Predictions of reaction rates: Statistical Methods

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The basic physical question

$$r_{12} = \frac{1}{1+\delta_{12}} n_1 n_2 \left\langle \sigma^* v \right\rangle_{12} = \frac{1}{1+\delta_{12}} \rho^2 Y_1 Y_2 N_A^2 \left\langle \sigma^* v \right\rangle_{12}$$

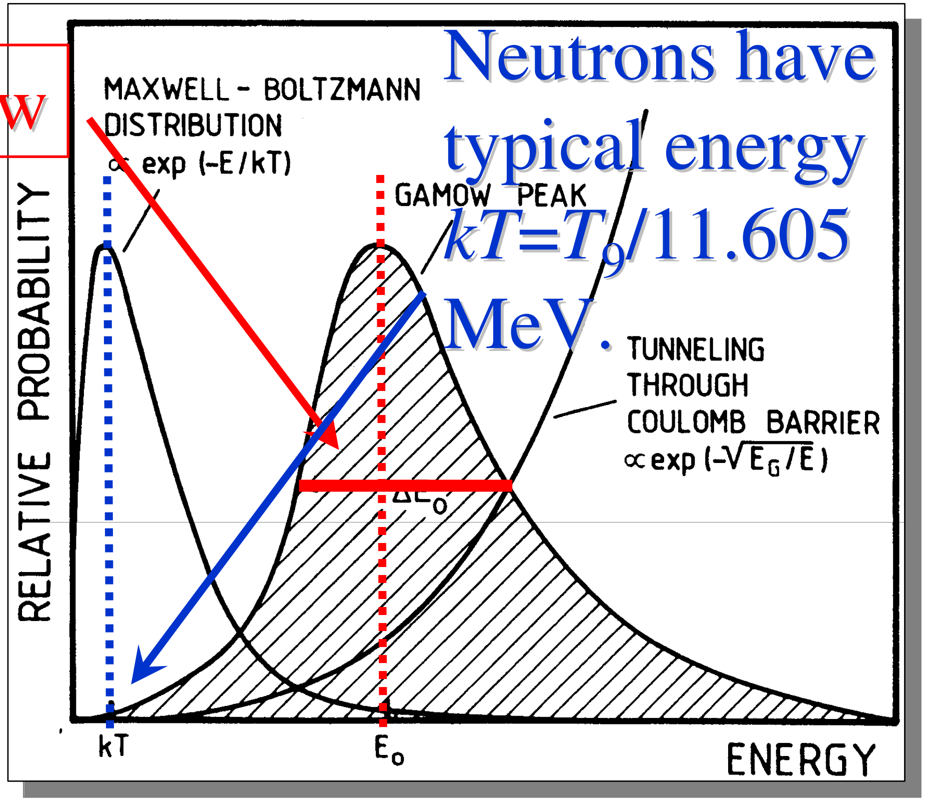
Number of reactions per time and volume

$$\sigma^* = \frac{\sum_i (2J_i + 1)\sigma_i e^{-E_i/kT}}{\sum_i (2J_i + 1) e^{-E_i/kT}}$$

Stellar cross section

Reaction Rate (MB) Per Particle Pair (Nucleus-Nucleus/Nucleon)

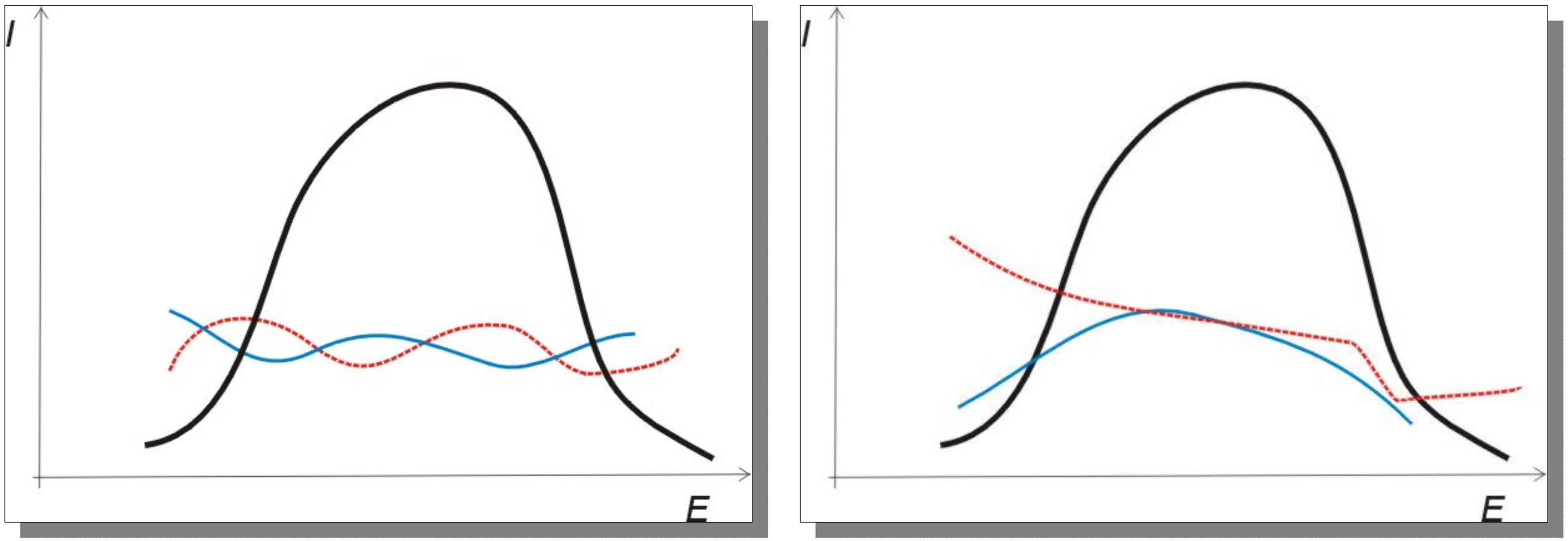
Gamow window



Rolfs & Rodney 1985

$$\langle \sigma^* v \rangle = \sqrt{\frac{8}{\mu\pi}} \frac{1}{(kT)^{3/2}} \int_0^\infty E\sigma^*(E) e^{-E/kT} dE$$

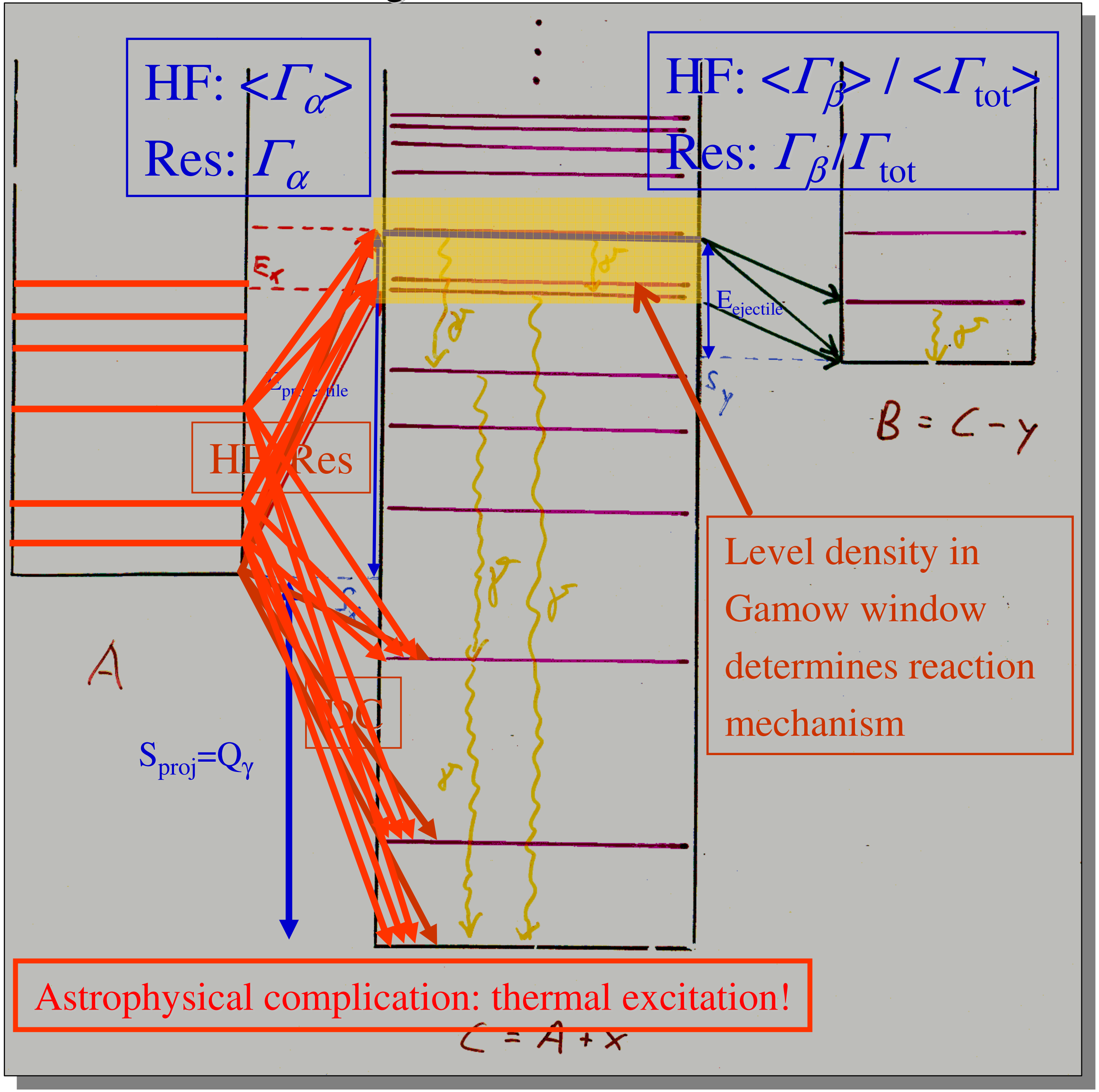
Accuracy considerations



• Due to integration (averaging) over Gamow peak, inaccuracies in the calculated cross sections do not enter the rates at the same level (Sargood 1982).

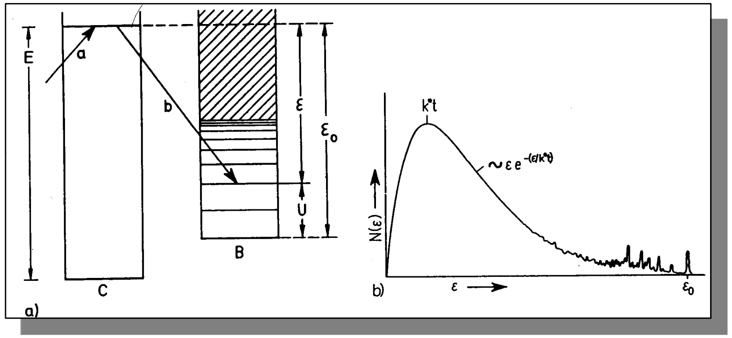
• However, a realistic minimum uncertainty for *global* predictions in the Hauser-Feshbach model may be on the level of 10-20%.

Energetics in Nuclear Reactions



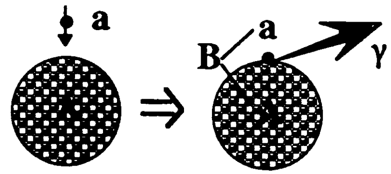
Reaction Mechanisms

Statistical Model (Hauser-Feshbach):



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

Direct Reaction (capture):



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

A ... target nucleus

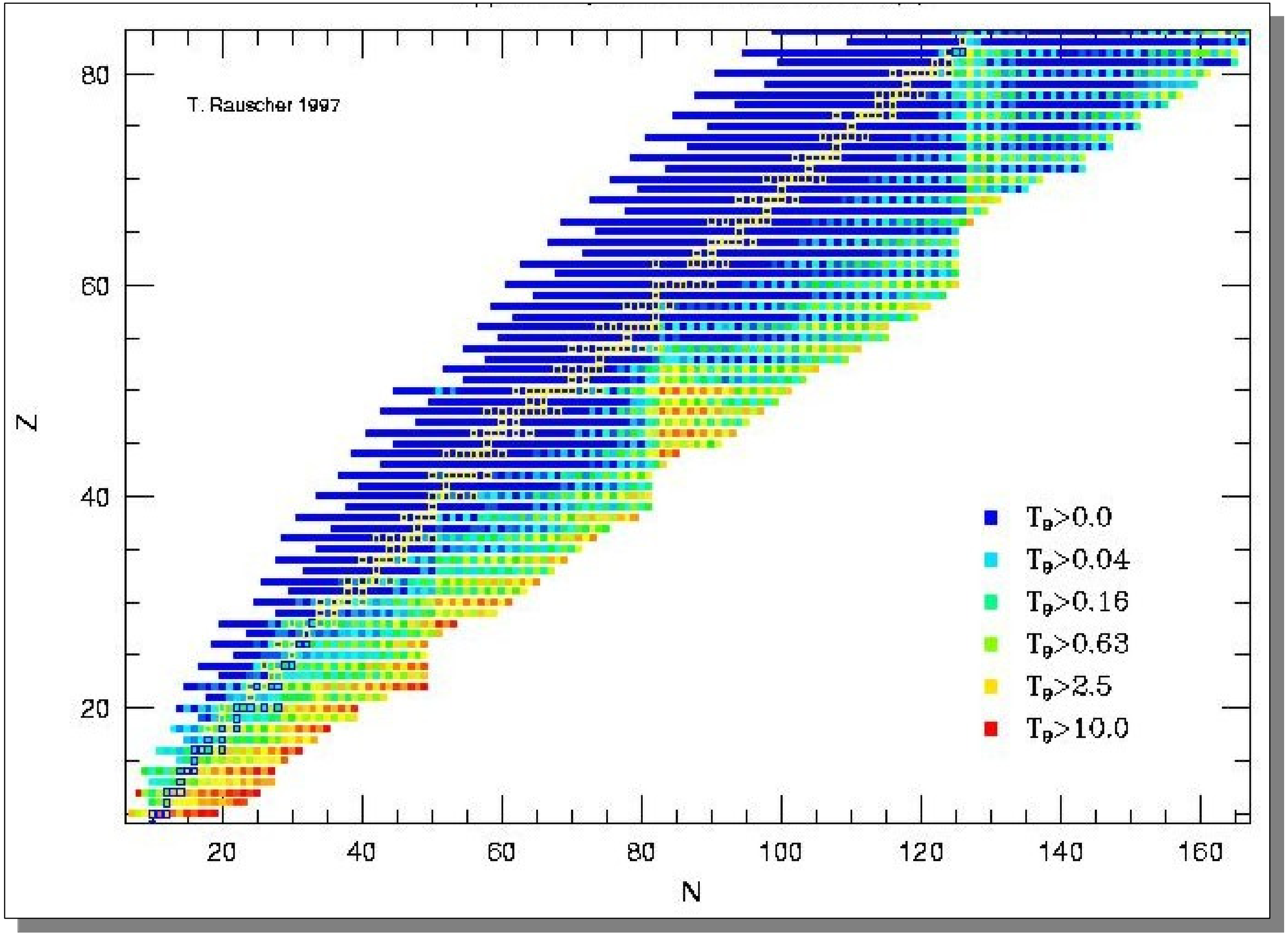
a ... projectile

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

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

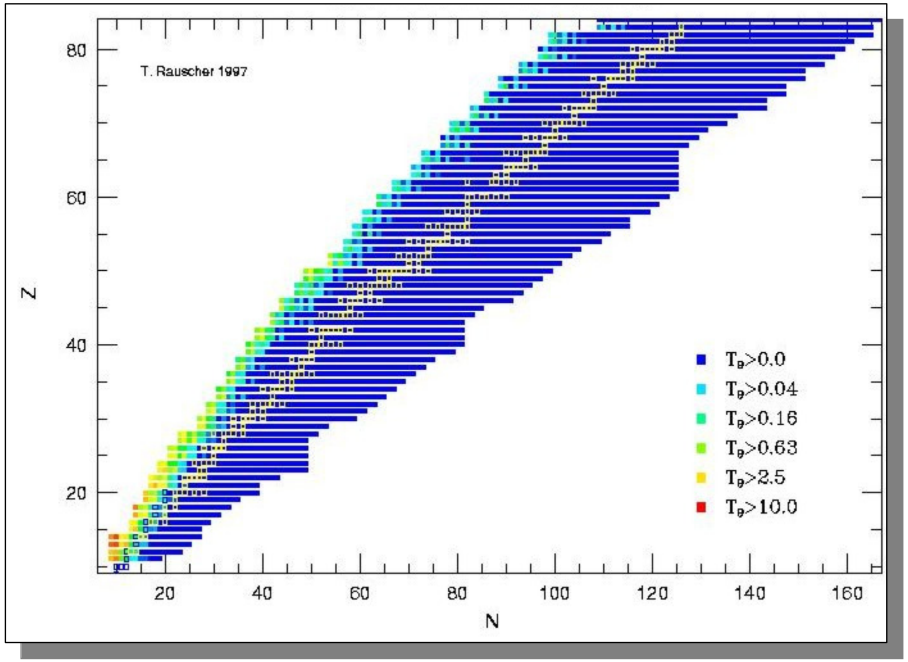
Applicability of the Statistical Model

Neutron induced reactions



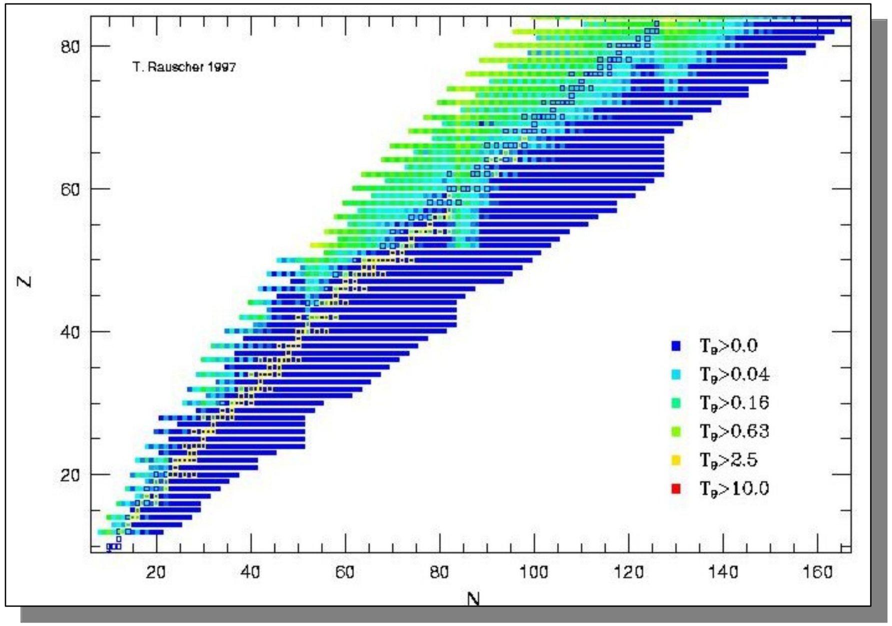
Rauscher et al. 1997

Applicability of Statistical Model



Proton induced reactions

α-induced reactions



Rauscher et al. 1997

Hauser-Feshbach Codes

• NEA search: 29 hits, including HAUSER-5, STAPRE, GNASH, Empire-II

• Not including recent ones: e.g. Thalys, McGNASH

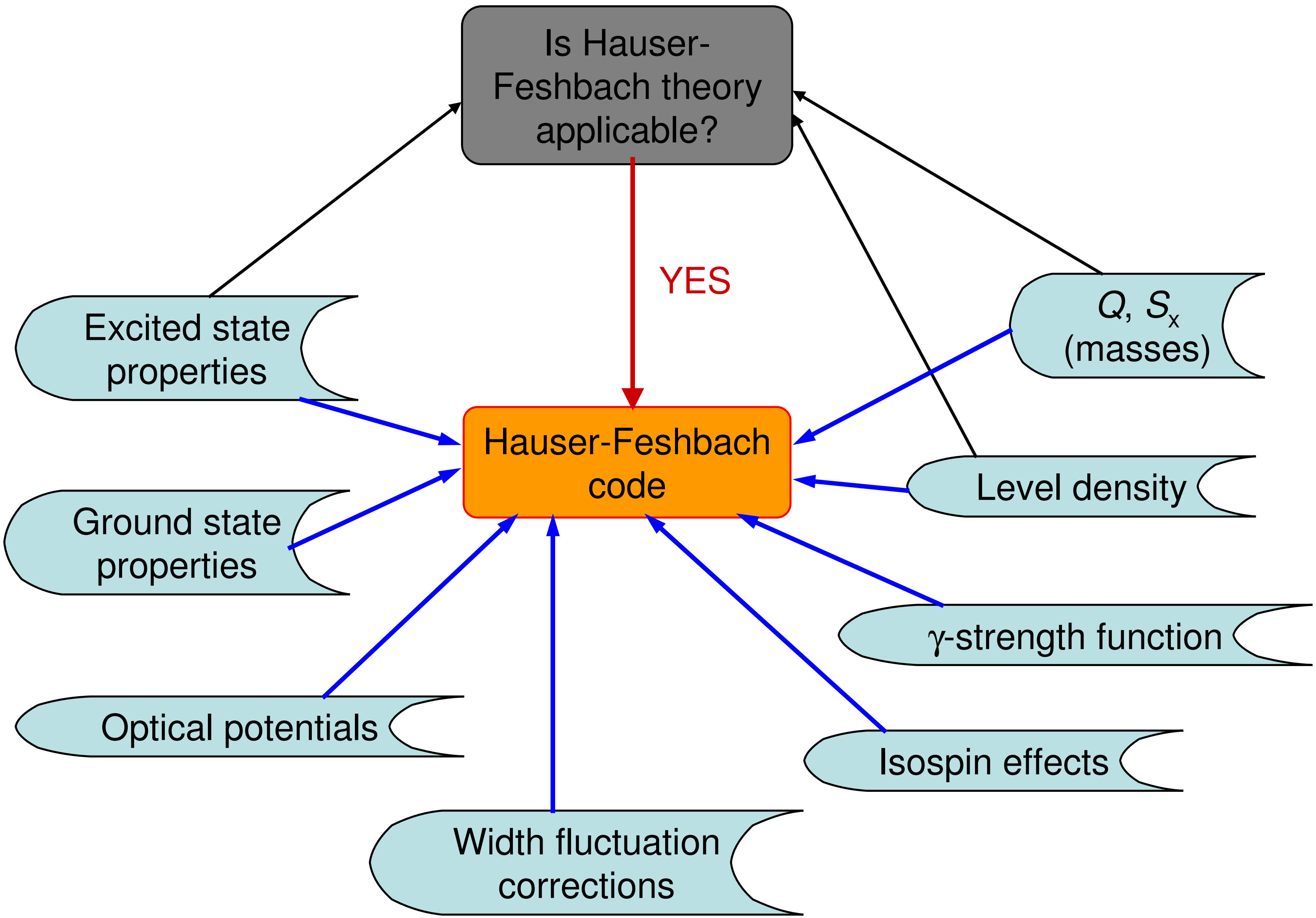
Older and newer codes for astrophysics: OAP-422, KGHFP, HAUSER-4, CRSEC, SMOKER, MOST, NON-SMOKER

Obvious differences:

• Astro-codes are for low-energy; do not include multistep, precompound processes

• Astro-codes include thermal excitation of the target and compute reaction rate directly

• Astro-codes use *global* input parameters; regular codes need tailored parameter set for each calculation


Is Hauser-Feshbach theory applicable?
YES
Hauser-Feshbach code
Excited state properties
Ground state properties
Optical potentials
Width fluctuation corrections
Isospin effects
γ-strength function
Level density
Q, S_x (masses)

Interesting Nuclear Properties

(in no particular order!)

- Nuclear level density (stat. mod. input)
  - Also single low-lying states important (DC+stat. mod.)
  - Systematics
  - Shell quenching?
- Masses (Q-values, sep. energies, equilibria path location)
- Optical Potentials (stat. mod. inp., DC)
- γ-Transitions: Giant resonances (stat. mod. inp.)
  - Low energy behavior
  - Pygmy Resonances?
- Nucleon density distribution (folding potentials, LDA)
- Fission barriers

Description of Required Nuclear Properties

microscopic

macroscopic-microscopic

phenomenological

Semi-microscopic

"Scientific approach"

"Engineering approach"

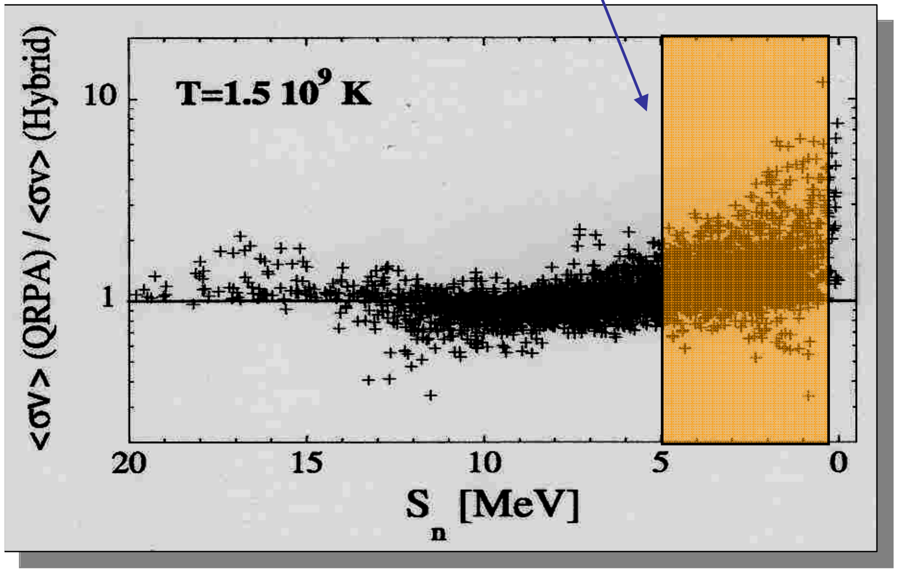
Globally more trustworthy?

Local fit, globally doubtful?

Some thoughts

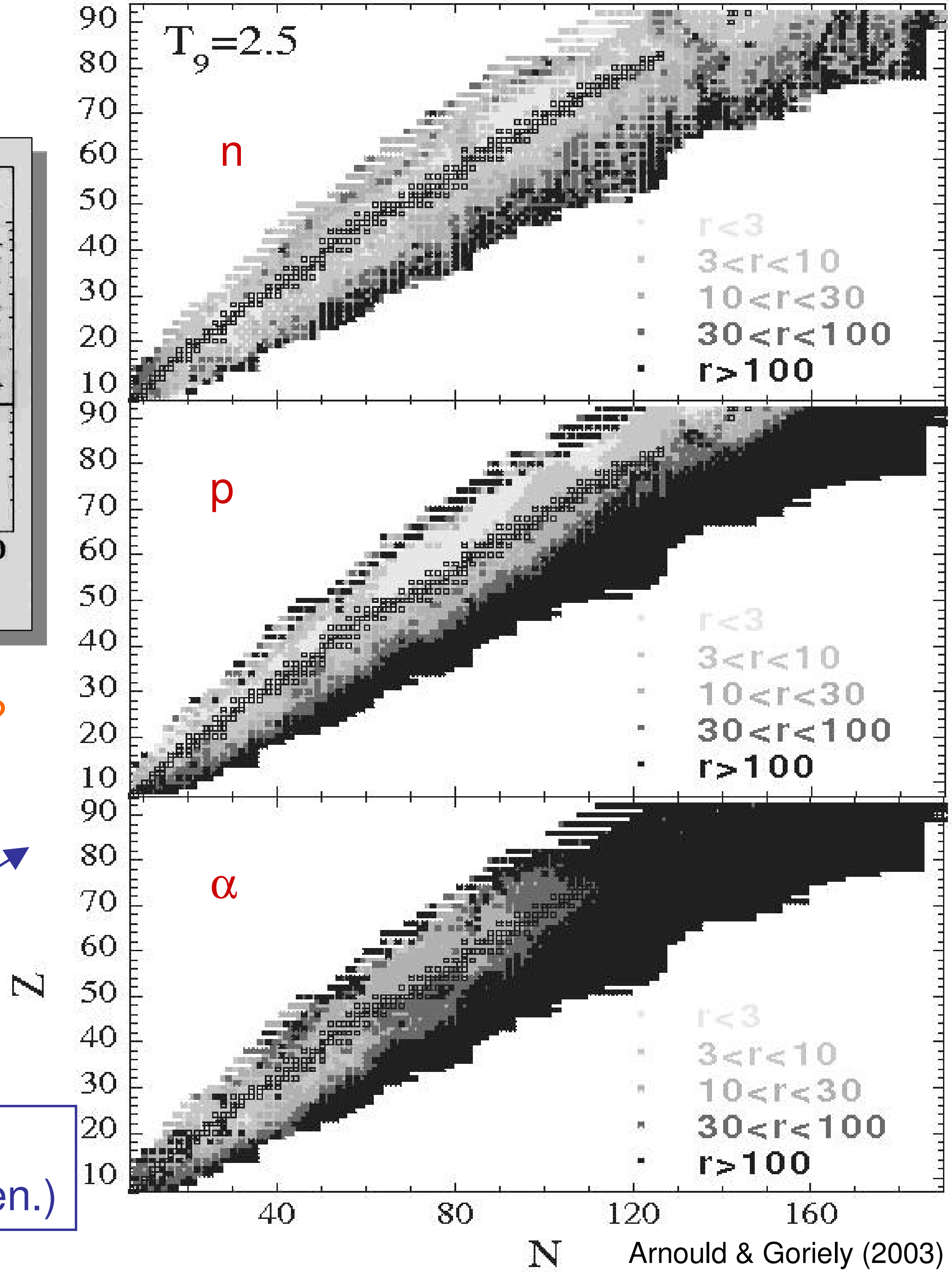
- *Microscopic approaches*
  - Limited availability
  - Accuracy locally lower than semi-microscopic or phenomenological methods
  - Different models do not agree, especially when dealing with exotic nuclei
- *Other approaches (mac-mic, semi-mic, phen)*
  - By no means, “stupid” fitting of functions (e.g. Fermi-gas; low-energy mod. of E1 Lorentzian)
  - Inclusion of microscopic effects by appropriate parametrization possible (e.g. pygmy resonances)
  - For example, in predicting masses, a mac-mic model (FRDM) is the most successful up to now
  - Finite number of nuclei, i.e. we do not have to extrapolate to infinity

Effect of (QRPA) pygmy resonances



Goriely & Khan (2002)

(n,γ)-(γ,n) equilibrium?



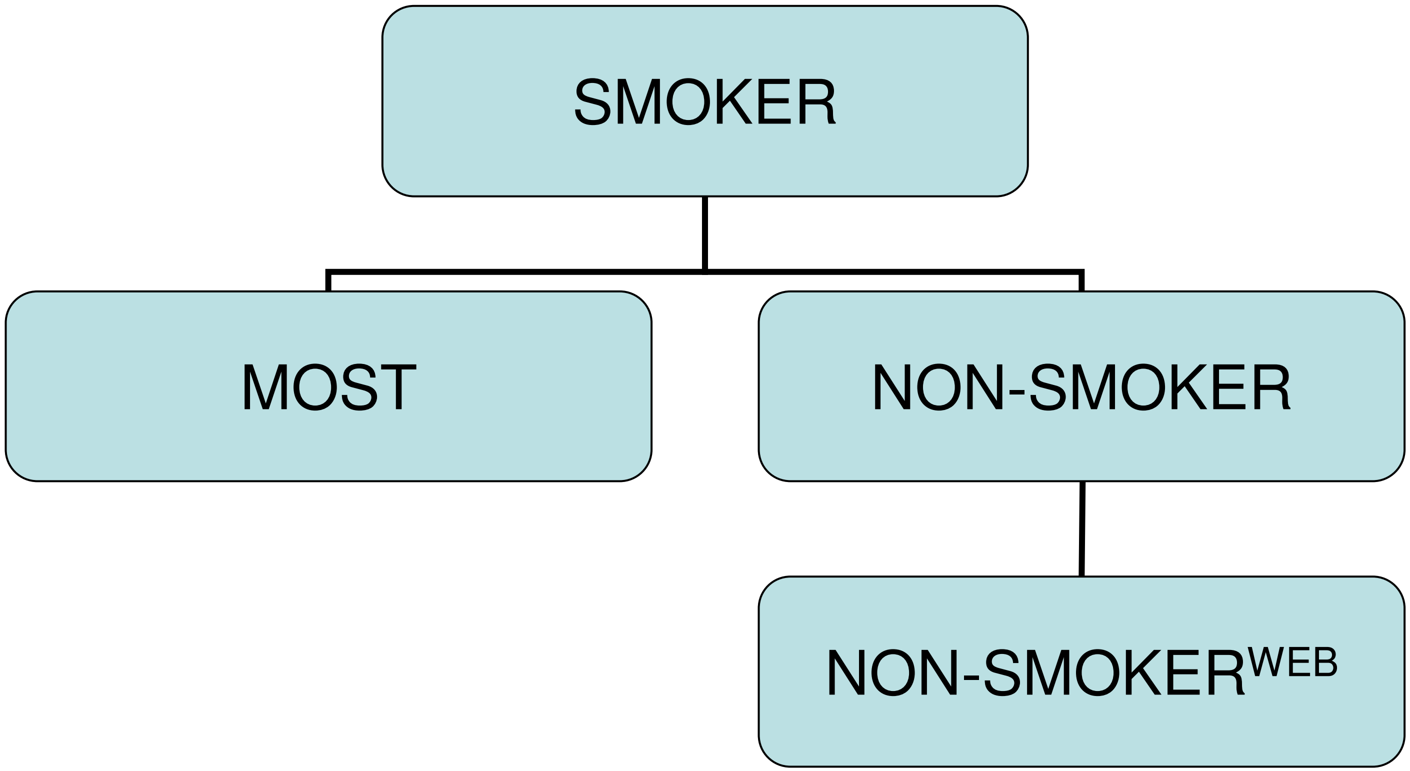
Arnould & Goriely (2003)

Effect of wide variation of inputs
(including different micr., mac-mic, phen.)

Prediction of Nuclear Properties Near To And Far From Stability

- Global models necessary for large-scale calculations
  - Microscopic, macroscopic-microscopic
  - Parameterized
- Parameterized models should be derived from basic understanding and/or microscop. models $\rightarrow$ then often better suited for large-scale calculations
- Situation not dramatic for regions of interest where Hauser-Feshbach is applicable
- We need pragmatic, “engineer” solutions …
- Biggest problem, even at stability: low-energy α+nucleus optical potential for intermediate and heavy nuclei!!

A code family



Difference in the used global parameters and the availability and documentation of results for cross sections and reaction rates.

Accessibility and User-Friendliness

- NON-SMOKER
  - www.nucastro.org
  - Tables of reaction rates (single access and complete file)
  - Tables of partition functions (complete file)
  - Tables of cross sections (single access and complete file)
  - Fits of rates in REACLIB format (complete file)
  - Temperature/energy applicability limits given!!
  - Version history on website
  - Published, peer-reviewed standard sets
- MOST
  - www-astro.ulb.ac.be/Html/hfr.html
  - Tables of reaction rates (isotopic chains and complete file)
  - Tables of partition functions (isotopic chains and complete file)

Final remarks I

- User advice: When comparing results of different codes, do not just look at the name, check which inputs were used!

- Recommended inputs are also provided by nuclear physics community (RIPL); but of limited use for astrophysics (too confined in selection, too local).

- Current uncertainties at stability: around 30% *on average* for neutron-induced reactions, slightly worse for proton-induced ones, and largest uncertainties for α-induced reactions on intermediate and heavy targets

- Large number of experimental data needed for improvement of inputs (optical potentials)

Final remarks II

- Online databases or compilations (of whatever kind) *always need*:
  - Version numbers and version history
  - Archive of previous versions
  - Preferrably at least one “standard” version in a public repository (journal data)

- Apart from numerical details all codes should be able to achieve the same results $\Rightarrow$ possibility to create unique code into which users can plug in desired inputs as “modules” (subroutines) (example: NON-SMOKER^{WEB} for optical potentials) $\Rightarrow$ truly global code…
  [however, this would just shift the decision problem on what to use in a recommended reaction rate set (experimental+theoretical)]

Have a lively discussion!

Level density in the back-shifted Fermi-gas model

$$\rho(U,J,\pi) = \frac{1}{2} f(U,J)\rho(U)$$

$$\rho(U) = \frac{1}{\sqrt{2\pi}} \frac{\sqrt{\pi}}{12 a^{1/4}} \frac{\exp(2\sqrt{aU})}{U^{5/4}}$$

$$f(U,J) = \frac{2J+1}{2\sigma^2} \exp\left(\frac{-J(J+1)}{2\sigma^2}\right)$$

$$\sigma^2 = \frac{\Theta_{\mathrm{rigid}}}{\hbar^2}\sqrt{\frac{U}{a}} \qquad \Theta_{\mathrm{rigid}} = \frac{2}{5} m_{\mathrm{u}} A R^2 \qquad U = E - \delta .$$

$$a(U,Z,N) = \tilde{a}(A)\left[1 + C(Z,N)\frac{f(U-\delta)}{U-\delta}\right] ,$$

$$\tilde{a}(A) = \alpha A + \beta A^{2/3} \quad ,$$

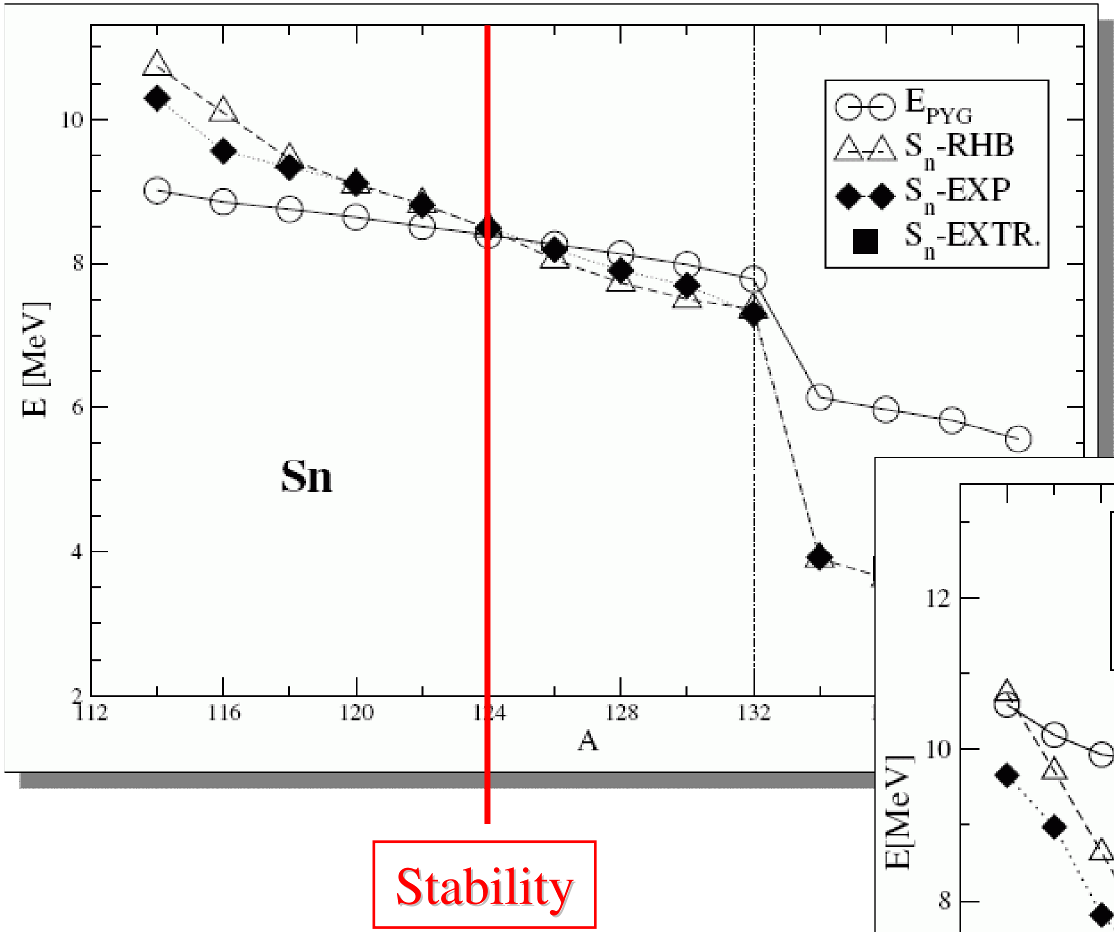
$$f(U) = 1 - \exp(-\gamma U) \quad .$$

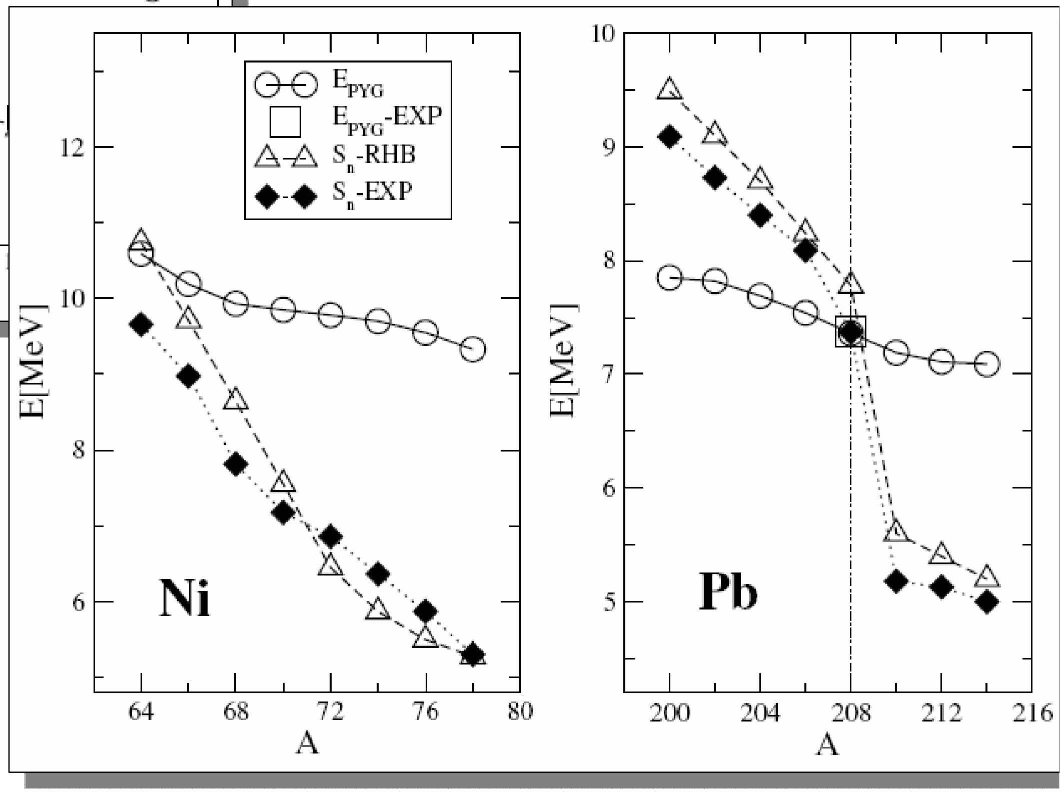
$$\delta(Z,N) = \Delta_{\mathrm{n}}(Z,N) + \Delta_{\mathrm{p}}(Z,N)$$

$$\Delta_{\mathrm{n}}(Z,N) = \frac{1}{4}[E^G(Z,N-2) - 3E^G(Z,N-1) + $$
$$+3E^G(Z,N) - E^G(Z,N+1)]$$

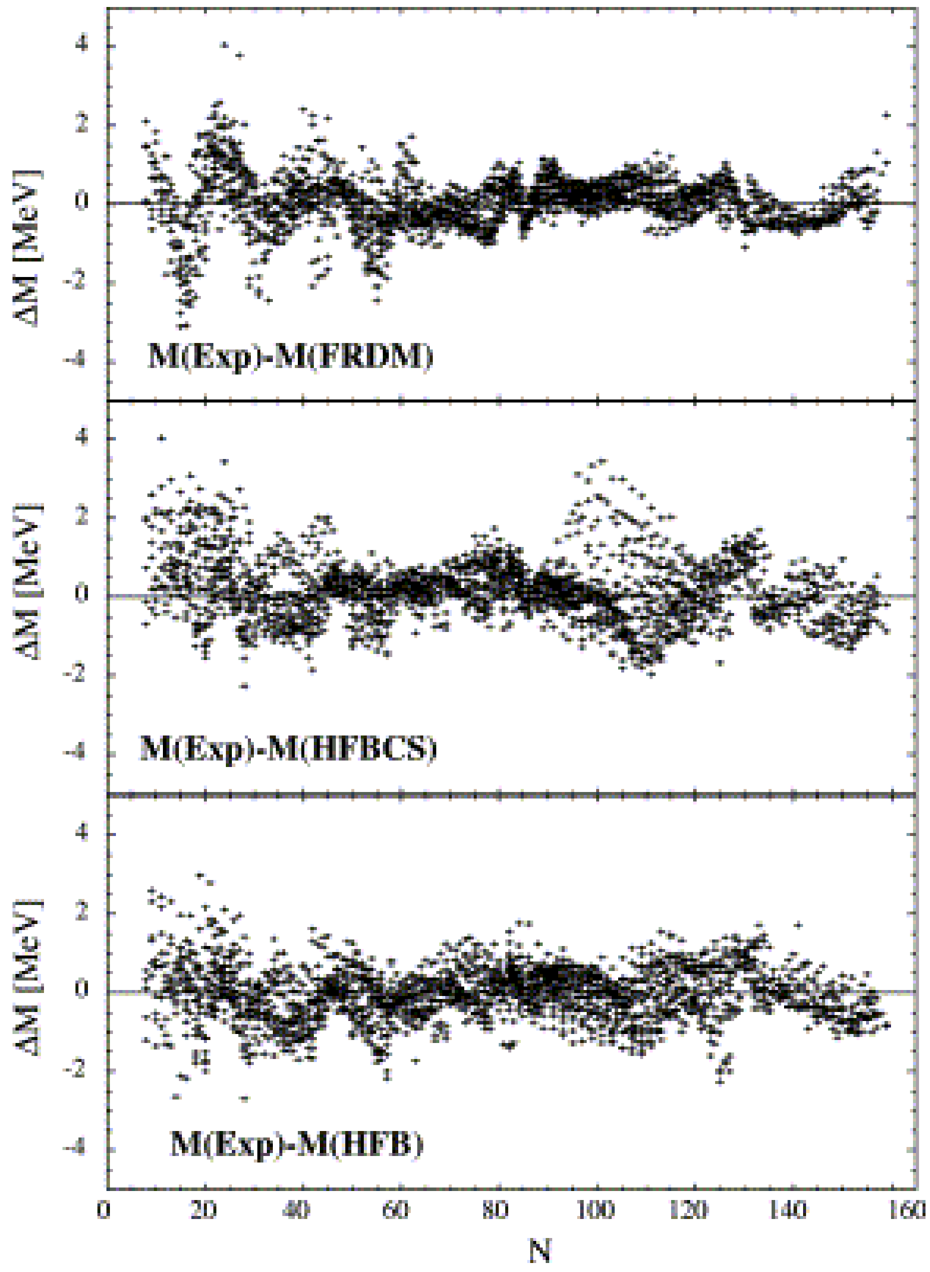
- Bethe's BSFG description is derived from basic principles, also valid far off stability
- Correctness of shape confirmed by many modern mic. calc., also for exotic nuclei and to high excitation energies [e.g. Dean et al (1995), Paar et al (1997), Alhassid et al (2000), Van Isacker (2002), Alhassid et al (2003)]
- Two parameters account for shell effects and can be determined, e.g., from nuclear mass differences
- At low excitation energies it is smoothly supplemented by a constant temperature formula

Pygmy Predictions

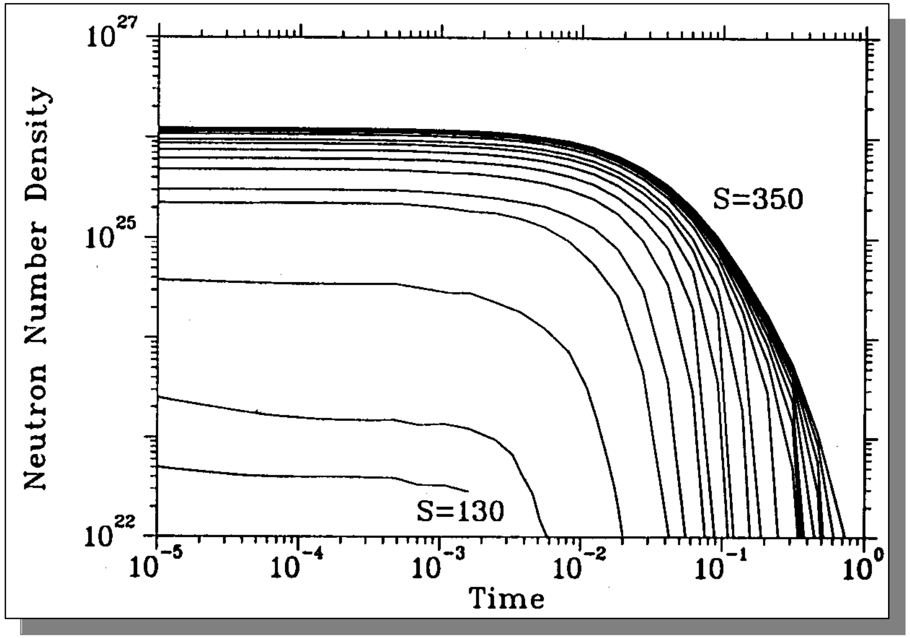




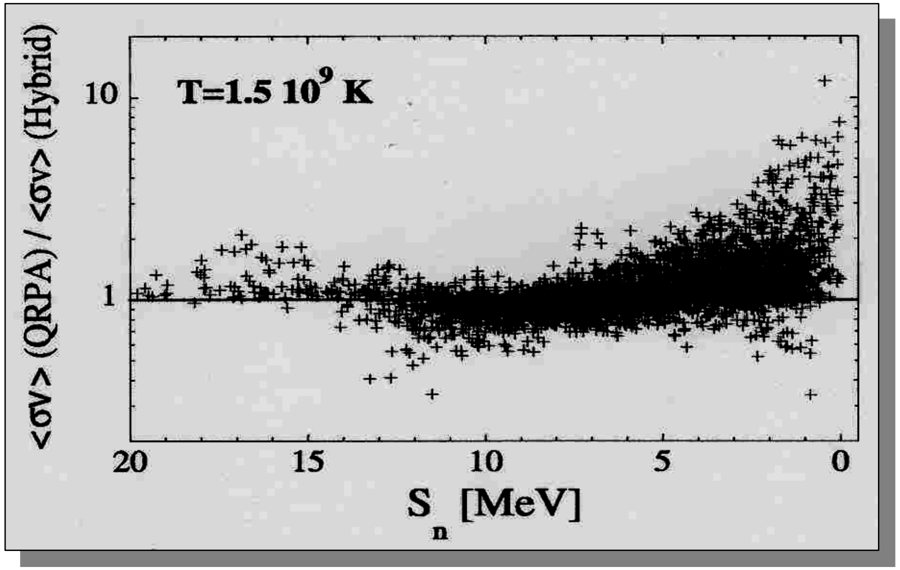
Paar, Nikšić, Vretenar, Ring 2005


ΔM [MeV]
M(Exp)-M(FRDM)
ΔM [MeV]
M(Exp)-M(HFBCS)
ΔM [MeV]
M(Exp)-M(HFB)
N

Impact of rate uncertainties



Freiburghaus et al. (2002)



Goriely & Khan (2002)

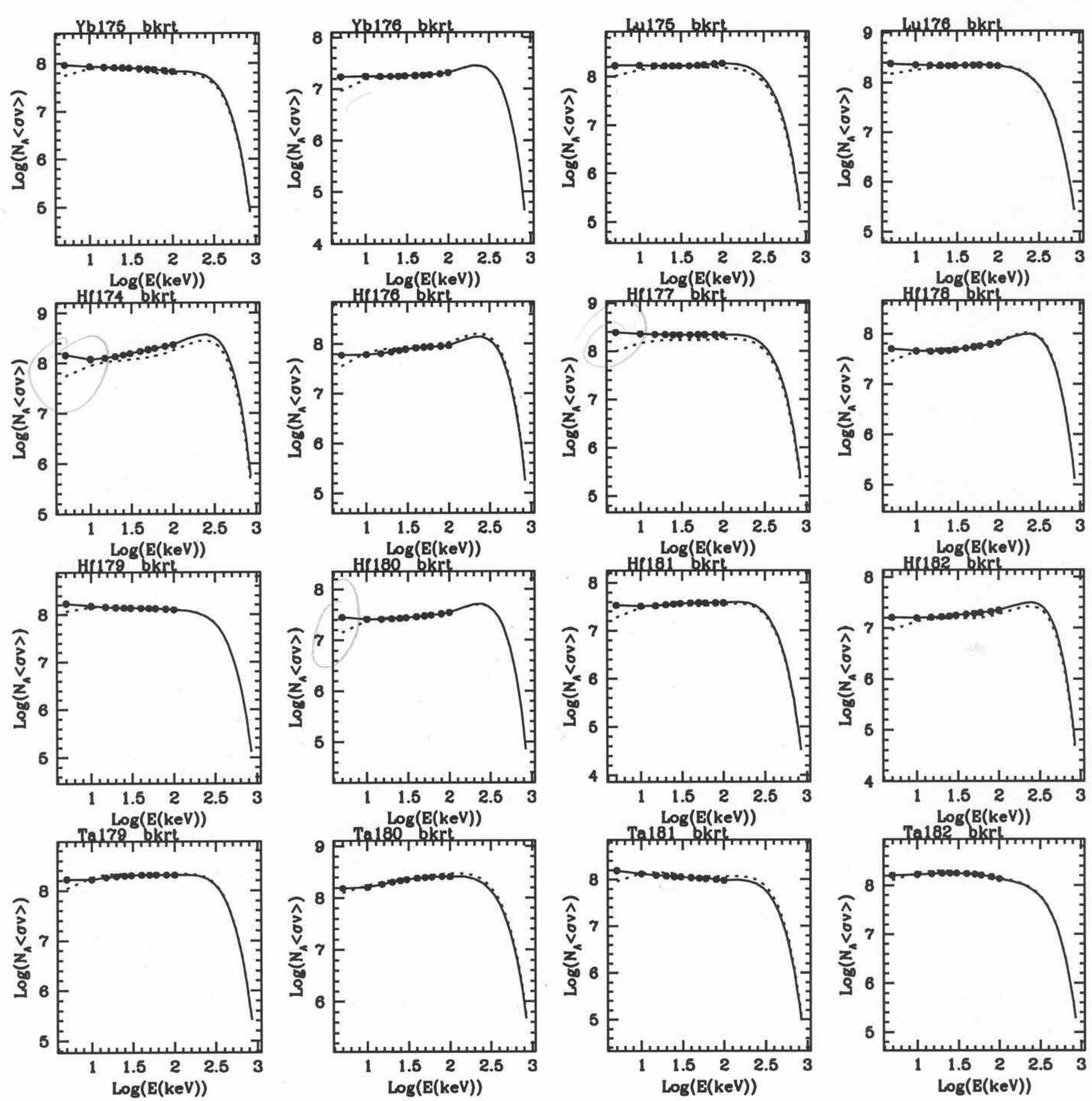
- T ↑↑⇒ (γ,n) rate ↑↑
- n_n ↑↑⇒ (n,γ) rate ↑↑
- Mult. factor ↑↑⇒ (n,γ) ↑↑, (γ,n) ↑↑
- Freeze-out:
  - Low entropy: instantaneous
  - High entropy: final neutron captures
  - Mult. fact. does not change „scissor gap“, entropy scaling
  - Capture later: different equil. abundances, less time(?)
  - Speculations: small impact of rates, perhaps suppression of captures with higher rates??
- Freeze-out dependent; model dependent?

Reaction Rates From The Statistical Model

- Standard rates from NON-SMOKER code
- Rate library with fits
  (5000 targets, 30000 reactions)
  Rauscher & Thielemann, ADNDT 75 (2000) 1
- Temperature/Energy applicability limits given!!
- Tables of rates, cross sections, inputs
  Rauscher & Thielemann, ADNDT 79 (2001) 47
- Available on-line
  ADNDT web site or
  http://nucastro.org/reaclib.html

Comparison to (n,γ) Experiment I

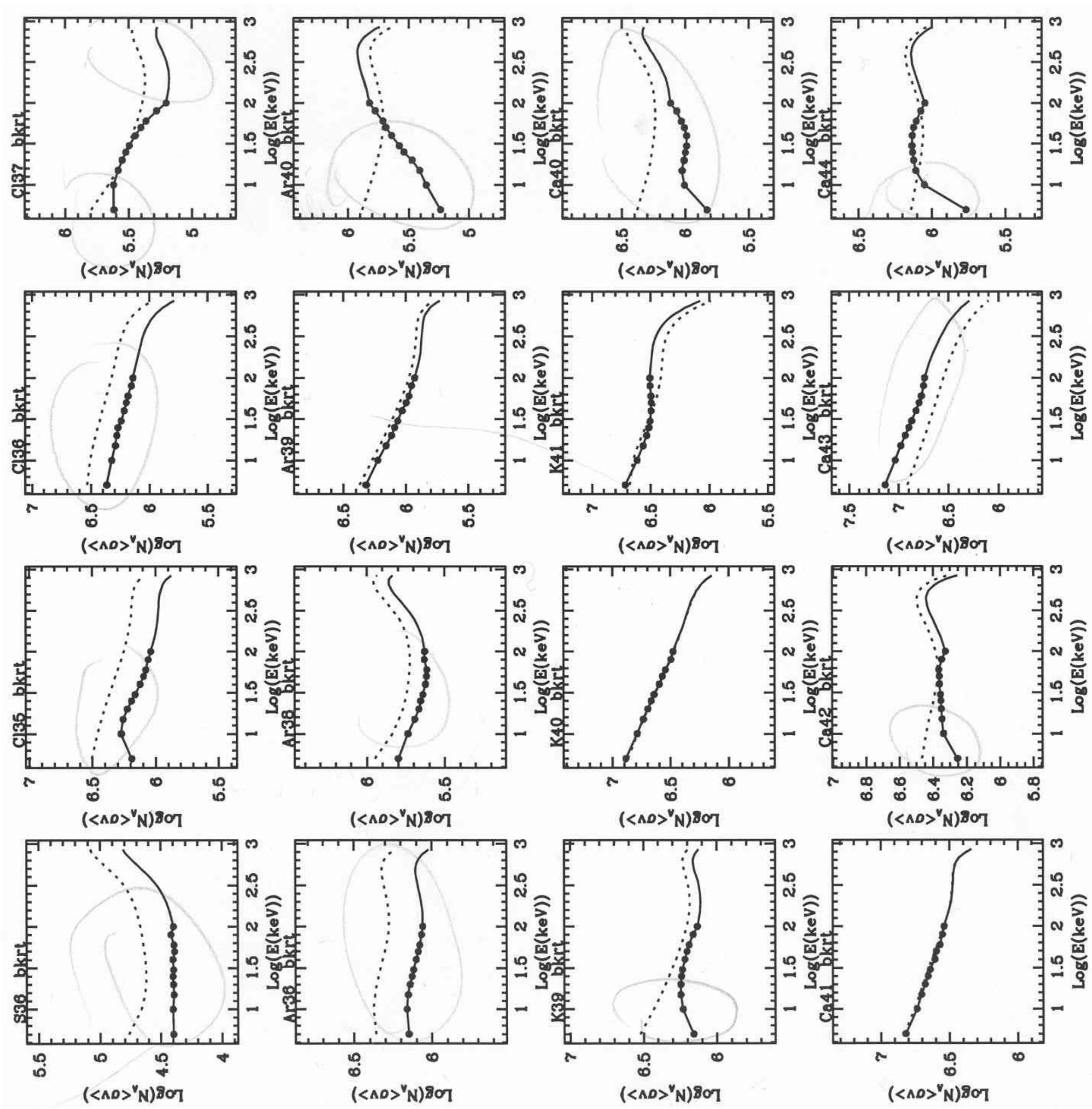
Comparison with Bao et al. 2000



Plots provided by R. Gallino, M. Limongi, F. Käppeler, S. Cristallo

Comparison to (n,γ) Experiment II

Plots provided by R. Gallino, M. Limongi, F. Käppeler, S. Cristallo



Comparison with Bao et al. 2000