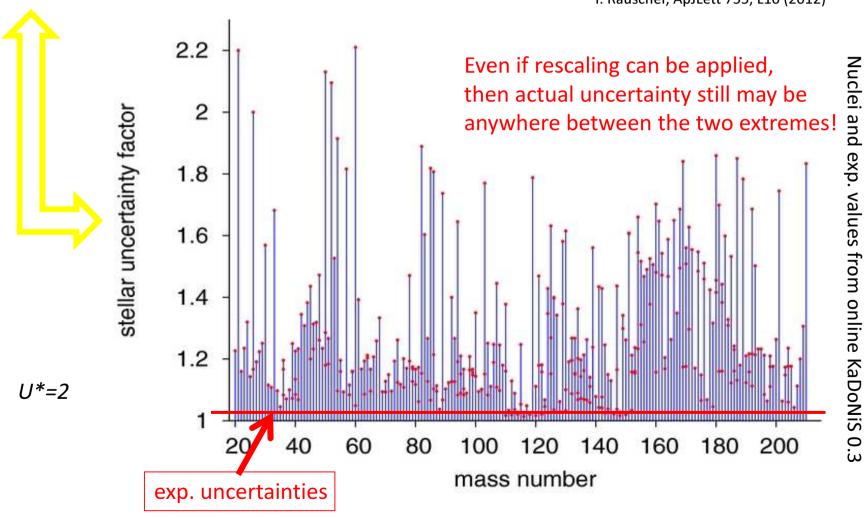
predicted + exp.

$$R_{\text{new}}^* = R_0^{\text{exp}} f_{\text{SEF}}$$

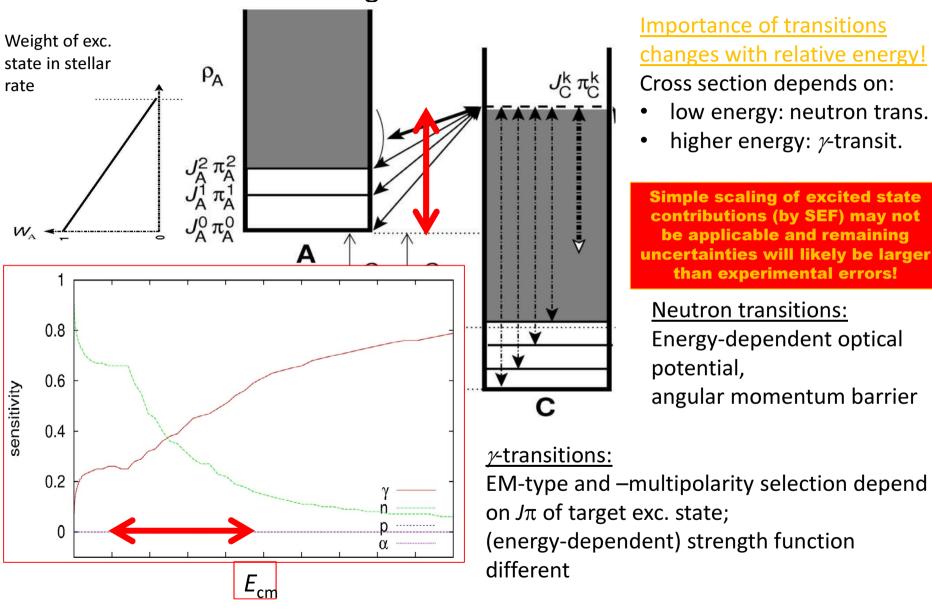
Realistic uncertainties in stellar (n, γ) rates close to stability (for s-process)

$$U_{\text{new}}^* = U_{\text{exp}} + (U^* - U_{\text{exp}})(1 - X_0)$$

T. Rauscher, ApJLett 755, L10 (2012)



Differences in uncertainties of neutron captures from g.s. and excited states



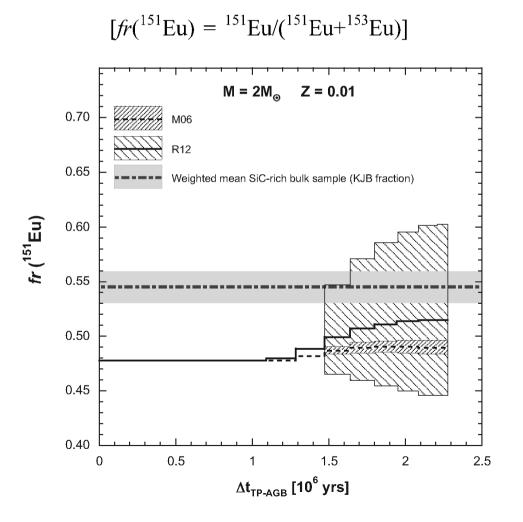
A practical application:

The ¹⁵¹Eu/Eu ratio in stars and meteoritic grains

Isotopic information from 2 CEMP(r+s) stars (Aoki et al, 2003).

New meteoritic data: individual mainstream grains (LS+LU) and SiC-enriched bulk sample (KJB) from Murchison meteorite (Avila et al, 2013).

J. N Avila et al; Ap. J. Lett. 768 (2013) L18



CEMP stars have low metallicity, meteorite data from close to solar metallicity star: both show *fr* higher than solar!

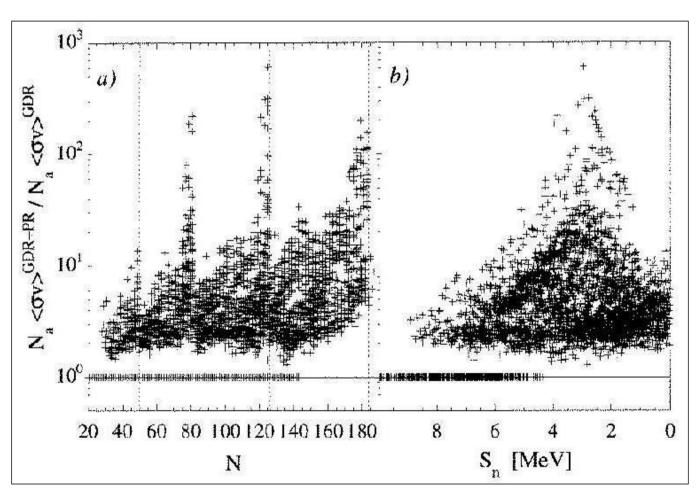
$$fr \propto \frac{1}{\left\langle 151 \operatorname{Sm}(n,\gamma) \right\rangle}$$

- M06...Marrone et al (2006) rate with exp. uncertainties
- R12...Rate including Marrone et al (2006) for the g.s. cross section but using the prescription as given by Rauscher (2012) for the stellar rate and its uncertainty



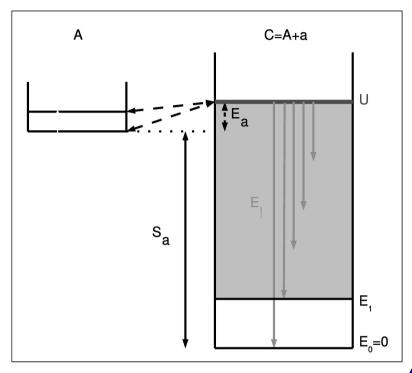
Pygmy resonance

Possible Impact of Pygmy Resonances Far Off Stability?



Goriely 1999 Rauscher 1999

Relevant γ -transition energies for capture



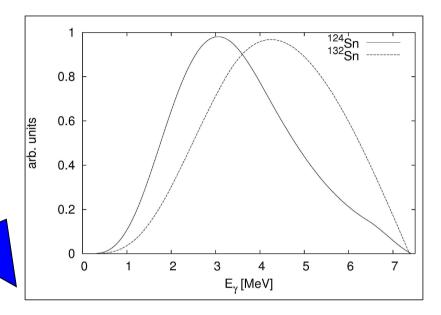
Competition between level density increase and decrease of transition strength:

$$\rho \propto \frac{\mathrm{e}^{2\sqrt{aU}}}{U^{5/3}}$$

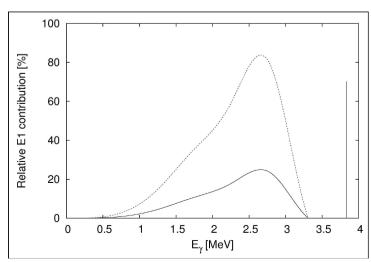
$$T_{\rm E1} \propto \frac{\Gamma_{\rm GDR} E_{\gamma}^{\ 4}}{\left(E_{\gamma}^{\ 2} - E_{\rm GDR}^{\ 2}\right)^2 + \Gamma_{\rm GDR}^{\ 2} E_{\gamma}^{\ 2}}$$

$$T_{\rm M1} \propto E_{\gamma}^{-3}$$

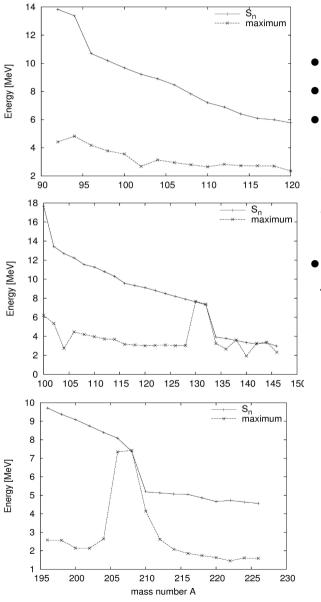
Rauscher, PRC 78 (2008) 032801(R)



Transition to g.s. or isolated excited states often suppressed by selection rules:

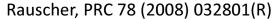


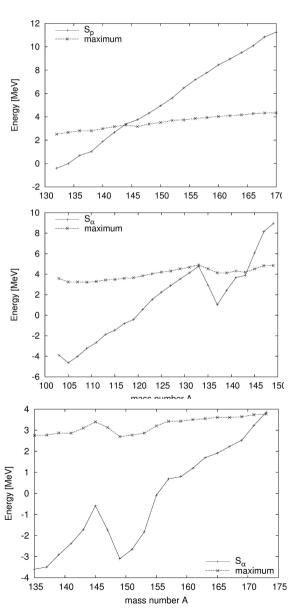
Location of maximum contribution at astrophysically relevant reaction energies



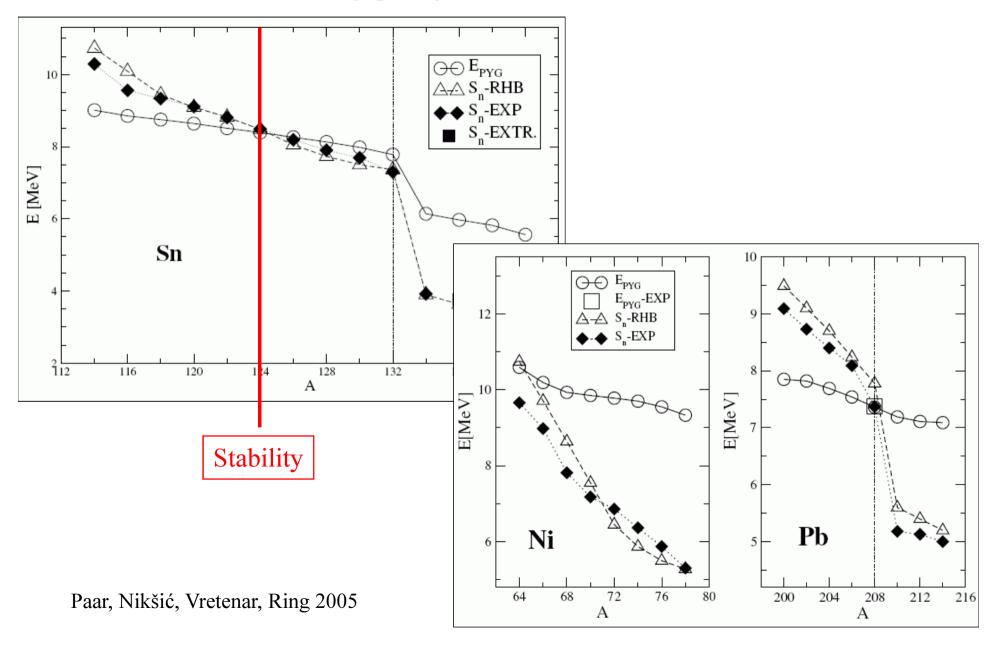
- Maxima located at 2-4 MeV
- quite independent of reaction
- Exception: nuclei with low level density (magic numbers or close to drip) → maximum shifted to higher energies (isolated states)
- Hauser-Feshbach not valid for exceptions

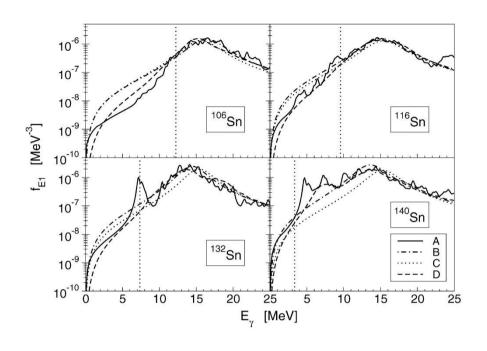
Important to judge relevance of modification of γ transition strength (e.g. pygmy resonance)



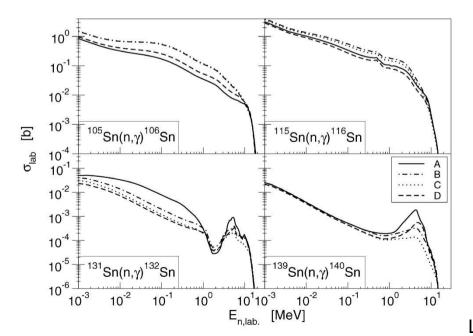


Pygmy Predictions





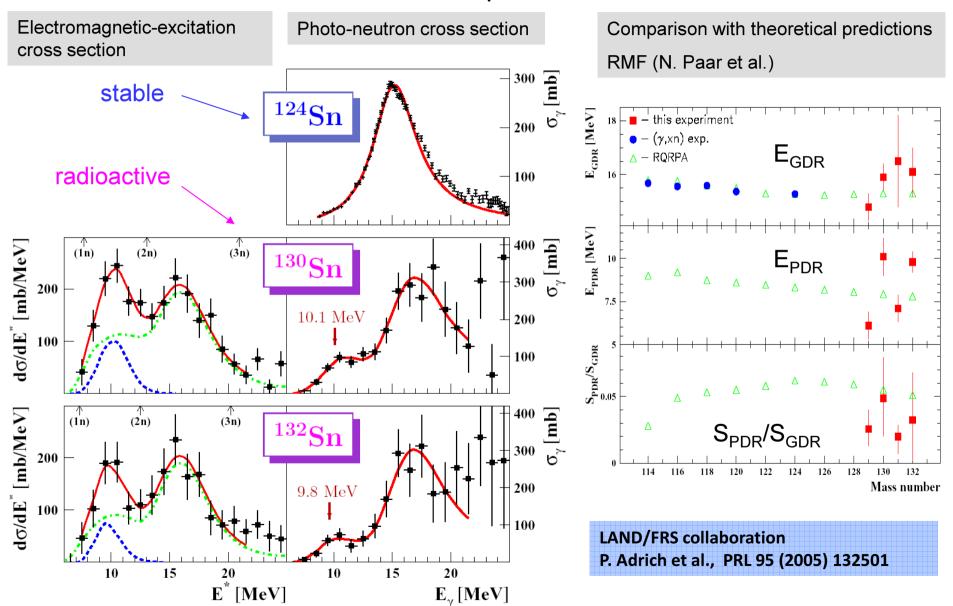
γ-Strengths and Pygmy Resonances in Neutron Captures



- Captures on ^{105,115}Sn: $E_{\gamma} \approx E_{\rm n} + 3 \text{ MeV}$
- Captures on ^{131,139}Sn: $E_{\gamma} \approx E_{\rm n} + S_{\rm n}$

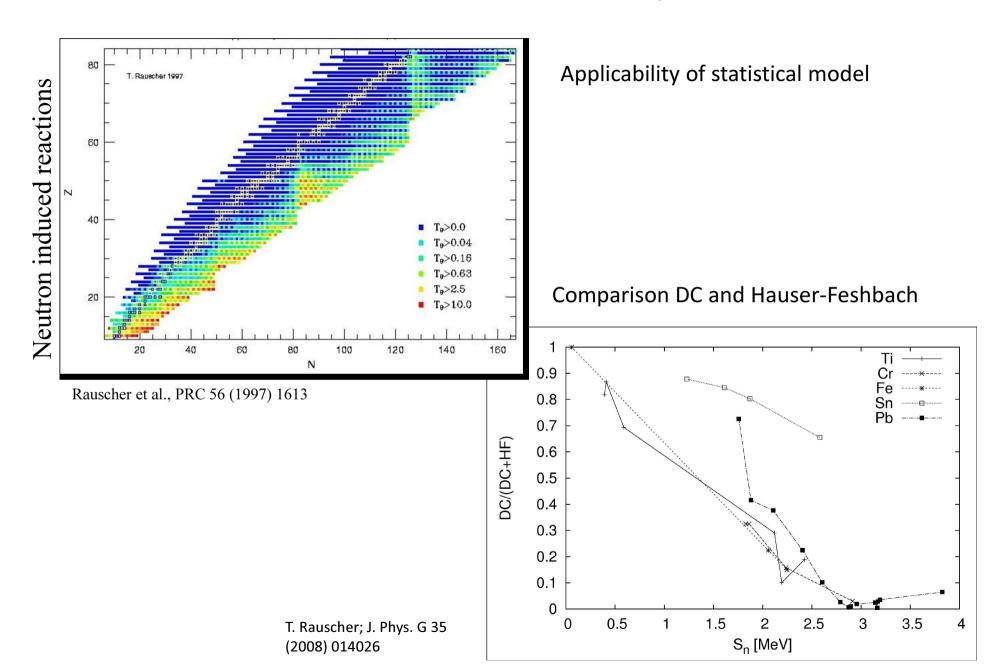
Litvinova et al, NP A823 (2009) 26

Results: Dipole-strength distributions in neutron-rich Sn isotopes

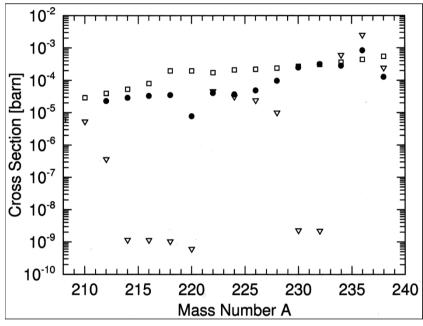


Direct Capture Far Off Stability

Reaction Mechanism Comparison



Direct Neutron Capture On Pb- and Sn-Isotopes



10⁻³
10⁻⁴
10⁻⁴
10⁻⁴
10⁻⁴
10⁻⁴
10⁻⁴
10⁻⁴
10⁻⁴
10⁻⁴
1125
130
135
140
145

(30 keV neutrons)

Pb

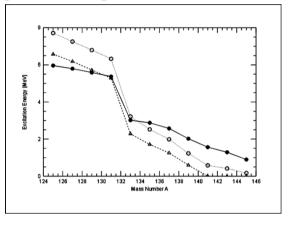
- >HFB: Squares
- >RMFT: Triangles
- >FY: Dots

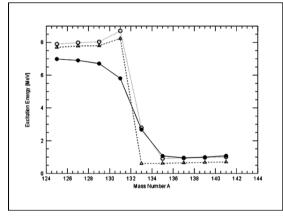
Large differences in predictions due to differences in predicted spectroscopy and masses (separation energies)

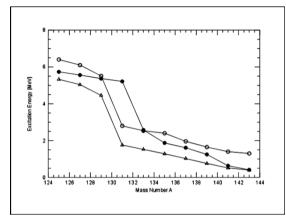
Sn

Nuclear Structure Characteristics of Sn-Isotopes

triangles: $1/2^-$, open circles: $3/2^-$, full dots : S_n





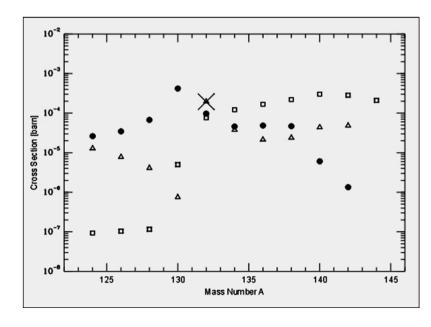


HFB

RMFT (NL-SH)

FY (FRDM)

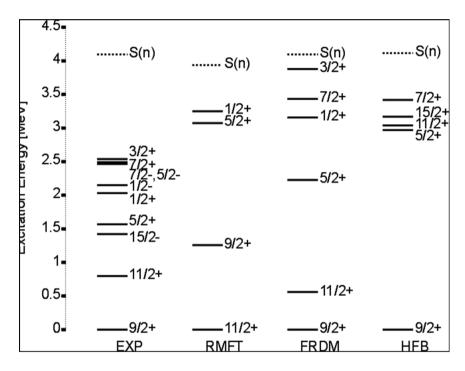
Direct neutron capture (30 keV)

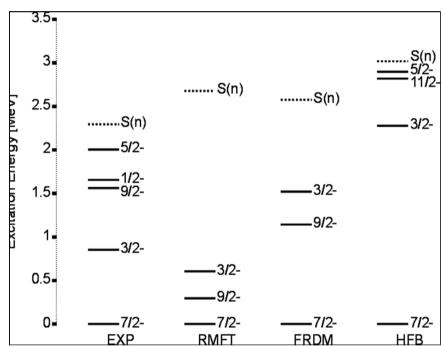


- >HFB: Squares
- >RMFT: Triangles
- >FY: Dots
- >Exp. levels: Cross

Rauscher et al. 1998

Comparison With Experimental Levels



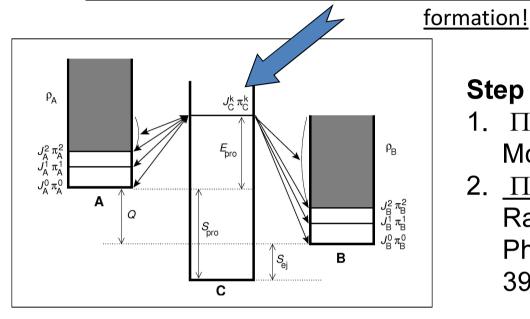


²⁰⁹Pb

¹³³Sn

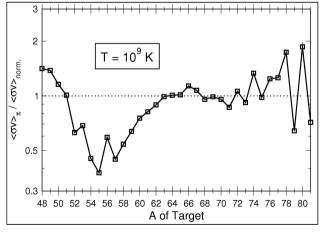
Modified Hauser-Feshbach model

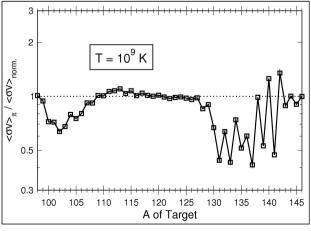
<u>Lifting assumption that all spins and parities are available for compound nucleus</u>



Step A: Parity dependence

- 1. Π -dep. in initial/final channels: Mocelj et al., PRC 75, 045805
- 2. <u>Π-dep. of compound formation!</u> Rauscher 2007; Loens et al., Phys. Lett. B 666, 395 (2008)

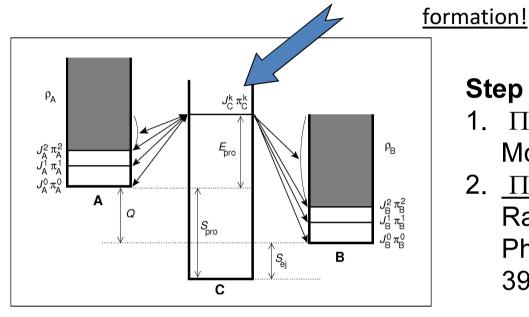




Factor of 2 effect; largest factors for nuclei with low level densities (far off stability)

Modified Hauser-Feshbach model

<u>Lifting assumption that all spins and parities are available for compound nucleus</u>



Step A: Parity dependence

- 1. Π -dep. in initial/final channels: Mocelj et al., PRC 75, 045805
- 2. <u>Π-dep. of compound formation!</u> Rauscher 2007; Loens et al., Phys. Lett. B 666, 395 (2008)

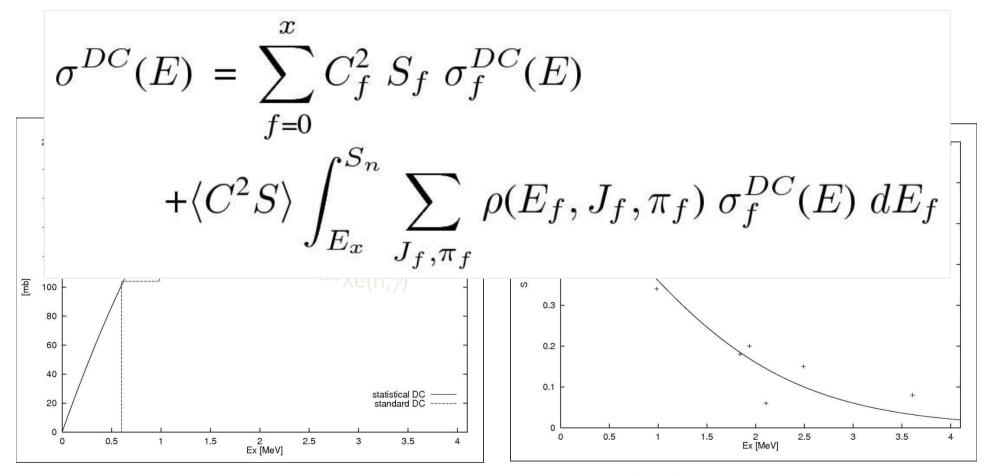
Step B: Spin dependence

- 1. Spin distribution at compound formation energy
- Dependence on level density in compound nucleus → suppression factor

(Rauscher 2007, 2009, 2010)

Averaged DC

- Average over levels (level density) instead of discrete states
- Spectroscopic factors: constant or averaged



Rauscher 1996; Hauser et al. 1997; Goriely 1997; Rauscher; J. Phys. G 35 (2008) 014026

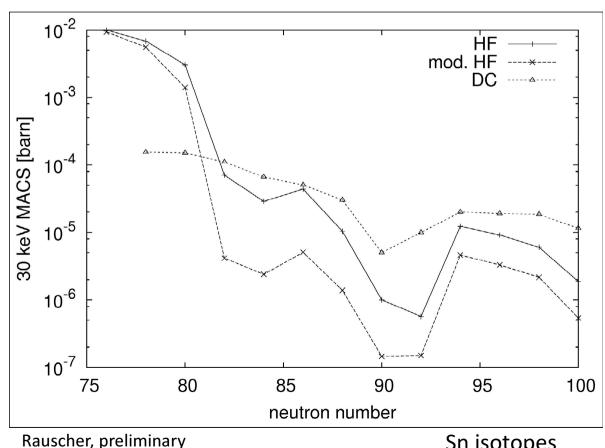
DC vs Statistical Model

Compound formation is overestimated at low level density: modification of stat. model (Hauser-Feshbach) rates necessary! Renormalization scales with NLD in compound nucleus at formation energy.

So far, unmodified stat. mod. rates are also employed in astrophysical calculations far off stability without (or only in few cases) consideration of DC.

Considering uncertainties, this may not be completely wrong:

- 1. If Nuclear Statistical Equilibrium is achieved, rates far off stability (where DC dominates) are not relevant (only masses)
- 2. DC may compensate for overestimated stat. rate



Sn isotopes

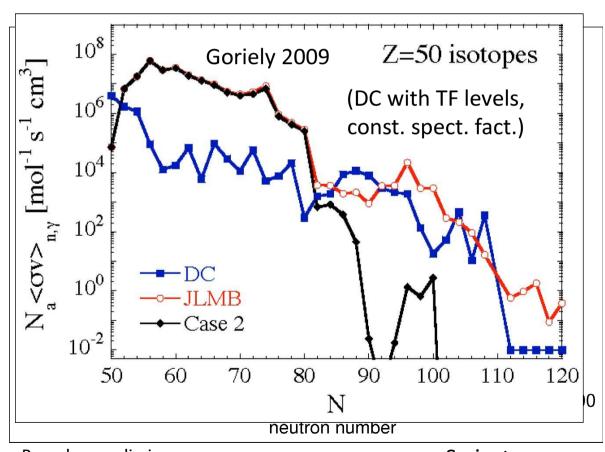
DC vs Statistical Model

Compound formation is overestimated at low level density: *modification of stat. model* (Hauser-Feshbach) rates necessary! Renormalization scales with NLD in compound nucleus at formation energy.

So far, unmodified stat. mod. rates are also employed in astrophysical calculations far off stability without (or only in few cases) consideration of DC.

Considering uncertainties, this may not be completely wrong:

- 1. If Nuclear Statistical
 Equilibrium is achieved,
 rates far off stability
 (where DC dominates)
 are not relevant (only
 masses)
- 2. DC may compensate for overestimated stat. rate



Rauscher, preliminary

Sn isotopes

DC vs Statistical Model

Compound formation is overestimated at low level density: *modification of stat. model* (Hauser-Feshbach) rates necessary! Renormalization scales with NLD in compound nucleus at formation energy.

So far, unmodified stat. mod. rates are also employed in astrophysical calculations far off stability without (or only in few cases) consideration of DC.

Considering uncertainties, this may not be completely wrong:



- If Nuclear Statistical Equilibrium is achieve rates far off stability (where DC dominates are not relevant (only masses)
- 2. DC may compensate overestimated stat. ra

Additional complication:

Spectroscopic factors for transitions from (thermally populated) excited states!

Perhaps small in most cases (because overlap wavefunction small) but never calculated.

neutron number

Rauscher, preliminary

Sn isotopes

Possible (simple) Modifications of Reaction Theory

- Modification of Hauser-Feshbach (H-F) model to account for incomplete spin and parity distribution at compound formation energy
- Modification of direct capture calculation by using "Averaged Direct Capture" (inspired by statistical model)
- Improved spectroscopic factors for DC
 - from BCS population of states
 - "Averaged" spectroscopic factor (but excitation energy dependent)
 - Spectroscopic factors also for transitions initiated on excited states
 - usual spectroscopic factors are measured/calculated relative to target ground state!
- Calibration of H-F relative to DC from absorptive part of global optical potential

Some of these things have already been tried locally but global calculation still missing; planned for inclusion in the SMARAGD code.

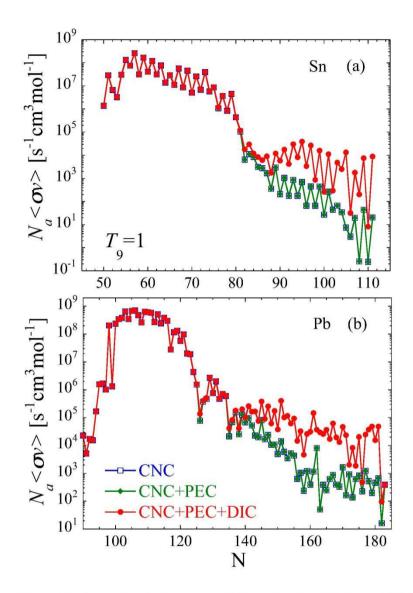


FIG. 3. (Color online) Total (CNC + PEC + DIC), CNC + PEC, and CNC reaction rates for (a) Sn and (b) Pb isotopic chains (from the proton to the neutron drip lines) at $T_9 = 1$ (T_9 denotes the temperature in 10^9 K).

Neutron Capture Predictions

Xu et al, PRC 90, 024604 (2014)

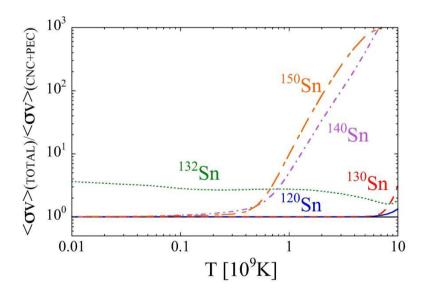
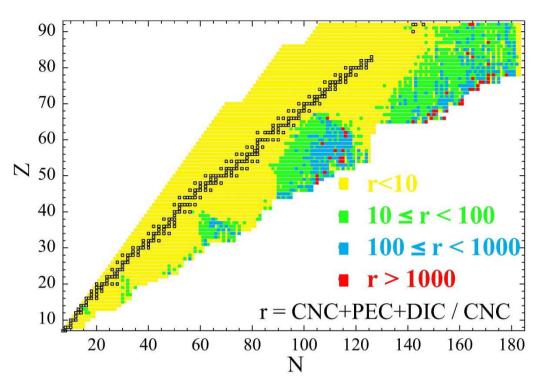
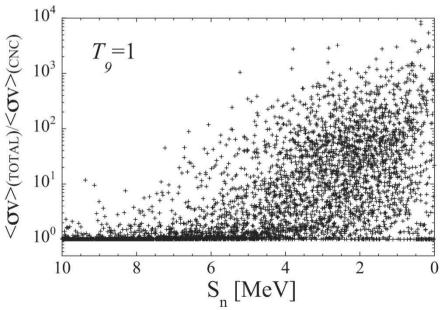


FIG. 4. (Color online) Ratio between the total (CNC + PEC + DIC) and CNC + PEC reaction rates for five Sn isotopes as a function of the temperature.



Neutron Capture Predictions

Xu et al, PRC 90, 024604 (2014)



r-Process yields (neutrino-driven wind)

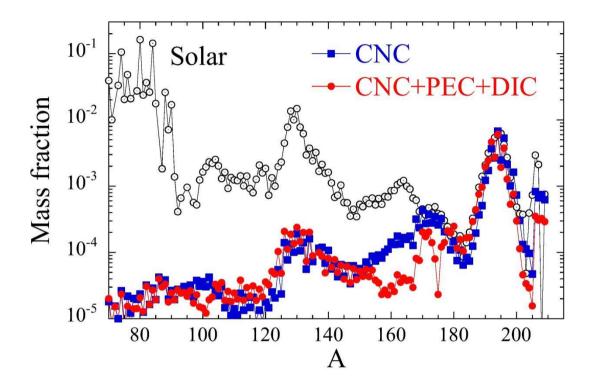


FIG. 7. (Color online) Distributions of the r-nuclide abundances obtained within the neutrino-driven wind corresponding to an entropy S = 200, electron fraction $Y_e = 0.41$, mass-loss rate $dM/dt = 6 \times 10^{-7} M_{\odot} \text{ s}^{-1}$, and breeze solution $f_w = 3$ (see Refs. [1,67] for more details). The distributions are compared with the solar r-abundance distribution (dotted circles).

r-Process yields (neutron star merger)

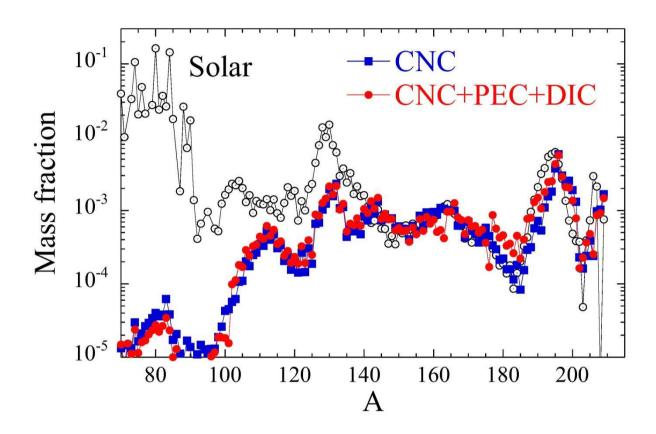
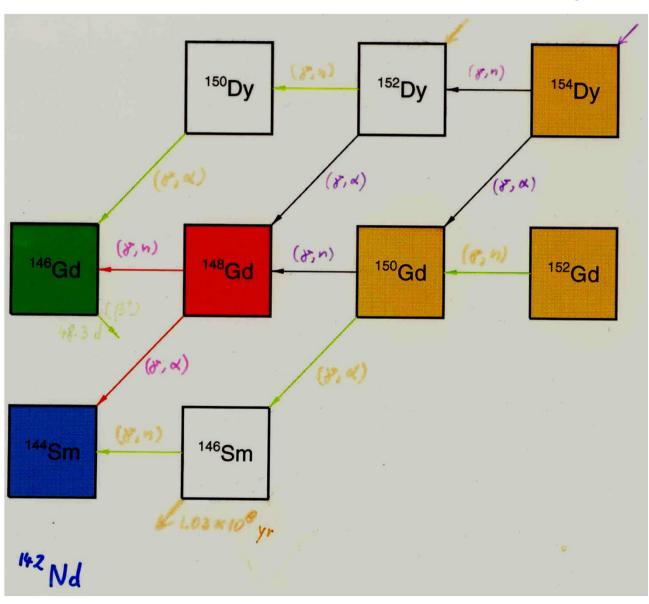


FIG. 8. (Color online) Final nuclear-abundance distributions of the ejecta from a $1.35-1.35M_{\odot}$ (squares) neutron star merger as functions of atomic mass. The distributions are normalized to the solar r-abundance distribution (dotted circles).

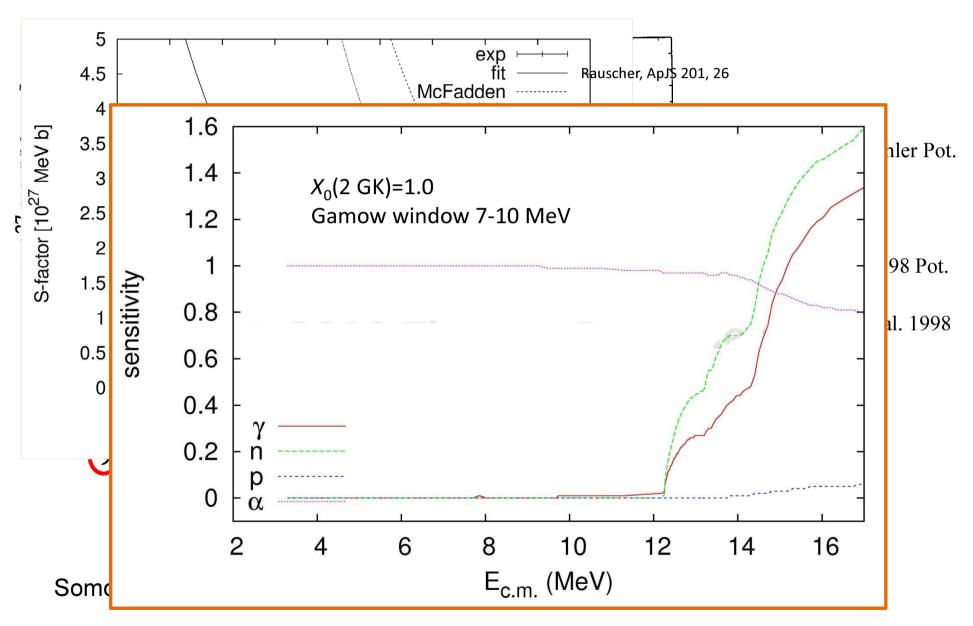
Studies of the α +nucleus optical potential for the γ -process

Network for Nd/Sm

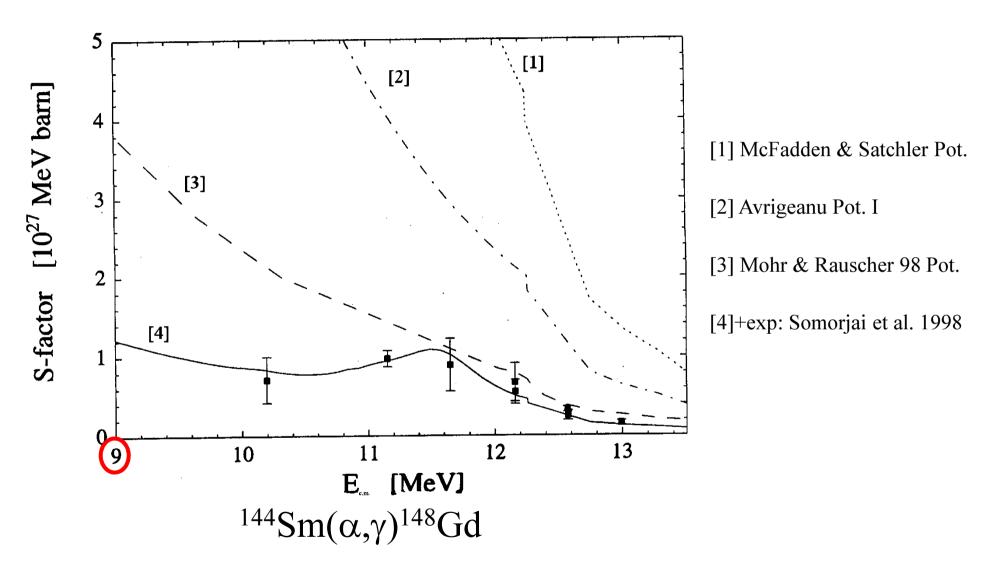


- Ratio ¹⁴⁴Sm/¹⁴²Nd in the early solar system can be studied in meteoritic material.
- Allows inference of production ratio in ccSN.
- Production ratio depends only on (γ,α)/(γ,n) branching on
 148Gd.
- 148 Gd(γ,α) can be computed from 144 Sm(α,γ)!

Problem with α +144Sm Potential

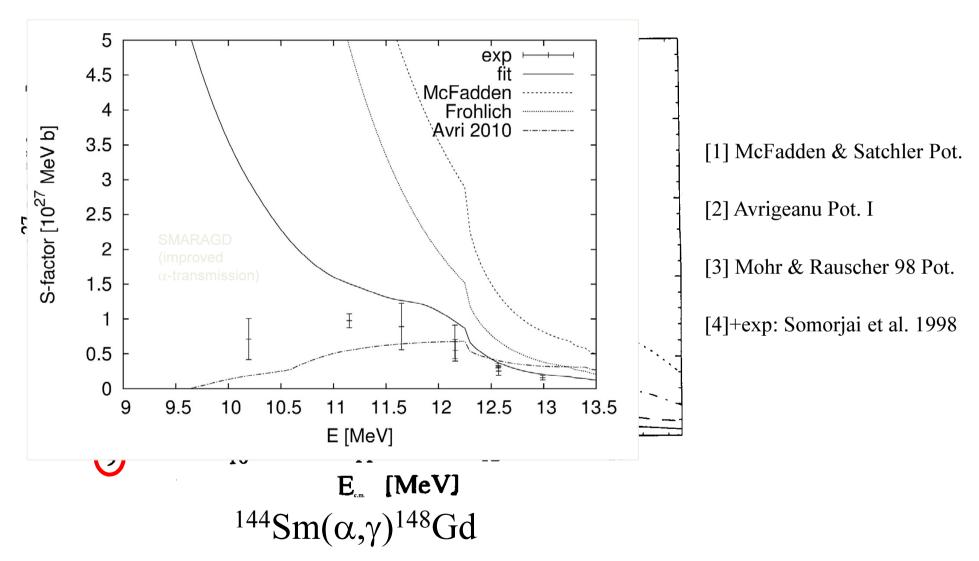


Problem with α +144Sm Potential



Somorjai et al, A&A 333, 1112 (1998)

Problem with α +144Sm Potential



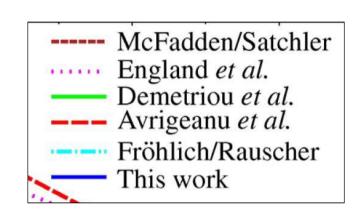
Somorjai et al, A&A 333, 1112 (1998)

Problem with optical α +nucleus potential at subCoulomb energies

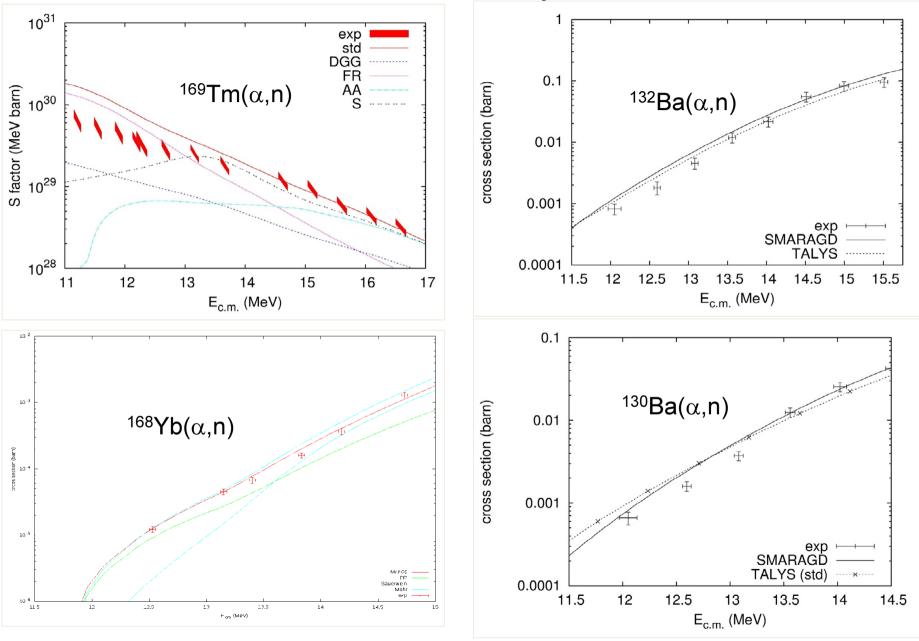
- General factor 2-3 overprediction of exp. cross section found for p-rich nuclei at low energy
- Can translate into up to a factor of 10 difference at astrophysical energy
- Phenomen. potential fitted to reaction cross sections (Frohlich et al 2003) can reproduce c.s. over wide range of masses; but does not describe scattering
- Local potentials can be constructed describing reaction and scattering
- Global solution??
 - Many attempts but not really successful so far
- Recent idea: Perhaps not problem of potential but of reaction model, not all channels included in compound reaction?

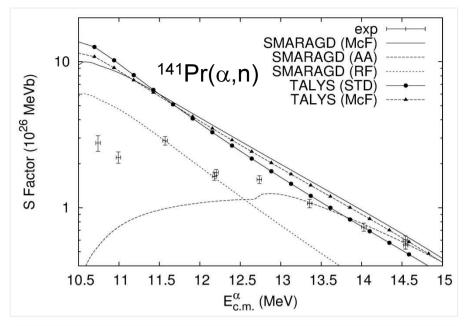
Various approaches for "global" optical α +nucleus potential were tried

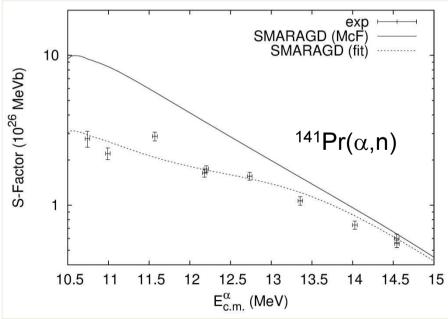
- Real part:
 - Folding
 - E-independent Woods-Saxon
 - E- , A-, Z-dependent Woods-Saxon
- Imaginary part:
 - constant Woods-Saxon
 - volume+surface W-S with E-, A-, Z-dependence
- Parameters derived from
 - fit to scattering data
 - fit to reaction data
 - theoretical considerations
- Strong sensitivity to Coulomb radius parameter
 - often not discussed



Some examples



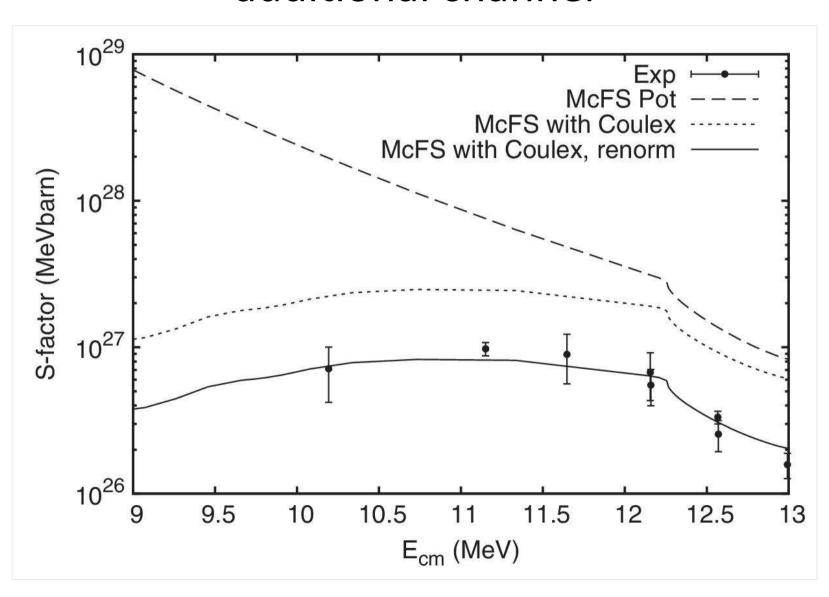


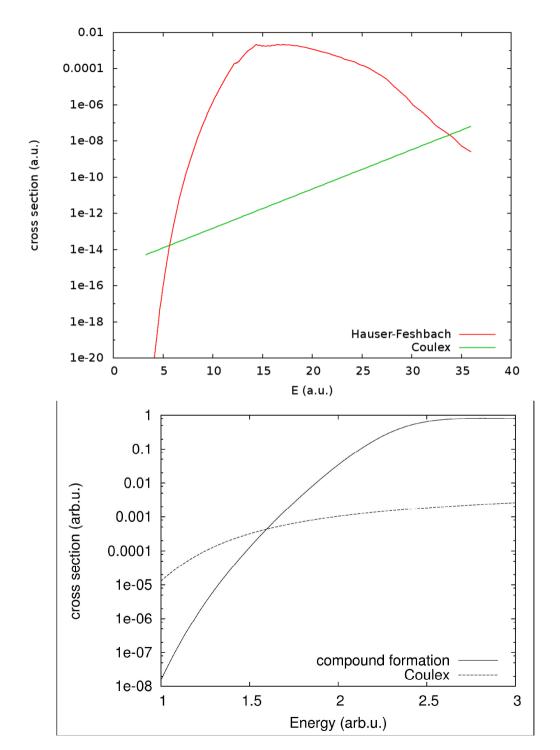


Data Summary:

- Data are scarce, mostly known at either lower charge and/or higher energy
- Only few cases known with:
 - Large Z
 - Low energy (close to astrophysical region or region where α-width is dominating)
 - Or low-energy (α, n)
- No scattering data at low energy
- Above Sn: Some deviations found but not consistently; some reactions can still be described with standard McFadden/Satchler potential, others show factor of 2-3 overprediction (144Sm is extreme case!)
- Local potentials in principle possible but do not provide much information for astrophysics rates
- "Global" potentials cannot globally describe data

With low-energy Coulomb excitation as additional channel





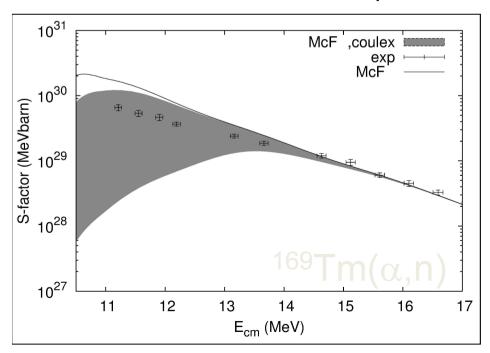
- Coulex well known and used at "high" energies
- Energy dependence of Coulex cross section weaker than that of alpha-capture
- Coulex may become important again when going to very low, subCoulomb energies
- Question: At which energy?
- Depends on nucleus
- Coherent summation of transmission coefficients

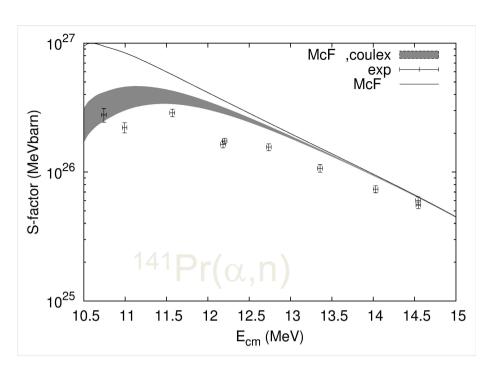
Low-Energy Coulex with α -Particles

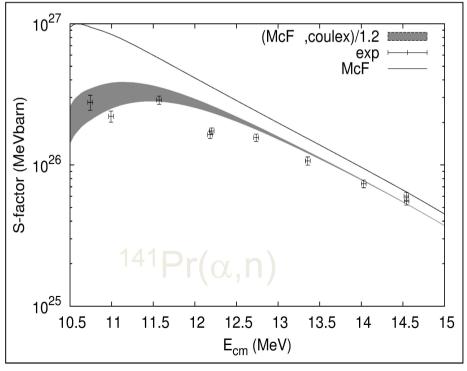
- Can well describe 144 Sm (α,γ) data with standard potential (McFadden & Satchler, 1966)
- Only very few data for other reactions
- Coulex effect seems to be compatible with available data
- B(E2) values uncertain (or mixed B(E2) and B(E2)↑ values!) in ENSDF

Testing with other reactions:

- Only few available at low E and "high" Z (above Sn)
- 130 Ba, 132 Ba(α ,n)
 - No effect seen previously, stand.pot. OK
 - OK, because low B(E2), no Coulex
- odd nuclei are more complicated

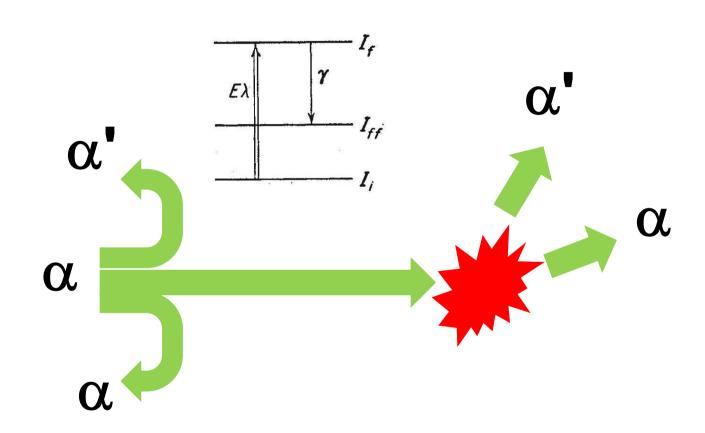






Implication for γ -process rates

- Laboratory effect in α -induced reactions
- Does NOT affect α -emission, does not affect photodisintegration rates!
- But when checking validity of optical α +nucleus potential against low-energy (reaction or scattering) data, this effect has to be taken into account.



- Direct elastic scattering is included in optical model calculation of compound formation
- Direct inelastic is not included

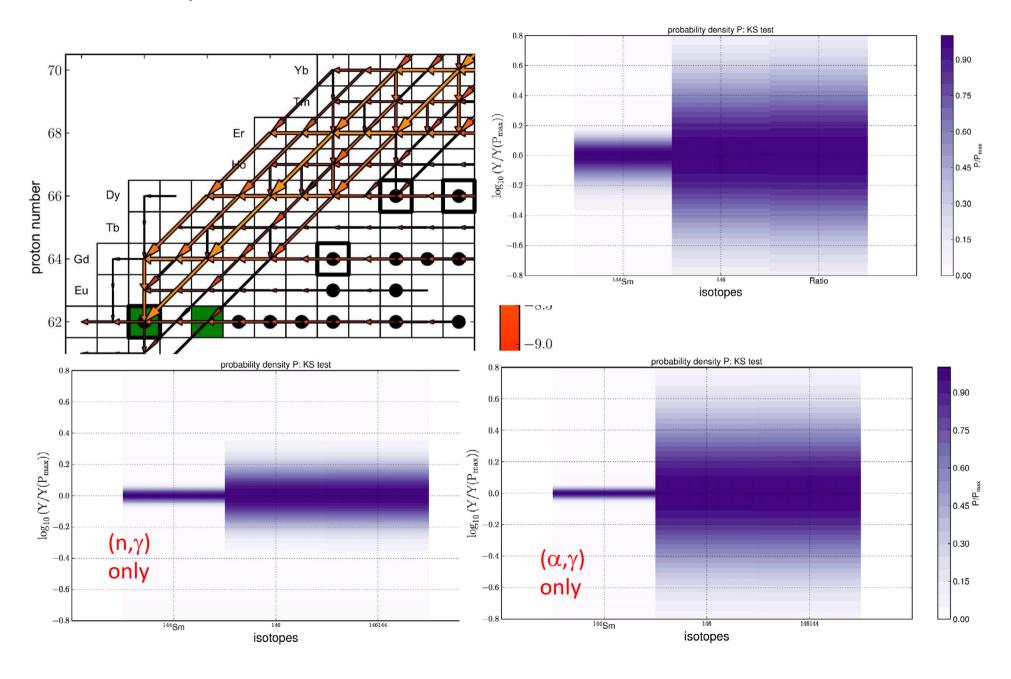
Monte Carlo \gamma-process studies to identify reactions for experiments

PizBuin Monte Carlo Framework

- Monte Carlo driver + fast, parallelized reaction network
- Hertfordshire-Keele collaboration (with Nishimura, Hirschi), within ERC project and the BRIDGCE consortium (UK)
- using computing clusters at Keele and Hertfordshire
- ability to study 10000s of reactions simultaneously in post-processing
- Goal: large scale study of nuclear uncertainties in various nucleosynthesis processes, mainly in massive stars but also SNIa, X-ray bursts
- Will be able to follow detailed uncertainties in nuclear input (different for different nuclei) to final abundances, sensitivity and correlation information will enter individual uncertainty estimates for the reactions
- Focus on nucleosynthesis beyond Fe, (weak) s-process, p/ γ -process, r-process, rp-process, vp-process, (v-driven winds)

Project recently started, first test results available

γ -process for ¹⁴⁶Sm/¹⁴⁴Sm ratio in SNIa



Conclusion

Heavy element nucleosynthesis compared to that of light nuclei

- Sites less well known (although required conditions can be constrained)
- Explosive environments lead to higher nucleosynthesis temperatures (except sprocess)
 - unstable nuclei (also s-process branchings)
 - considerable excited state contributions to stellar rate
 - equilibria may help (e.g., rp-, 1/p-, r-process)
- Heavier nuclei with higher nuclear level density
 - High Coulomb barriers, sensitivities strongly energy dependent
 - considerable <u>excited state contributions</u> to stellar rate (also at low *T*), direct measurements do not include this
 - many transitions between nuclear levels have to be considered
 - indirect experiments only probe few, mostly irrelevant ones
 - somewhat simpler to calculate (average level properties)?
 - large number of resonances <u>allow application</u> of averaged reaction models (Hauser-Feshbach) for majority of reactions (except close to driplines or at magic numbers)
- Experimental techniques which work well for light nuclei (direct + indirect methods)
 provide only limited information here

Theory Requirements in Nuclear Astrophysics

• Specific topics:

- Large-scale prediction of cross sections, reaction rates
- Interplay of different reaction mechanisms
- Population of excited states, stellar cross sections, stellar decays
- Plasma screening
- $-\beta$ -delayed fission
- and many more (see before)…

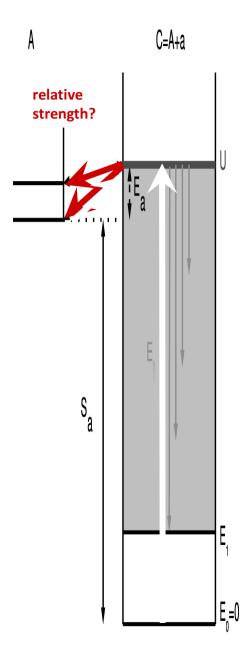
• General approach:

- Fine-tuning of established phenomenological models (CPU "friendly")
- Large-scale microscopic calculations (CPU "expensive")
- <u>Parameterized ↔ microscopic</u> (currently there is no "winner", especially at higher mass range)

Limitations of indirect experimental approaches

- Indirect: reverse reaction, photodisintegration, Coulomb break-up, (d,p) or (d,n) reactions
- Work well for light nuclei but catch only very limited set of information for intermediate and heavy nuclei
 - e.g., (d,p) only spectroscopic information (levels, spec. fact.);
 other nuclear properties required for (d,p) theory are not necessarily related to stellar rate calculations
- Do not measure stellar reaction rates
- Useful to determine certain properties to test theory but have to be selected carefully!

How to make use of experimental data



Most stellar rates have considerable contributions from excited states at γ -process temperatures

theoretical prediction required

Only few reactions (on low mass p-nuclei) have large g.s. contributions to stellar rate

- measured cross section has direct impact
- but many relevant reactions on unstable nuclei

Experiments can be used to constrain certain inputs (optical potentials, γ —strength)

- Important: measure at relevant energies!
- Low energies, quite sensitive to parameters, extrapolations difficult

Experiments (including photodisintegration, (n,n')) can be used to test relative strengths of transitions to g.s. and excited states (g.s. contribution, stellar enhancement)

Caution: partial wave selection

Problems in prediction of transitions from g.s. and excited states may be correlated

- g.s. correction also applicable to excited states?
- Ratios R_x/R_0 better predicted than R_0 alone?

Challenges

Relevant Energies

- Neutron Capture important in
 - s-Process (at stability, 5-50 keV)
 - Hydrostatic Burning of Stars (around stability, 1-100 keV)
 - r-Process (very n-rich, 80-120 keV)
 - γ-Process (p-rich, 100-300 keV)
- Further reactions with neutrons
 - (n,α) to study optical α potentials (stable, p-rich, <10 keV)
 - (n,p) in γ -process (p-rich, 1-300 keV)
 - (n,p) in *v*p-process (unstable p-rich, 200-400 keV)
- Reactions with protons
 - Hydrostatic burning: (p, γ) on light nuclei, 10-300 keV
 - rp-process: (p, α) on light & intermediate p-rich nuclei, (p, γ) on intermediate nuclei close to p-drip (up to A=120), 0.5-2 MeV
 - γ -process: (p, γ) on intermediate & heavy stable and p-rich nuclei (up to Pb), 1-4 MeV
- Reactions with alphas
 - Hydrostatic burning: $(\alpha, \gamma/p/n)$ on light nuclei, 250-1000 keV
 - High-T and explosive burning: (α, γ) on N=Z nuclei, 7-9 MeV
 - γ -process: (α, γ) on stable and p-rich nuclei from Mo to Bi, 8-12 MeV

Nuclear Physics Problems

- Reactions: Low energies, 0-10 MeV (reaction rates, <u>mechanisms</u>?)
- Exotic Nuclei (properties needed for reactions, 6000 nuclei, 60000 reactions)
- Stellar Rates (thermal excitation, screening, β -decay in plasma)
 - (De)population of isomers (²⁶Al, ¹⁸⁰Ta)

Differences in heavy element nucleosynthesis compared to that of light nuclei

- Sites less well known (although required conditions can be constrained)
- Explosive environments lead to higher nucleosynthesis temperatures (except sprocess)
 - unstable nuclei (also s-process branchings)
 - considerable excited state contributions to stellar rate
 - equilibria may help (e.g., rp-, 1/p-, r-process)
- Heavier nuclei with higher nuclear level density
 - High Coulomb barriers, sensitivities strongly energy dependent
 - considerable <u>excited state contributions</u> to stellar rate (also at low T)
 - many transitions between nuclear levels have to be considered
 - indirect experiments only probe few, mostly irrelevant ones
 - somewhat simpler to calculate (average level properties)?
 - large number of resonances <u>allow application</u> of averaged reaction models (Hauser-Feshbach) for majority of reactions (except close to driplines or at magic numbers)
- Experimental techniques which work well for light nuclei (indirect methods) provide only limited information here

Available data at low energies

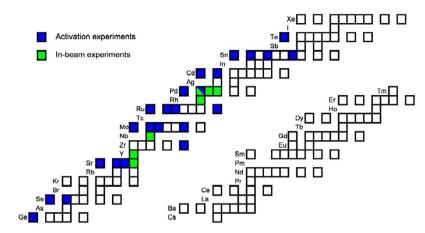


Figure 14. Isotopes on which (p,γ) cross sections relev been measured. The upper part of the p-isotope mass there are no data available there. The measured cross ϵ in [144, 150, 151, 155–167].

- charged particle reactions:
 - scarce at low energy, even at stability!
 - still not in astrophysically relevant energy range!

 neutron capture: well covered along stability for 30 keV g.s. cross sections (compilations: Bao et al 2000, KADoNiS) but need high resolution measurements up to 200 keV

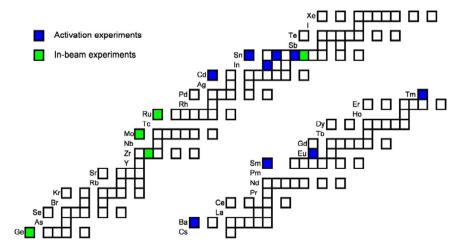


Figure 15. Isotopes on which (α, γ) cross sections relevant for the γ -process have been measured. The upper part of the p-isotope mass region is not shown since there are no data available there with the exception of the ¹⁹⁷Au $(\alpha, \gamma)^{201}$ Tl [168]. The measured cross section data can be found in [139–143, 169–178].