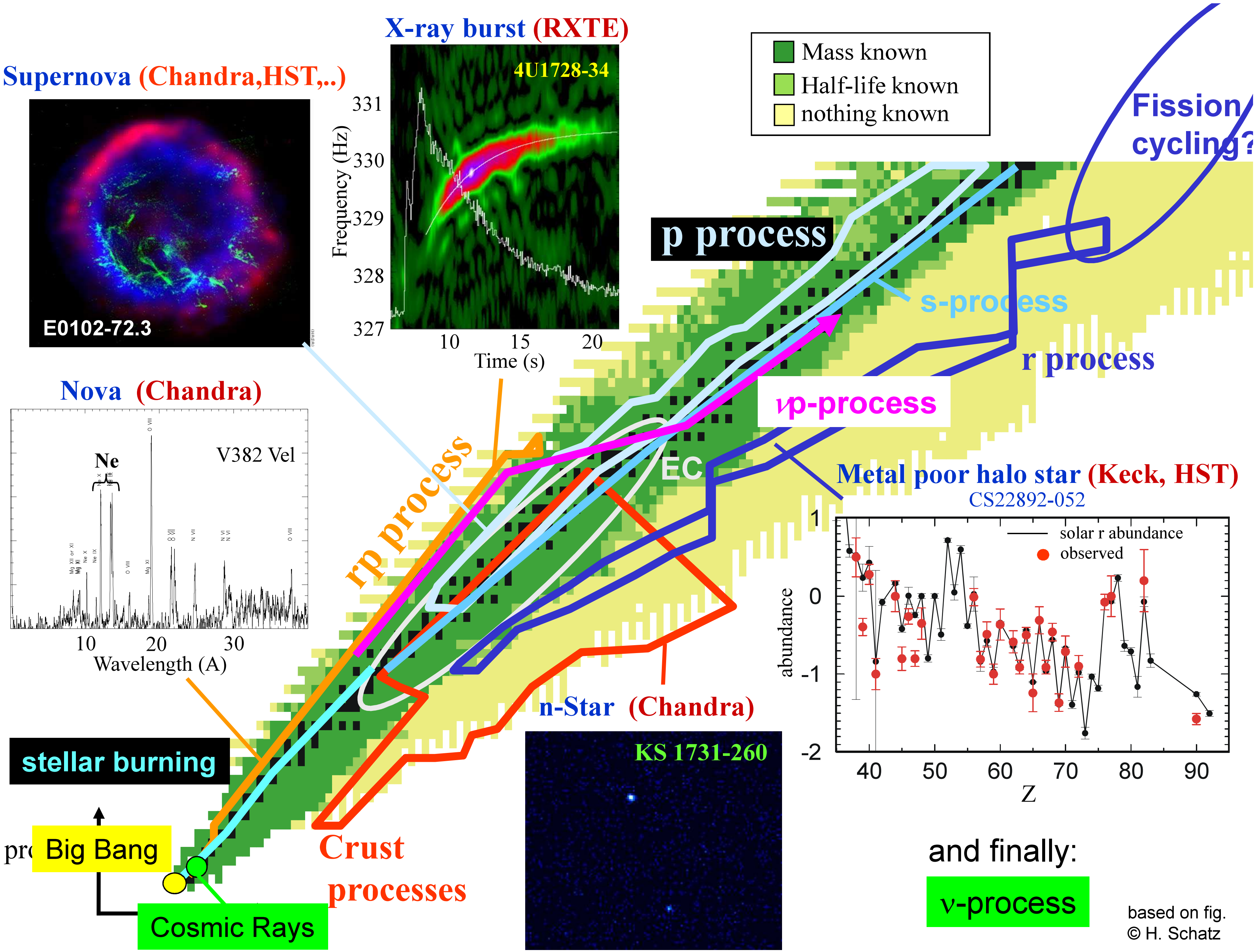
Challenges in prediction and measurements of stellar rates for heavy element nucleosynthesis

T. Rauscher

University of Hertfordshire, UK

TOC



X-ray burst (RXTE)
4U1728-34
Frequency (Hz)
Time (s)
Supernova (Chandra,HST,..)
E0102-72.3
Mass known
Half-life known
nothing known
Fission cycling?
p process
s-process
r process
νp-process
rp process
EC
Metal poor halo star (Keck, HST)
CS22892-052
solar r abundance
observed
abundance
Z
Nova (Chandra)
Ne
V382 Vel
Wavelength (A)
n-Star (Chandra)
KS 1731-260
stellar burning
Big Bang
Cosmic Rays
Crust processes
and finally:
ν-process
based on fig.
© H. Schatz

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 νp-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: (α,γ/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, mechanisms?)
- Exotic Nuclei (properties needed for reactions, 6000 nuclei, 60000 reactions)
- Stellar Rates (thermal excitation, screening, β-decay in plasma)
  - (De)population of isomers (^{26}Al, ^{180}Ta)
- Nuclear equation of state
  - Early core collapse phase (e^- captures, ν trapping, collective effects)
  - Late core collapse phase
  - Neutron star properties
  - Neutron star merger

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
  - β-delayed fission
  - and many more (see before)...
- General approach:
  - Fine-tuning of established phenomenological models (CPU „friendly")
  - Large-scale microscopic calculations (CPU "expensive")
  - Parameterized ↔ microscopic (currently there is no "winner", especially at higher mass range)

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 s-process)
  - unstable nuclei (also s-process branchings)
  - considerable excited state contributions to stellar rate
  - equilibria may help (e.g., rp-, νp-, r-process)
- Heavier nuclei with higher nuclear level density
  - High Coulomb barriers, sensitivities strongly energy dependent
  - considerable excited state contributions 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 allow application 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

- 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

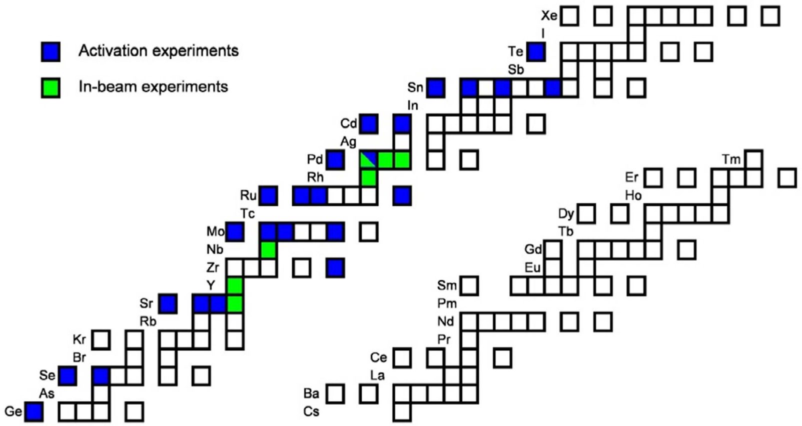


Figure 14. Isotopes on which (p,γ) cross sections relev
been measured. The upper part of the p-isotope mass
there are no data available there. The measured cross s
in [144, 150, 151, 155–167].

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

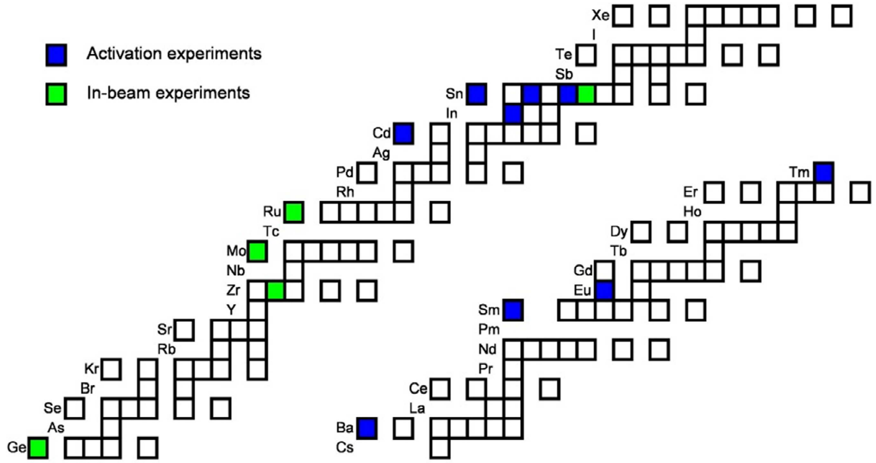
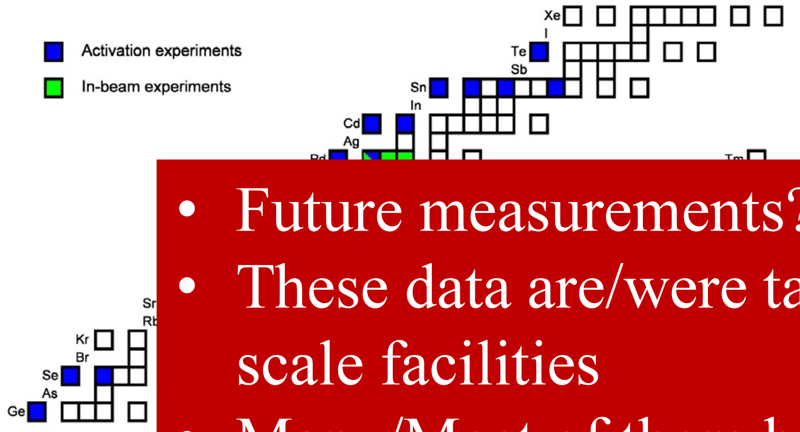


Figure 15. Isotopes on which (α,γ) cross sections relevant for the γ-process have been measured. The upper part of the p-isotope mass region is not shown since there are no data available there with the exception of the $^{197}Au(\alpha,\gamma)^{201}Tl$ [168]. The measured cross section data can be found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

Available data at low energies



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

- Future measurements??
- These data are/were taken by dedicated efforts at small scale facilities
- Many/Most of them have been shut down because money moves to large scale (RIB) facilities
- Also person-power moved there (and is currently often blocked by commissioning work

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

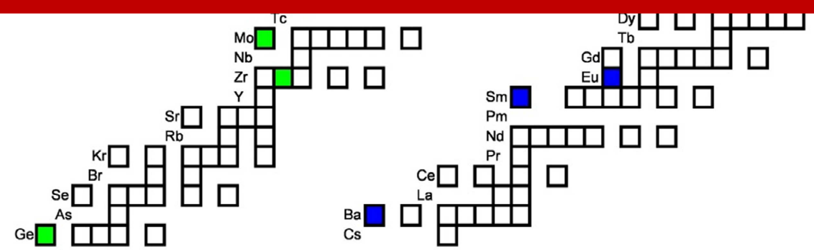


Figure 15. Isotopes on which (α, γ) cross sections relevant for the γ-process have been measured. The upper part of the p-isotope mass region is not shown since there are no data available there with the exception of the ^{197}Au$(\alpha, \gamma)^{201}$Tl [168]. The measured cross section data can be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

Reaction Mechanisms

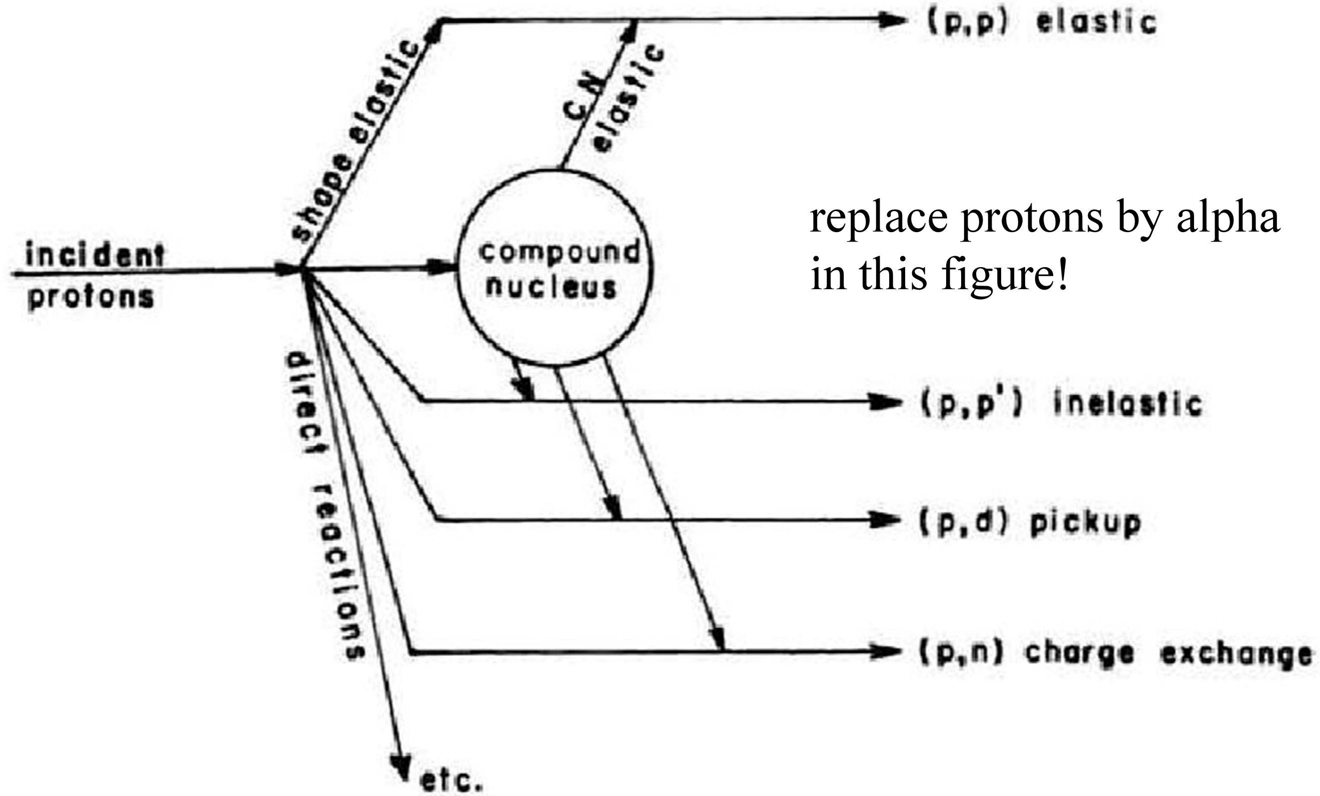
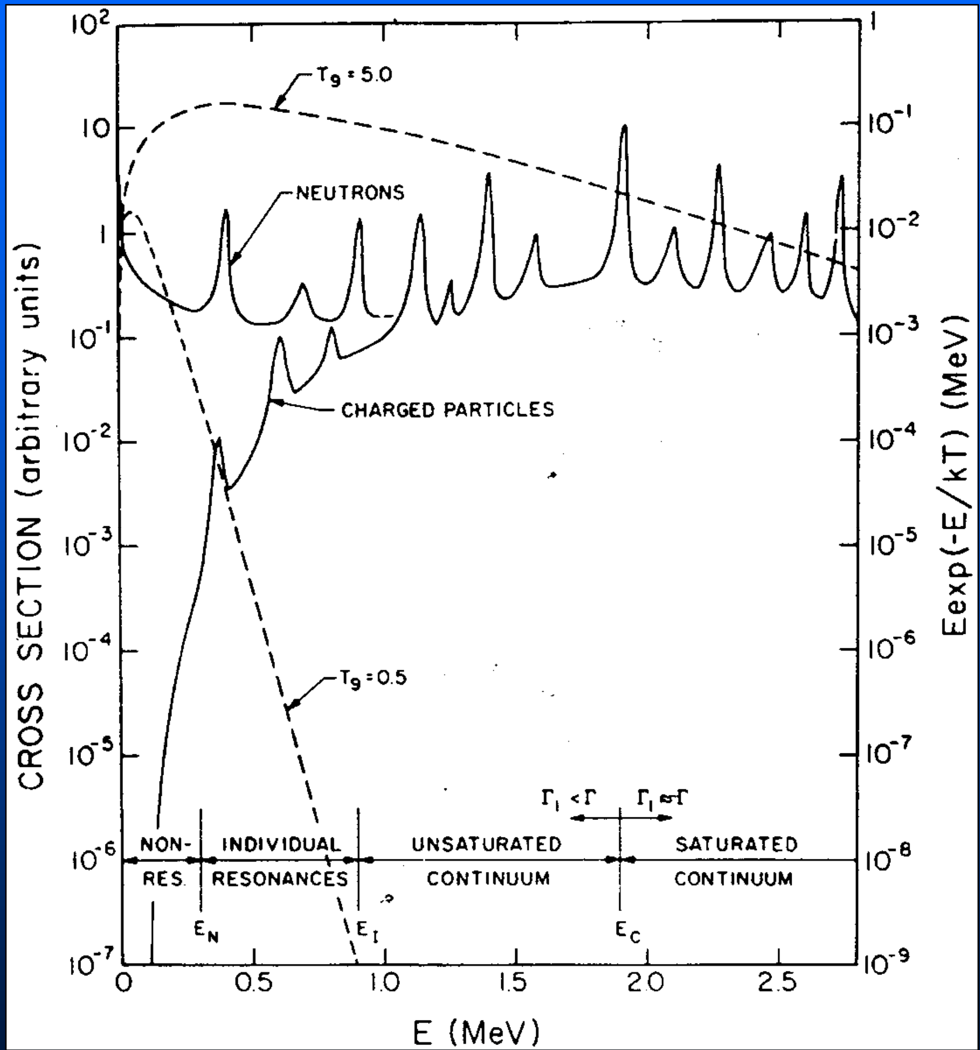


Fig. 1.2. Depiction of the processes that are typical of proton–nucleus interactions. (Adapted from P. E. Hodgson, 1971.)

replace protons by alpha
in this figure!

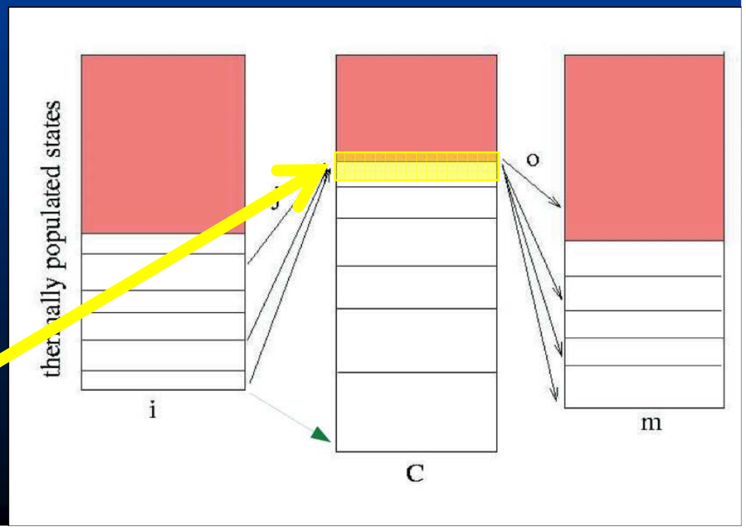
Reaction Mechanisms



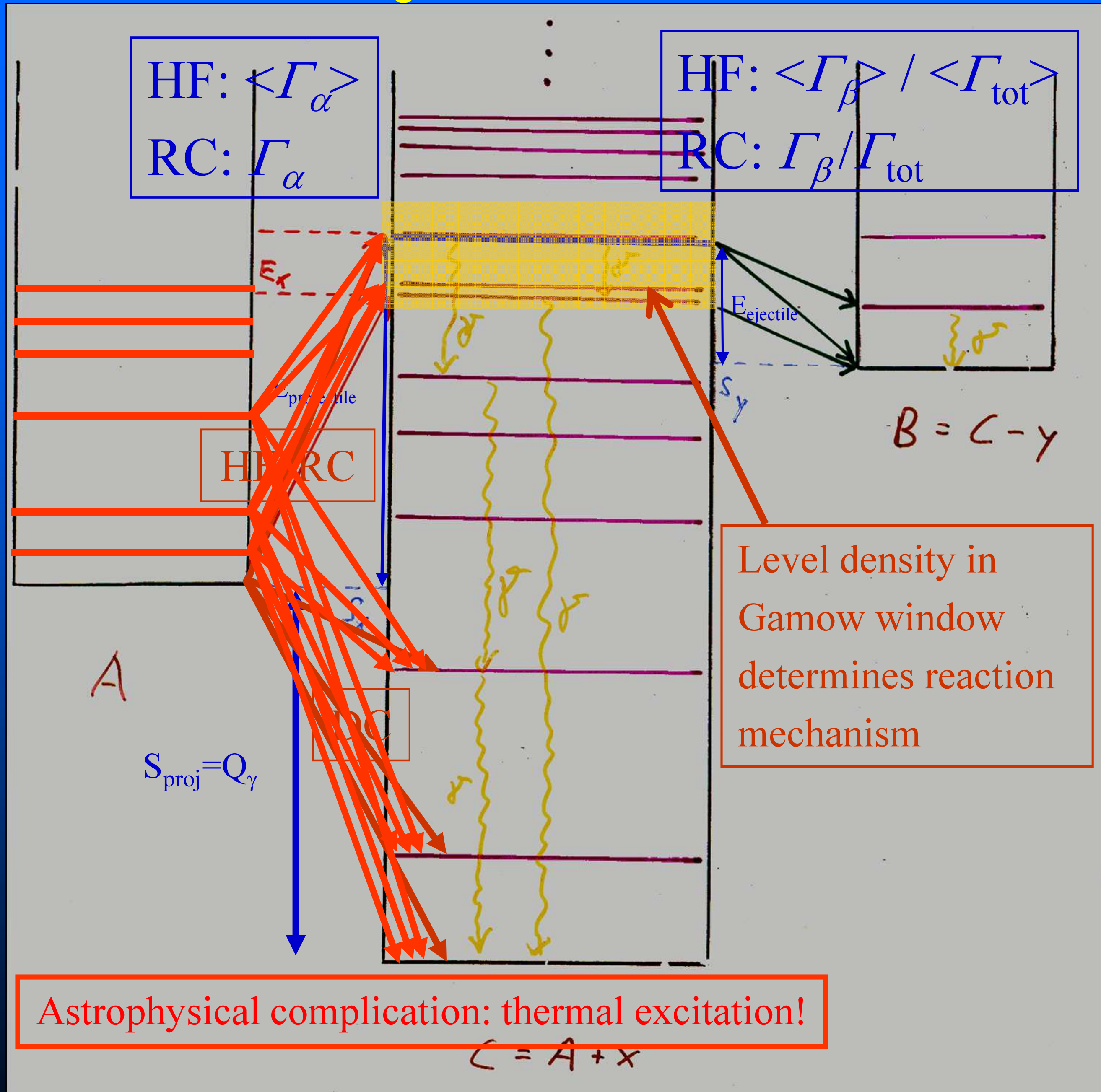
Regimes:

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

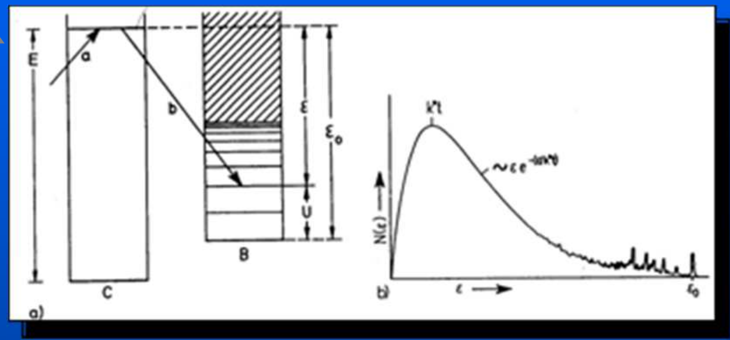


Reaction Mechanisms II

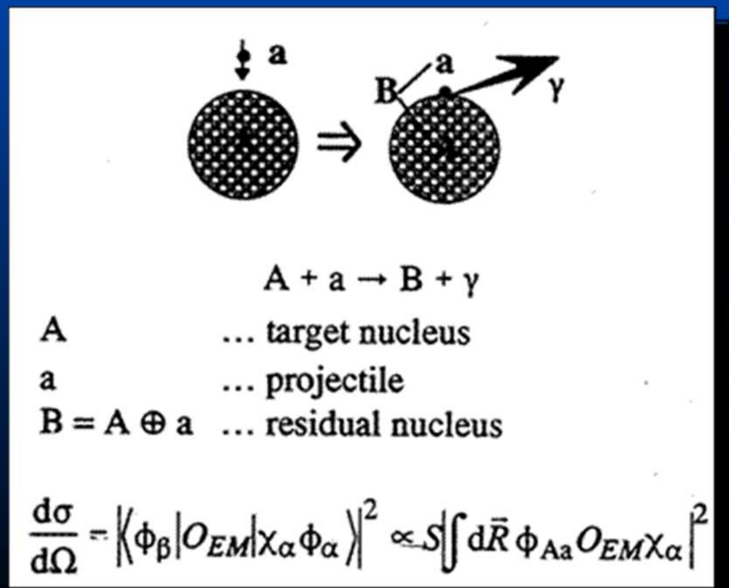
Statistical Model (Hauser-Feshbach):

$$\sigma^{\mathrm{CN}}_{\alpha\to\beta} = \sigma^{\mathrm{form}}_{\alpha} b_{\beta} = \sigma^{\mathrm{form}}_{\alpha} \frac{\langle \Gamma_{\beta} \rangle}{\langle \Gamma_{\mathrm{tot}} \rangle} \propto \frac{\langle \Gamma_{\alpha} \rangle \langle \Gamma_{\beta} \rangle}{\langle \Gamma_{\mathrm{tot}} \rangle}$$

Compound Reaction



Direct Reaction



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

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

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

stat. model

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

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

Breit-Wigner

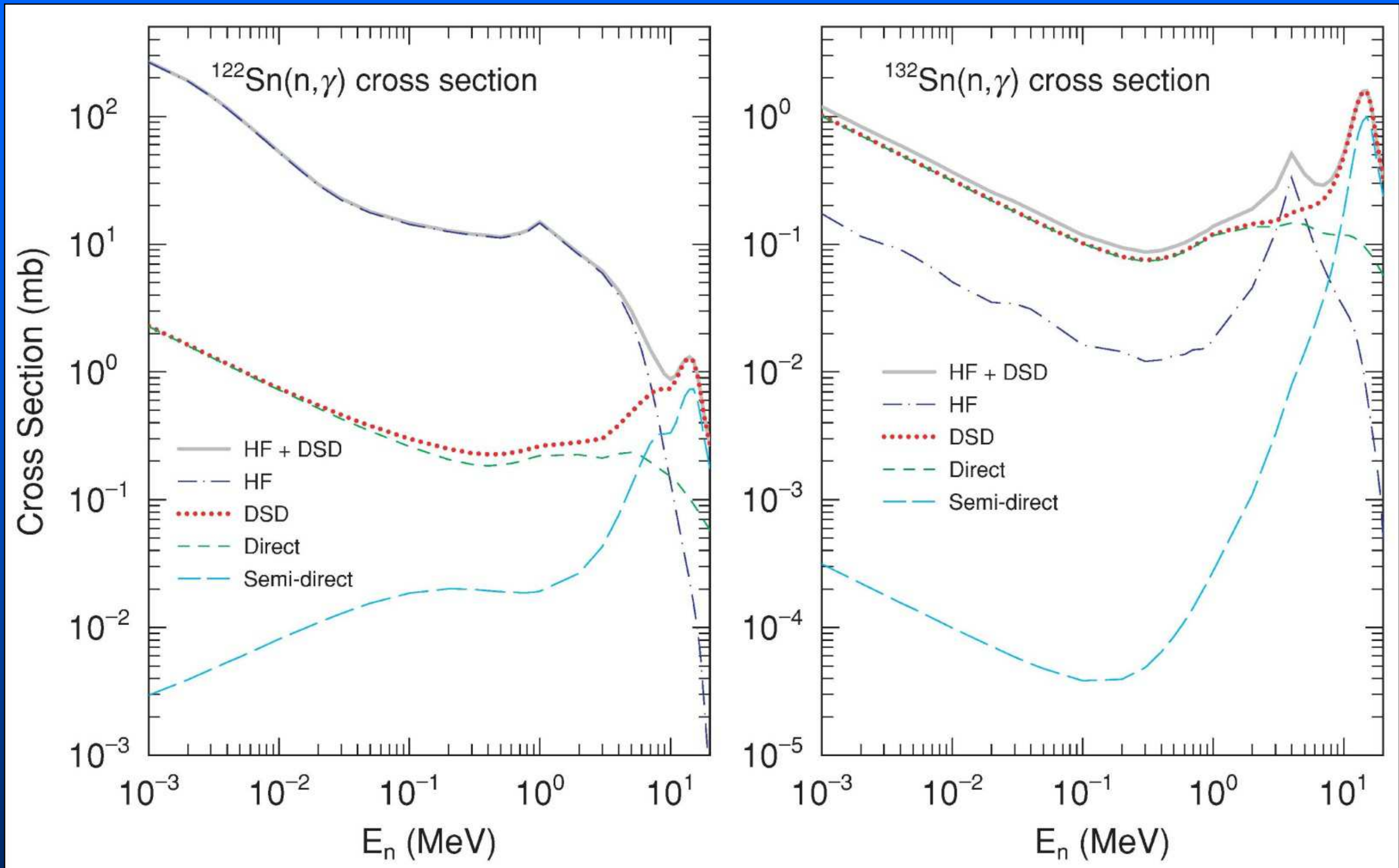
$$T_j(E,J,\pi) = \frac{2\pi}{D(E,J,\pi)}\langle \Gamma_j(E,J,\pi) \rangle$$

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?

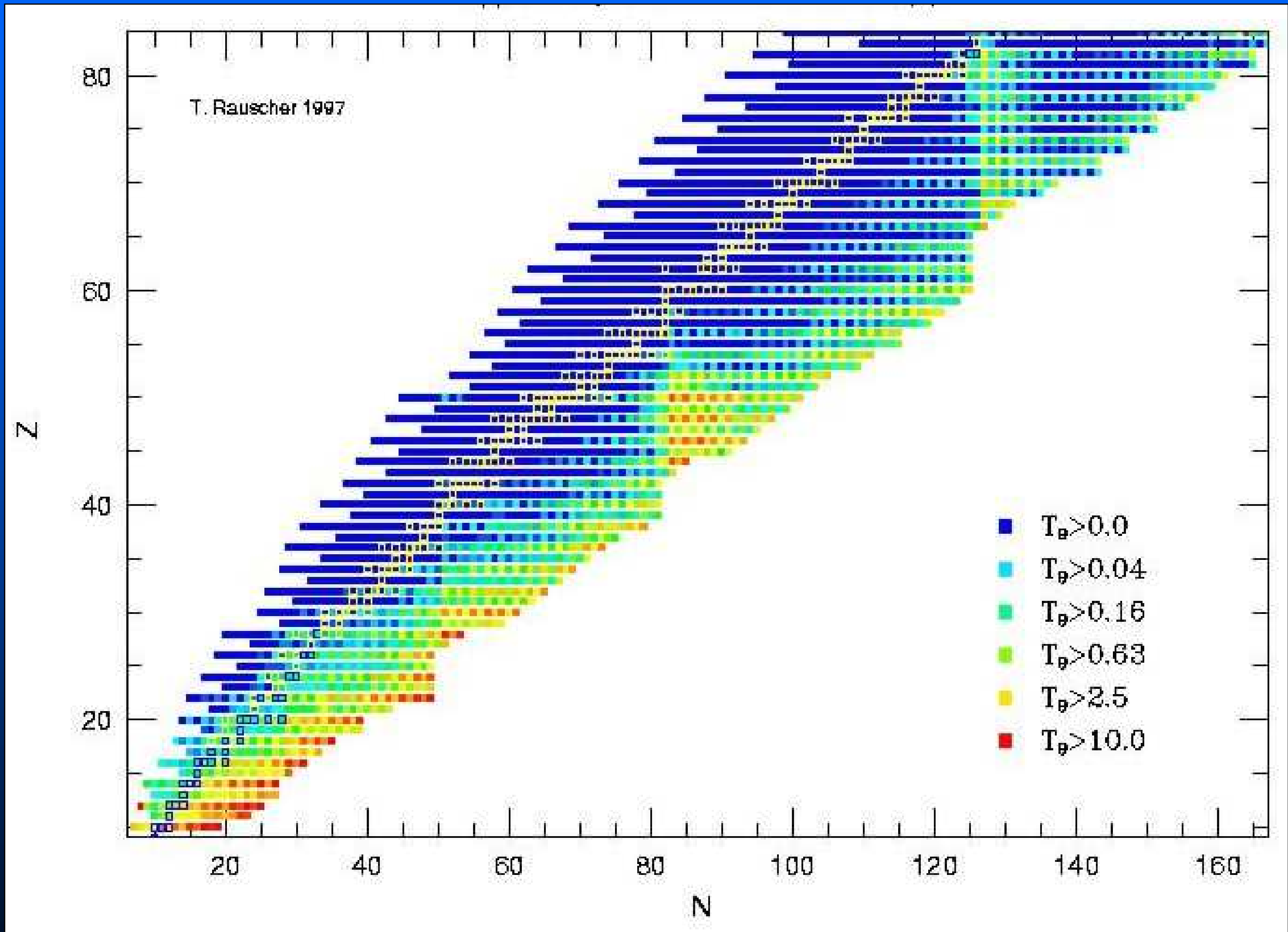


Chiba et al, PRC 77 (2008) 015809

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

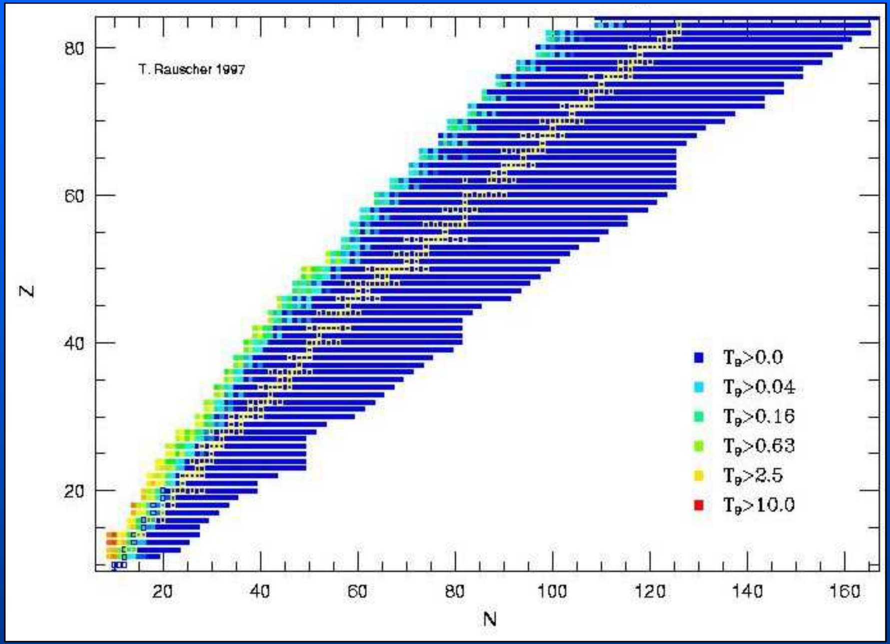
Applicability of the Statistical Model

Neutron induced reactions



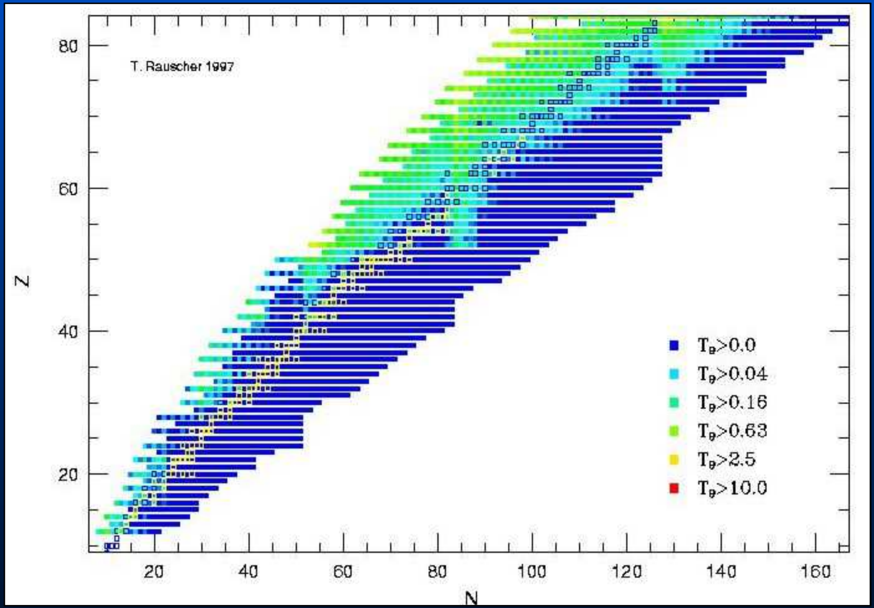
Rauscher et al. 1997

Applicability of Statistical Model



Proton induced reactions

α-induced reactions



Rauscher et al. 1997

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

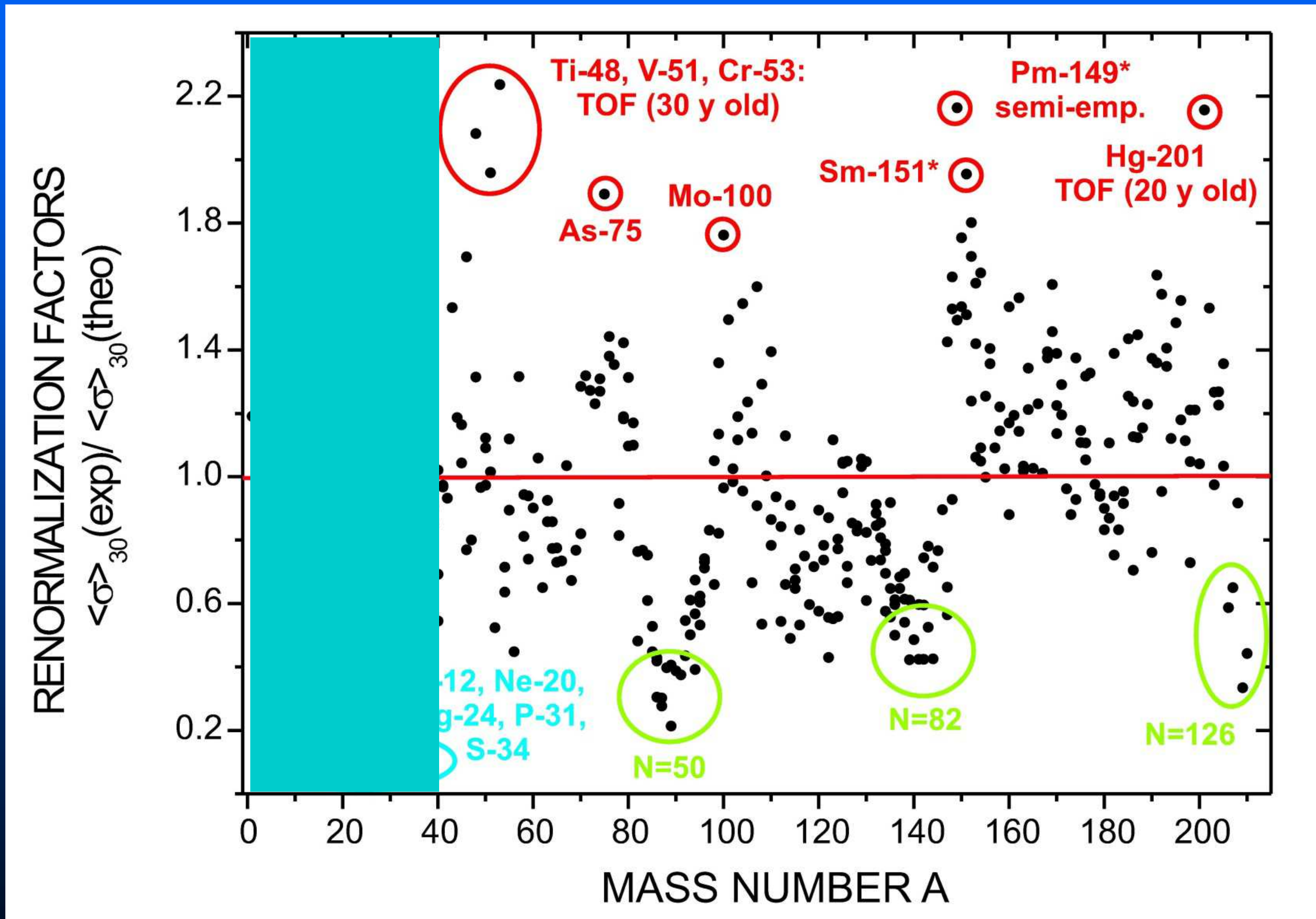
Reaction Rates From A Statistical Compound Reaction Model

- Standard rates from NON-SMOKER code
- Rate library with fits
  (5000 targets, 30000 reactions)
  At. Data Nucl. Data Tabl. 75 (2000) 1
- *(Among top 1% papers in its field according to ESI !)*
- Worldwide most widely used rate set for astrophysical applications
- Temperature/Energy applicability limits given!!
- Beyond Stat. Model: new SMARAGD code
  - (in development)
  - contains *modified* stat. mod. (lifts previous assumptions of spin and parity distributions at low compound formation energy)
  - includes direct capture + averaged direct capture (ADC) far from stability
    - » impact on explosive nucleosynthesis far from stability (r-process, rp-process)

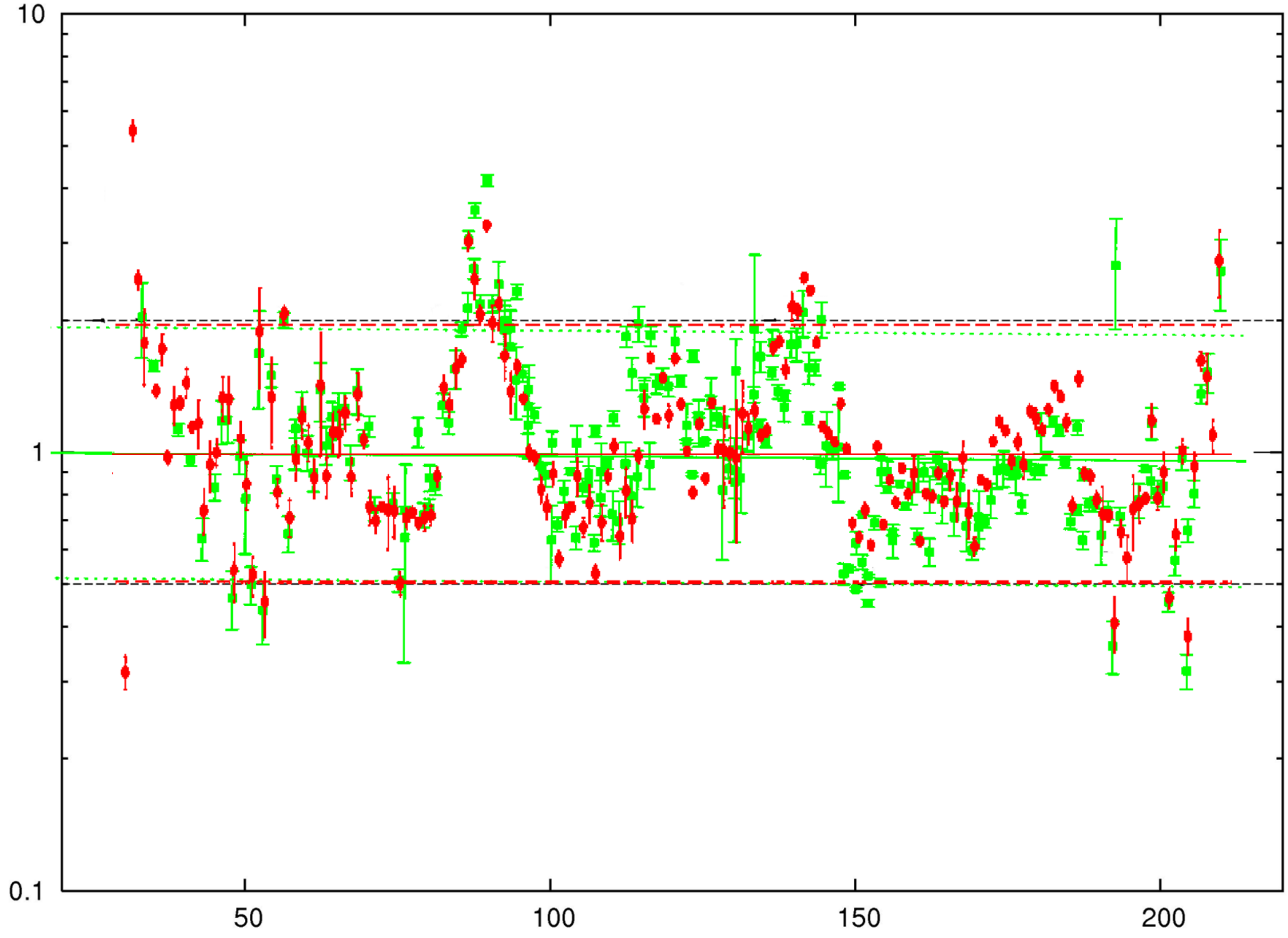
Code Timeline

1. NON-SMOKER (1998-2002)
   - ADNDT rate sets published 2000, 2001
2. NON-SMOKER^{WEB} (2004-2009)
   - Improved Hauser-Feshbach code; easy web interface
   - input updates
   - used in many calculations; comparison to and analysis of experimental results
3. SMARAGD (2009-) (see http://nucastro.org/forum)
   - Hauser-Feshbach: further improvements (treatment of properties, numerics, modified mechanism)
   - input updates
   - multiple particle emission
   - (Fission)
   - Direct Reactions (consistently implemented with optical model)
   - New rate library in preparation

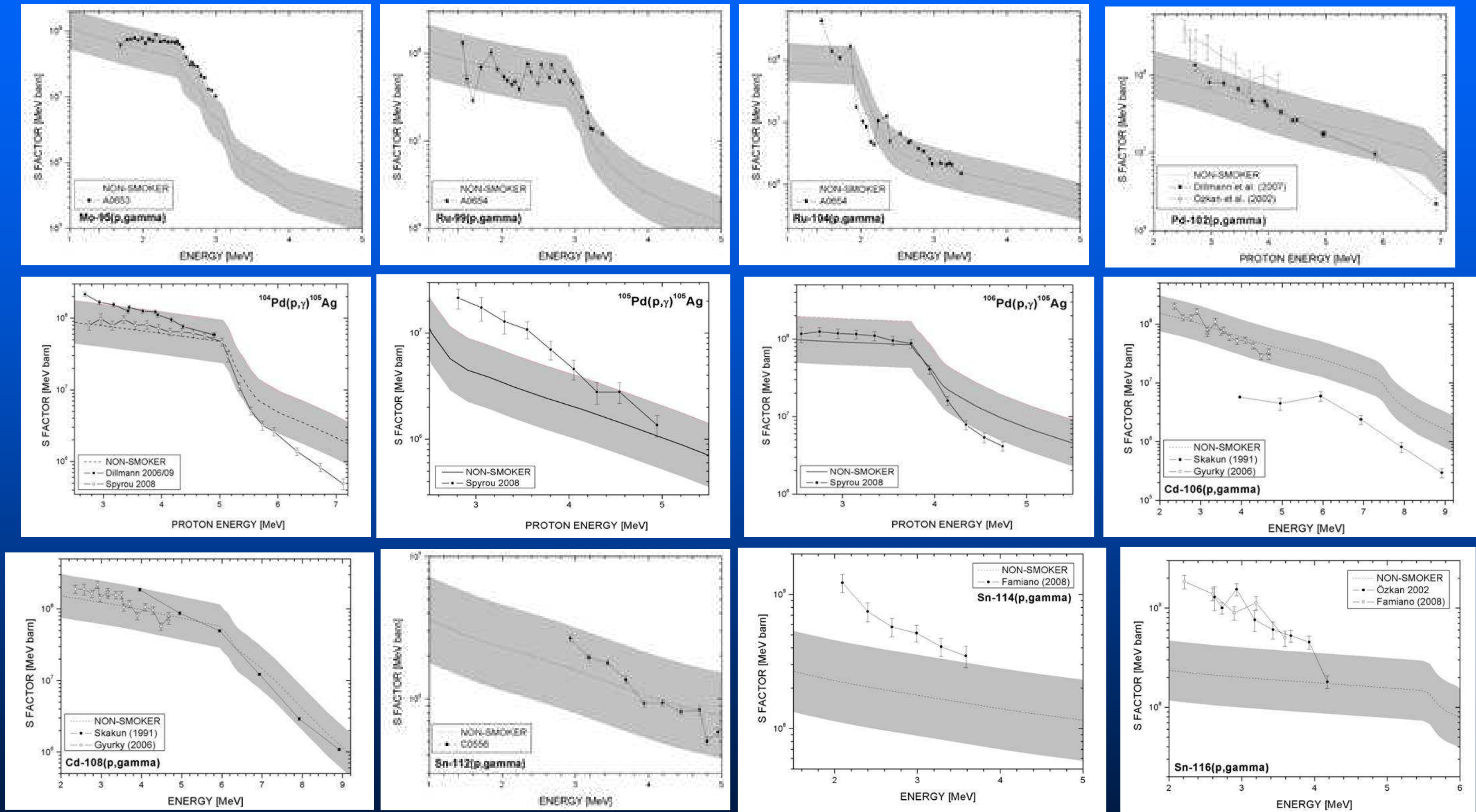
Comparison of ***global*** NON-SMOKER Hauser-Feshbach Theory to (n,γ) Experiment (Status: Bao et al 2000)



Historical change due to change in exp. data



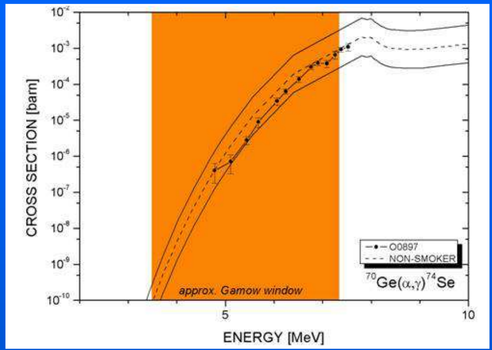
(p,γ) Comparison

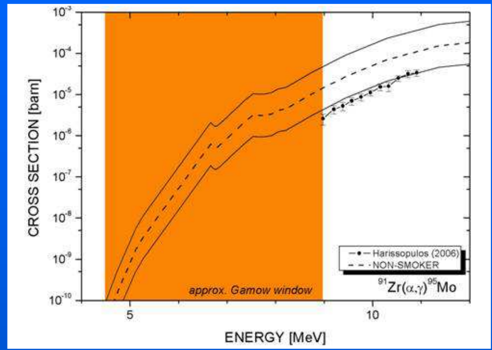


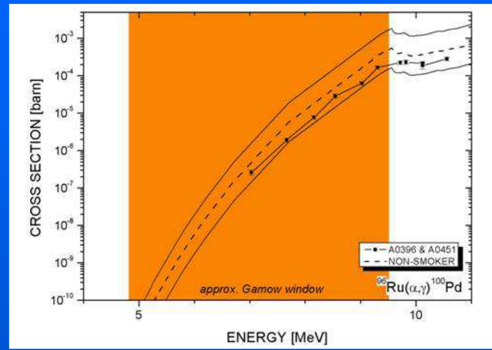
From I. Dillmann

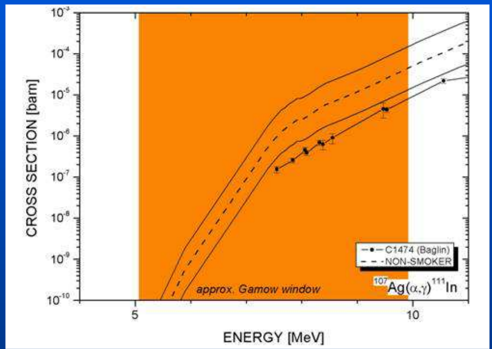
Sometimes reasonable agreement, no obvious trend

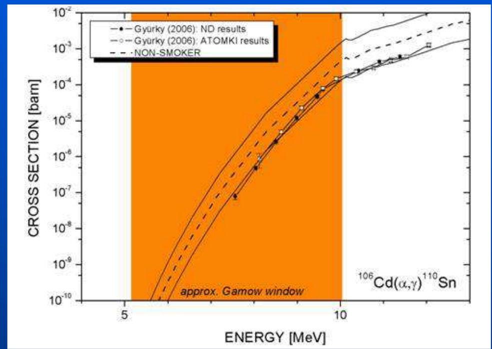
(α,γ) Comparison

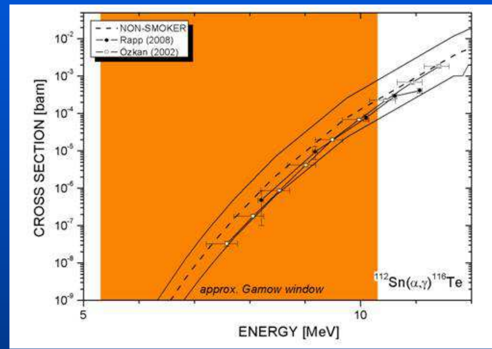


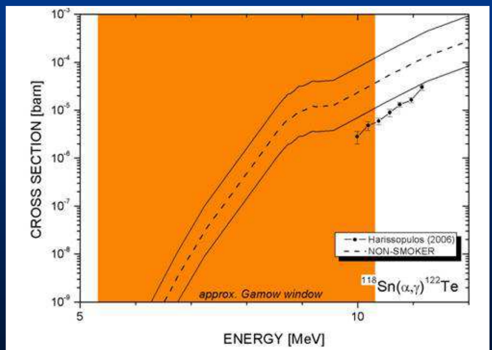


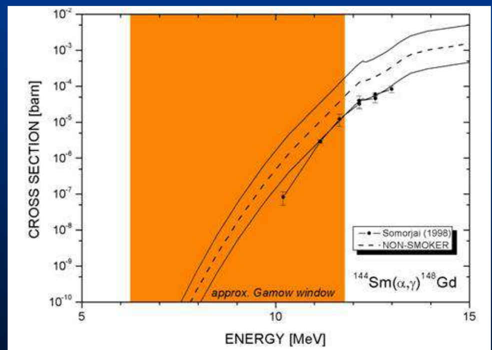












All experimental data systematically LOWER than theory (OMP: McFadden-Satchler)

From I. Dillmann

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 low-lying states important (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)

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

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

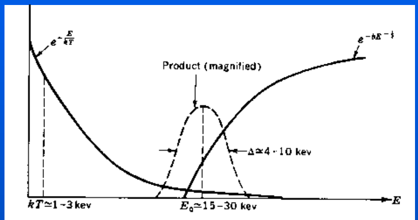
Detailed discussion in: ApJL 755, L10 (2012); ApJS 201 (2012) 26;
AIP Advances 4 (2014) 041012.

Uncertainties in “input quantities”

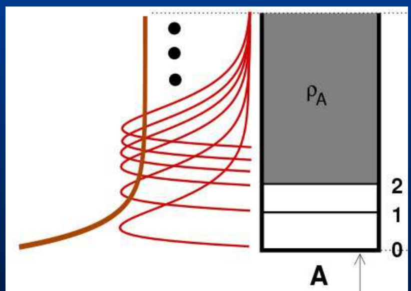
Nuclear property → Reaction model → Cross section, Rate → Astrophysical model → Reaction network → Abundances

- Distinction between:
  - Measured input or input derived from measurements (type I)
    - Experimental errors, propagated and convoluted
    - Statistical and systematic error
    - Probability distribution functions (from MC, first attempts)
  - Calculated (predicted) properties (type II)
    - Contains type I errors which can be propagated
    - But model error not really quantifiable (or only crudely, “systematic error”)
- Things to be considered:
  - Model sensitivities can help to disentangle input and model uncertainties
  - *Correct treatment of experimental constraints on rates*
  - ***Systematic variations of input are required to study uncertainties!!!***
    - not enough to just play around by plugging in different descriptions of properties (e.g., different GDR, level density descriptions, optical potentials)
    - This shows disagreement between theories but not real uncertainty range
    - Different models can fortuitously agree at relevant energies
    - Monte Carlo? Also cannot capture model uncertainties

When assessing impact of nuclear physics, pay attention to:



$$\sigma \propto \frac{\langle T_{\text{entrance}}\rangle\langle T_{\text{exit}}\rangle}{\langle T_{\text{total}}\rangle}$$



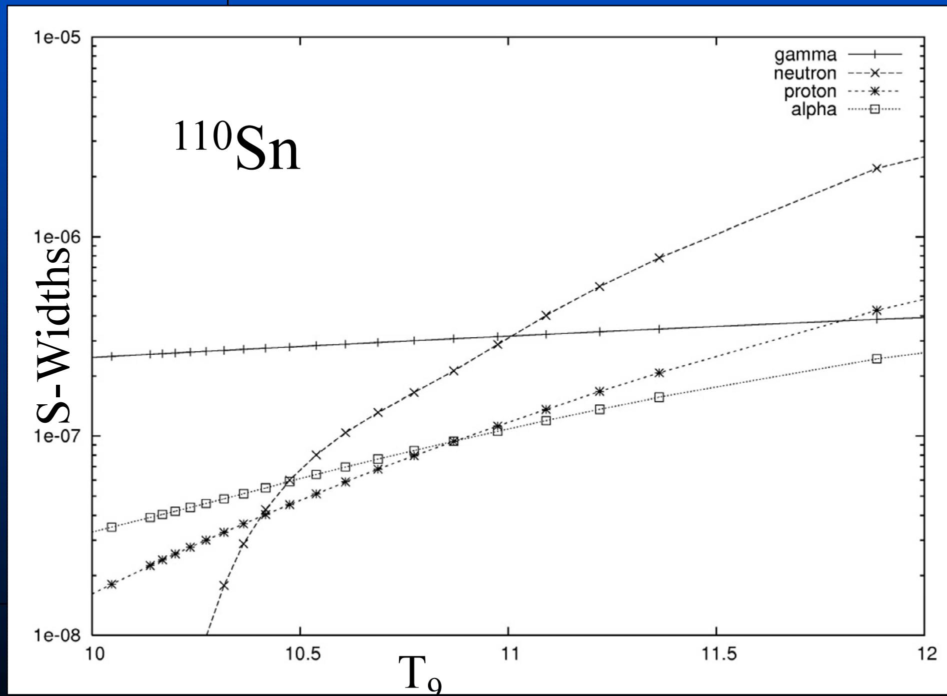
- Relevant energy range!
  - simple Gamow peak formula NOT correct!
  - determines reaction mechanism
- Sensitivities to nuclear properties
  - different at astrophysical energy than at energies accessible in the lab!
- Stellar modification of the rates
  - Many additional transitions from excited states!
  - NOT simple Boltzmann factor!

Sensitivities

Relative importance of widths

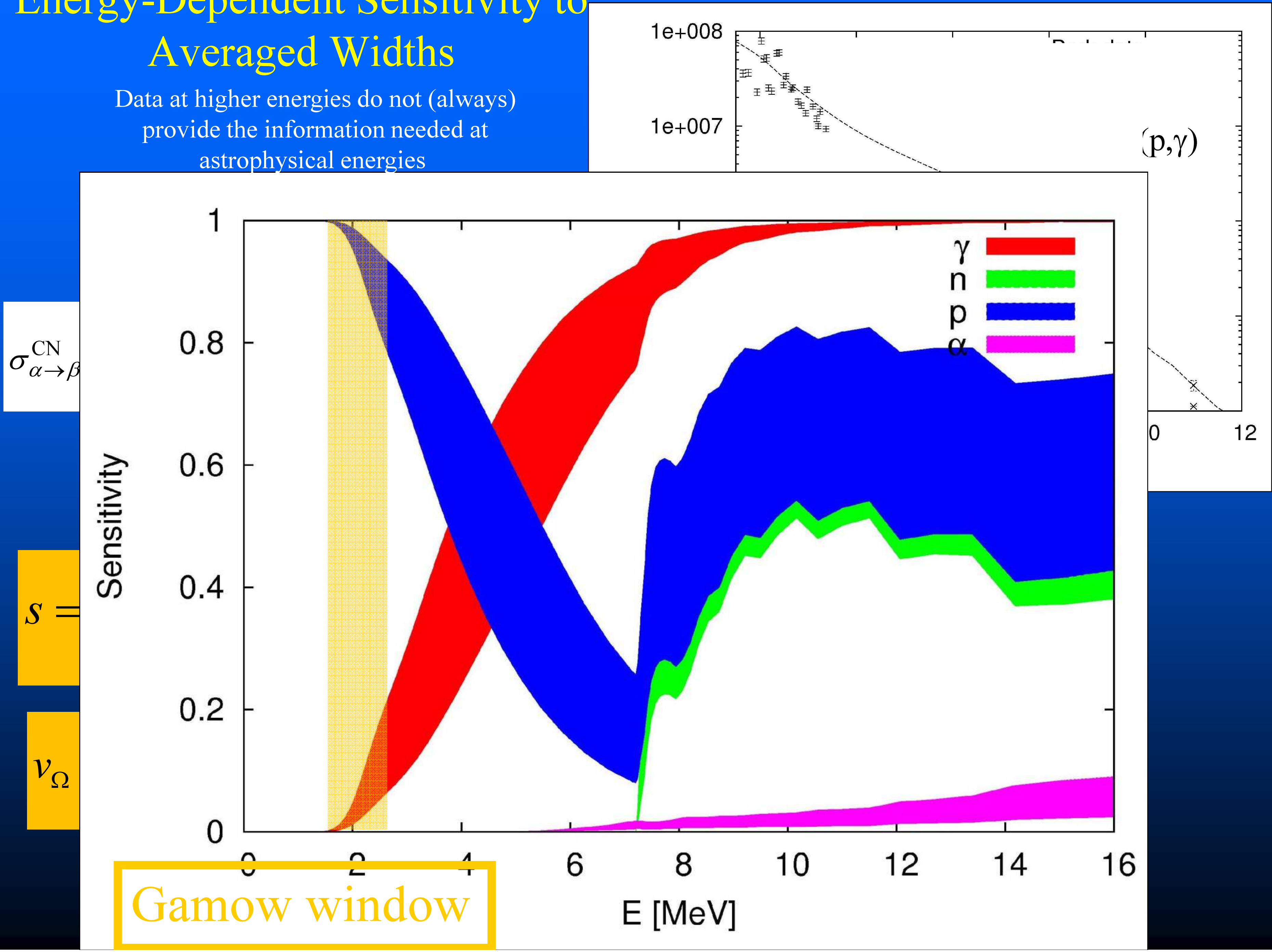
- Average widths (=transmission coefficients) determine the Hauser-Feshbach cross section
- γ-widths not necessarily the smallest ones at astrophysical energies!

$$\sigma \propto \frac{\langle T_{\text{entrance}} \rangle \langle T_{\text{exit}} \rangle}{\langle T_{\text{total}} \rangle}$$



Energy-Dependent Sensitivity to Averaged Widths

Data at higher energies do not (always) provide the information needed at astrophysical energies



Energy-Dependent Sensitivity to (Averaged) Widths

$$\sigma^{\mathrm{CN}}_{\alpha\rightarrow\beta} = \sigma^{\mathrm{form}}_{\alpha} b_{\beta} = \sigma^{\mathrm{form}}_{\alpha} \frac{\langle\Gamma_{\beta}\rangle}{\langle\Gamma_{\mathrm{tot}}\rangle} \propto \frac{\langle\Gamma_{\alpha}\rangle\langle\Gamma_{\beta}\rangle}{\langle\Gamma_{\mathrm{tot}}\rangle}$$

- 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)

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

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)

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:

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

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

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

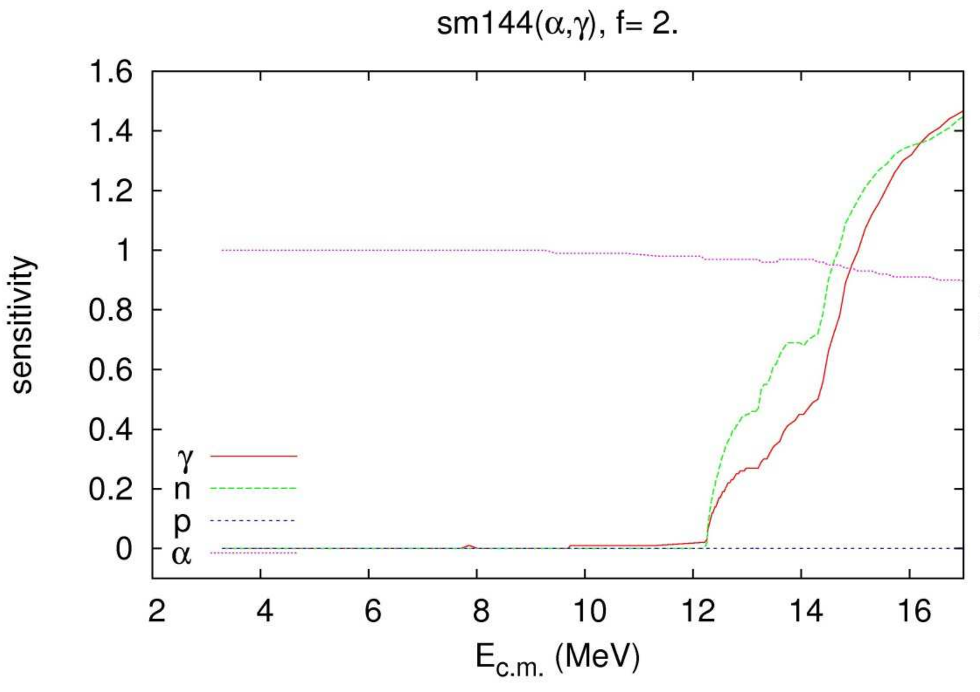
q…input (widths: NLD, opt. pot., GDR, spectroscopy)

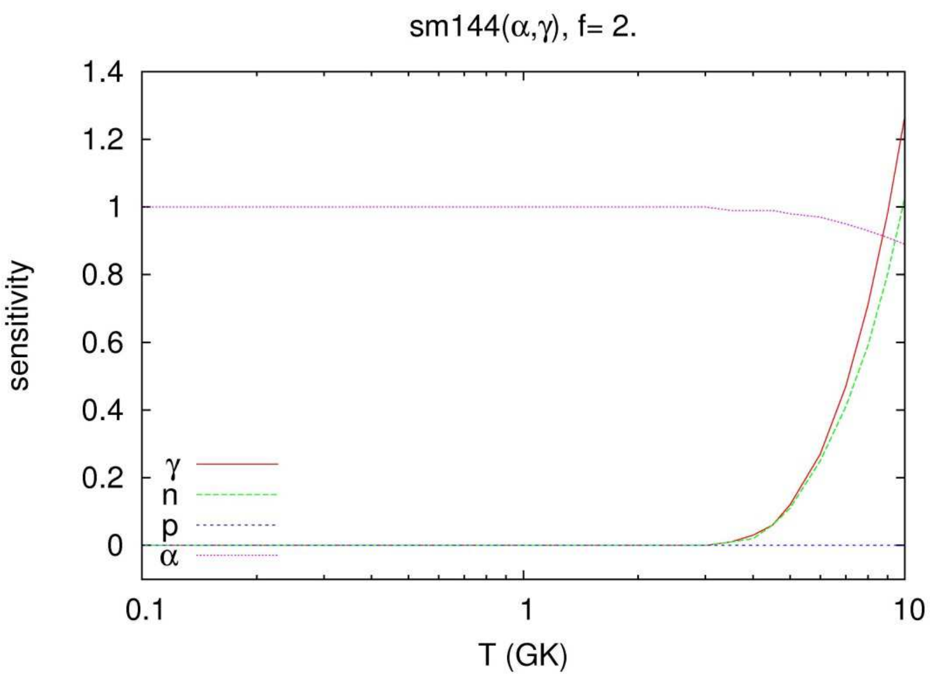
It is better to look at the rates than at the cross sections:

- Rates are the relevant quantities
- No need to separately compute the Gamow window

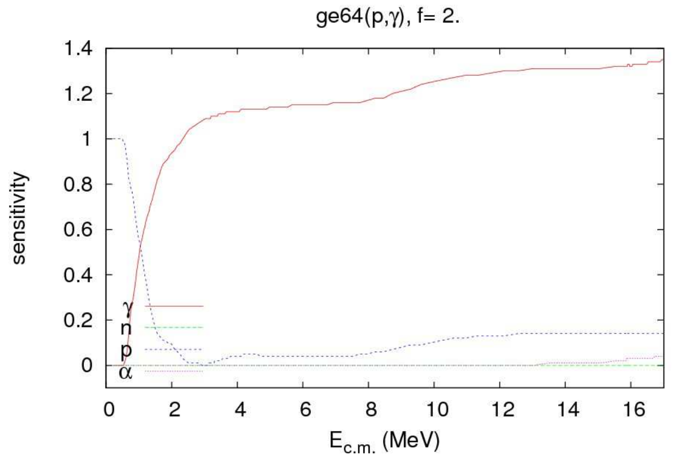
Examples relevant to the γ-process

cross section sensitivity | **rate sensitivity**

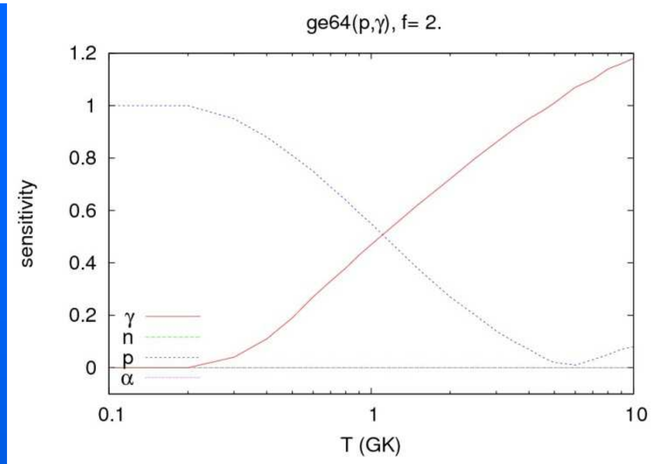


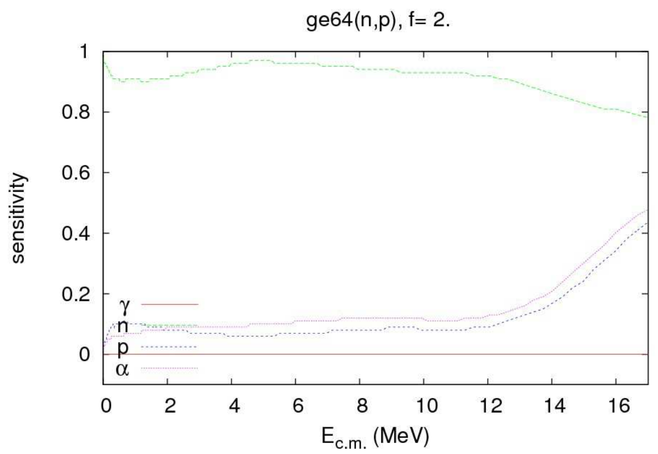


calculations performed with SMARAGD v0.8.1s

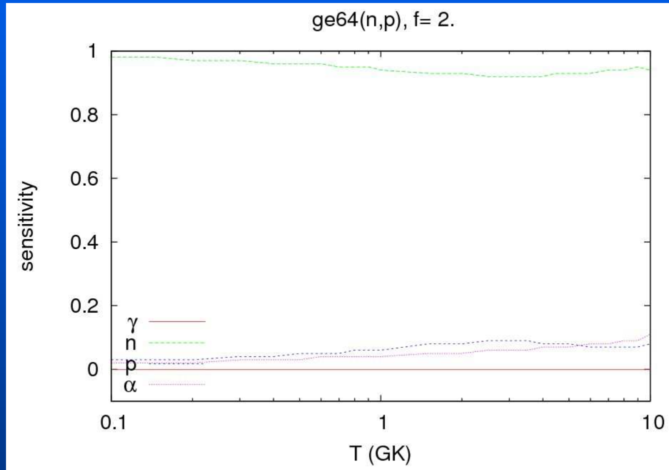


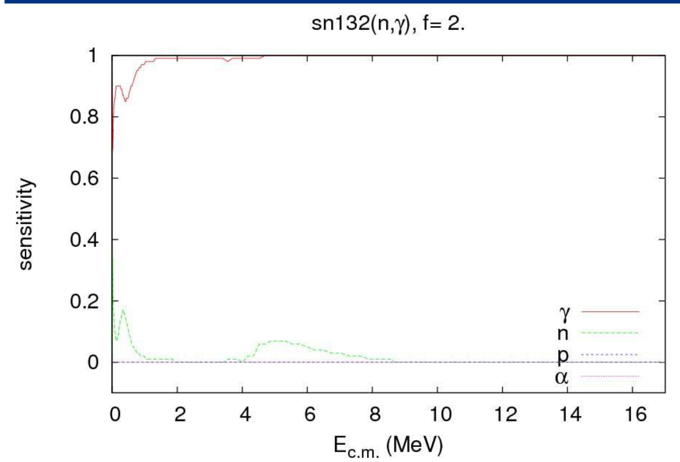
rp-process



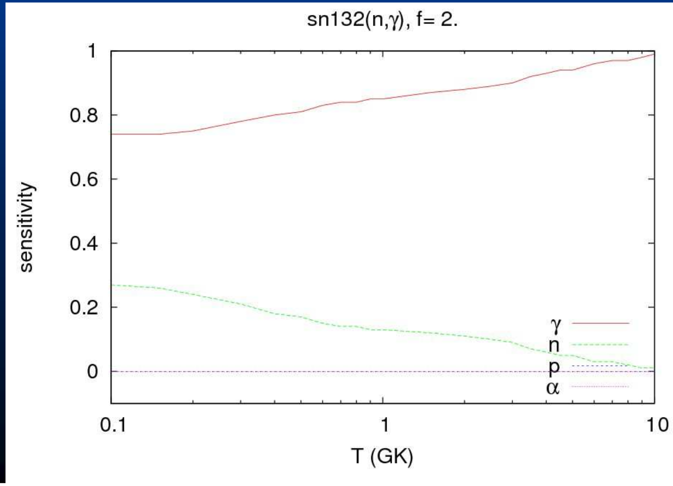


νp-process

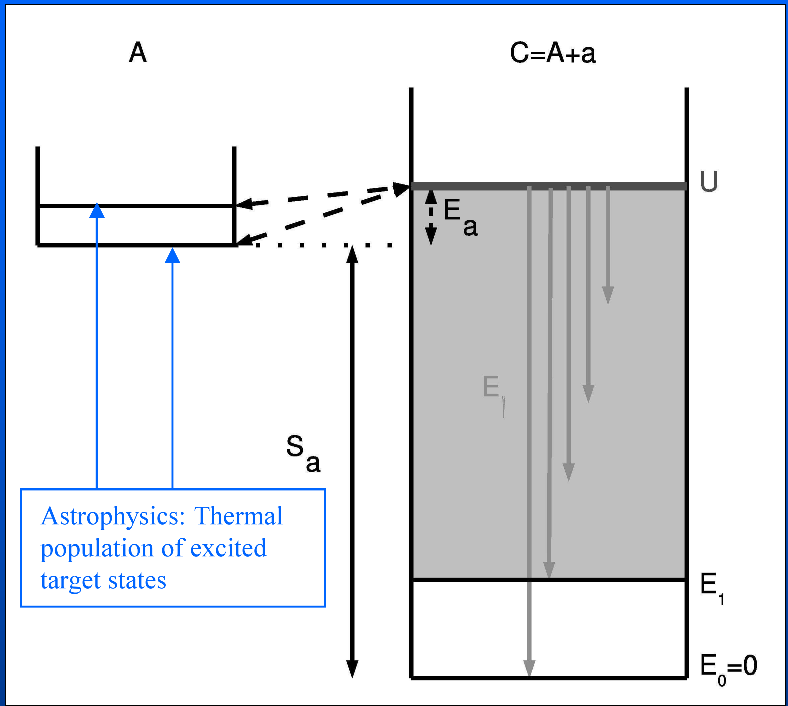




r-process



Relevant γ-transition energies for capture

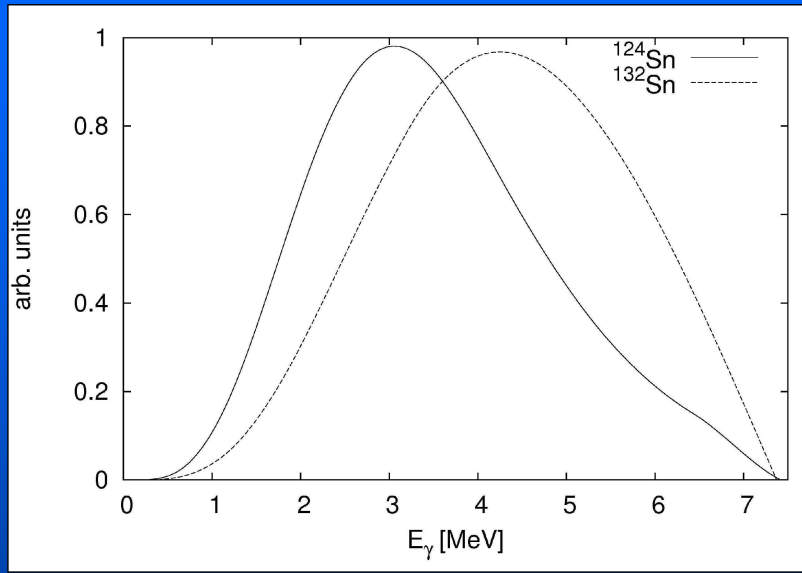


Competition between level density increase and decrease of transition strength:

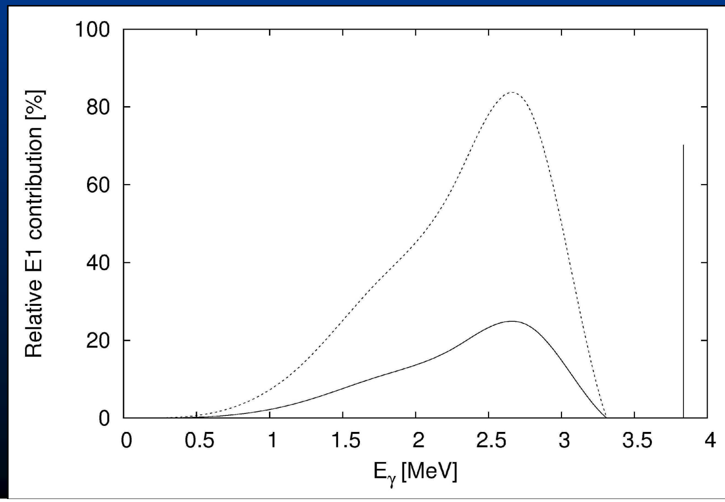
$$\rho \propto \frac{e^{2\sqrt{aU}}}{U^{5/3}}$$

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

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

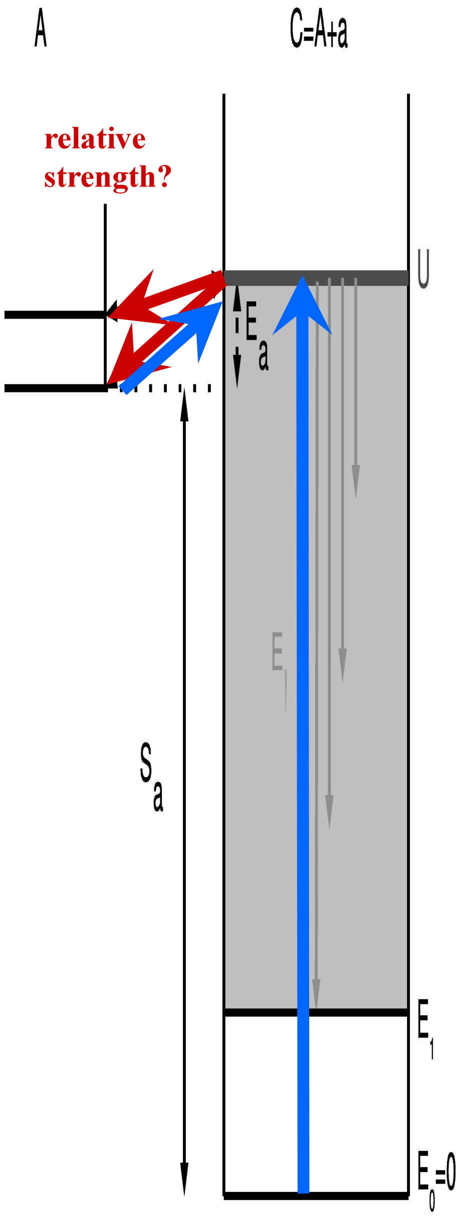


Transition to g.s. or isolated excited states often suppressed by selection rules:



Rauscher, PRC 78 (2008) 032801(R)

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?

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!

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

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

Stellar reactivity

$$R_i(T) = \int_0^\infty \sigma_i(E_i)\,\Phi(E_i,T)\,dE_i$$

$$w_i = (2J_i + 1)e^{-E_i/(kT)}$$

Boltzmann weights

The measured cross section σ_0 determines R_0

$$\sigma^*(E,T) = \frac{\sigma^{\mathrm{eff}}(E)}{G_0(T)} = \frac{1}{\sum_i P_i} \sum_i \sum_j \frac{2J_i+1}{2J_0+1} \frac{E-E_i}{E} \sigma^{i\to j}(E-E_i)$$

$$= \frac{1}{\sum_i P_i} \sum_i \sum_j \frac{2J_i+1}{2J_0+1} W_i \sigma^{i\to j}(E-E_i) \quad ,$$

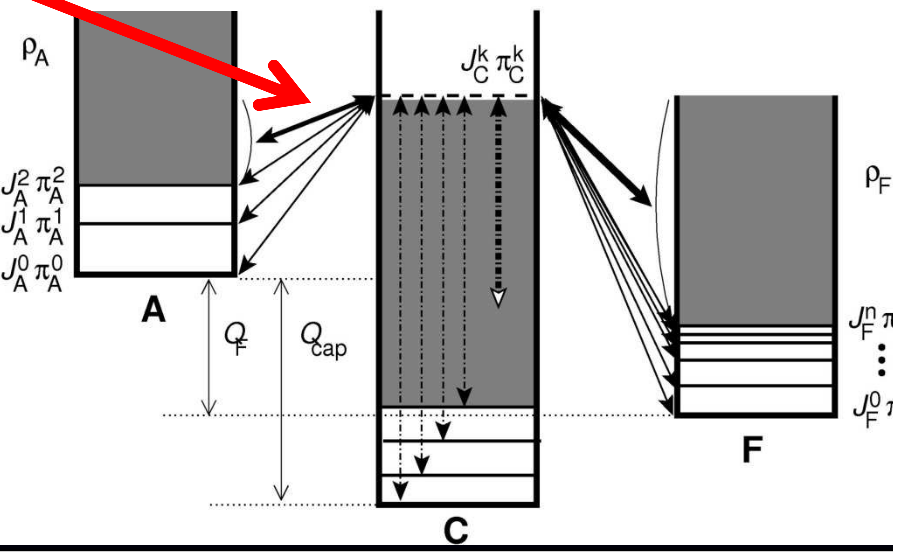
Stellar cross section

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

Population factor

$$W_i = \frac{E-E_i}{E} = 1 - \frac{E_i}{E}$$

Weight of excited state



T. Rauscher, Int. J. Mod. Phys. E 20, 1071 (2011)

Ground state contribution to stellar rate

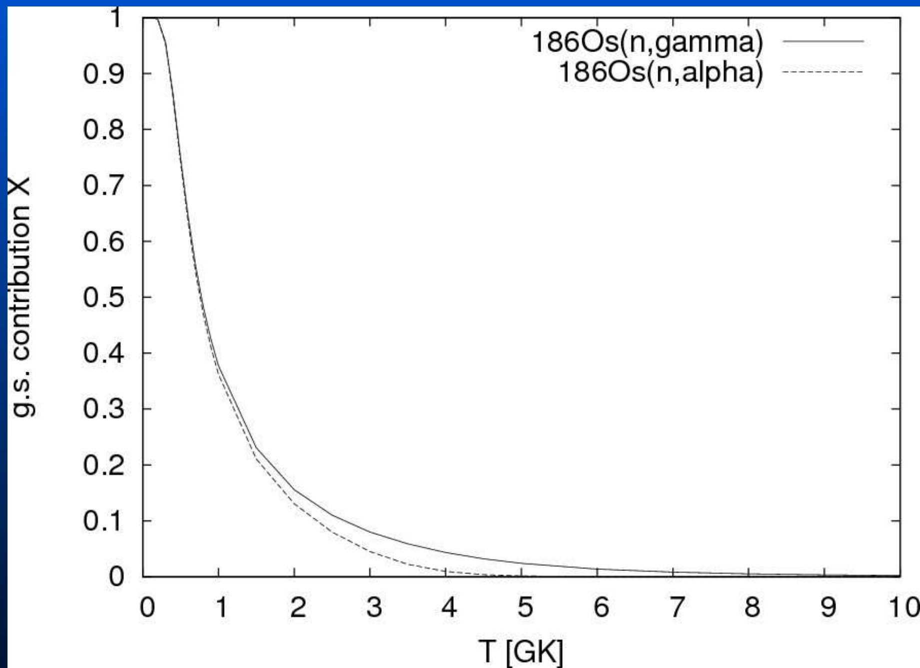
$$X = \frac{R_0}{R^* G_0} = \frac{\int \sigma^{\mathrm{lab}}(E)\Phi_{\mathrm{MB}}(E,T)dE}{\int \sigma^{\mathrm{eff}}(E)\Phi_{\mathrm{MB}}(E,T)dE}$$

Traditional Stellar Enhancement Factor is different:

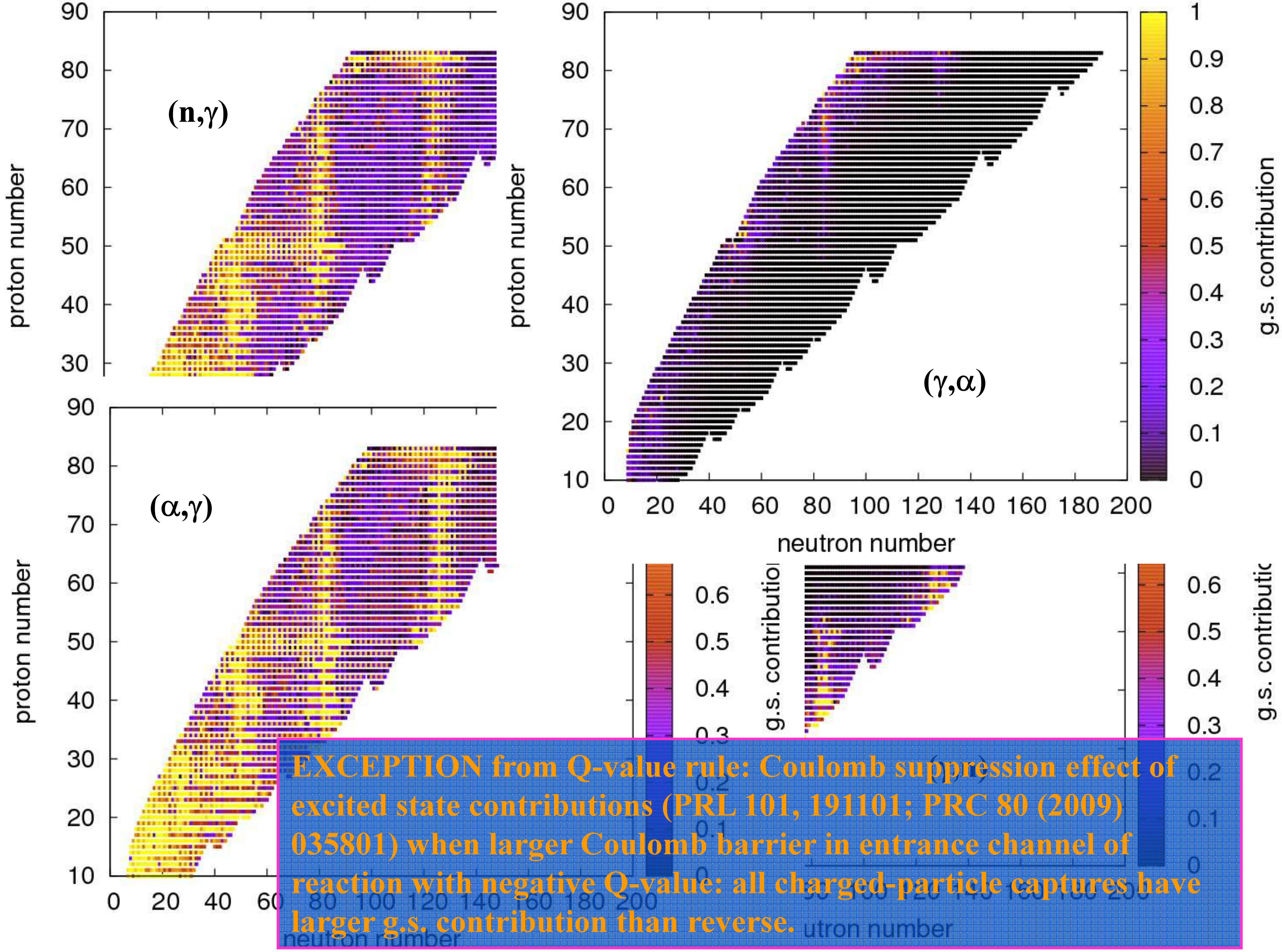
$$f_{\mathrm{SEF}} = \frac{R^*}{R_0}$$

(SEF does not give 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 G_0 and is related to X:
    - $u=(1-X)u'$



T. Rauscher, ApJLett 755, L10 (2012)   Rauscher et al, Ap. J. 738, 143 (2011)



EXCEPTION from Q-value rule: 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: all charged-particle captures have larger g.s. contribution than reverse.

How to combine theory and measurement in a revised stellar rate

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

Contribution of i-th excited state

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

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

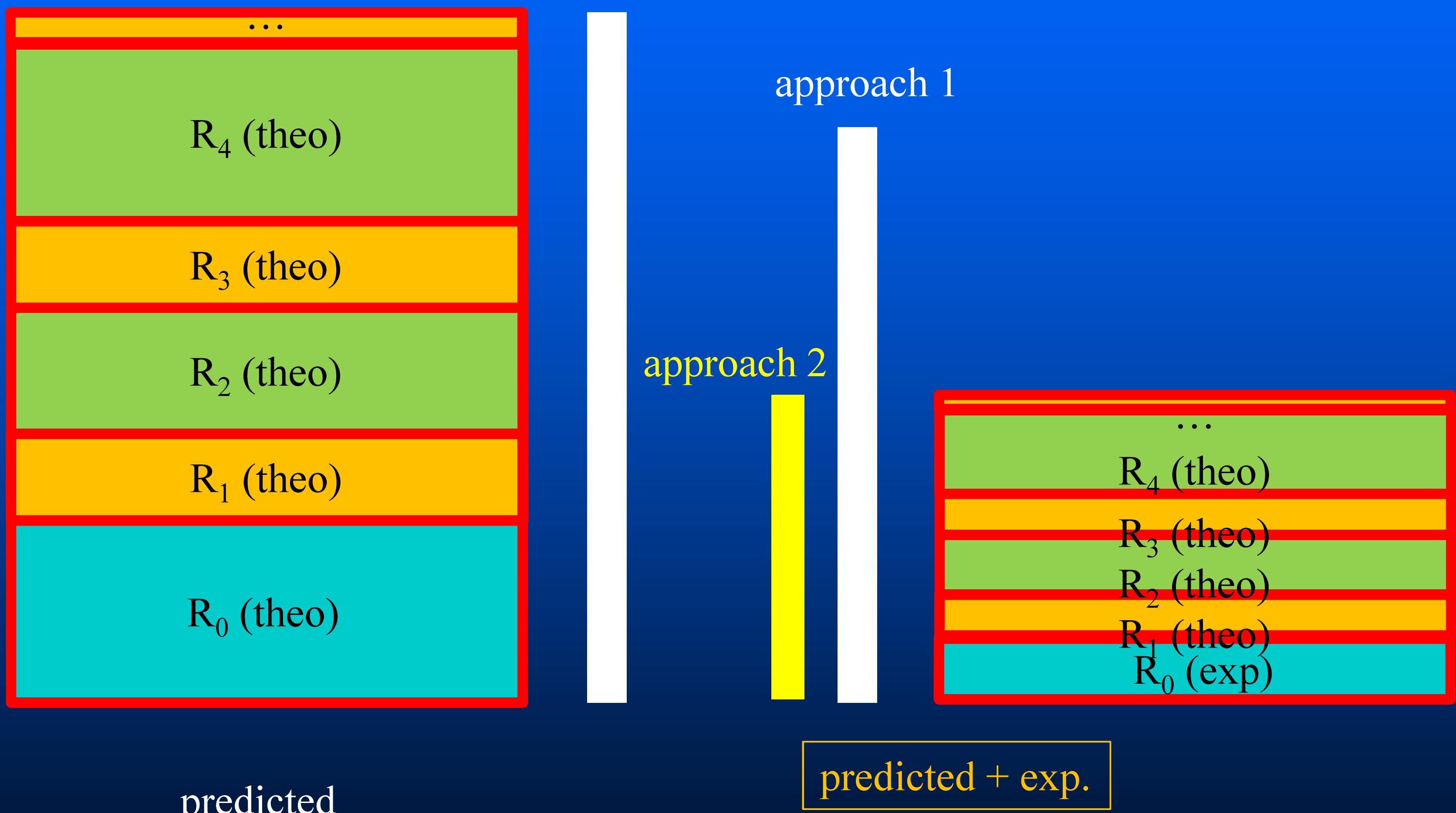
Contribution of g.s. state

One of two assumptions can be made, either:

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

(experimentalist's view OR include additional theory?)

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



R^*

$$R^*_{\mathrm{new}} = R_0^{\mathrm{exp}} f_{\mathrm{SEF}}$$

$$R^*_{\mathrm{new}} = f^* R^*$$

How to combine theory and measurement in a revised stellar rate

Approach 1: Use experimental information without further assumptions

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

Contribution of g.s. state

$$R^*_{\mathrm{new}} = f^* R^*$$

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

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

The factor contains the *theoretical* and the *experimental* g.s. reactivity and the g.s. contribution.

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

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

T. Rauscher, ApJLett 755, L10 (2012)

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 ?

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

Contribution of g.s. state

$$R^*_{\mathrm{new}} = f^* R^*$$

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

$$f^* = \frac{R_0^{\exp}}{R_0}$$

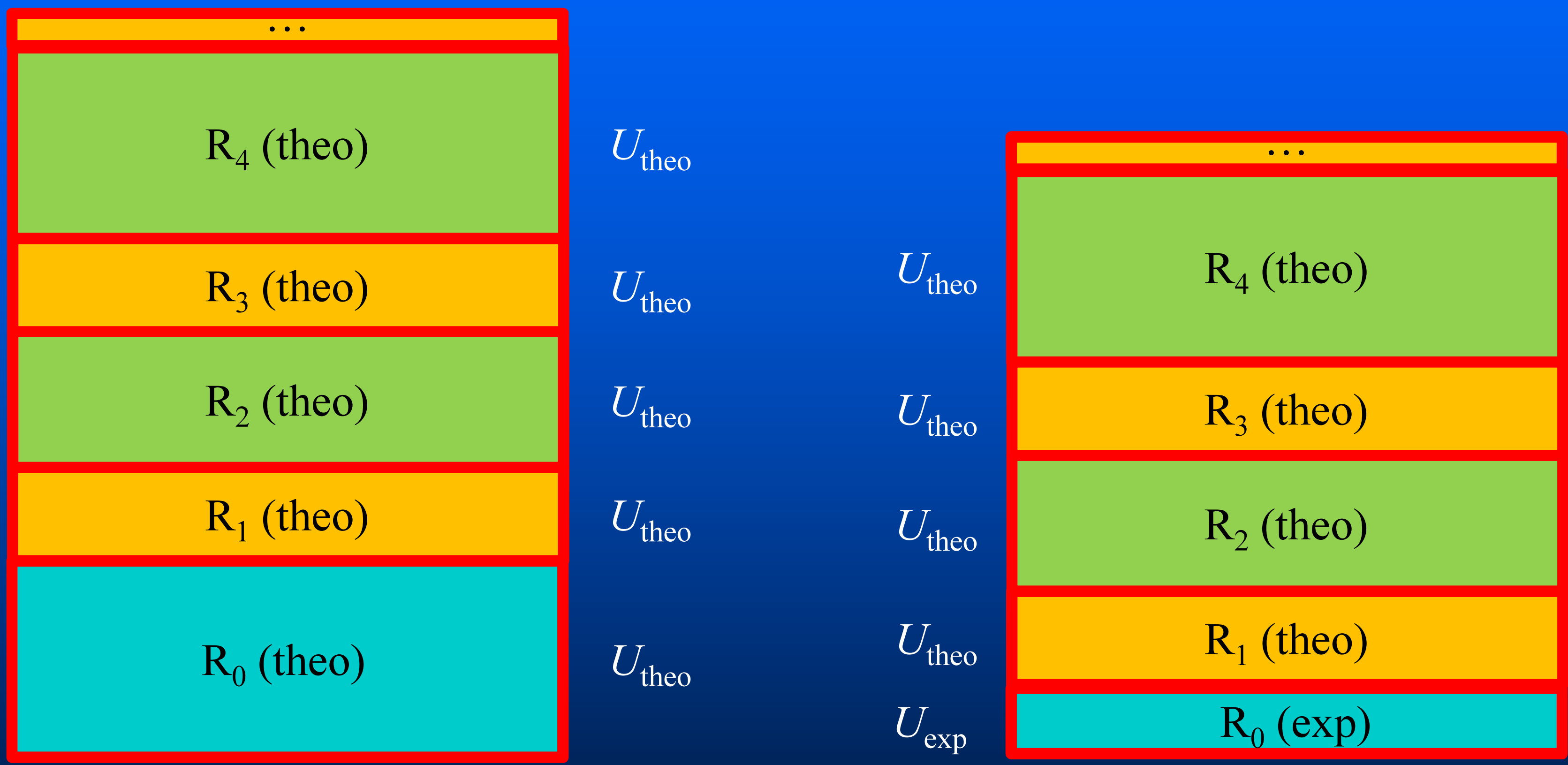
The factor contains the *theoretical* and the *experimental* g.s. reactivity.

$$U^*_{\mathrm{new}} = \mathbf{?}$$

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)



predicted

R^*

$U^* = U_{theo}$

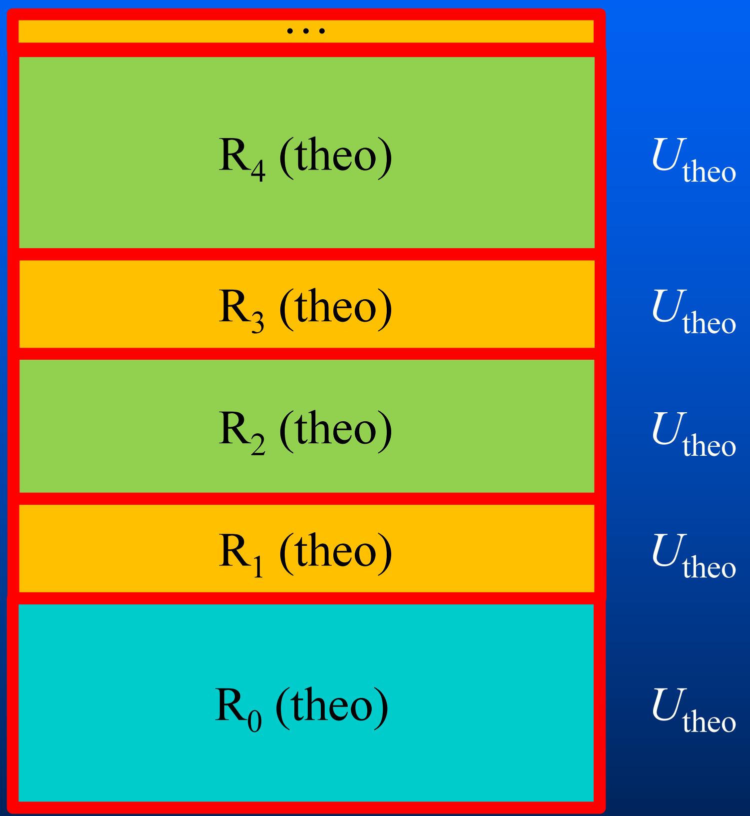
predicted + exp.

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

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??

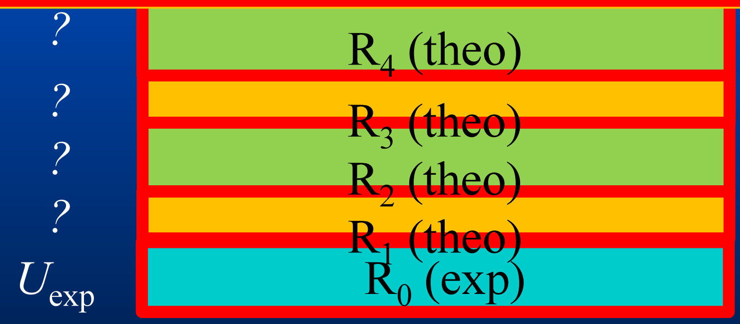
- If so, then $U^*_{new}=U_{exp}$
- If there are different sources of uncertainty, then scaling may remove theory uncertainty only partially or not at all! Then we are back to approach 1 (or in between approaches 1 and 2)…



predicted

R^*

$U^*=U_{theo}$



predicted + exp.

$U^*_{new}=?$

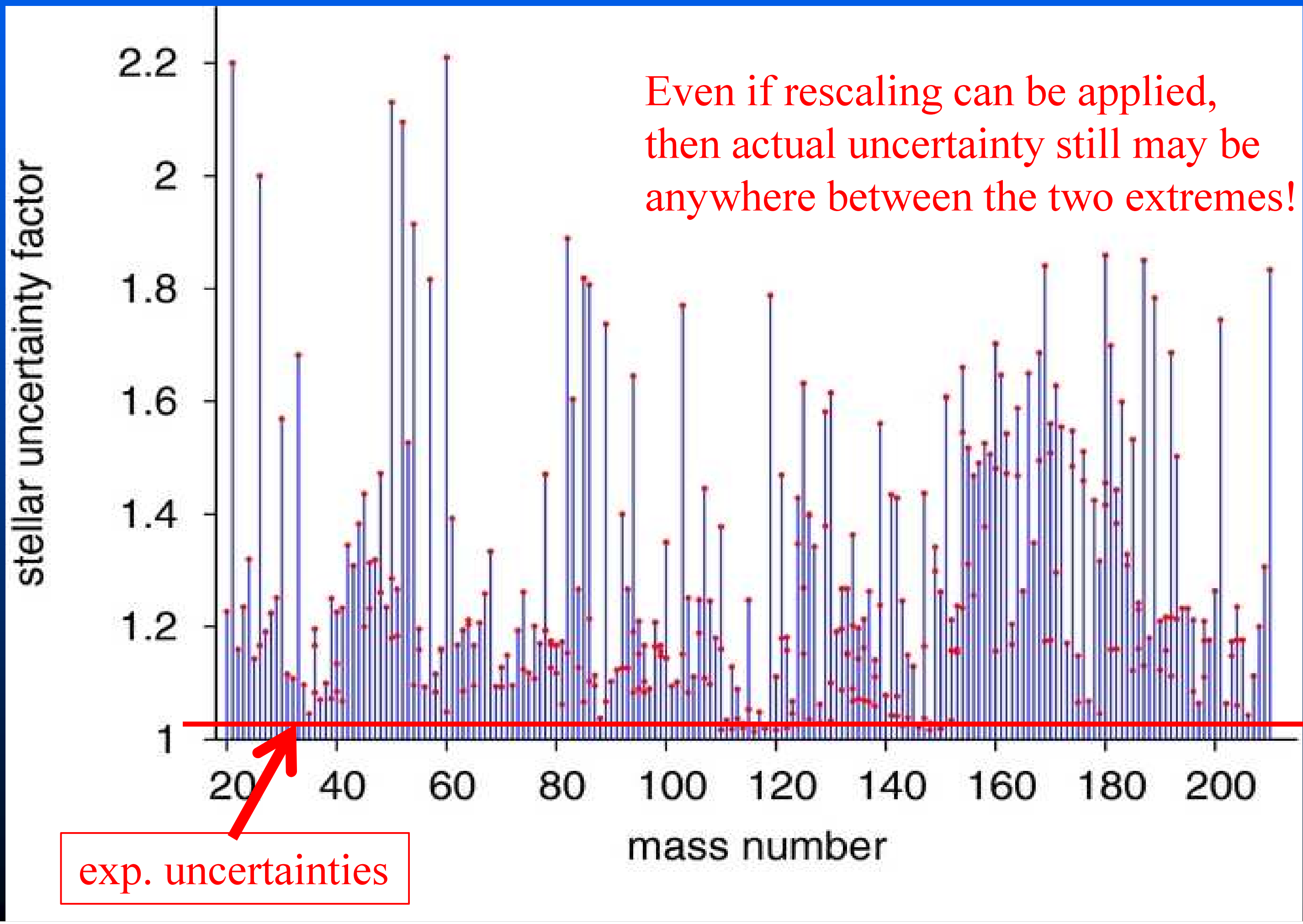
$$R^*_{new} = R_0^{exp} f_{SEF}$$

Realistic uncertainties in stellar (n,γ) rates close to stability

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

T. Rauscher, ApJLett 755, L10 (2012)

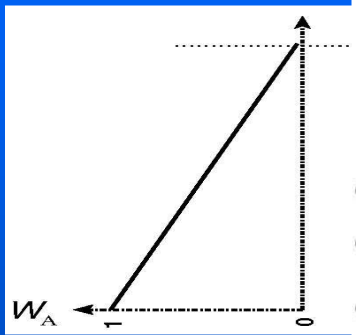
U=2*

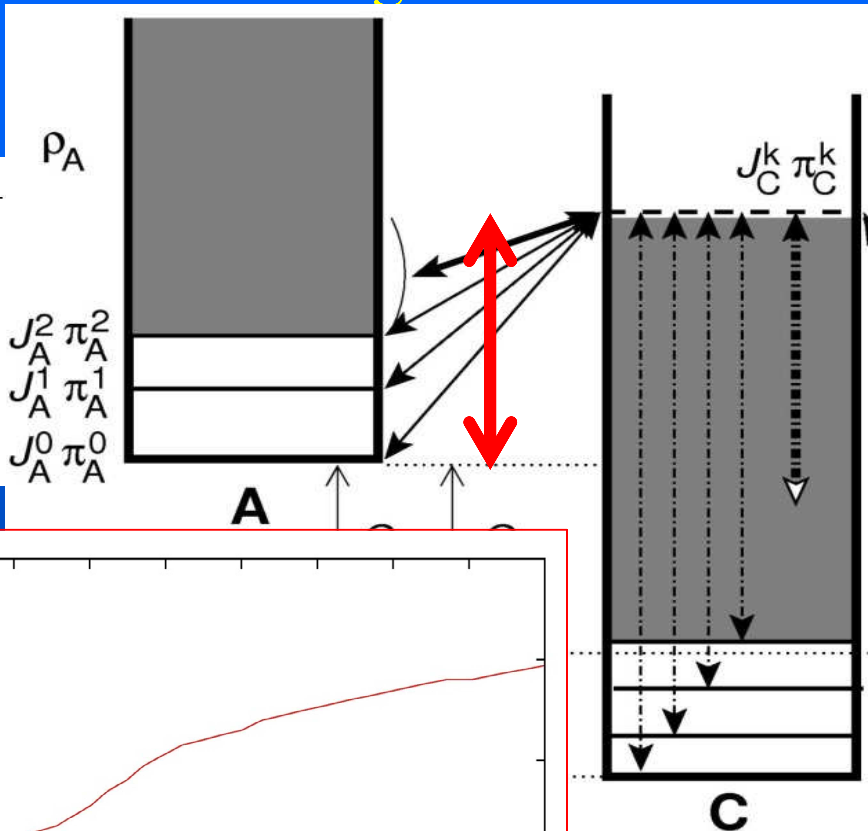


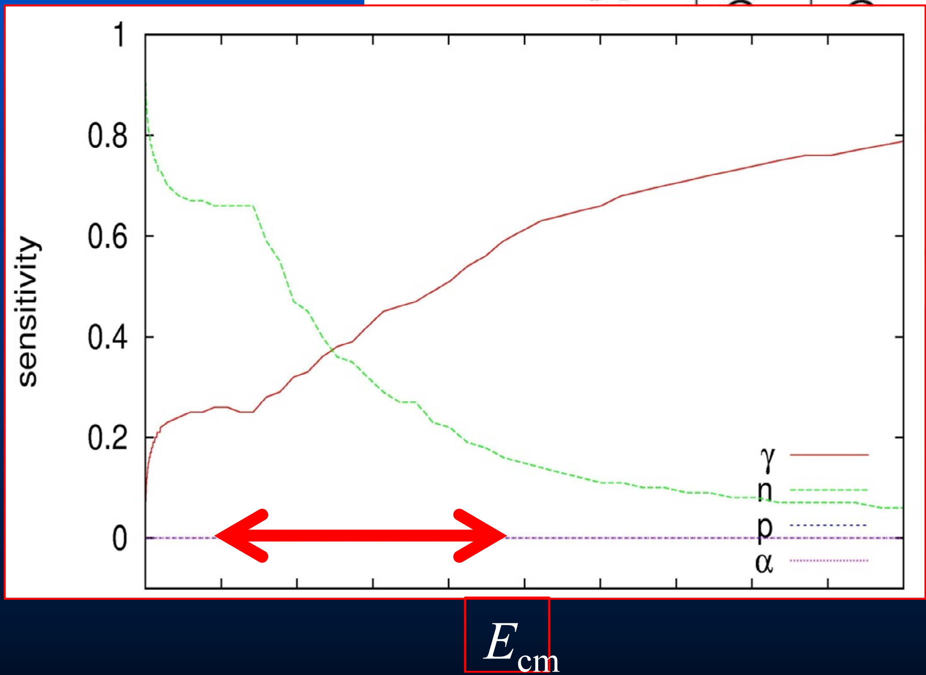
Nuclei and exp. values from online KaDoNiS 0.3

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

Weight of exc. state in stellar rate







<u>Importance of transitions changes with relative energy!</u>

Cross section depends on:

- low energy: neutron trans.
- higher energy: *γ*-transit.

Simple scaling of excited state contributions (by SEF) may not be applicable and remaining uncertainties will likely be larger than experimental errors!

<u>Neutron transitions:</u>
Energy-dependent optical potential,
angular momentum barrier

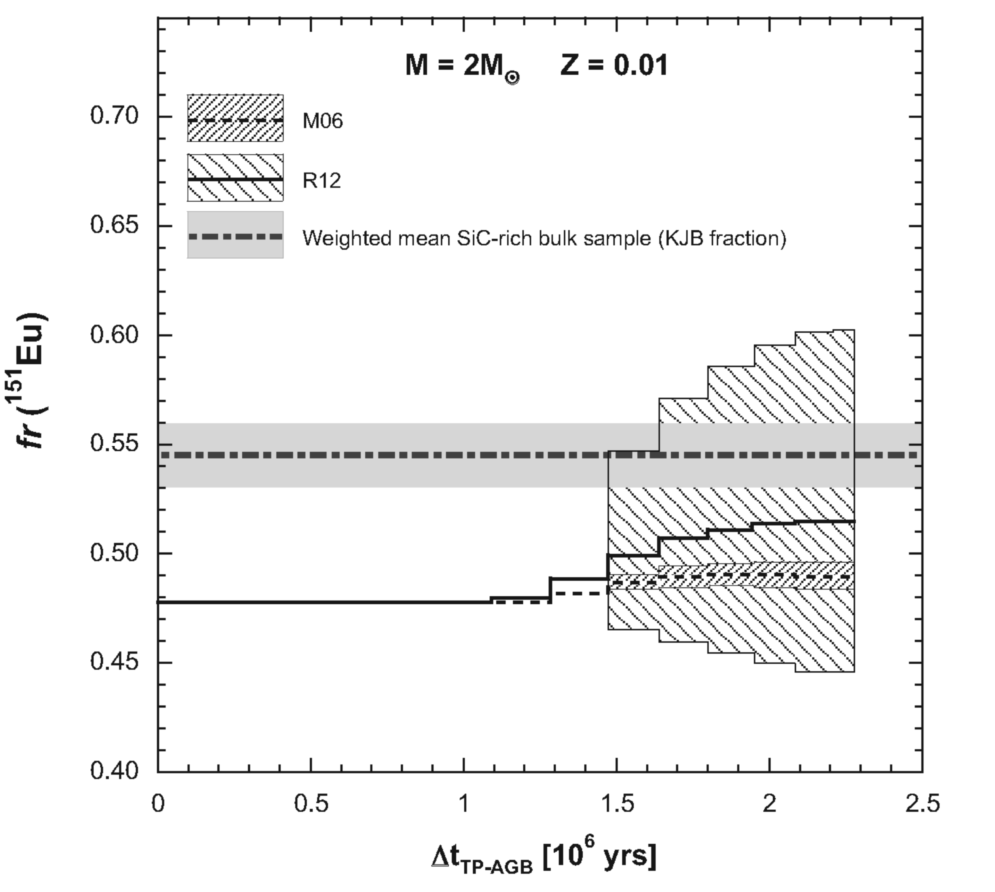
<u>*γ*-transitions:</u>
EM-type and –multipolarity selection depend on $J\pi$ of target exc. state;
(energy-dependent) strength function different

A practical application:
The ^{151}Eu/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).

$[fr(^{151}\mathrm{Eu}) = {}^{151}\mathrm{Eu}/({}^{151}\mathrm{Eu}+{}^{153}\mathrm{Eu})]$



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

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

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

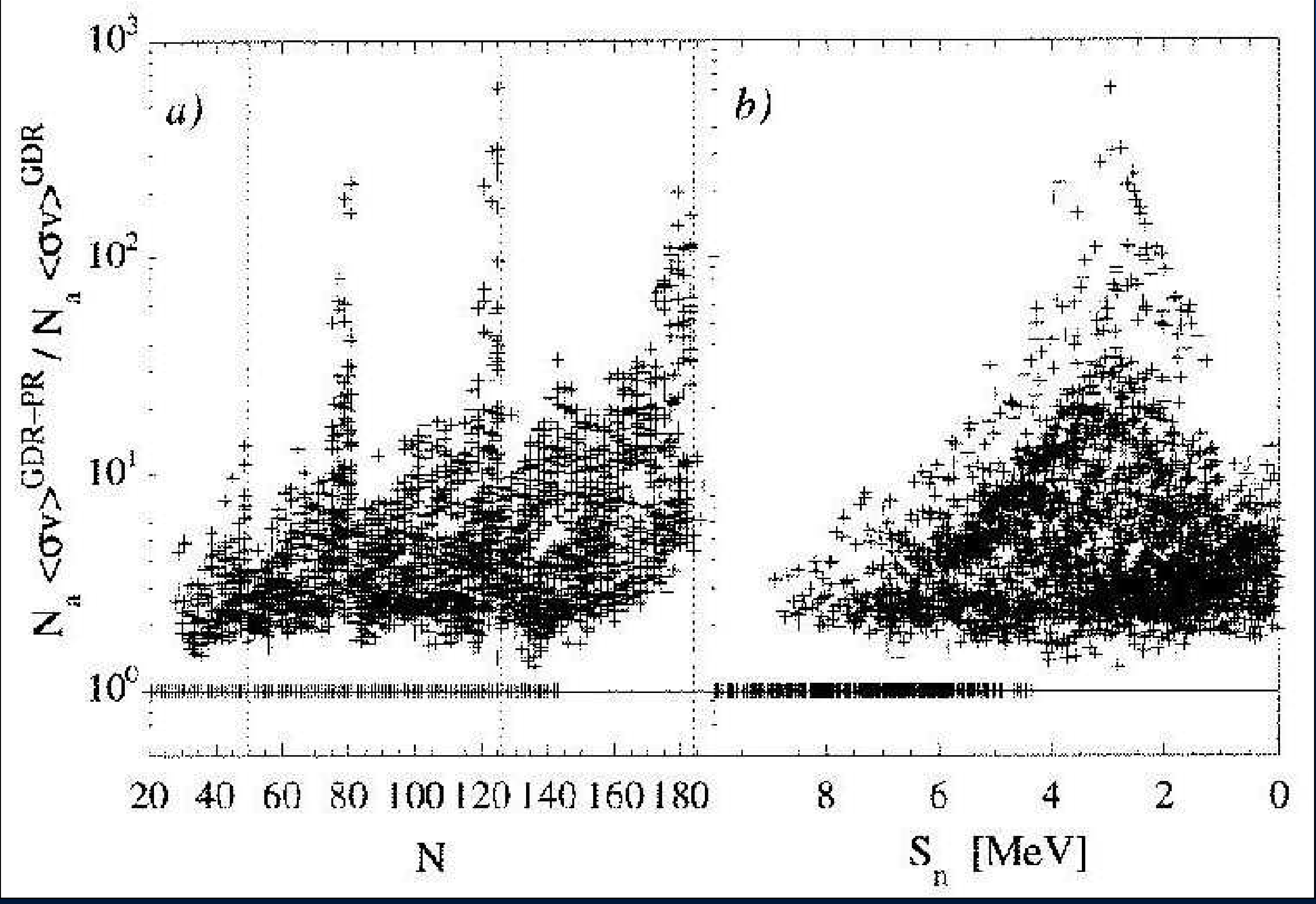
- M06…Marrone et al (2006) rate with exp. uncertainties
- R12…Rate including Marrone et al (2006) for the g.s. cross section but using the prescription as given by Rauscher (2012) for the stellar rate and its uncertainty

Which approach for rates and uncertainties?

- Scaling by SEF and assigning exp. error to full stellar rate is too simplistic (unless $X_0 \approx 1$), especially for (n,γ)!
  - underestimation of actual remaining uncertainty
  - works better for charged particle reactions
- If $X_0 \approx 1$, don't bother! (experiment determines rate completely)
  - n.b.: this cannot be seen from the SEF!!
- Otherwise, this has to be investigated for each reaction separately
  - Theory analysis required
  - Compare excited state reaction cross sections:
    - » e.g., sensitivity to entrance or exit channel, selection of EM multipoles for γ-transitions, etc
- To be safe, apply approach 1 (only g.s. transition is replaced by experiment, no SEF scaling) and its uncertainty estimate
  - within error, this encompassed the values obtained with any other approach

Possible Complications Far Off Stability

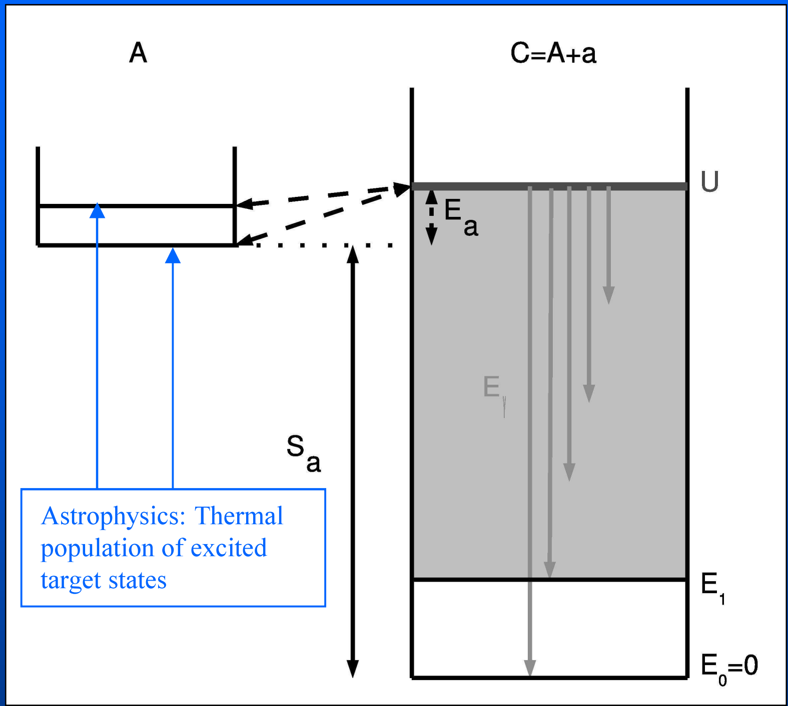
Possible Impact of Pygmy Resonances Far Off Stability?



Goriely 1999

Rauscher 1999

Relevant γ-transition energies for capture

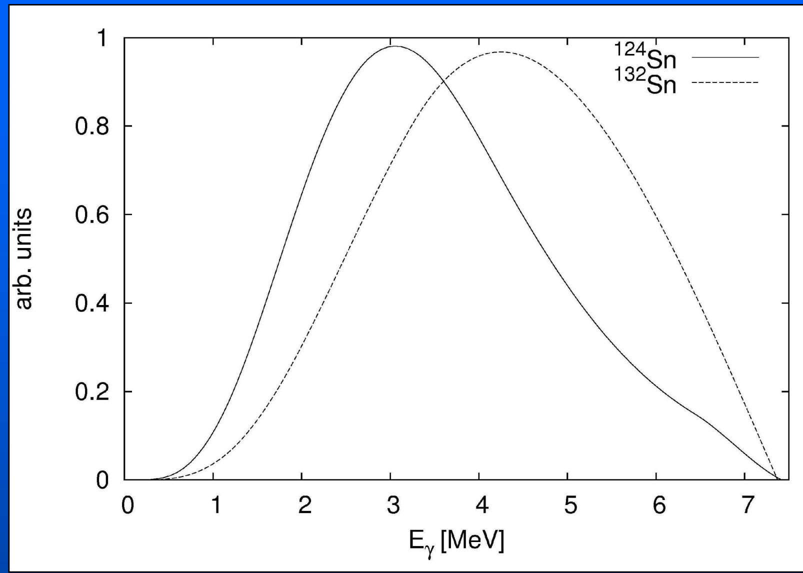


Competition between level density increase and decrease of transition strength:

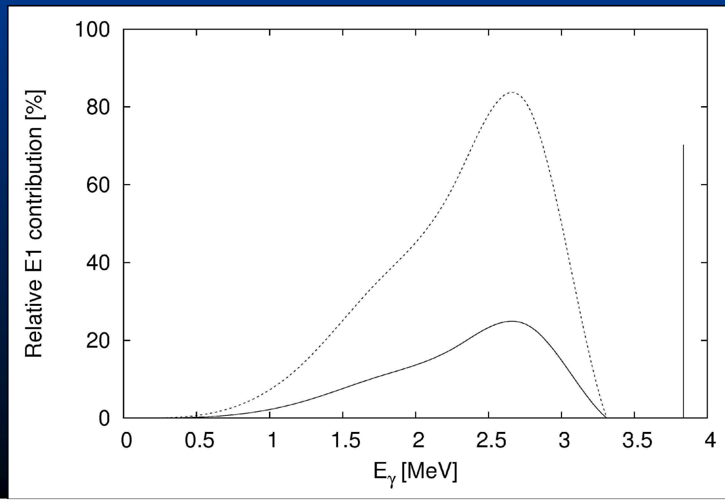
$$\rho \propto \frac{e^{2\sqrt{aU}}}{U^{5/3}}$$

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

$$T_{\mathrm{M1}} \propto E_\gamma^{\;3}$$

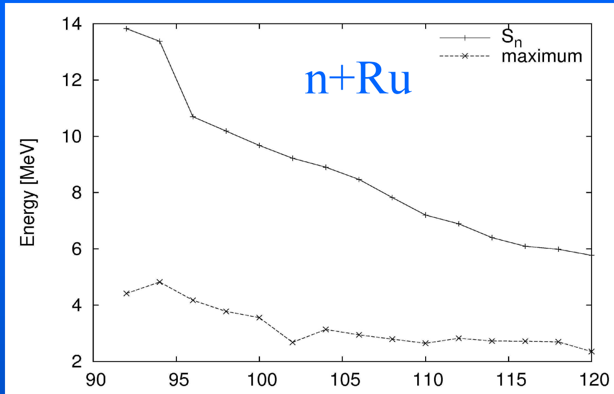


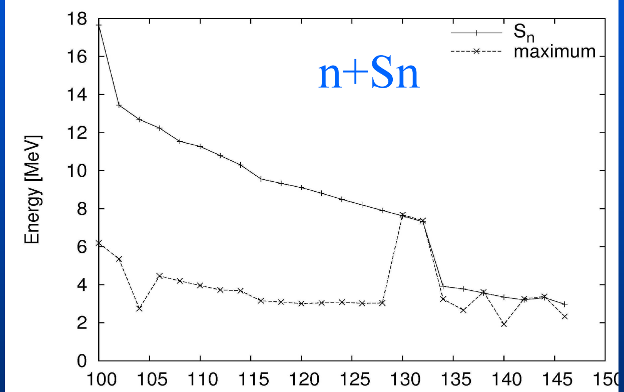
Transition to g.s. or isolated excited states often suppressed by selection rules:

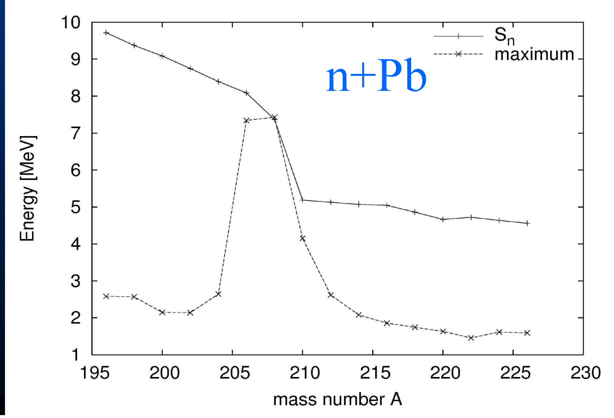


Rauscher, PRC 78 (2008) 032801(R)

Location of maximum contribution at astrophysically relevant reaction energies

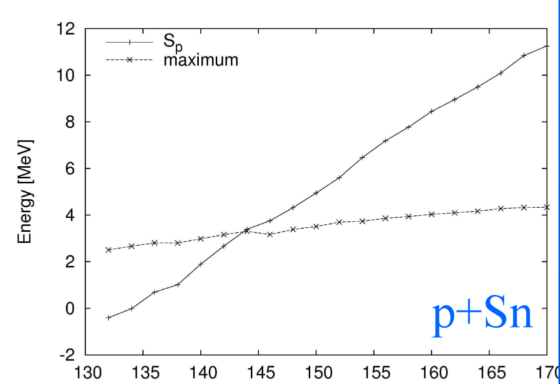


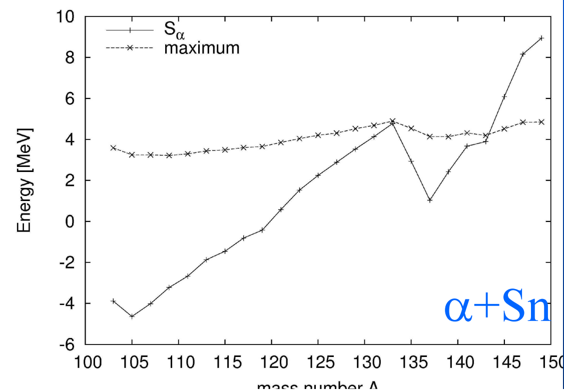


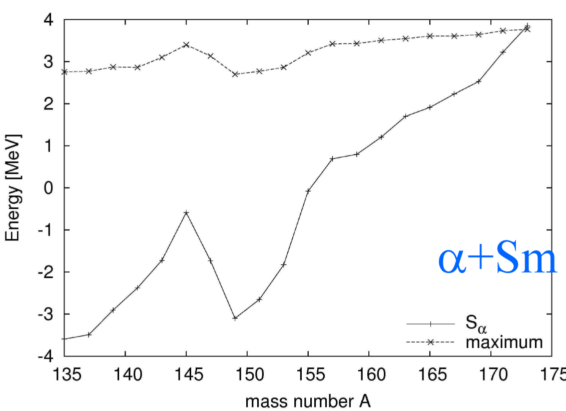


- Maxima located at 2-4 MeV
- quite independent of reaction
- Exception: nuclei with low level density (magic numbers or close to drip) → maximum shifted to higher energies (isolated states)
- Hauser-Feshbach not valid for exceptions

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

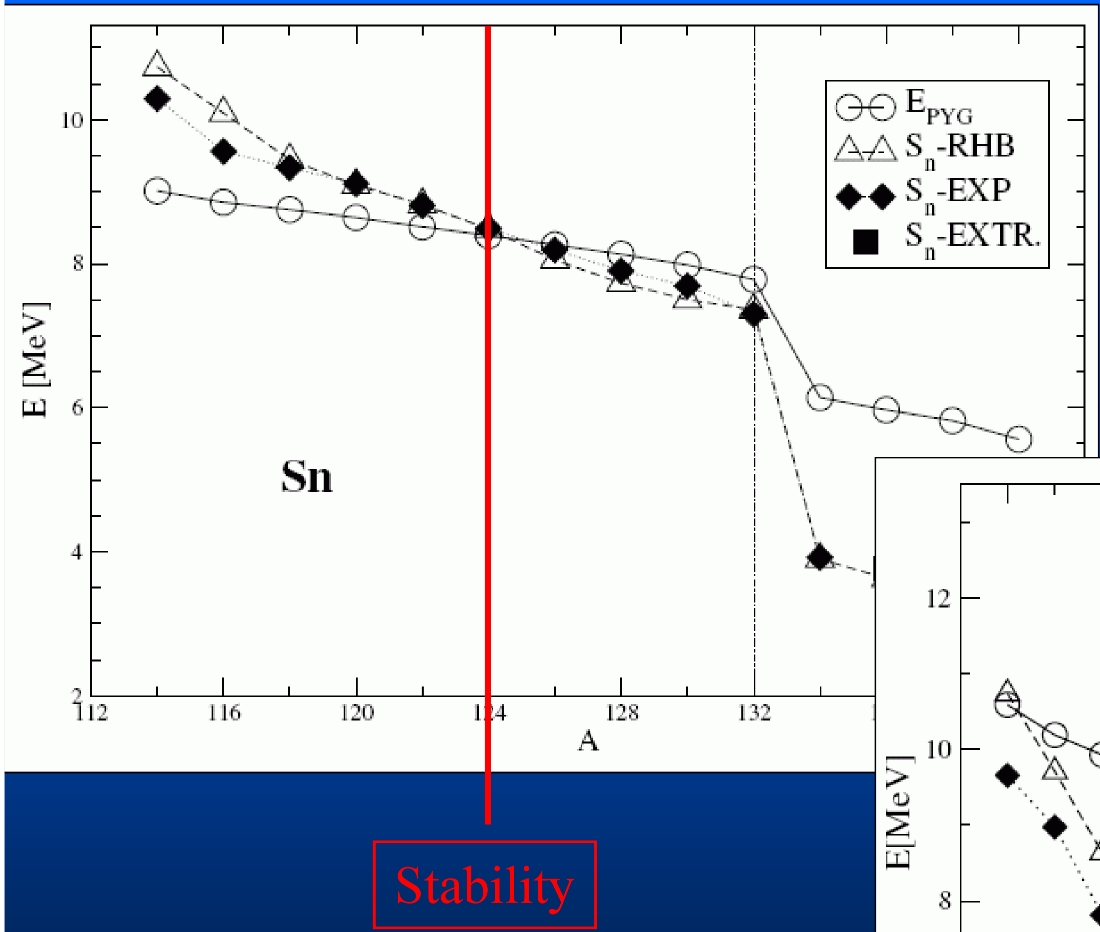


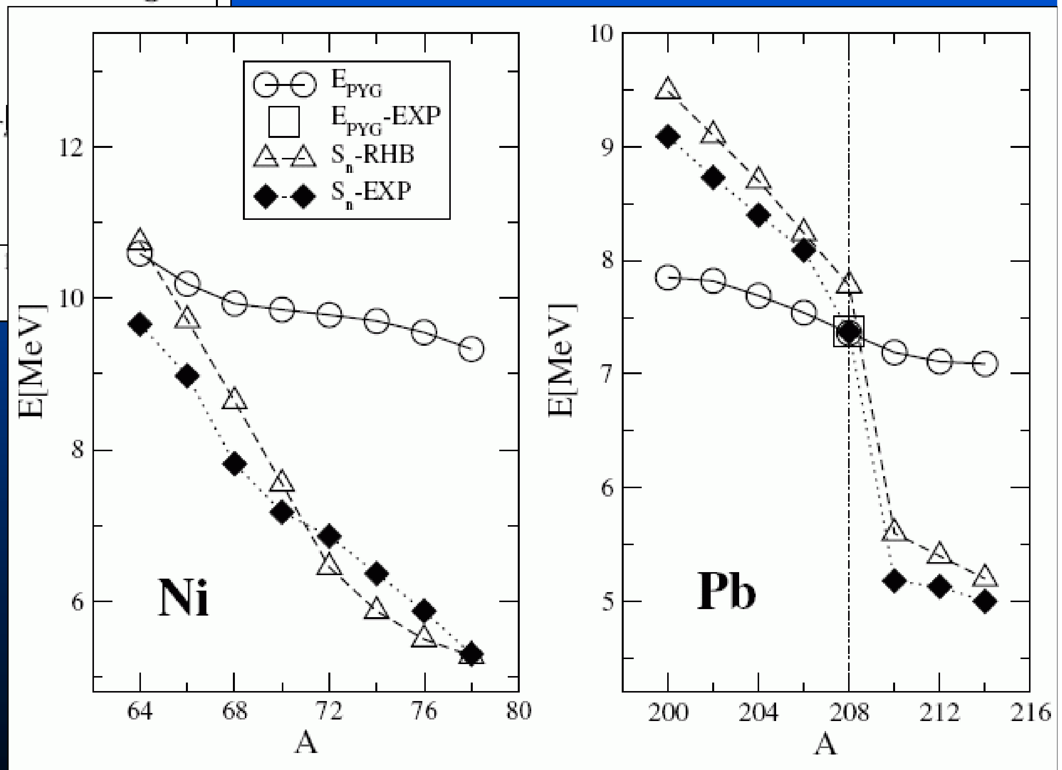




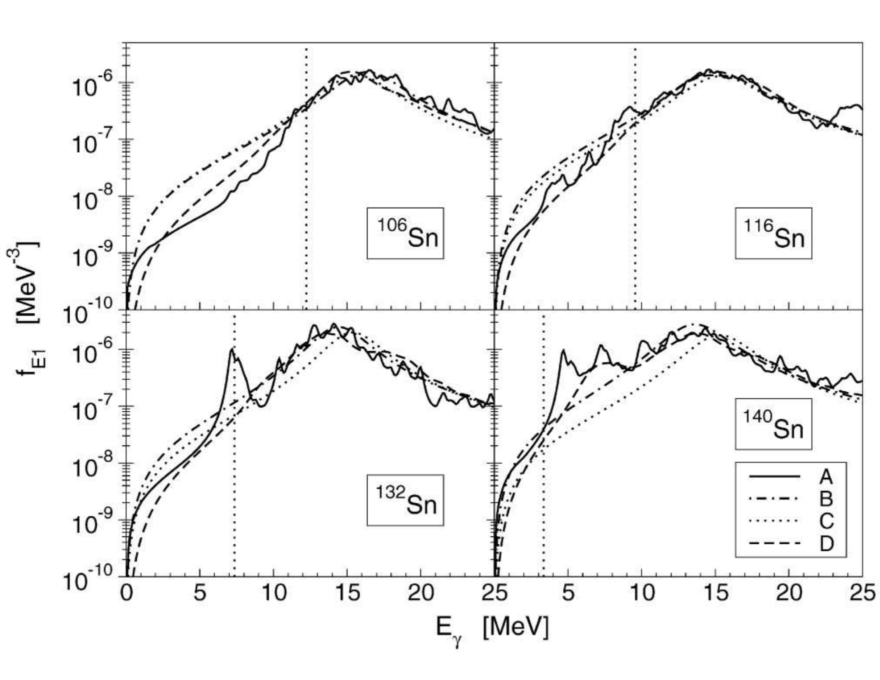
Rauscher, PRC 78 (2008) 032801(R)

Pygmy Predictions

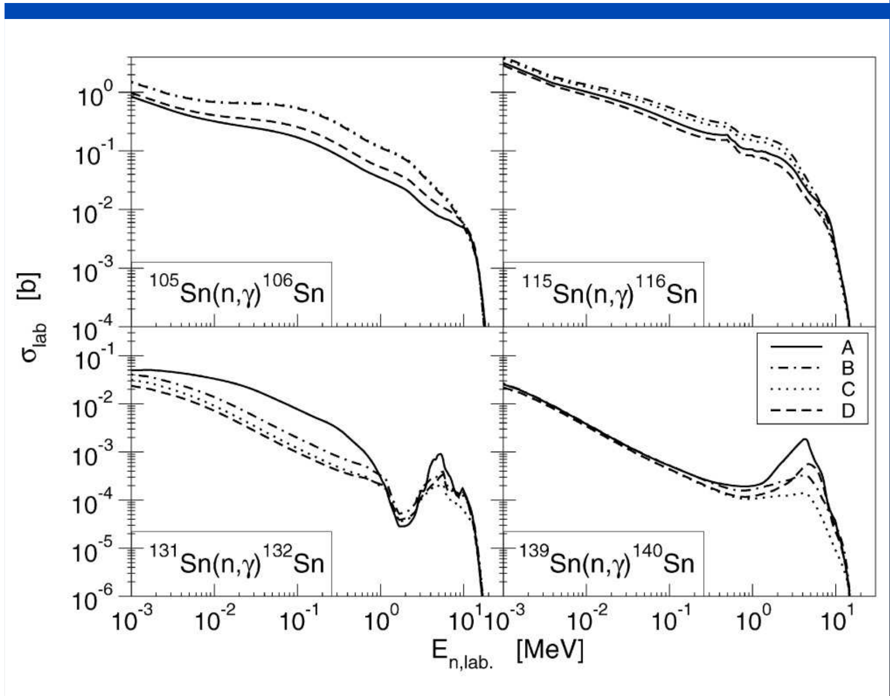




Paar, Nikšić, Vretenar, Ring 2005



γ-Strengths and Pygmy Resonances in Neutron Captures



- Captures on ^{105,115}Sn: $E_\gamma \approx E_n + 3$ MeV
- Captures on ^{131,139}Sn: $E_\gamma \approx E_n + S_n$

Litvinova et al, NP A823 (2009) 26

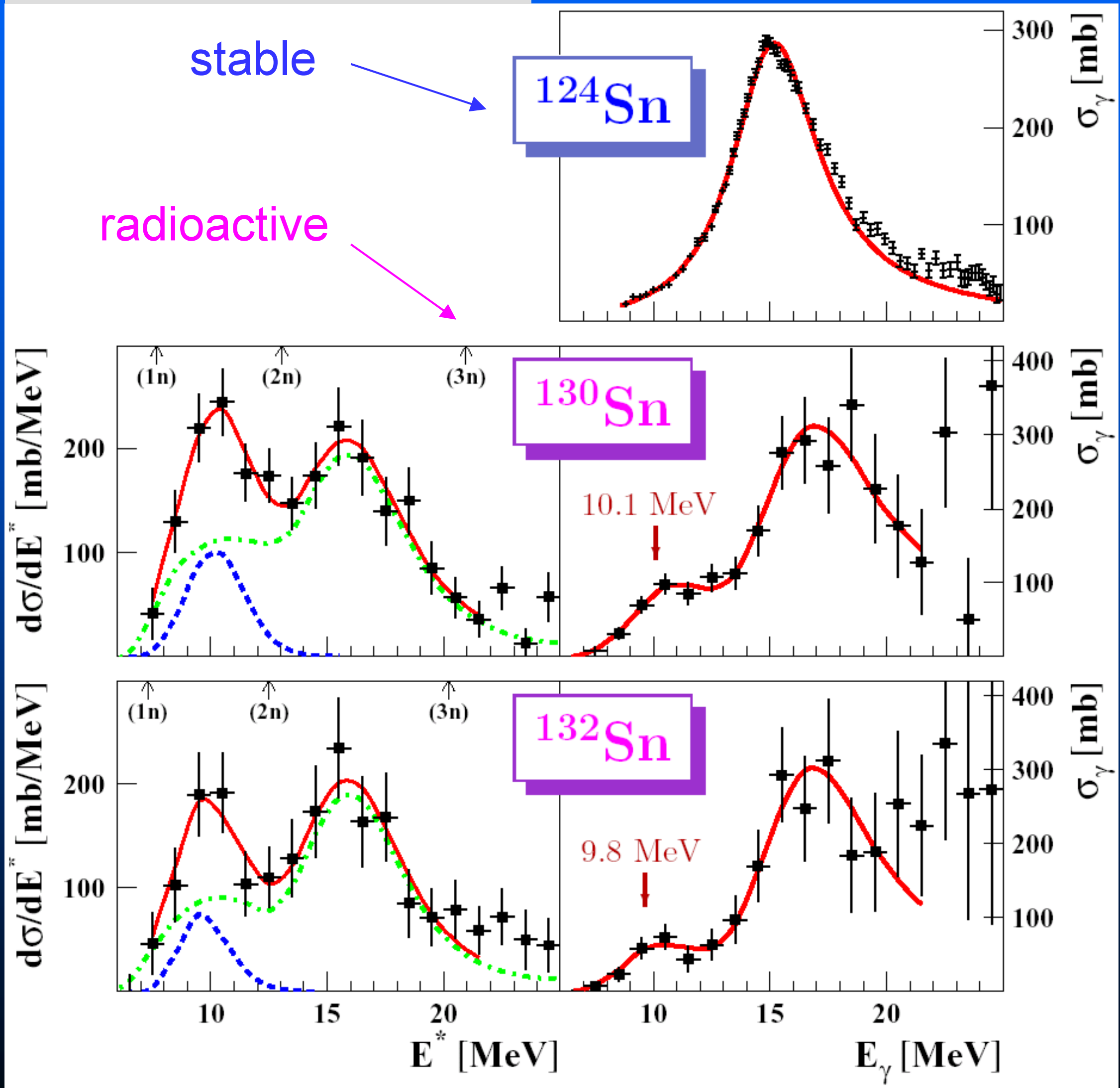
Results: Dipole-strength distributions in neutron-rich Sn isotopes

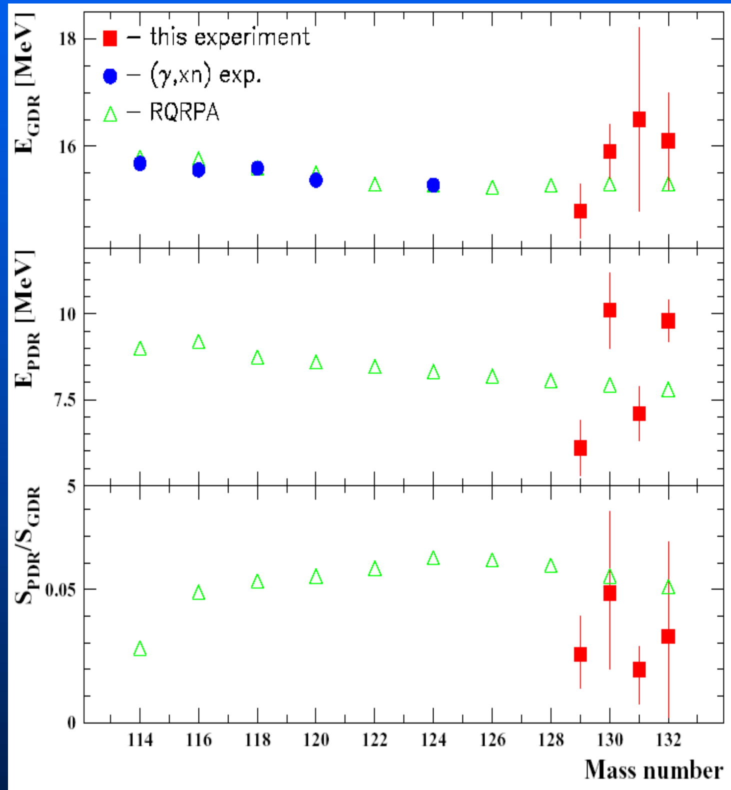
Electromagnetic-excitation cross section

Photo-neutron cross section

Comparison with theoretical predictions

RMF (N. Paar et al.)

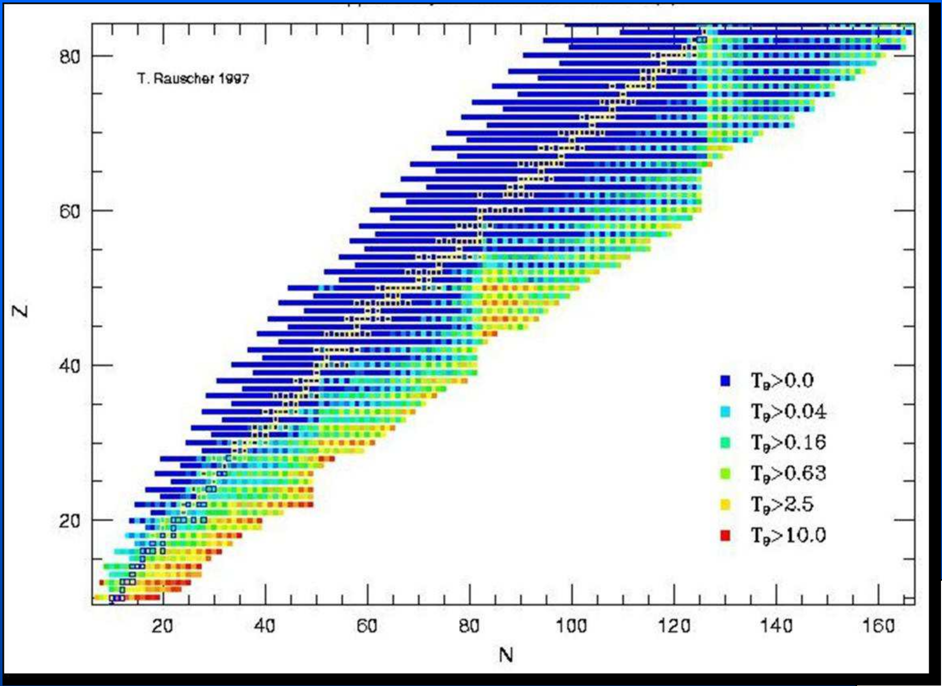




LAND/FRS collaboration
P. Adrich et al., PRL 95 (2005) 132501

Reaction Mechanism Comparison

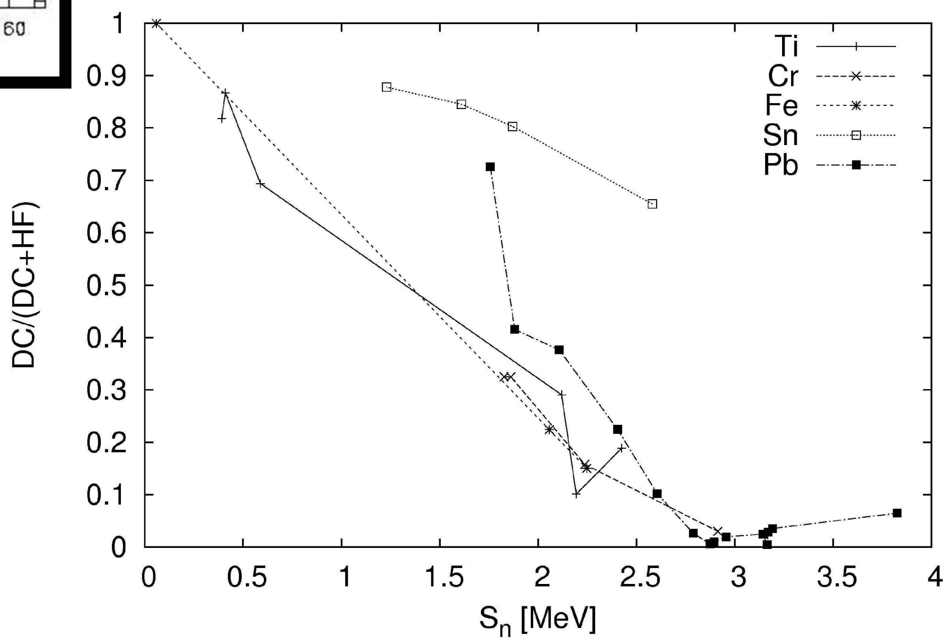
Neutron induced reactions



Rauscher et al., PRC 56 (1997) 1613

Applicability of statistical model

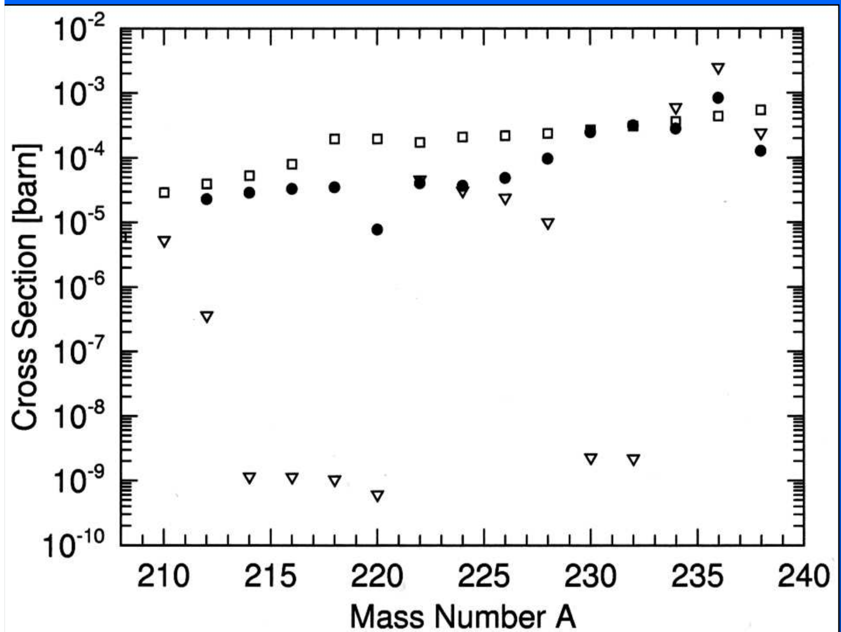
Comparison DC and Hauser-Feshbach



T. Rauscher; J. Phys. G 35 (2008) 014026

Direct Neutron Capture On Pb- and Sn-Isotopes

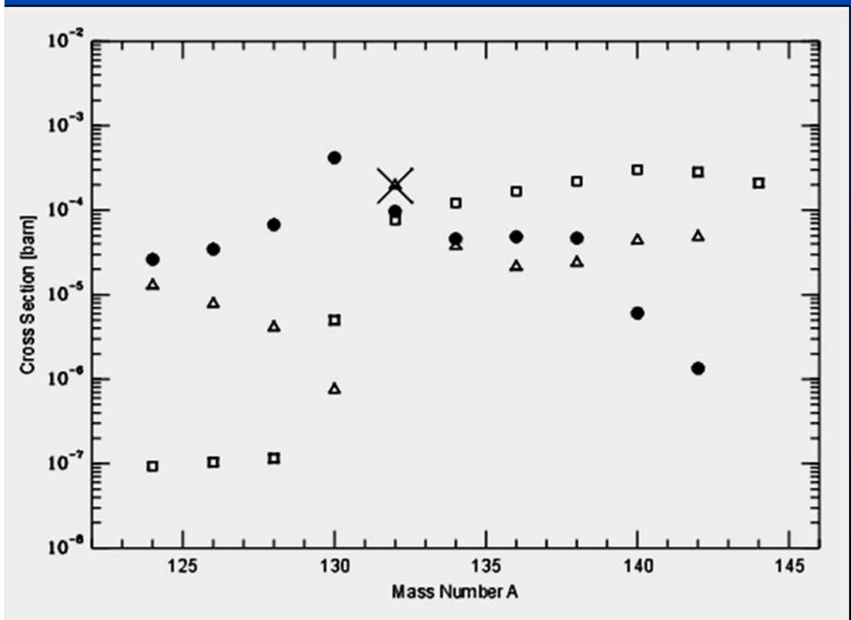
(30 keV neutrons)



Pb

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

Large differences in predictions due to differences in predicted <u>spectroscopy and masses</u> (separation energies)

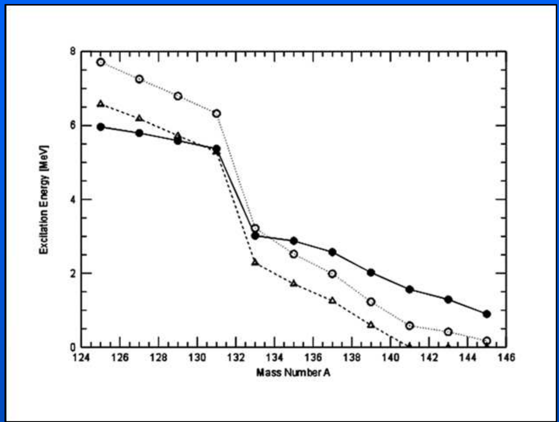


Sn

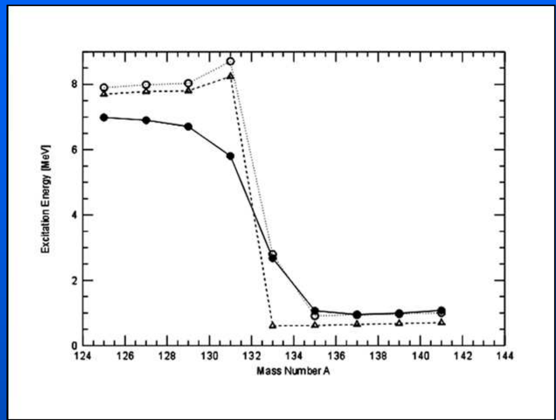
Rauscher et al., PRC 57 (1998) 2031

Nuclear Structure Characteristics of Sn-Isotopes

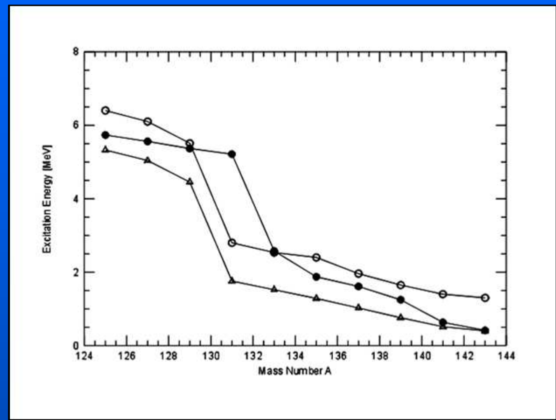
triangles: 1/2$^-$, open circles: 3/2$^-$, full dots □: S_n



HFB

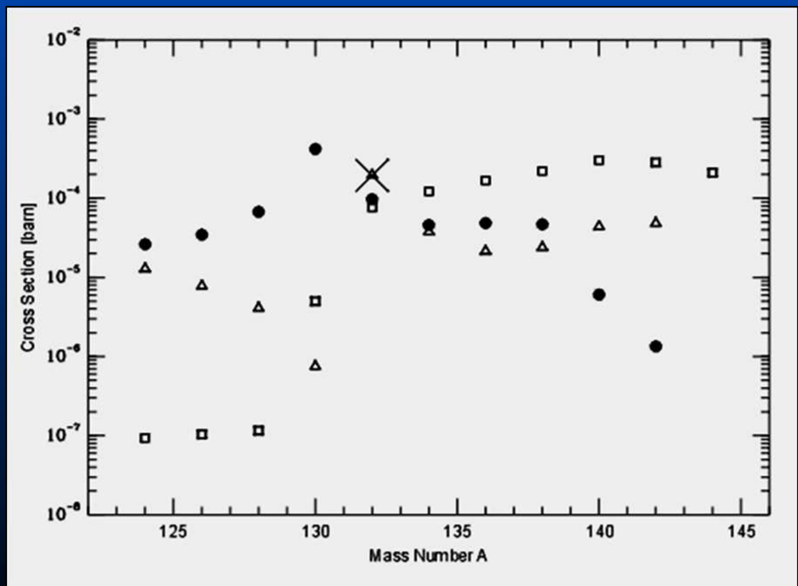


RMFT (NL-SH)



FY (FRDM)

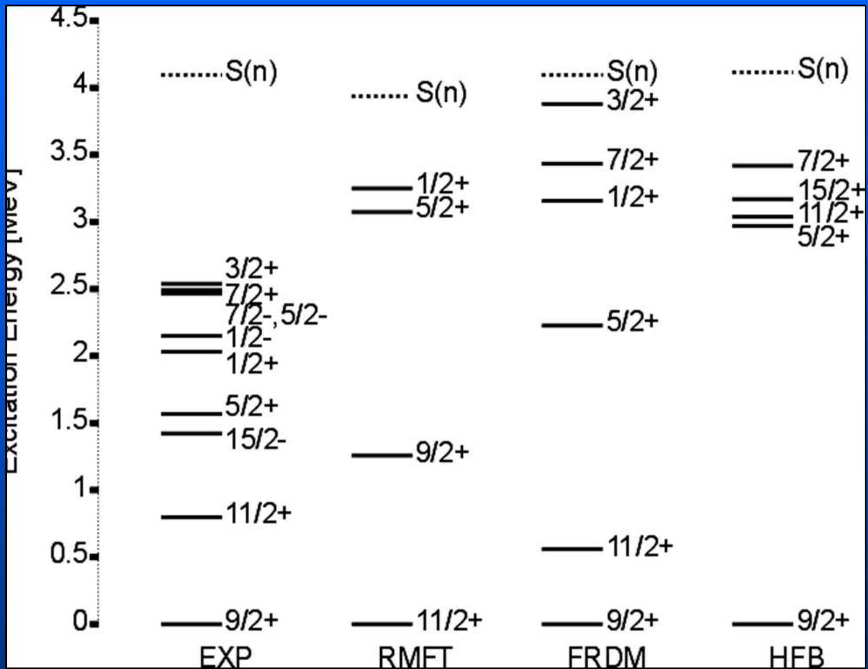
Direct neutron capture (30 keV)



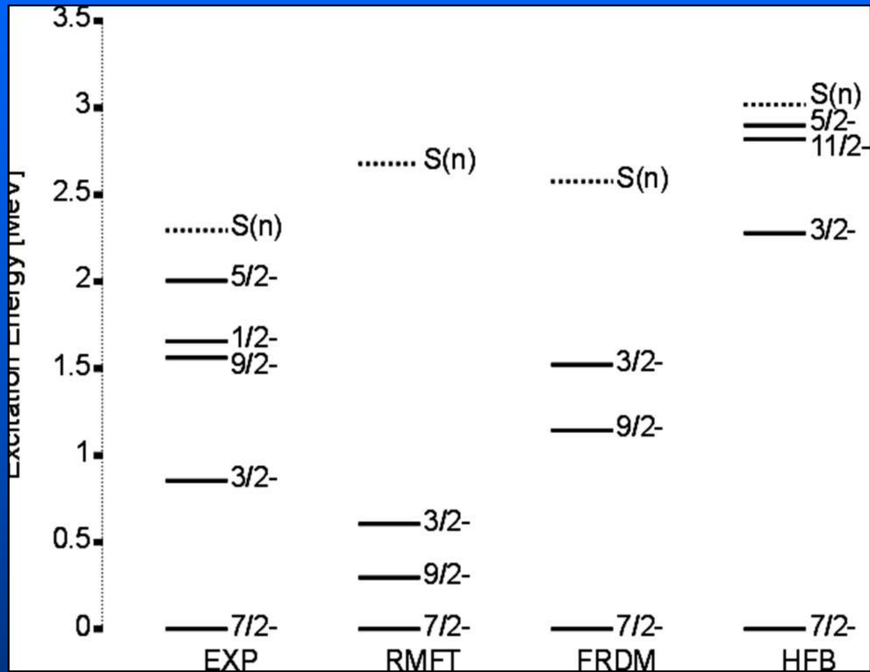
- HFB: Squares
- RMFT: Triangles
- FY: Dots
- Exp. levels: Cross

Rauscher et al. 1998

Comparison With Experimental Levels



^{209}Pb

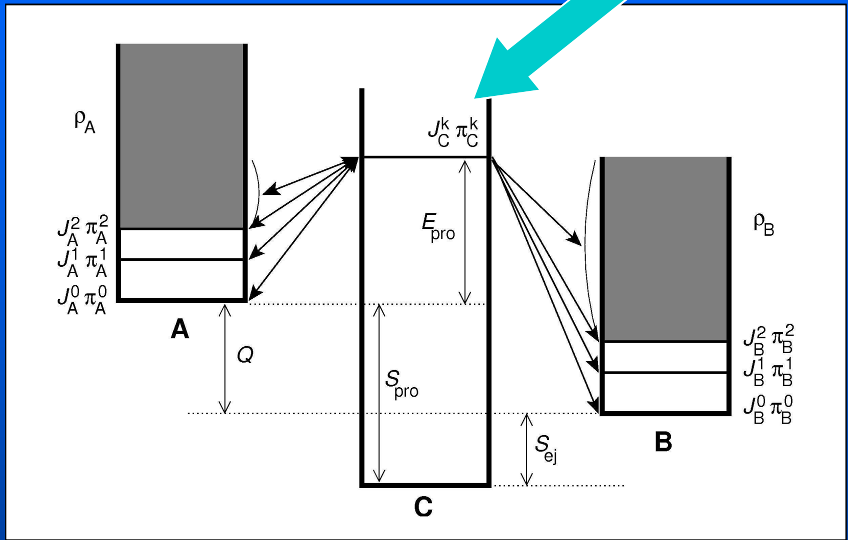


^{133}Sn

Rauscher et al. 1998

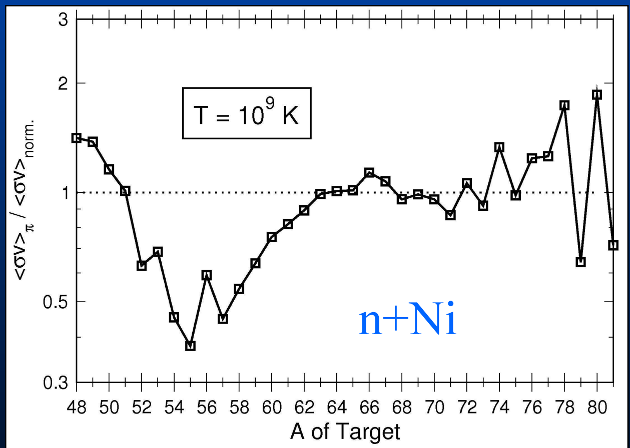
Modified Hauser-Feshbach model

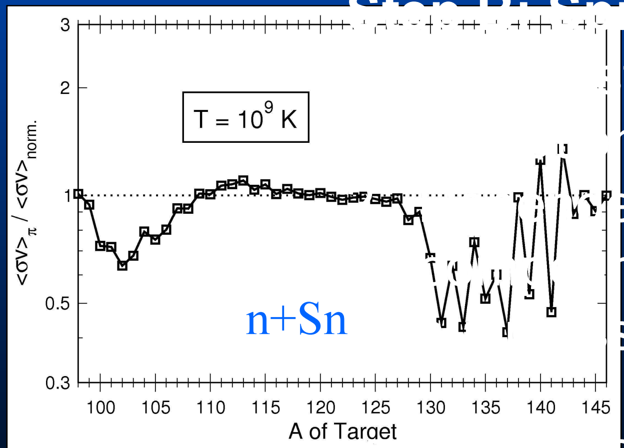
Lifting assumption that all spins and parities are available for compound nucleus formation!



Step A: Parity dependence

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





Step B: Spin dependence

...tribution at compound ... n energy ... ence on level density in ... nd nucleus → ... sion factor

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

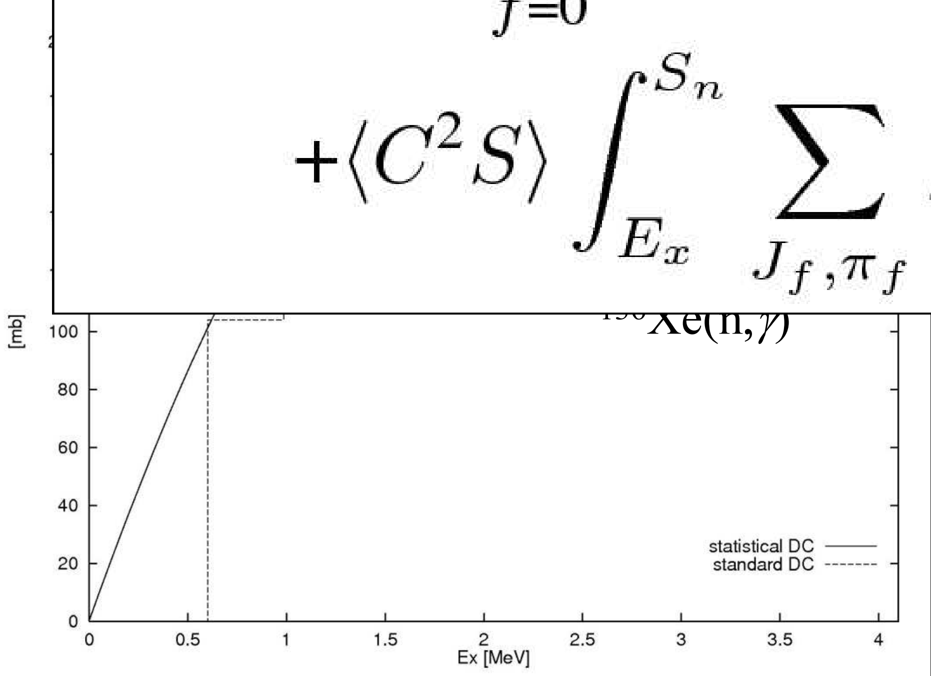
(Rauscher 2007, 2009, 2010)

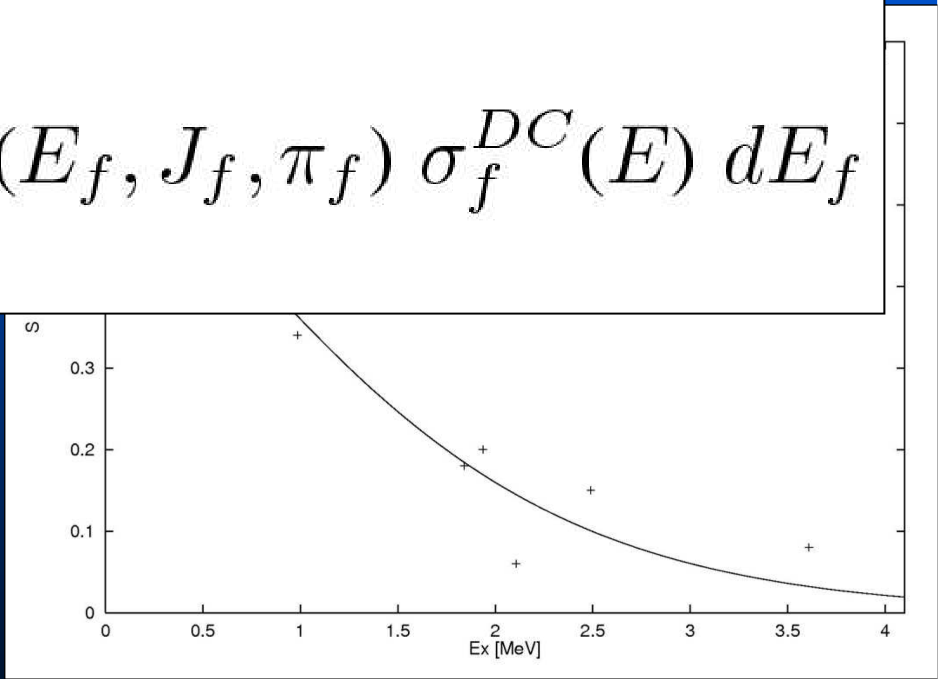
Averaged DC

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

$$\sigma^{DC}(E) = \sum_{f=0}^{x} C_f^2 \, S_f \, \sigma_f^{DC}(E)$$

$$+\langle C^2 S \rangle \int_{E_x}^{S_n} \sum_{J_f,\pi_f} \rho(E_f, J_f, \pi_f) \, \sigma_f^{DC}(E) \, dE_f$$





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

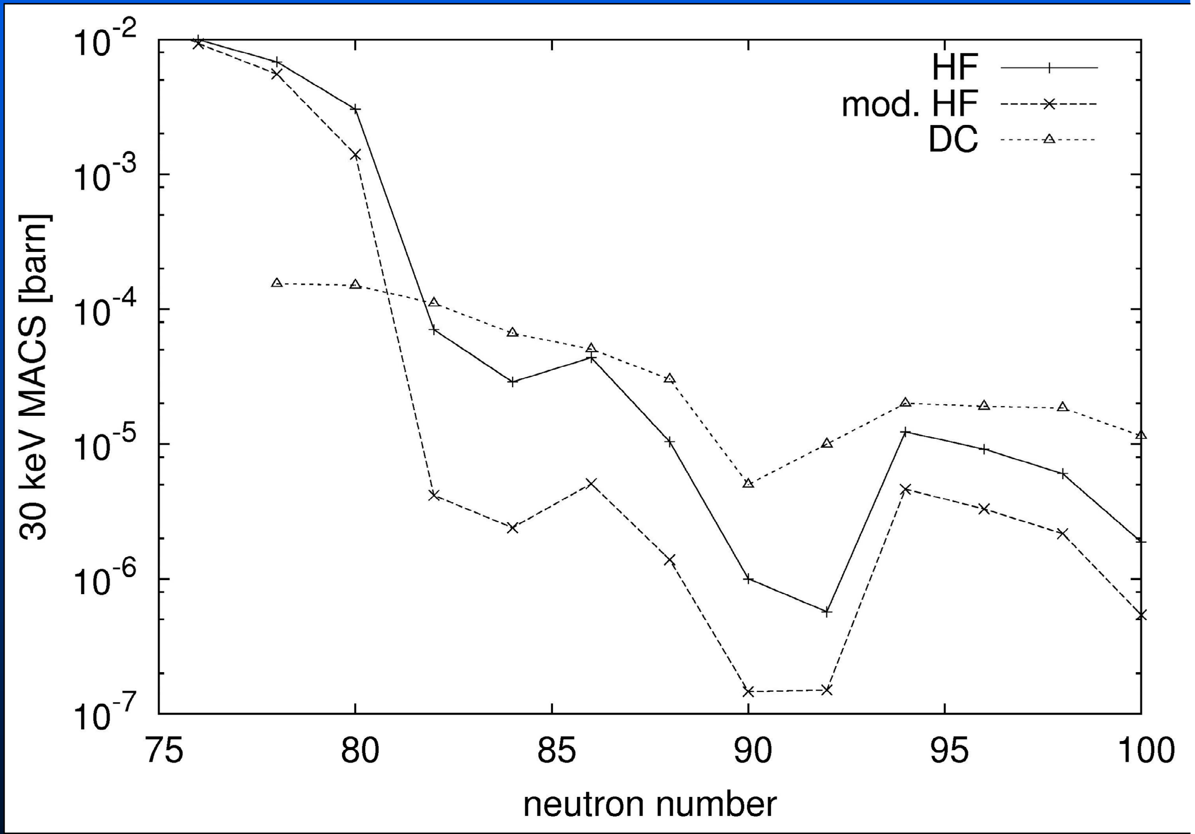
DC vs Statistical Model

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



Rauscher, preliminary

Sn isotopes

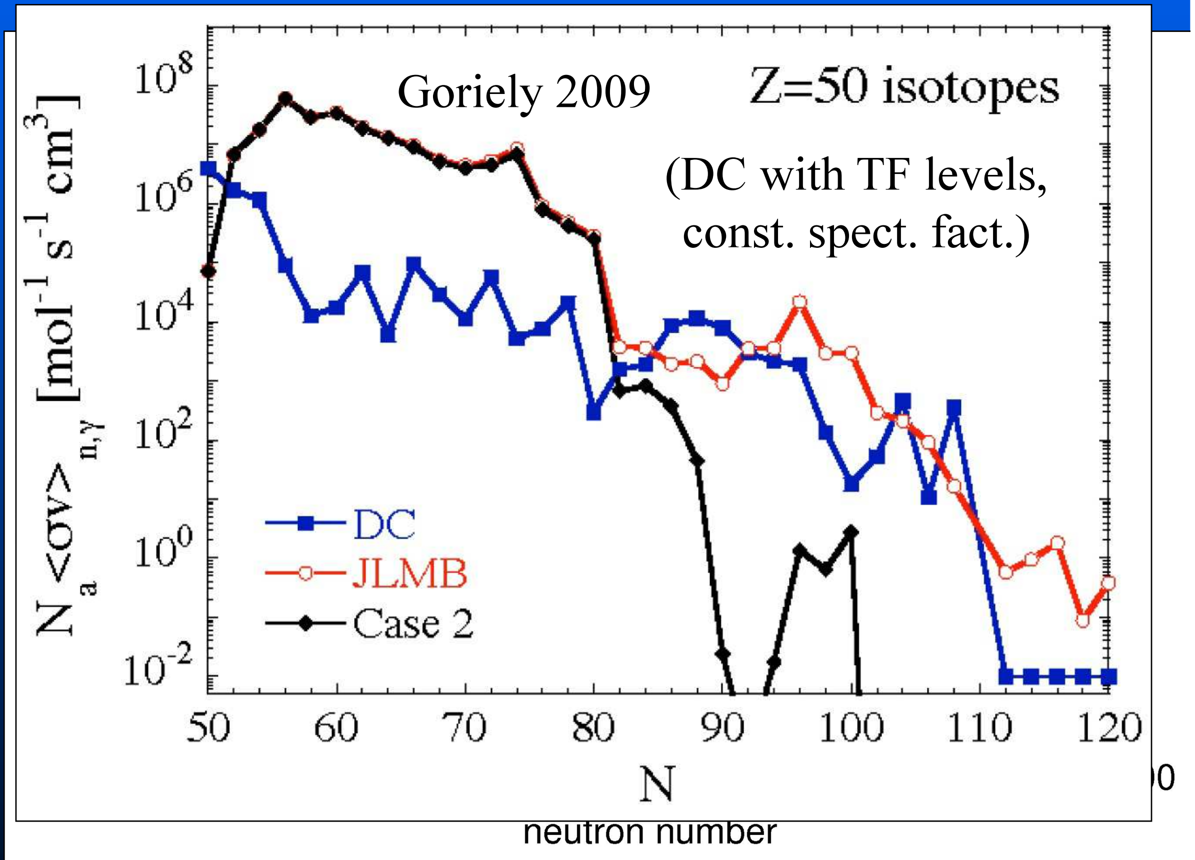
DC vs Statistical Model

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:

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

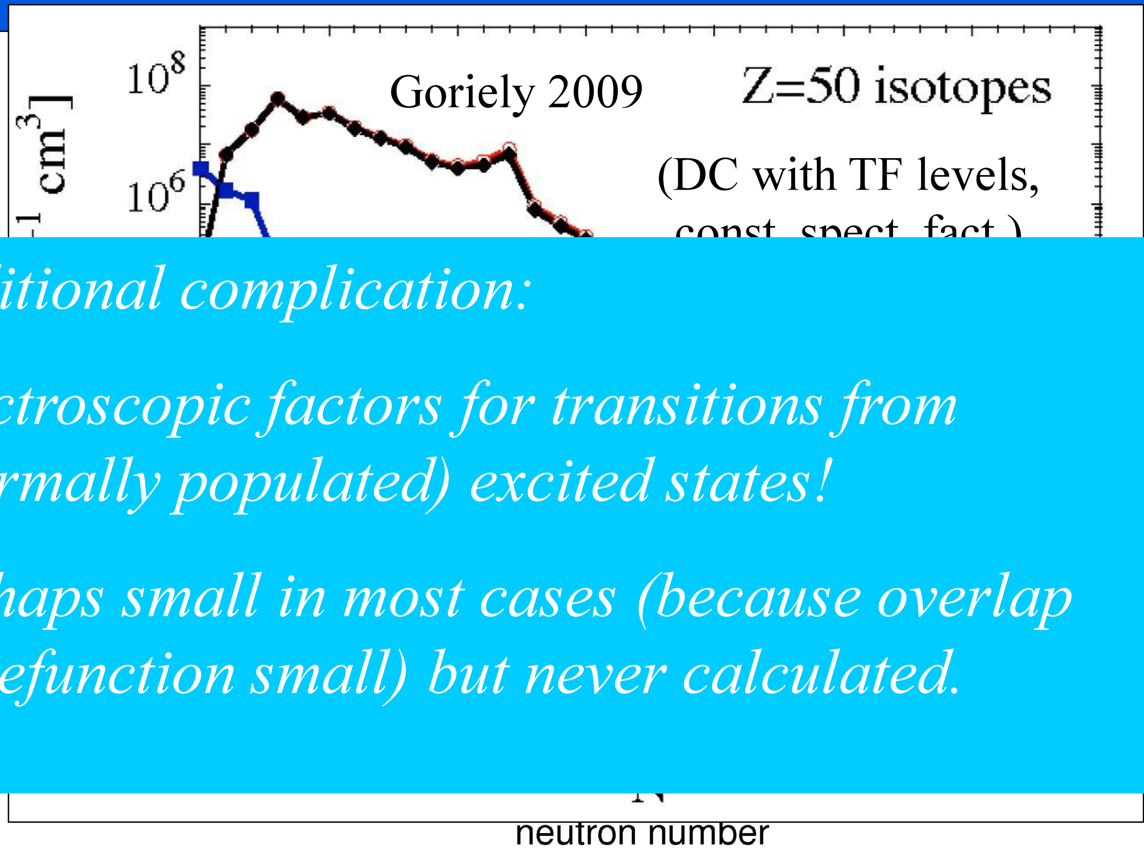
DC vs Statistical Model

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:

1. 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



Rauscher, preliminary

Sn isotopes

Additional complication:

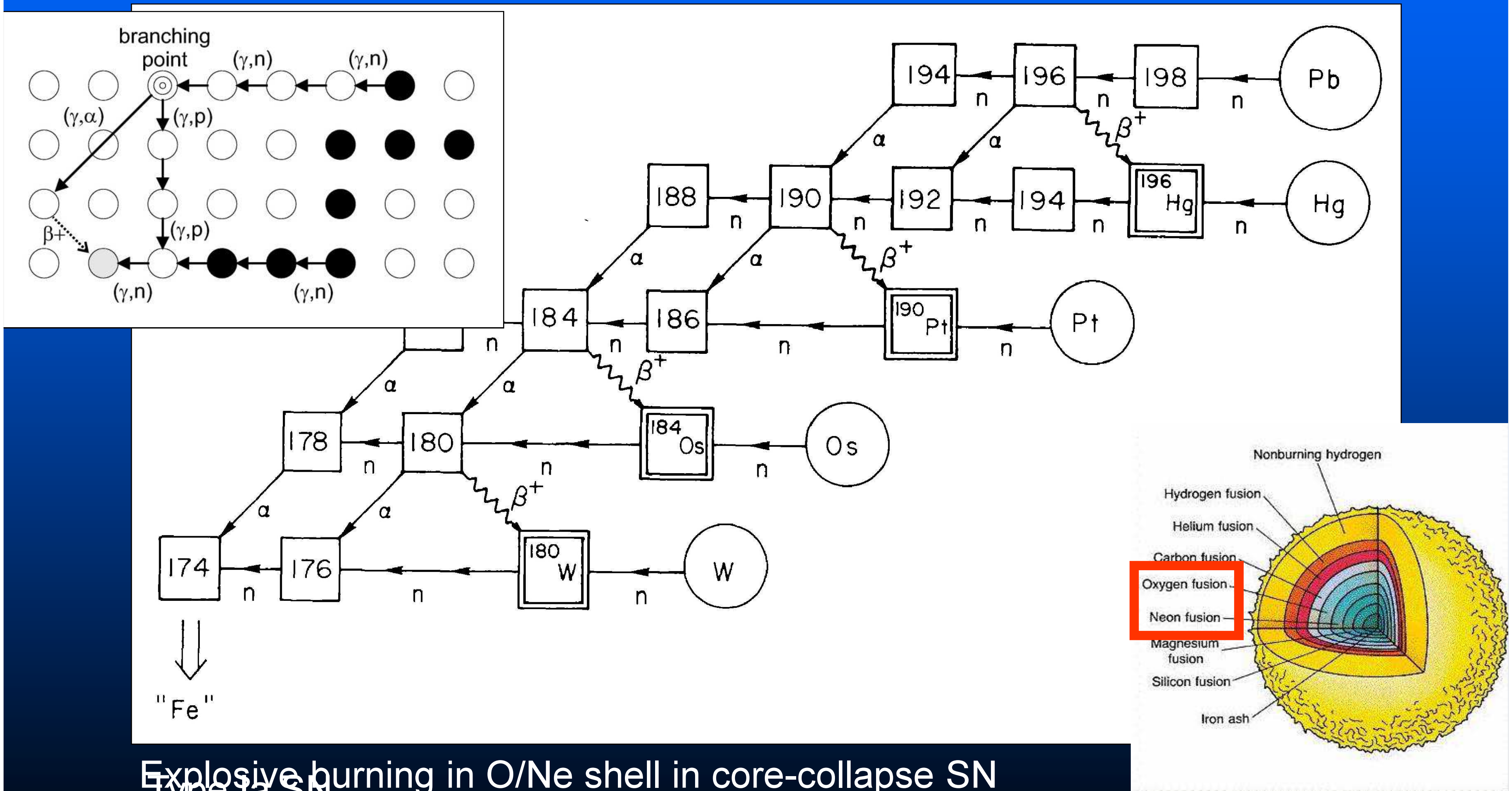
Spectroscopic factors for transitions from (thermally populated) excited states!

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

Dedicated γ-process studies in collaboration with experimentalists

The γ-Process

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



Explosive burning in O/Ne shell in core-collapse SN

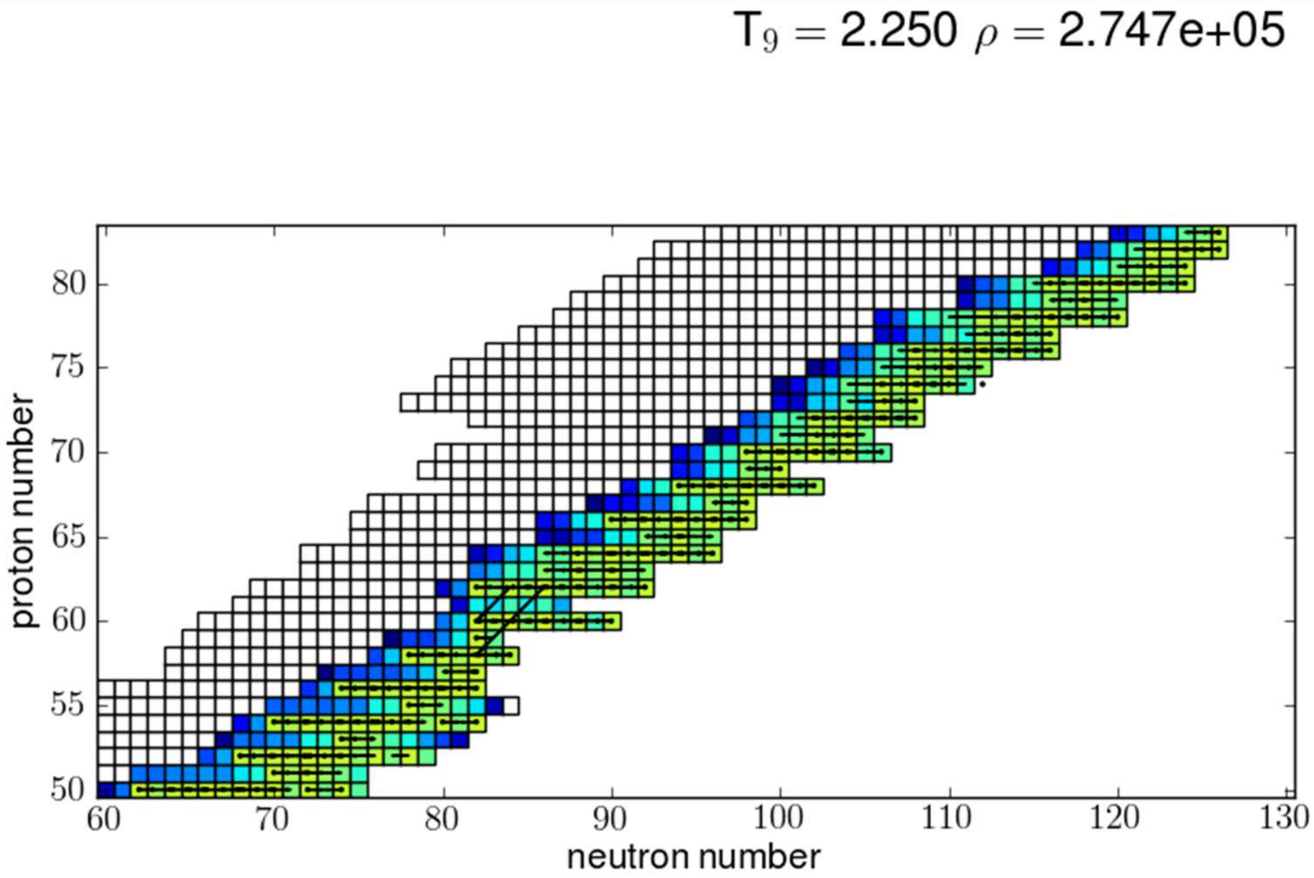
Type Ia SN

Howard, Meyer & Woosley 1991; Travaglio et al 2010; Nomoto et al 2011

Woosley & Howard 1978; Prantzos et al 1990; Rayet et al 1995

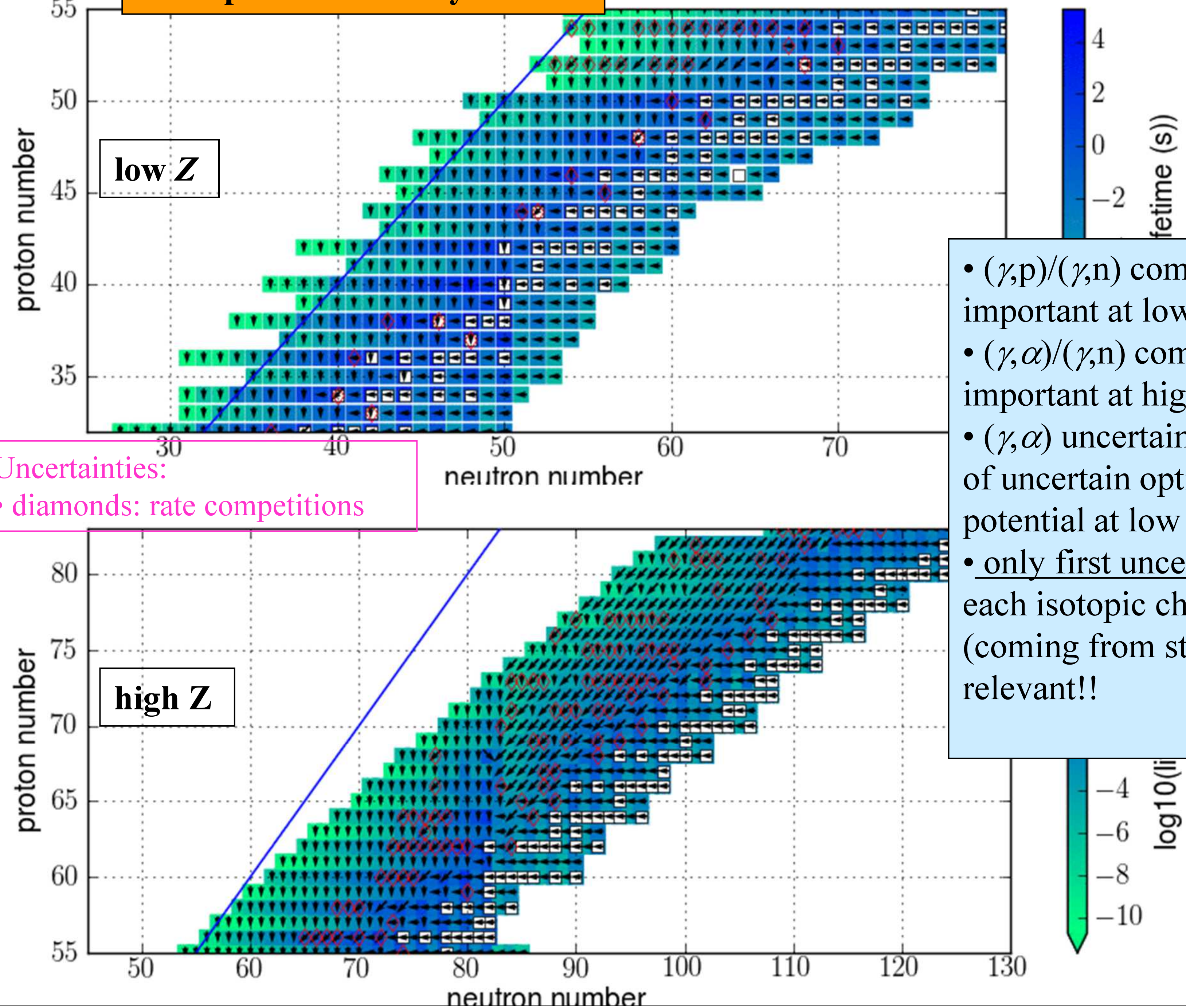
Photodisintegration of stable seed nuclei

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



(animation)

Example of Reactivity Field



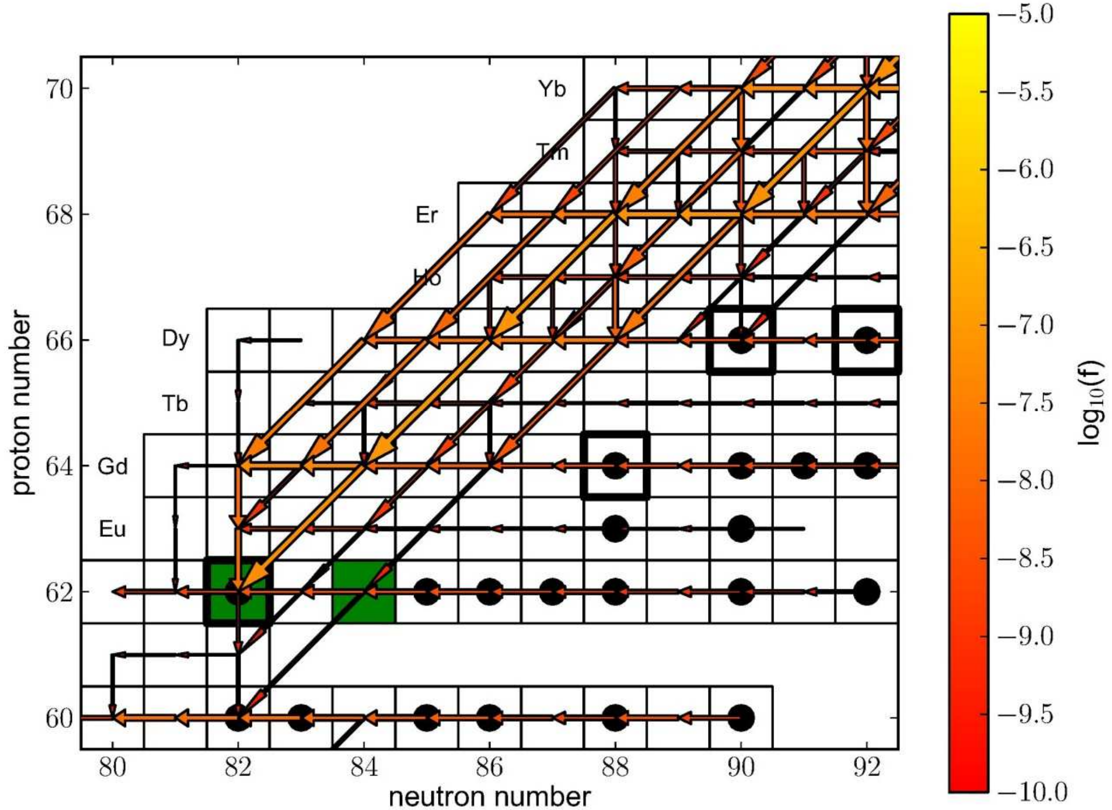
Uncertainties:

- diamonds: rate competitions

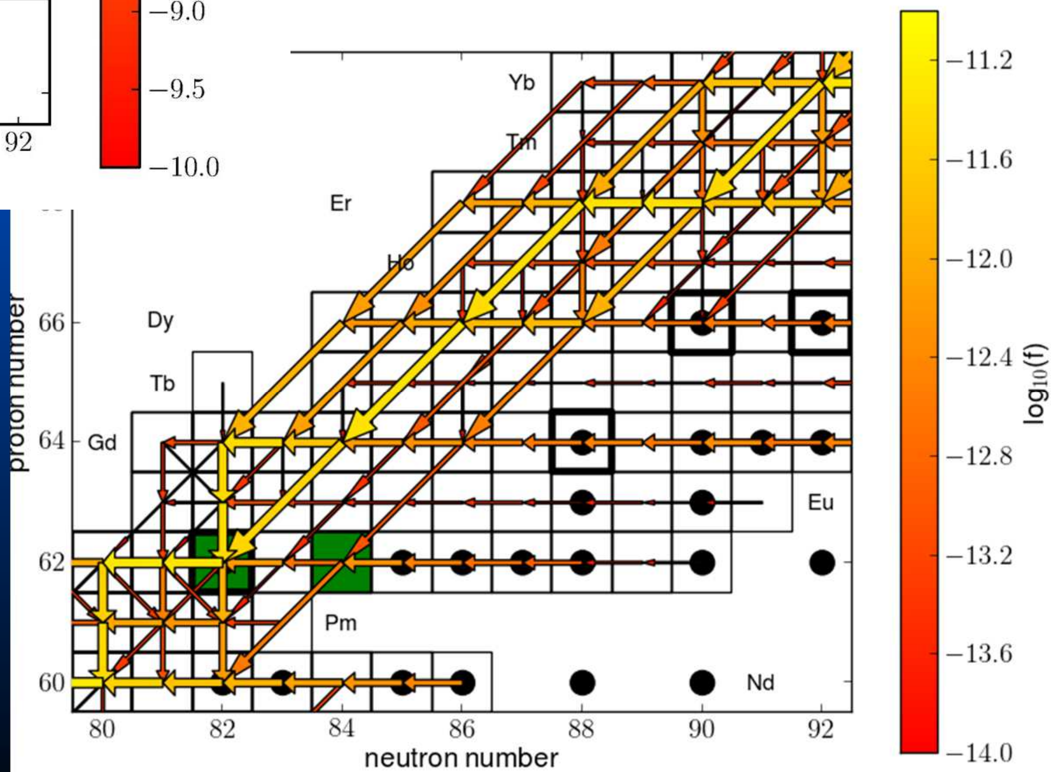
- (γ,p)/(γ,n) competition important at low Z
- (γ,α)/(γ,n) competition important at high Z
- (γ,α) uncertain because of uncertain optical potential at low energy
- only first uncertainty in each isotopic chain (coming from stability) is relevant!!

γ-process in Sm region

ccSN



SNIa
(one tracer)

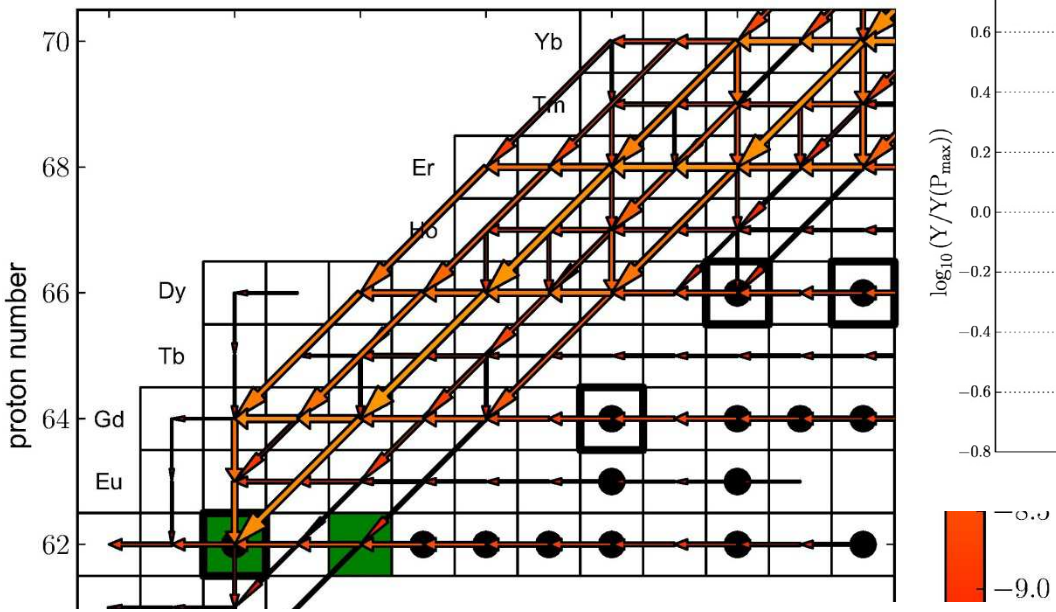


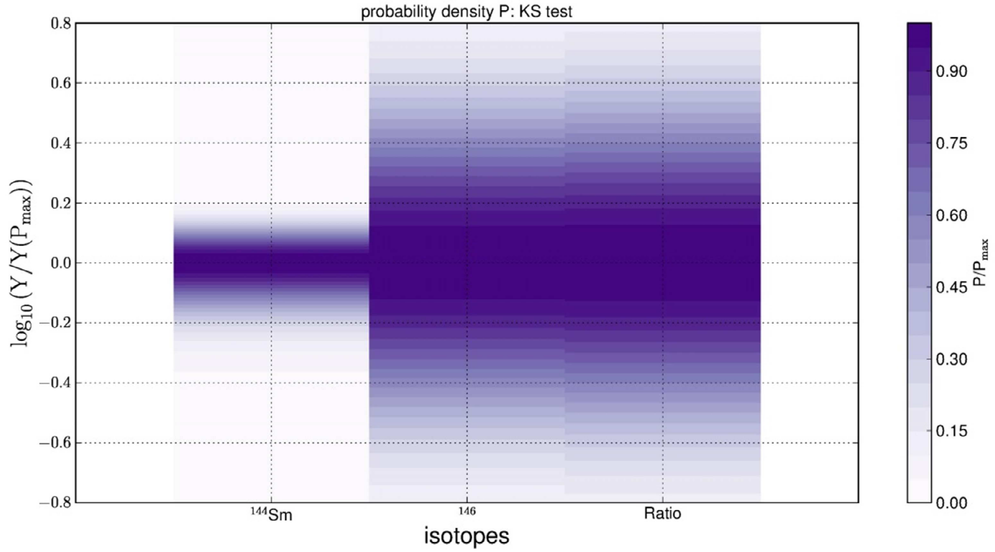
PizBuin Monte Carlo Framework

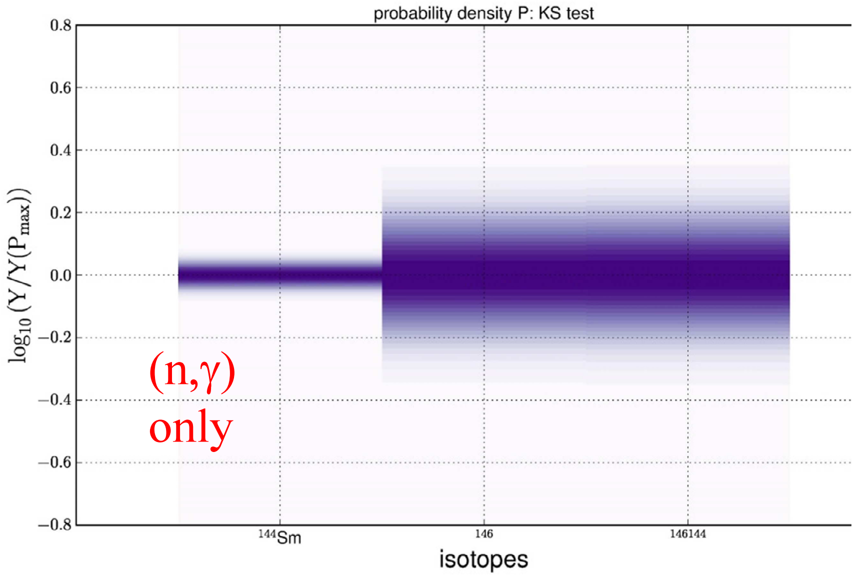
- Monte Carlo driver + fast, parallelized reaction network
- Hertfordshire-Keele collaboration (with Nishimura, Hirschi), within ERC project and the BRIDGCE consortium (UK)
- using computing clusters at Keele and Hertfordshire
- ability to study 10000s of reactions simultaneously in post-processing
- 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, νp-process, (ν-driven winds)

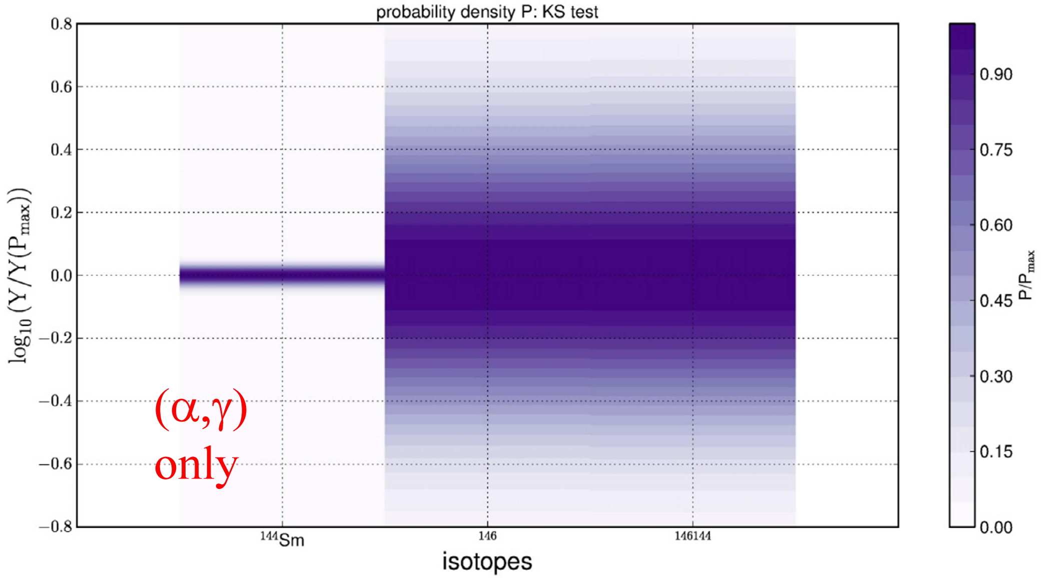
Project recently started, first test results available (see also posters by Nishimura, Rauscher)

γ-process for ^{146}Sm/^{144}Sm ratio in SNIa

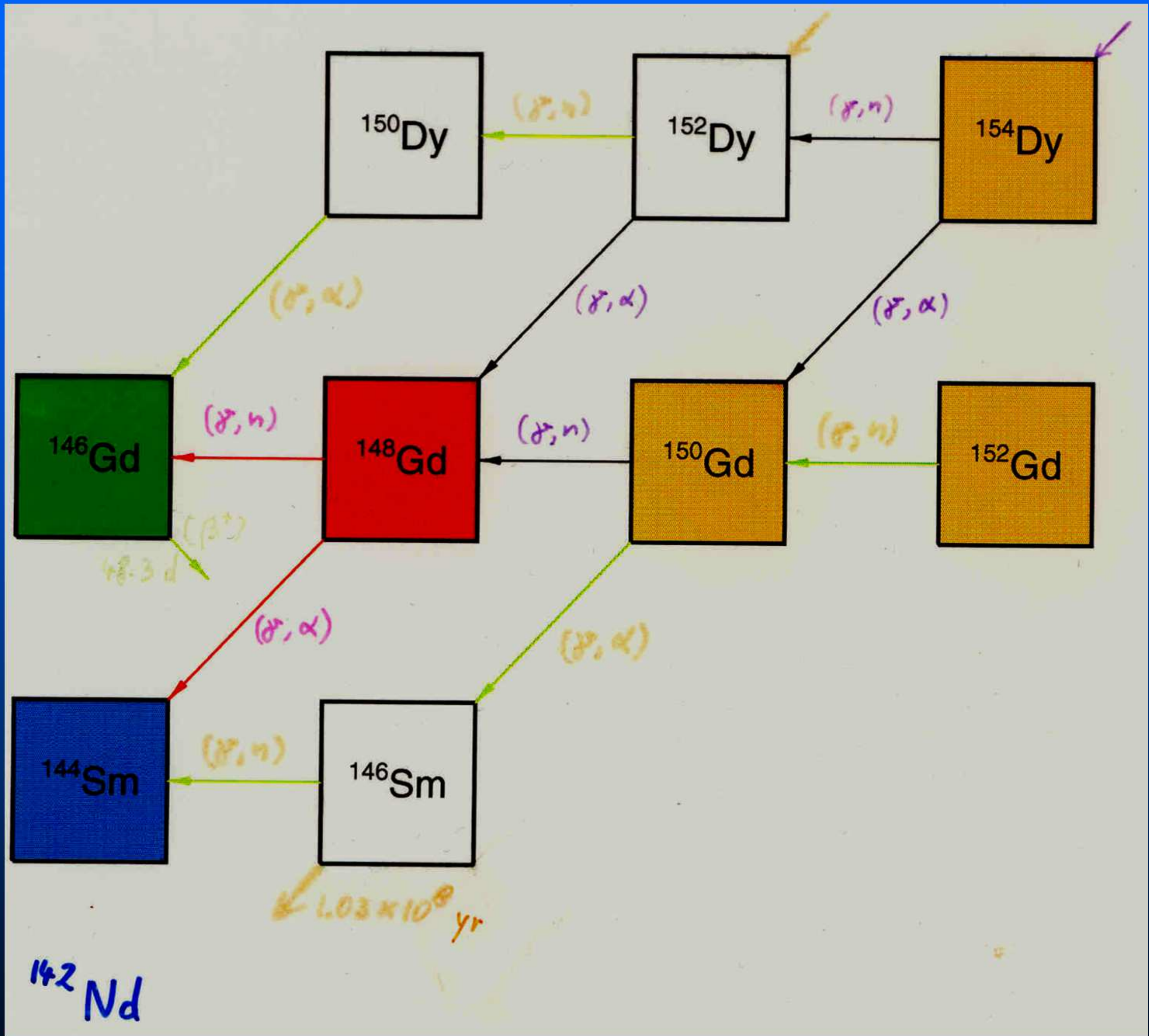






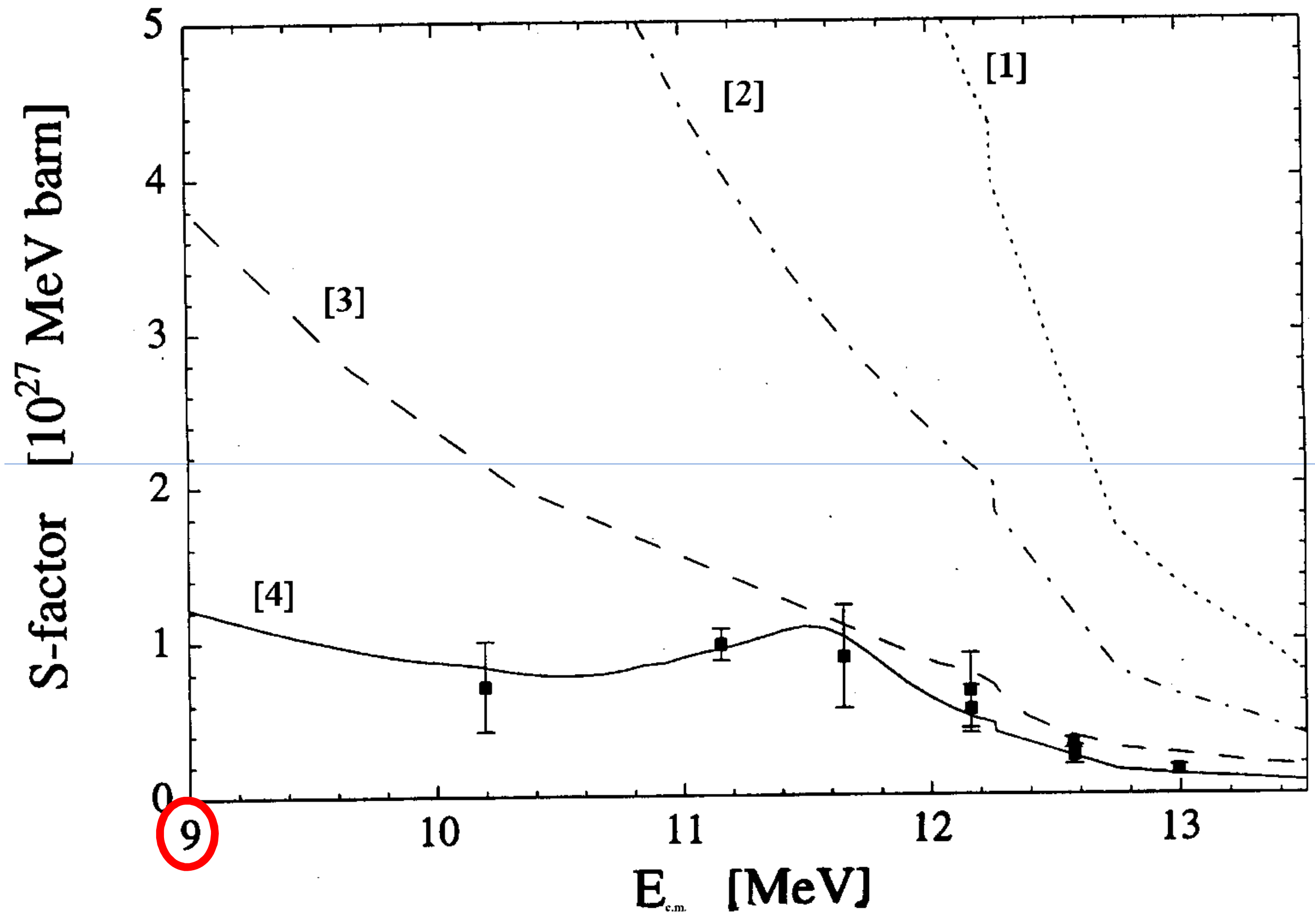


Network for Nd/Sm



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

Problem with $\alpha+^{144}Sm$ Potential



$^{144}Sm(\alpha,\gamma)^{148}Gd$

[1] McFadden & Satchler Pot.

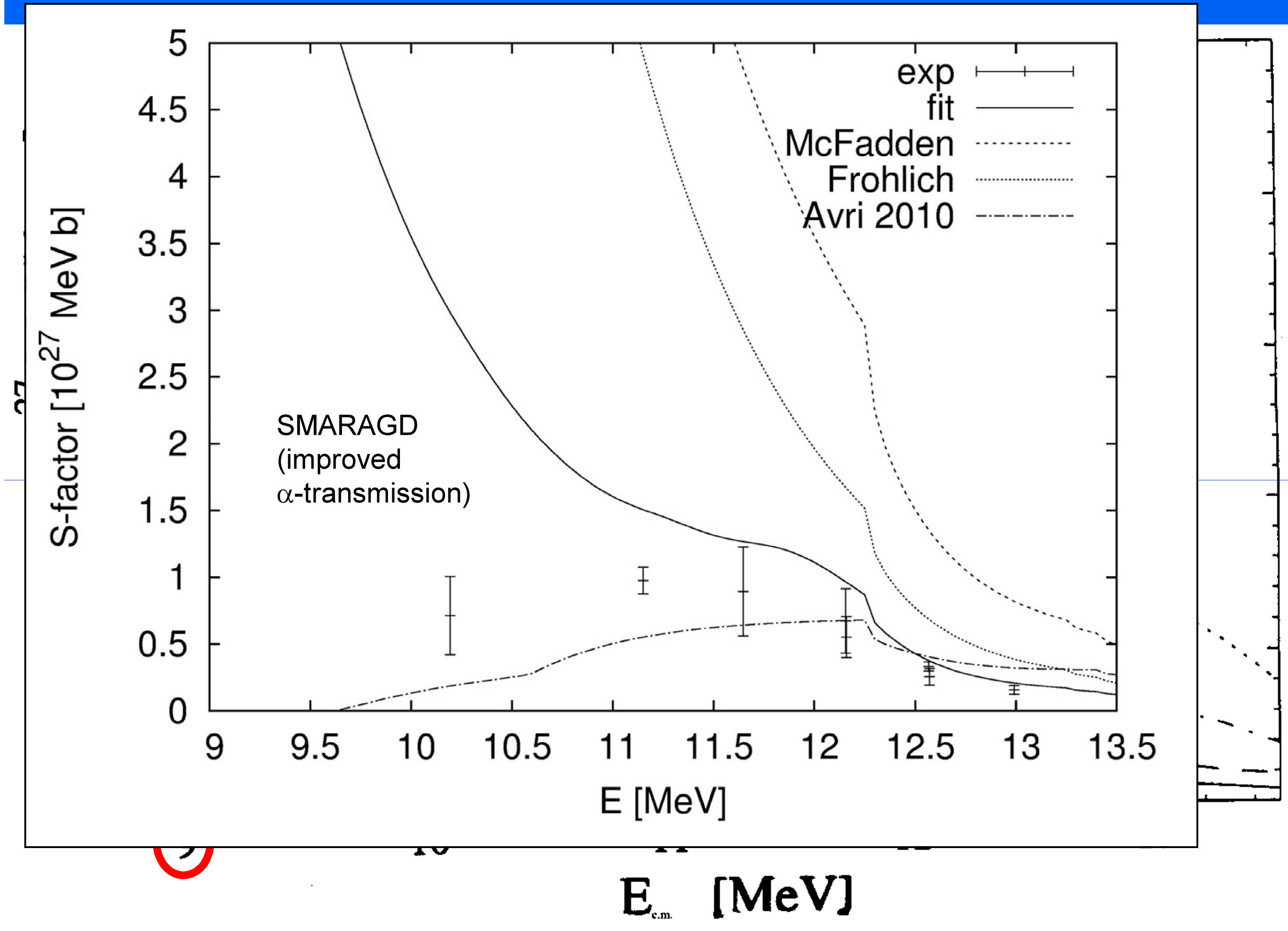
[2] Avrigeanu Pot. I

[3] Mohr & Rauscher 98 Pot.

[4]+exp: Somorjai et al. 1998

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

Problem with α+^{144}Sm Potential



^{144}Sm(α,γ)^{148}Gd

[1] McFadden & Satchler Pot.

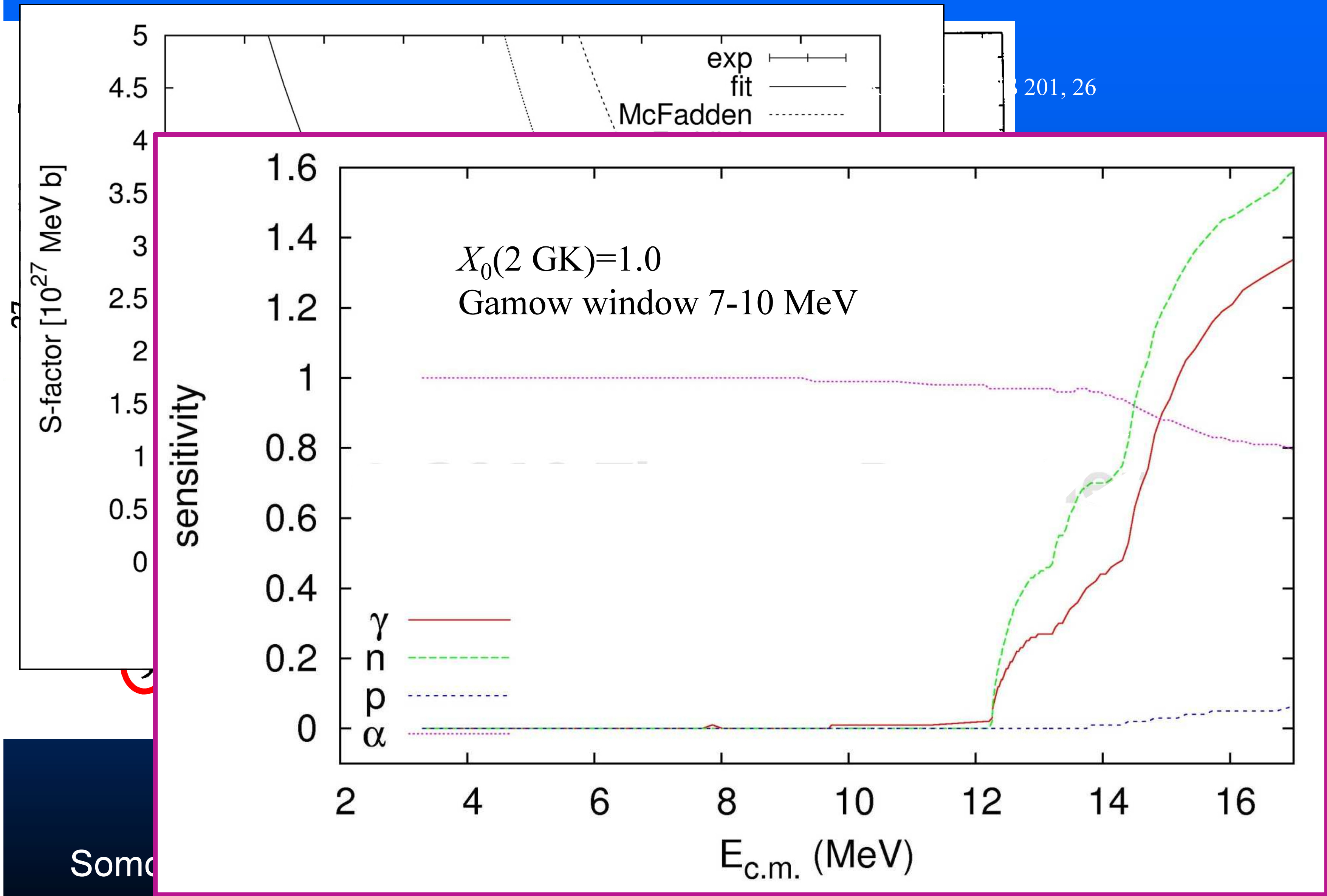
[2] Avrigeanu Pot. I

[3] Mohr & Rauscher 98 Pot.

[4]+exp: Somorjai et al. 1998

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

Problem with α+^{144}Sm Potential



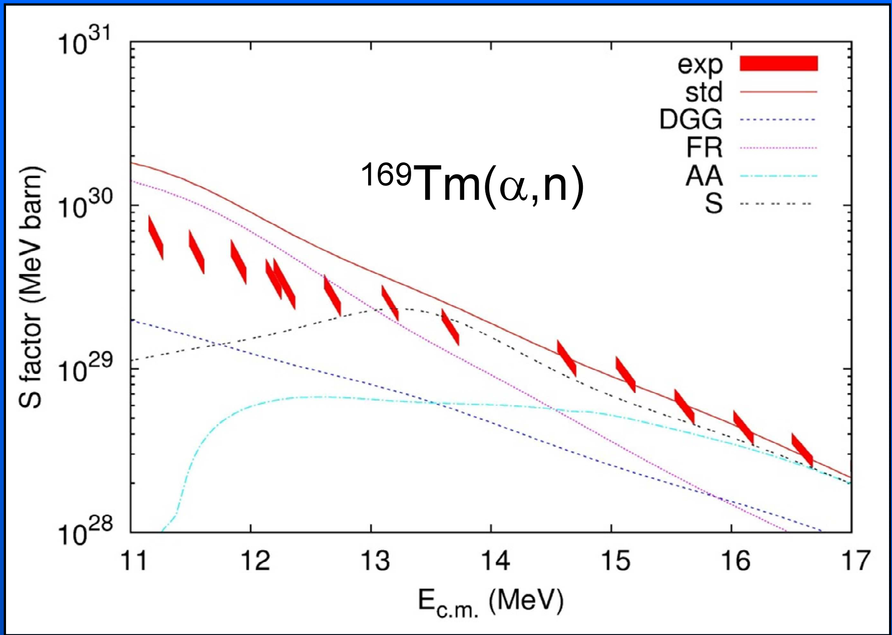
Problem with optical α+nucleus potential at subCoulomb energies

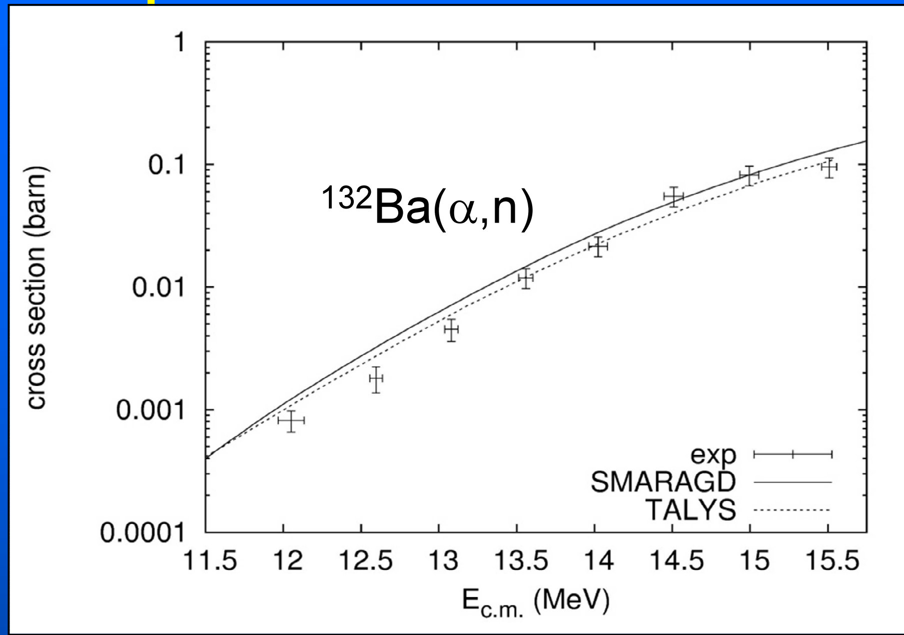
- General factor 2-3 overprediction of exp. cross section found for p-rich nuclei at low energy
- Can translate into up to a factor of 10 difference at astrophysical energy
- Phenomen. potential fitted to reaction cross sections (Frohlich et al 2003) can reproduce c.s. over wide range of masses; but 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?

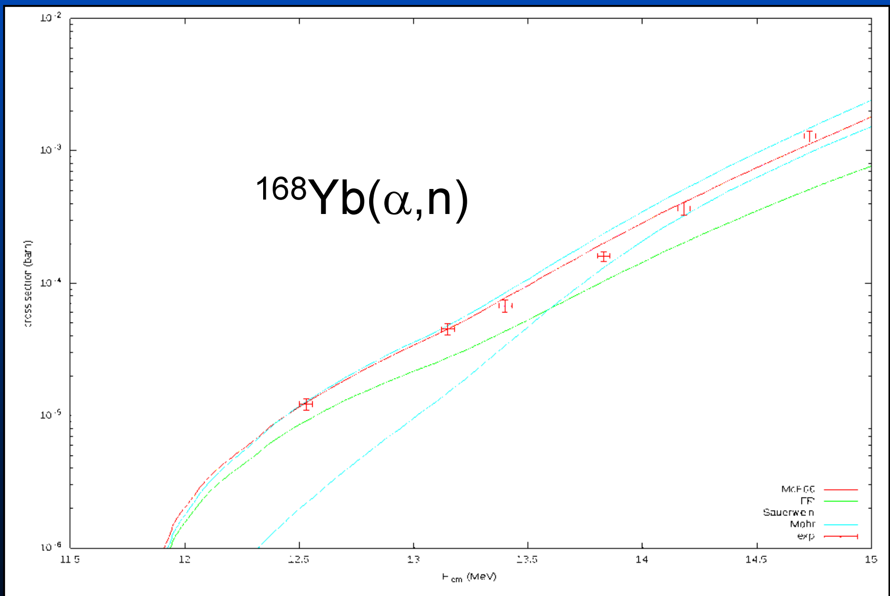
Various approaches for "global" optical α+nucleus potential were tried

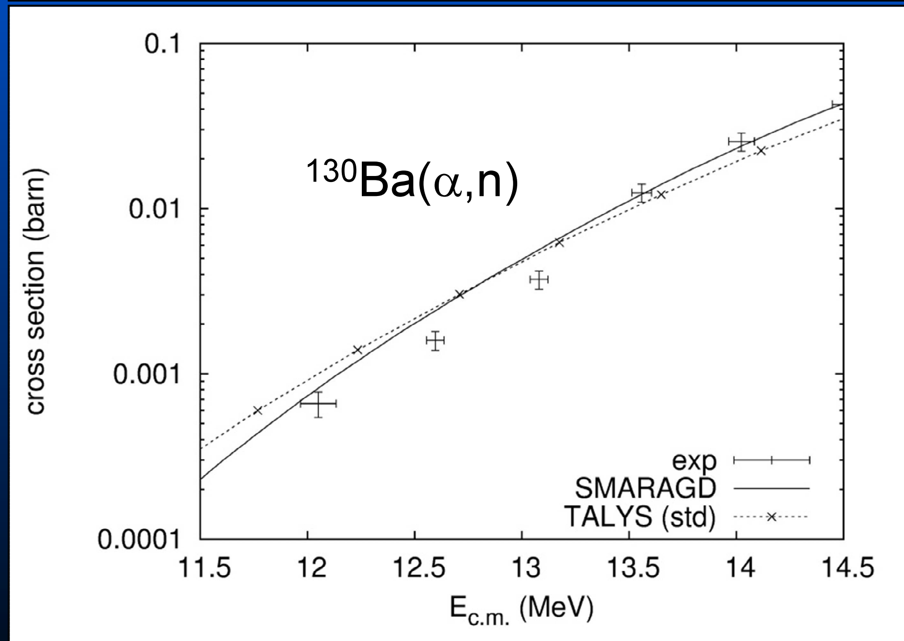
- Real part:
  - Folding
  - E-independent Woods-Saxon
  - E- , A-, Z-dependent Woods-Saxon
- Imaginary part:
  - constant Woods-Saxon
  - volume+surface W-S with E-, A-, Z-dependence
- Parameters derived from
  - fit to scattering data
  - fit to reaction data
  - theoretical considerations
- Strong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

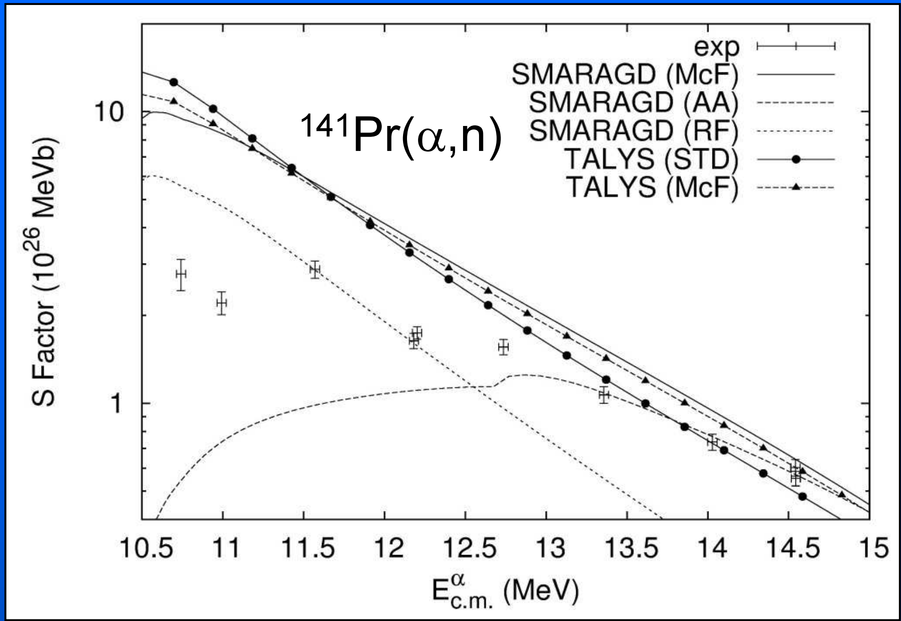
Some examples

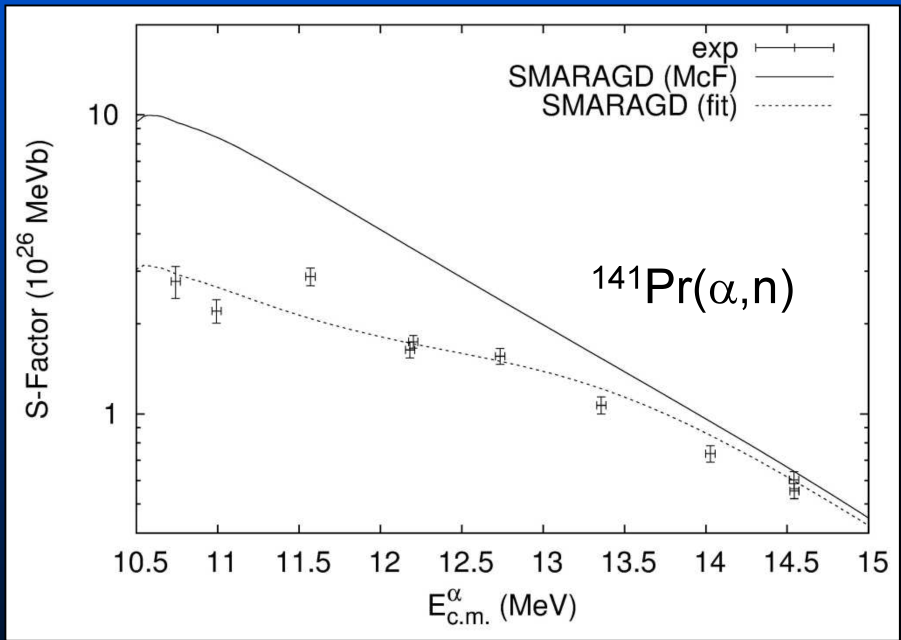












<u>Data Summary:</u>

- 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 (^{144}Sm is extreme case!)
- Local potentials in principle possible but do not provide much information for astrophysics rates
- „Global“ potentials cannot globally describe data

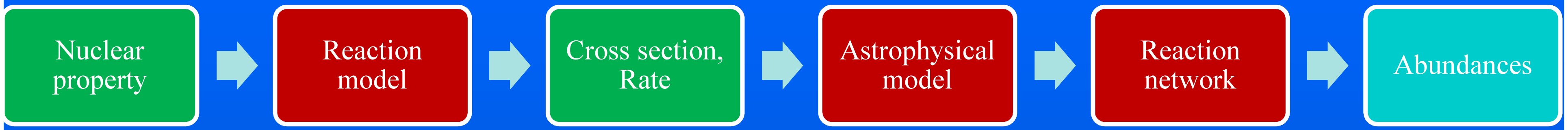
Discussion Slides

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

- Detailed discussion in:
- ApJL 755, L10 (2012) [g.s. contribution];
- ApJS 201 (2012) 26 [g.s. contributions, sensitivities];
- AIP Advances 4 (2014) 041012 [summary, strategies] .

Extensive review also in:
T. Rauscher, Int. J. Mod. Phys. E 20, 1071 (2011)
[including model input and model modifications]

Uncertainties in “input quantities”



- Distinction between:
  - Measured input or input derived from measurements (type I)
    - Experimental errors, propagated and convoluted
    - Statistical and systematic error
    - Probability distribution functions (from MC, first attempts)
  - Calculated (predicted) properties (type II)
    - Contains type I errors which can be propagated
    - But model error not really quantifiable (or only crudely, “systematic error”)
- Things to be considered:
  - Model sensitivities can help to disentangle input and model uncertainties
  - *Correct treatment of experimental constraints on rates*
  - ***Systematic variations of input are required to study uncertainties!!!***
    - not enough to just play around by plugging in different descriptions of properties (e.g., different GDR, level density descriptions, optical potentials)
    - This shows disagreement between theories but not real uncertainty range
    - Different models can fortuitously agree at relevant energies
    - Monte Carlo? Also cannot capture model uncertainties

Combining Rates & Uncertainties, Flowchart I

measure $\sigma_0(E)$

↓

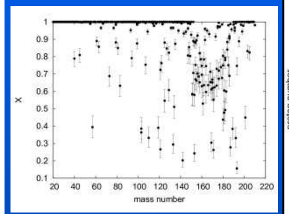
compute R_0^{exp}

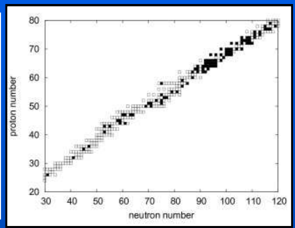
↓

$X_0 \approx 1$?

yes → $R^*_{new} = R_0^{exp}$, $U^*_{new} = U_{exp}$

no ↓





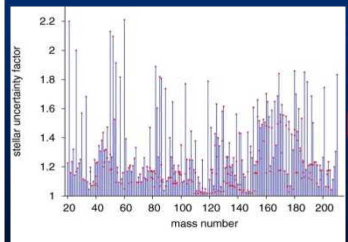
invoke theory?

yes → Further Analysis…

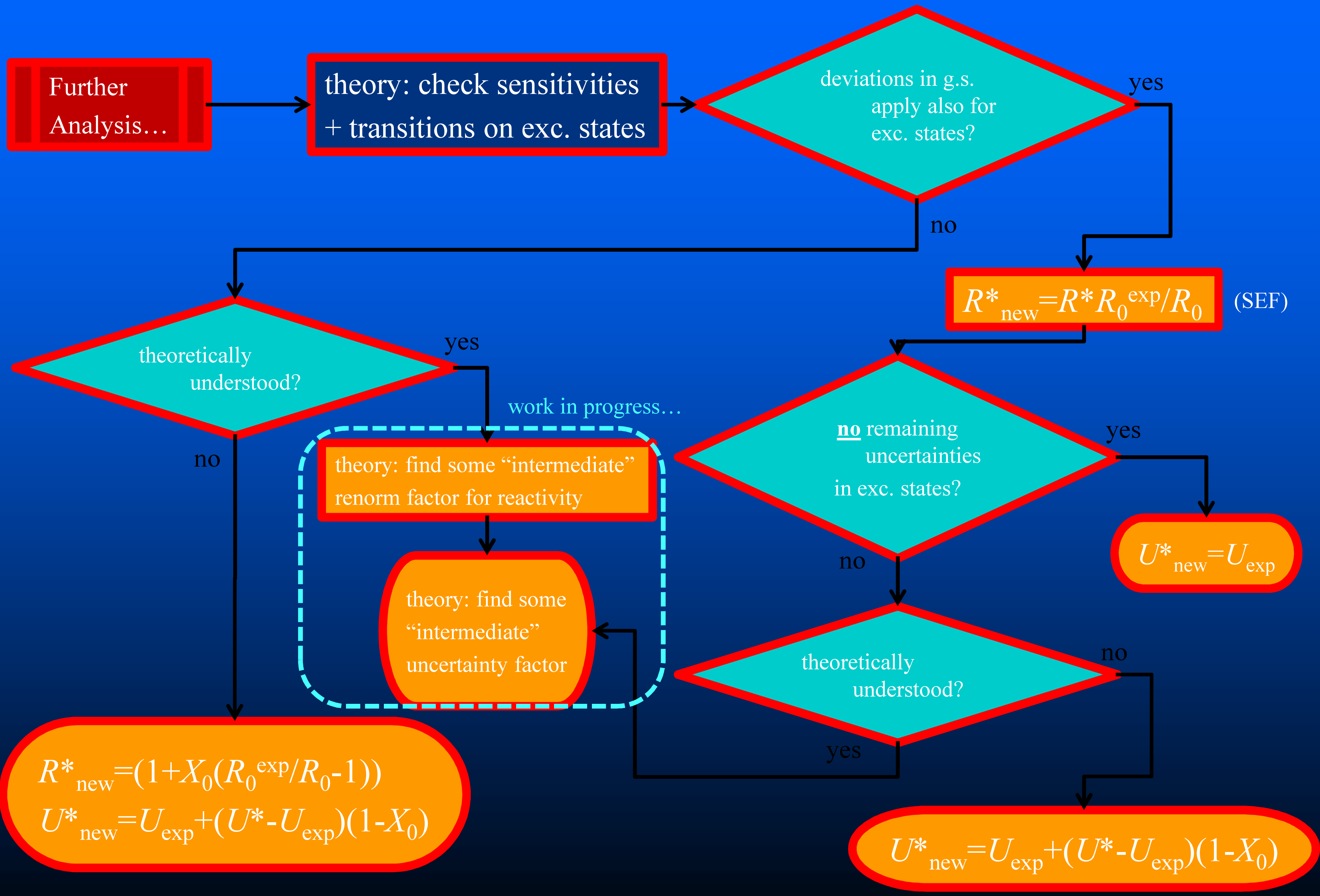
no ↓

$R^*_{new} = (1 + X_0(R_0^{exp}/R_0 - 1))$

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



Combining Rates & Uncertainties, Flowchart II



Instructions for Users of Reaction Rates and Data

- If theoretical rate:
  - Check *applicability limit* of model for desired plasma temperature range; Close to or outside the applicability limit?
    - If yes: Consider that the reaction model may be incorrect and expect larger uncertainties or do not use this rate at these temperatures
    - If no, use rate as advised
- If rate based on experiment:
  - Check *ground state contribution* X_0
    - If $X_0 \approx 1$, then rate is fully constrained by experimental cross section if measured in the relevant energy range; experimental uncertainty applies
    - If $X_0 < 1$, uncertainty is larger because partly determined by theory error
      - In this case, check how rate and uncertainty were constructed by combining experiment and theory (use *flowchart* for guidance)
      - If the flowchart procedure was not applied, to be sure make pessimistic assumption on uncertainty (see first part of *flowchart*)
- If you want to include a new cross section measurement (at relevant energy), start from theory rate R^* and follow procedure in *flowchart*

Instructions for planning experiments

- Determine range of temperatures (and therefore of the *relevant energies*), target nuclei, and the reaction type (e.g., neutron capture) for the nucleosynthesis process to be studied
- Direct measurement possible?
    - If yes, check *g.s. contribution* X_0
        - If $X_0 \approx 1$, then rate is fully constrained by experimental cross section if measured in the relevant energy range; experimental uncertainty applies
            - If cross section cannot be measured in relevant energy range, check *sensitivities* to see whether relevant properties (widths, input for widths) can be constrained by experiment
        - If $X_0 < 1$, combination with theory is required to determine stellar rate and stellar rate uncertainty, see *flowchart*
    - If no, check *sensitivities* to see whether relevant properties (widths, input for widths) can be constrained by experiment
- Remember the *Q-value rule:* the direction of positive reaction Q-value (almost) always has larger g.s. contribution X_0 !!
    - only exceptions are charged particle captures and a few (p,n) reactions
    - in the case of charged particle capture always the capture direction has the largest g.s. contribution (by far!)

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 $S_{\mathrm{proj}}+E_{\mathrm{proj}}$-3 MeV
  - Nuclear level density (or levels) at same energy
  - M1 strength functions

T. Rauscher, Int. J. Mod. Phys. E 20, 1071 (2011)

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

T. Rauscher, Int. J. Mod. Phys. E 20, 1071 (2011)

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.

T. Rauscher, Int. J. Mod. Phys. E 20, 1071 (2011)

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
  - photodisintegration does not measure relevant E1 strength (wrong energy)
- Do not measure stellar reaction rates
- Useful to determine certain properties to test theory but have to be selected carefully!

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.

T. Rauscher, Int. J. Mod. Phys. E 20, 1071 (2011)