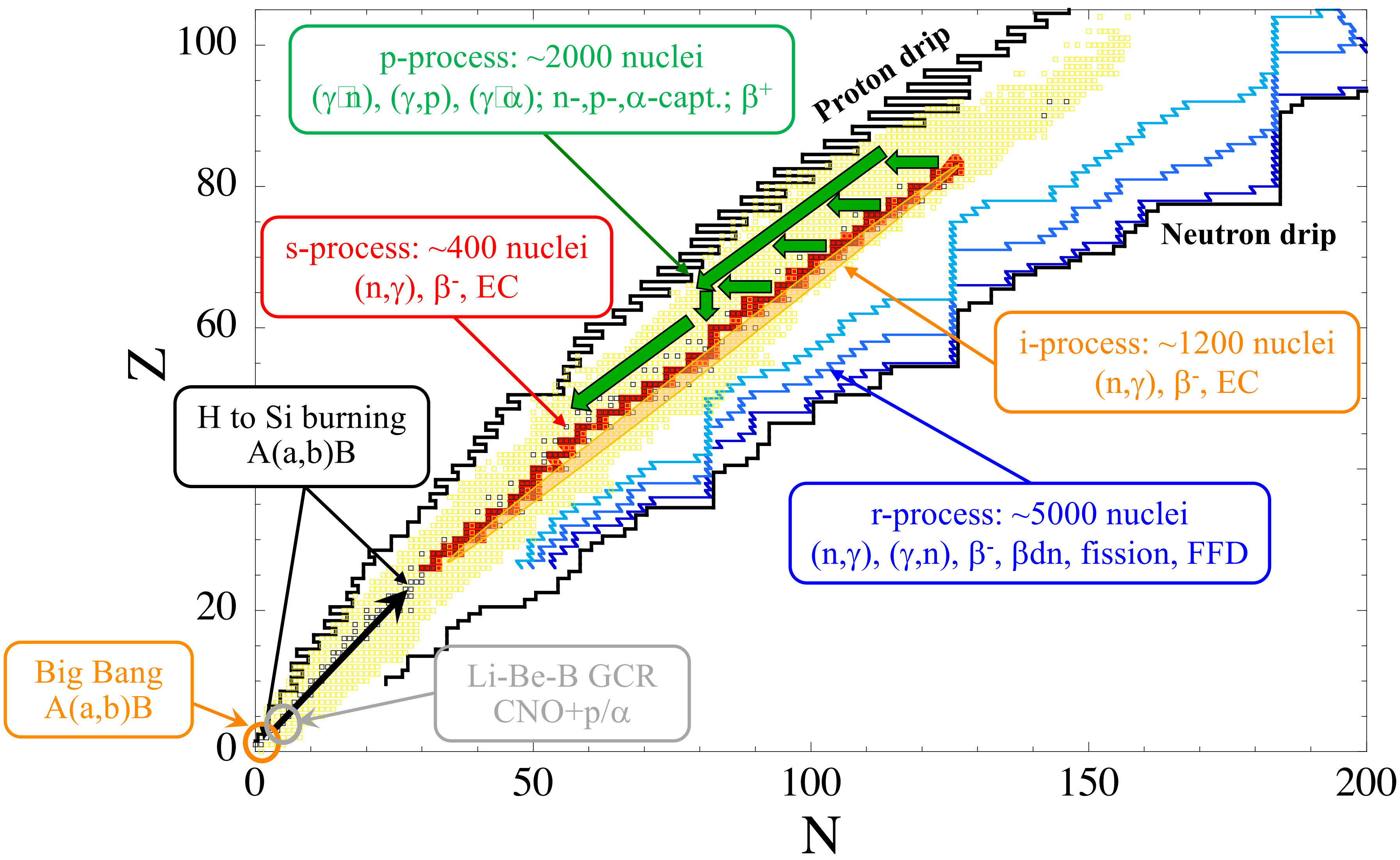
RELATED NUCLEAR DATA NEEDS

Lecture 3

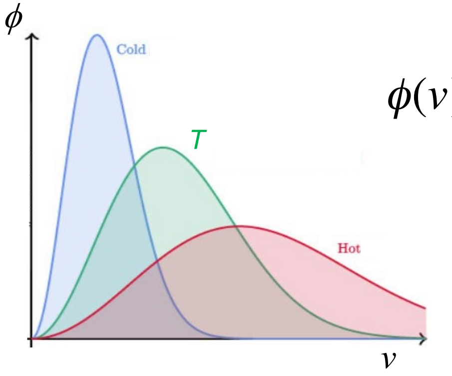
- Specificities of the stellar plasma
- Nuclear reaction rates
- Nuclear needs for the various nucleosynthesis processes

Many different nuclear needs for the various nucleosynthesis processes



Important needs for nuclear reaction rates

Reaction rate of astrophysical interest for a target in its GS



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

$$\mu = \frac{m_X m_a}{m_X + m_a}$$

The relative velocity distribution is a Maxwell-Boltzmann distribution based on the reduced mass □

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

Traditionally expressed in terms of

- $N_A<\sigma v>$ in mol^{-1} cm^3 s^{-1} (N_A = Avogadro nbr)
- $<\sigma>=<\sigma v>/v_T$ in mb for neutrons (MACS)

  where v_T is the thermal velocity

$$v_T = \sqrt{\frac{2k_B T}{\mu}}$$

For incident charged-particles

$$\sigma(E) = \pi\lambdabar^2 P(E) = \pi\frac{\hbar^2}{p^2}P(E) = \pi\frac{\hbar^2}{2mE}P(E)$$

The Coulomb penetration factor can be estimated in the case of a zero centrifugal barrier (l=0)

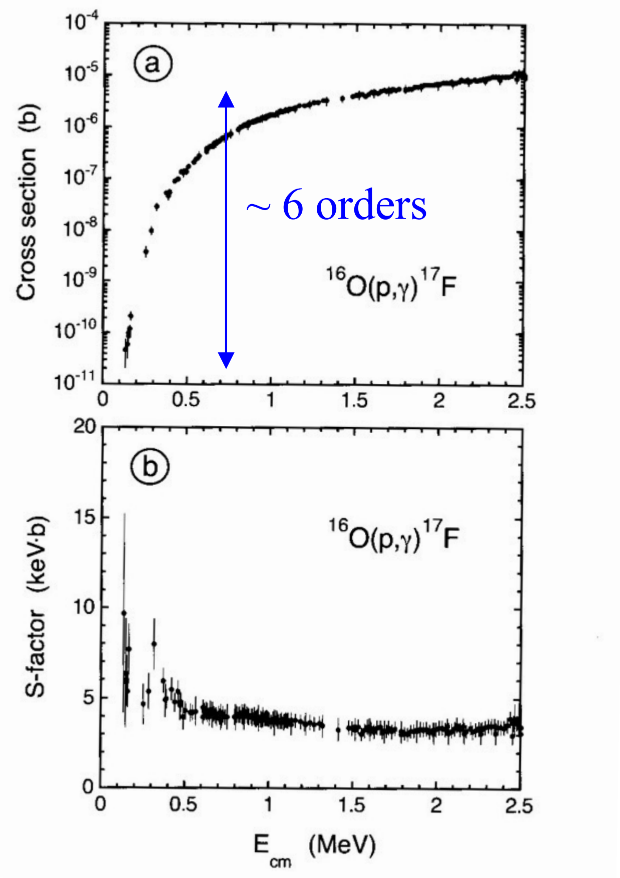
$$P(E) \propto \exp\left(-\frac{2\pi Z_X Z_a e^2}{\hbar v}\right) = \exp(-2\pi\eta)$$ where η is the Sommerfeld parameter

$$\boxed{\sigma(E) \equiv \frac{S(E)}{E}\exp\left(-bE^{-1/2}\right)}$$ where $b = 2\pi\eta E^{1/2}$

where $S(E)$ is called the *astrophysical S-factor* which presents the advantage of not being very much energy dependent (except for resonant reactions) since the geometrical ($1/E$) and the Coulomb repulsion [$\exp(-bE^{-1/2})$] factors have been explicitly extracted.

$S(E)$ represents the intrinsic nuclear part of the reaction probability:

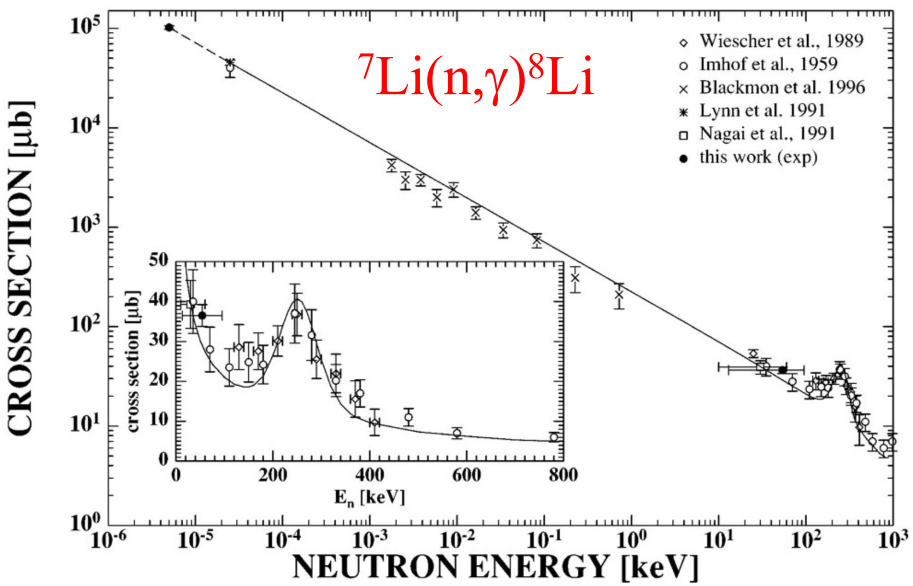
- $S(E)$ does not vary significantly in the energy region of astrophysics interest, and is therefore often expressed as $S(E)=S_0+S'_0(E-E_0)+\ldots$
- $S(E)$ may vary strongly on small energy scales due to the resonance phenomenon



For incident neutrons

$$\sigma(E) \approx \pi \lambda\!\!\!^{-2} P(E) \propto \frac{\sqrt{E}}{E} \propto \frac{1}{\sqrt{E}} \propto \frac{1}{v}$$

This relation is known as the **1/*v*-law**



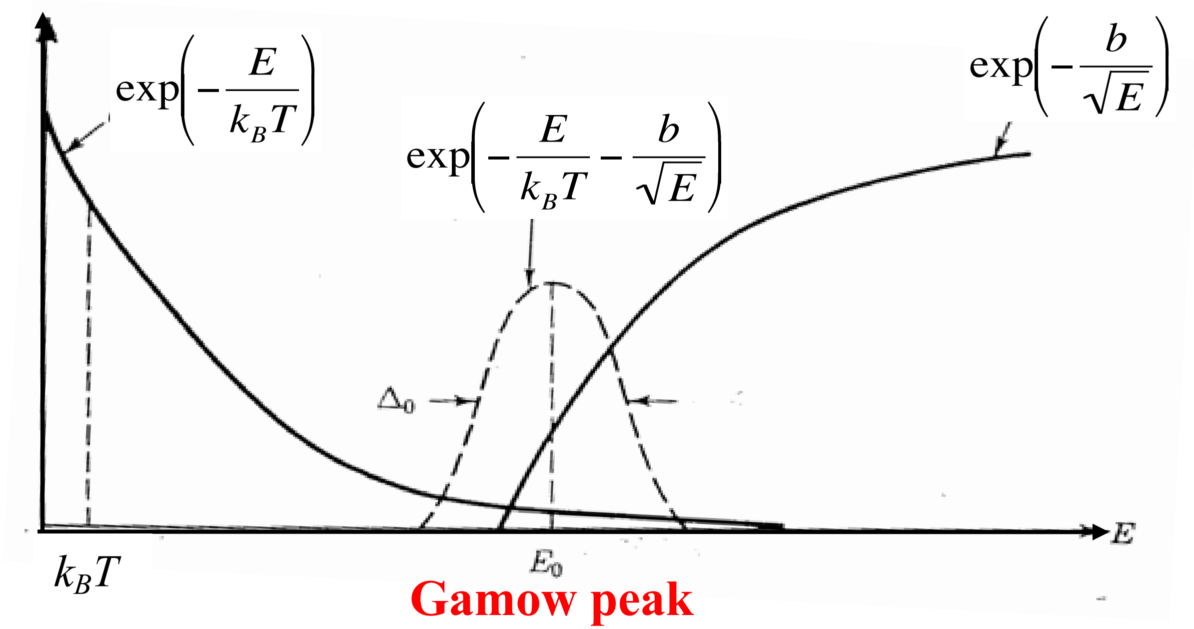
Due to the absence of the Coulomb barrier, reactions involving neutrons are extremely fast (by far faster than reactions with charged particles), so that the neutron half-life in a stellar plasma is extremely small (of the order of the micro- or milli-second). Neutrons can therefore not be found in traditional stellar medium, since as soon as they are produced, they are absorbed. They play a negligible role in the nuclear energy production. In contrast, they play a fundamental role in the nucleosynthesis of elements heavier than iron. Neutron captures are responsible for almost all nuclei heavier than iron (i.e about 2/3 of stable nuclei in the Universe).

Nuclear reaction rates in stellar plasmas

On the basis of the energy-dependent expression of the cross section *for charged-particle induced reactions*

$$\sigma(E) \equiv \frac{S(E)}{E}\exp\left(-bE^{-1/2}\right) \qquad \text{where } b = 2\pi\eta E^{1/2} = 31.28\ Z_X Z_a \square^{1/2}\ \text{keV}^{1/2}$$

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



The integrant is a strongly peaked function around the so-called Gamow energy E_0 defined from

$$\frac{d}{dE}\left(\frac{E}{k_B T}+bE^{-1/2}\right)_{E=E_0} = \frac{1}{k_B T}-\frac{1}{2}bE_0^{-3/2} = 0 \quad \Rightarrow \quad E_0 = \left(\frac{b k_B T}{2}\right)^{2/3}$$

$E_0 = 1.220(Z_X^2 Z_a^2 \square T_6^2)^{1/3}$ keV

For *radiative neutron captures* (with *l*=0), the cross section obeys the *1/v*-law, so that

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

And the integrant is maximum for

$$\frac{d}{dE}\left(\sqrt{E} \exp\left(-\frac{E}{k_B T}\right)\right)\Bigg|_{E=E_0} = \frac{1}{2\sqrt{E_0}} - \frac{\sqrt{E_0}}{k_B T} = 0 \quad \Rightarrow \quad \boxed{E_0 = \frac{k_B T}{2}}$$

so that

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

$$\int_0^\infty \sqrt{x}\, e^{-x} dx = 2\int_0^\infty y^2 e^{-y^2} dy = \int_0^\infty e^{-y^2} dy = \frac{\sqrt{\pi}}{2}$$

In such specific conditions, the neutron capture reaction *rate* is temperature and density independent !

Rem: It should be kept in mind that the results obtained here are based on a gross estimate of the energy dependence of the reaction cross section ($S(E)$ constant for charged particles, and the $1/v$-law for neutrons). Such a dependence can be drastically different in the neighbourhood of a resonance, leading to a very strong variation of σ on a very small energy range. These resonances, and most particularly those located in the Gamow energy range $E_0 \pm \Delta/2$ of astrophysical interest play a fundamental role and can strongly affect the nuclear reactions in a stellar plasma.

Contribution from thermally populated excited states

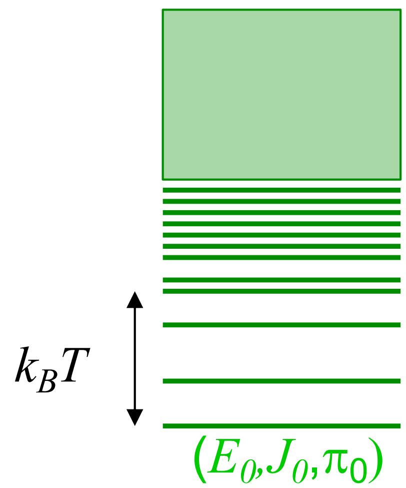
In hot astrophysical plasmas, *a target nucleus exists in its ground as well as excited states*.
In a thermodynamic equilibrium situation, the relative populations of the various levels of nucleus I^{μ} with excitation energies ε^{μ}_I obey a Maxwell-Boltzmann distribution.
The effective stellar rate of per pair of particles in the entrance channel at temperature T taking due account of the contributions of the various target excited states μ is thus expressed in a classical notation (in cm^3 s^{-1} mole^{-1}) as

$$N_A \langle \sigma v \rangle^*_{jl}(T) = \left(\frac{8}{\pi m}\right)^{1/2} \frac{N_A}{(kT)^{3/2}\ G_I(T)} \int_0^\infty \sum_\mu \frac{(2J_I^\mu + 1)}{(2J_I^0 + 1)} \sigma^\mu_{jl}(E) E \exp\left(-\frac{E + \varepsilon_I^\mu}{kT}\right) dE$$

where k is the Boltzmann constant, m the reduced mass of the $I^0 + j$ system, N_A the Avogadro number, and $G(T)$ the temperature-dependent normalised partition function given by

$$G_I(T) = \sum_\mu \frac{2J_I^\mu + 1}{2J_I^0 + 1} \exp\left(-\frac{\varepsilon_I^\mu}{kT}\right)$$

$$k_B T\ [\text{keV}] = 86.2\ T\ [10^9\text{K}]$$



No experimental cross section known on excited targets !

Only theory can fill the gap !

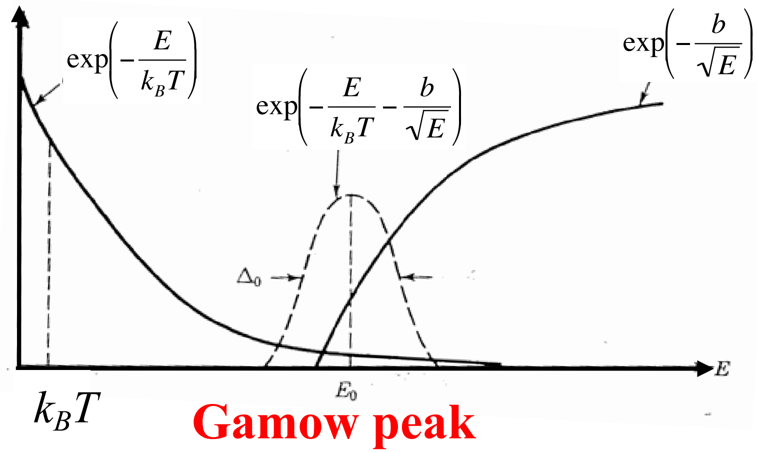
In Summary:

for all reacting species in the stellar plasma, we need to estimate experimentally or theoretically the astrophysical reaction rate at the temperature T of the plasma:

$$N_A \langle \sigma v \rangle^*_{jl}(T) = \left(\frac{8}{\pi m}\right)^{1/2} \frac{N_A}{(kT)^{3/2}\, G_I(T)} \int_0^\infty \sum_\mu \frac{(2J_I^\mu + 1)}{(2J_I^0 + 1)} \sigma^\mu_{jl}(E) E \exp\left(-\frac{E + \varepsilon_I^\mu}{kT}\right) dE$$

- For charged particles: around the Gamow energy E_0 (**far below the Coulomb barrier**)

$$\sigma(E) \equiv \frac{S(E)}{E} \exp\left(-bE^{-1/2}\right)$$



- For neutrons: around $k_B T$ (10-100 keV for s- or r-process nucleosynthesis)

$$\sigma(E) \approx \pi \lambda\!\!\!^{-2} P(E) \propto \frac{\sqrt{E}}{E} \propto \frac{1}{\sqrt{E}} \propto \frac{1}{v} \qquad (1/v\text{-law})$$

- Contribution from thermally excited states in target nuclei must be taken into account

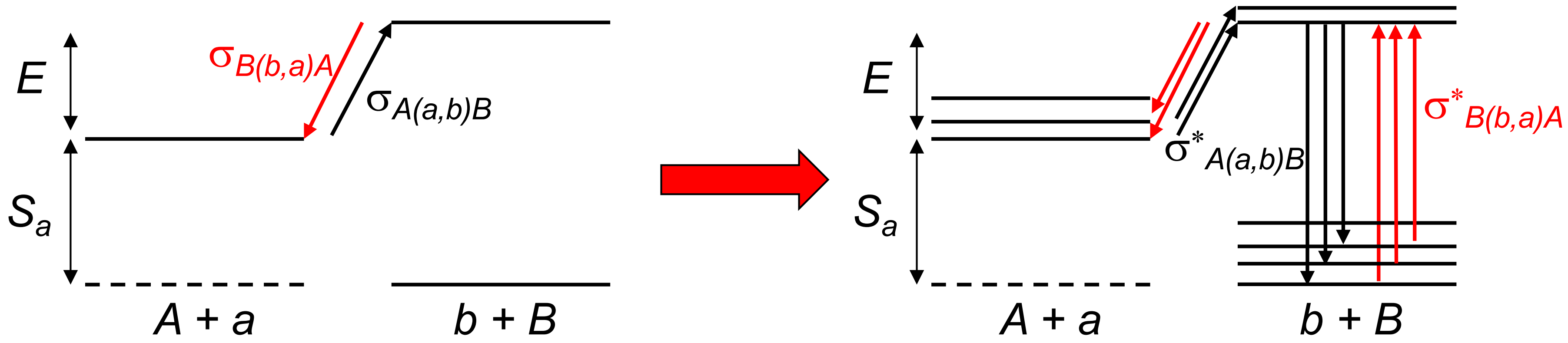
Detailed balance and reverse reactions in stellar conditions

Reverse reactions can be estimated with the use of the reciprocity theorem. In particular, the stellar photo-dissociation rates (in s^{-1}) are classically derived from the reverse radiative capture rates by

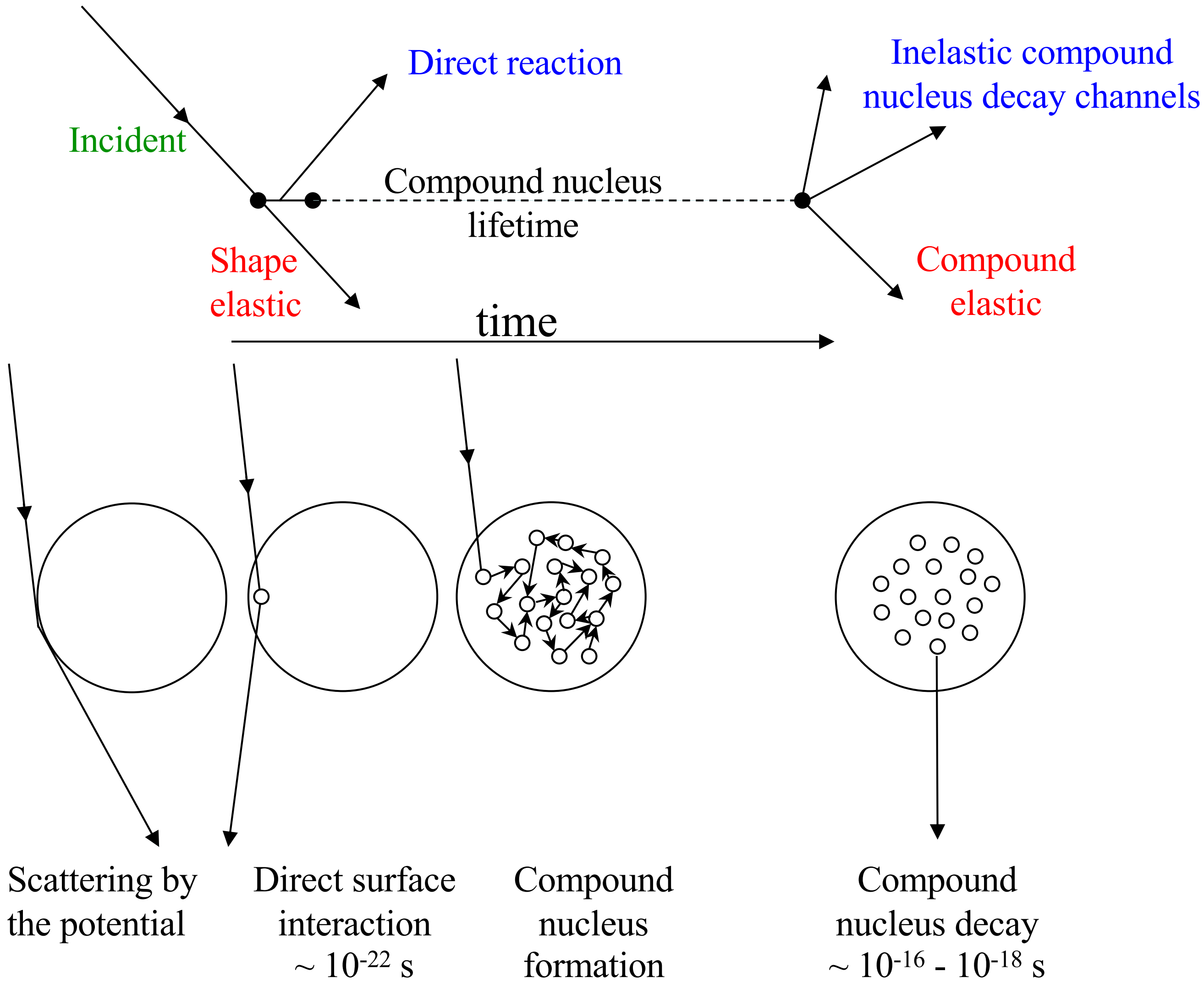
$$\lambda^*_{(\gamma,j)}(T) = \frac{(2J_I^0+1)(2J_j+1)}{(2J_L^0+1)} \frac{G_I(T)}{G_L(T)} \left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2} \langle\sigma v\rangle^*_{(j,\gamma)}\ \mathrm{e}^{-Q_{j\gamma}/kT}$$

where $Q_{j\gamma}$ is the Q-value of the $I^0(j,\gamma)L^0$ capture reaction.

Note that, in stellar conditions, the reaction rates for targets in thermal equilibrium obey reciprocity since the forward and reverse channels are symmetrical, in contrast to the situation which would be encountered for targets in their ground states only.

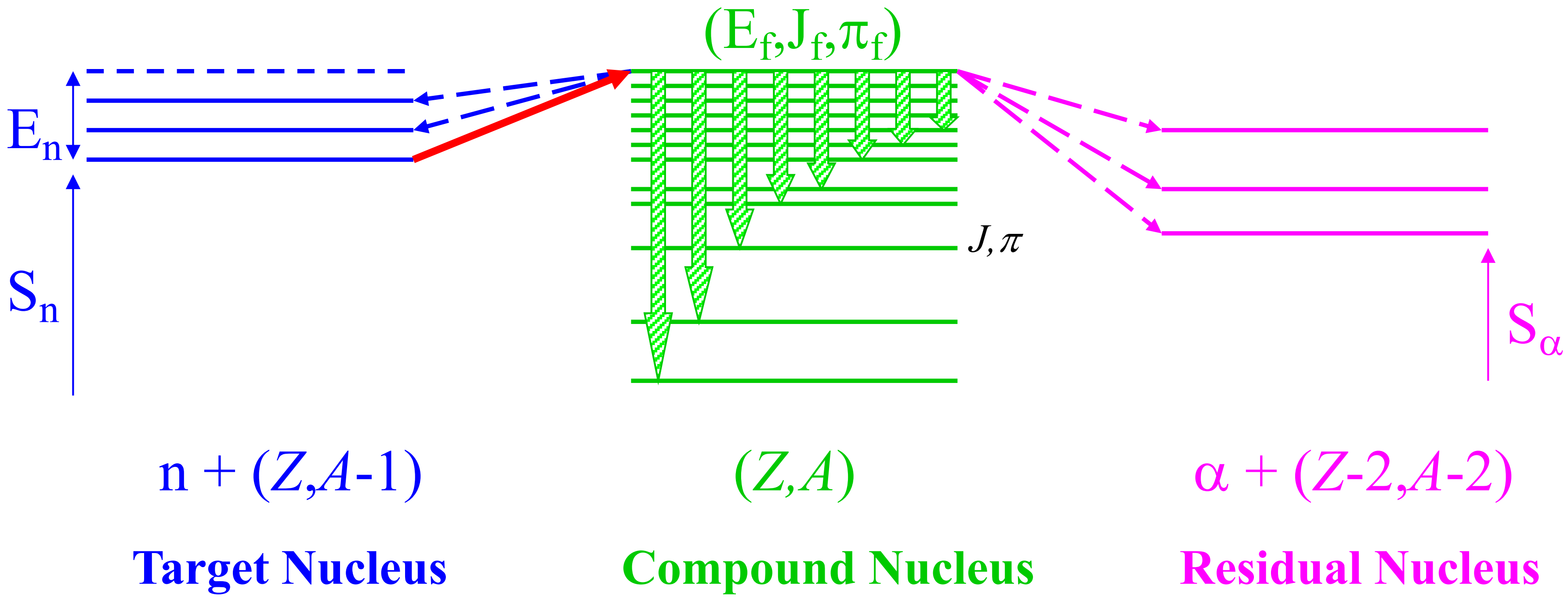


Nuclear reaction mechanism



At low energies ($E_n \sim kT;\ E_{p,\alpha} \sim E_G$), the compound nucleus mechanism dominates, at least for medium- and heavy-mass nuclei close to the valley of β-stability

The statistical Hauser-Feshbach reaction model

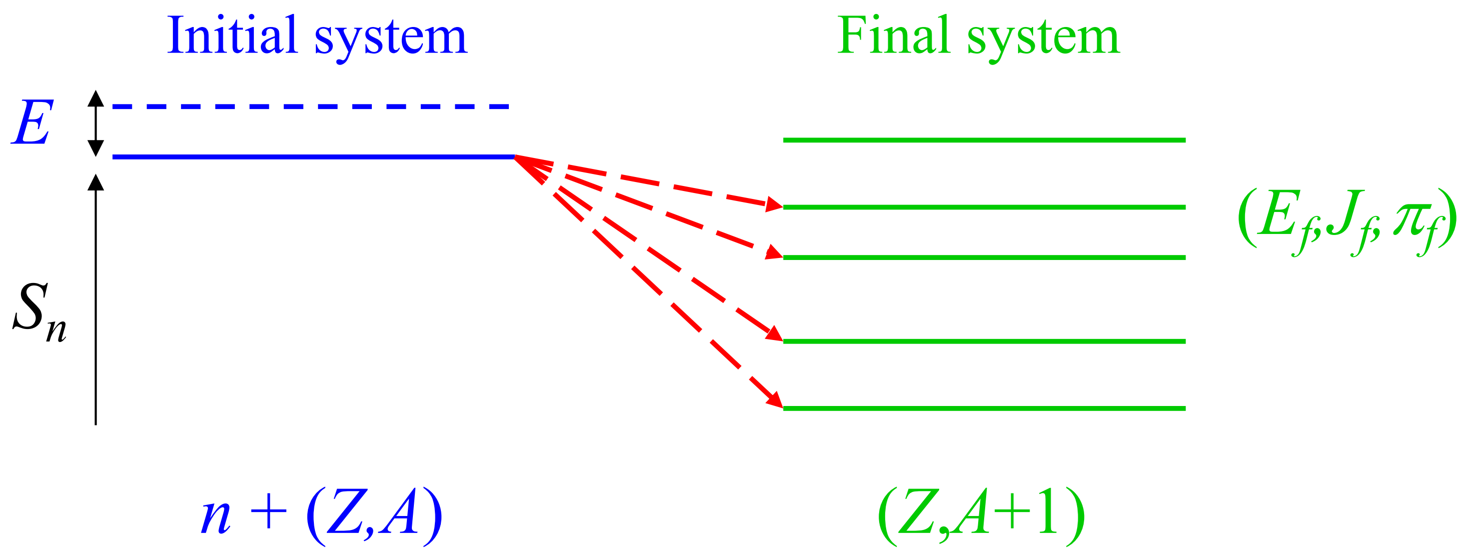


$$\sigma_{(a,b)} \propto \sum_{J,\pi} \frac{T_a(J^\pi)T_b(J^\pi)}{T_a(J^\pi) + T_b(J^\pi)}$$

T: Transmission coefficient, *i.e.* the probability to favour a given channel (***a,b***=n,p,α,γ)

Direct captures

Direct scatter of incoming neutrons into a bound state without formation of a Compound Nucleus (particularly important for light and low-S_n n-rich nuclei)

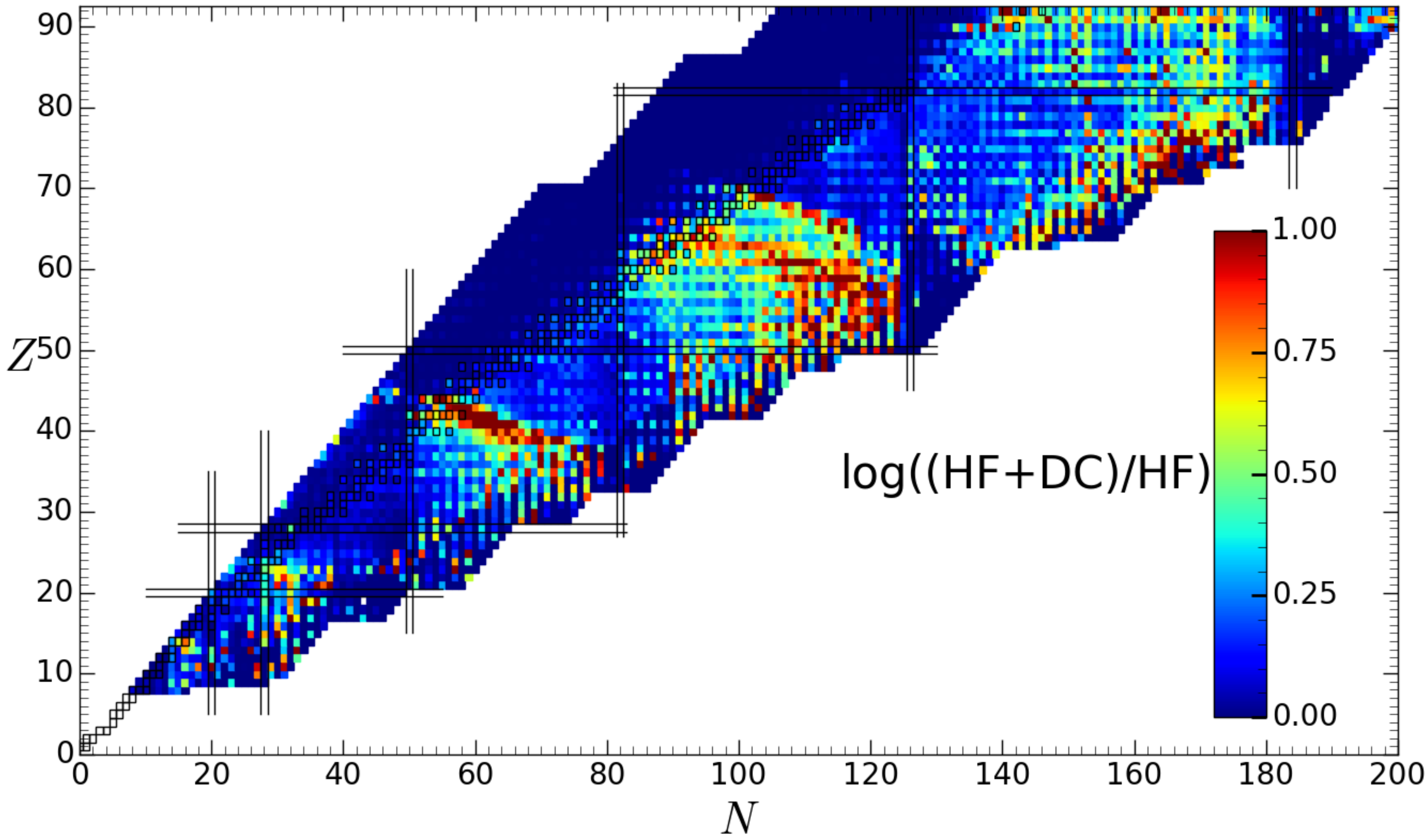


Different models exist (in particular the so-called potential model) but
Requires a detailed knowledge of

- detailed spectroscopy of low-excited states (E_f, J_f, π_f), including the spectroscopic factor of each excited state, describing the overlap between the antisymmetrized wave function of the initial system $(Z,N)+n$ and the final state f in $(Z,N+1)$
- n-nucleus interaction potential

Impact of the DC on the HF (n,γ) rates

TALYS calculation



Still many uncertainties in DC estimates (level scheme, SF, OMP…)

Some specificities of the astrophysical plasma

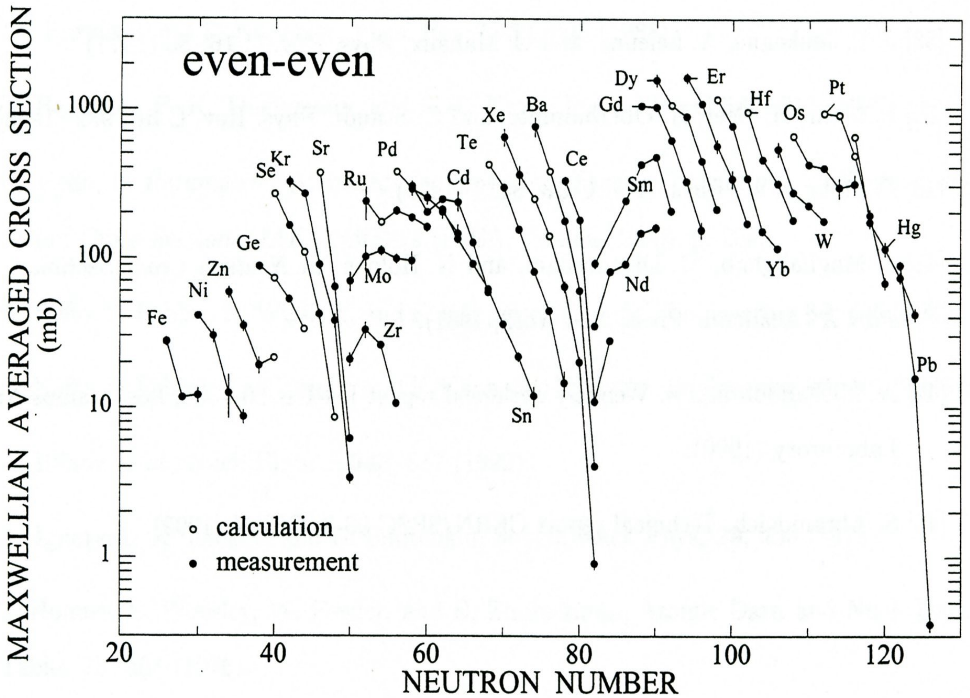
- Energy region of "almost no event" for charged-particle reactions:
  - low cross sections unreachable experimentally
- Unstable species involved:
  - limited experimental data are available
- Exotic species involved:
  - n-rich and n-deficient nuclei out of reach from experiment
- Large number of properties and nuclei involved
  - thousands of nuclei involved, tens of properties
- High-T environments:
  - thermalization effects of excited states by electron and photon interaction. Impact on reaction rates, β-decays
  - ionization effects: Impact on β-decays (bound state β-decay, continuum-$e^{-/+}$ capture); e^-- screening effects on reaction rates
- High-ρ environments (supernovae, neutron stars):

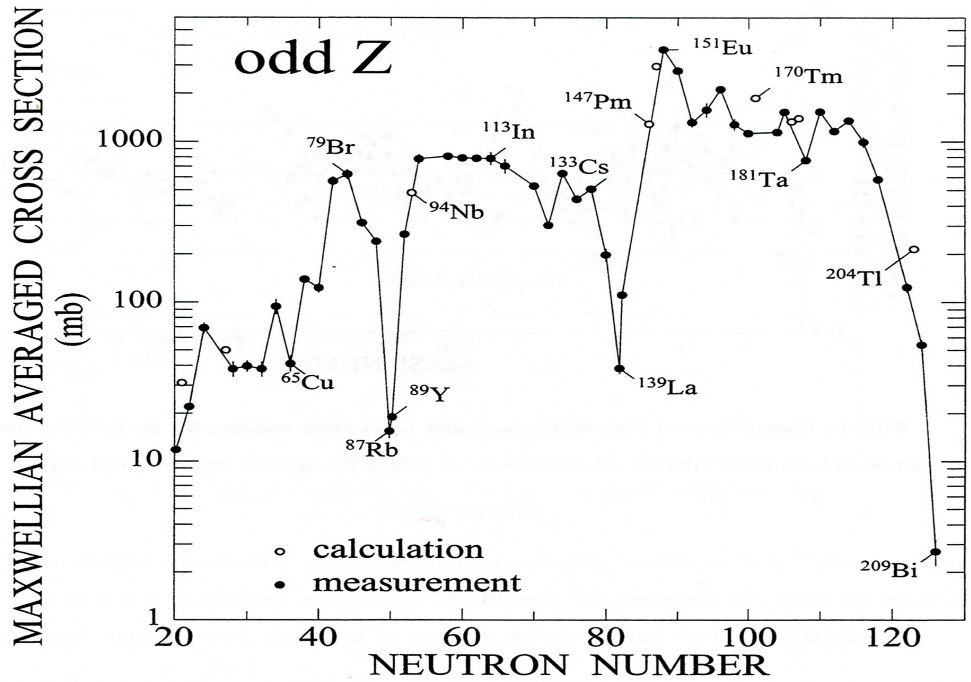
  nuclear binding understood in terms of a nuclear Equation of State (energy density and pressure of a system of nucleons as a function of matter density ρ□

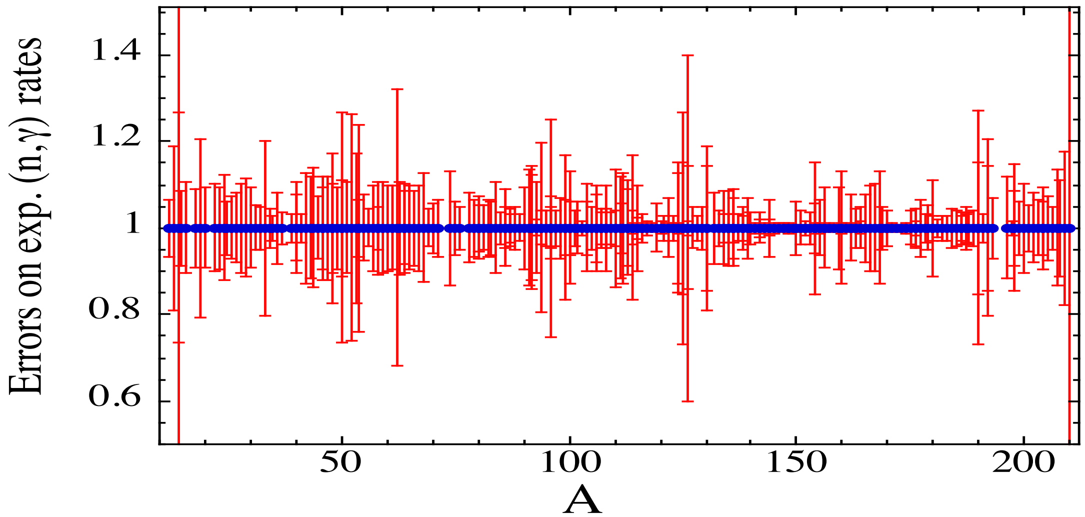
Experimental (n,γ) rates (MACS)

About 80% of the radiative neutron capture rates of relevance for the s-process are known experimentally

30 keV Maxwellian-averaged cross sections (T~3.5 10^8K)

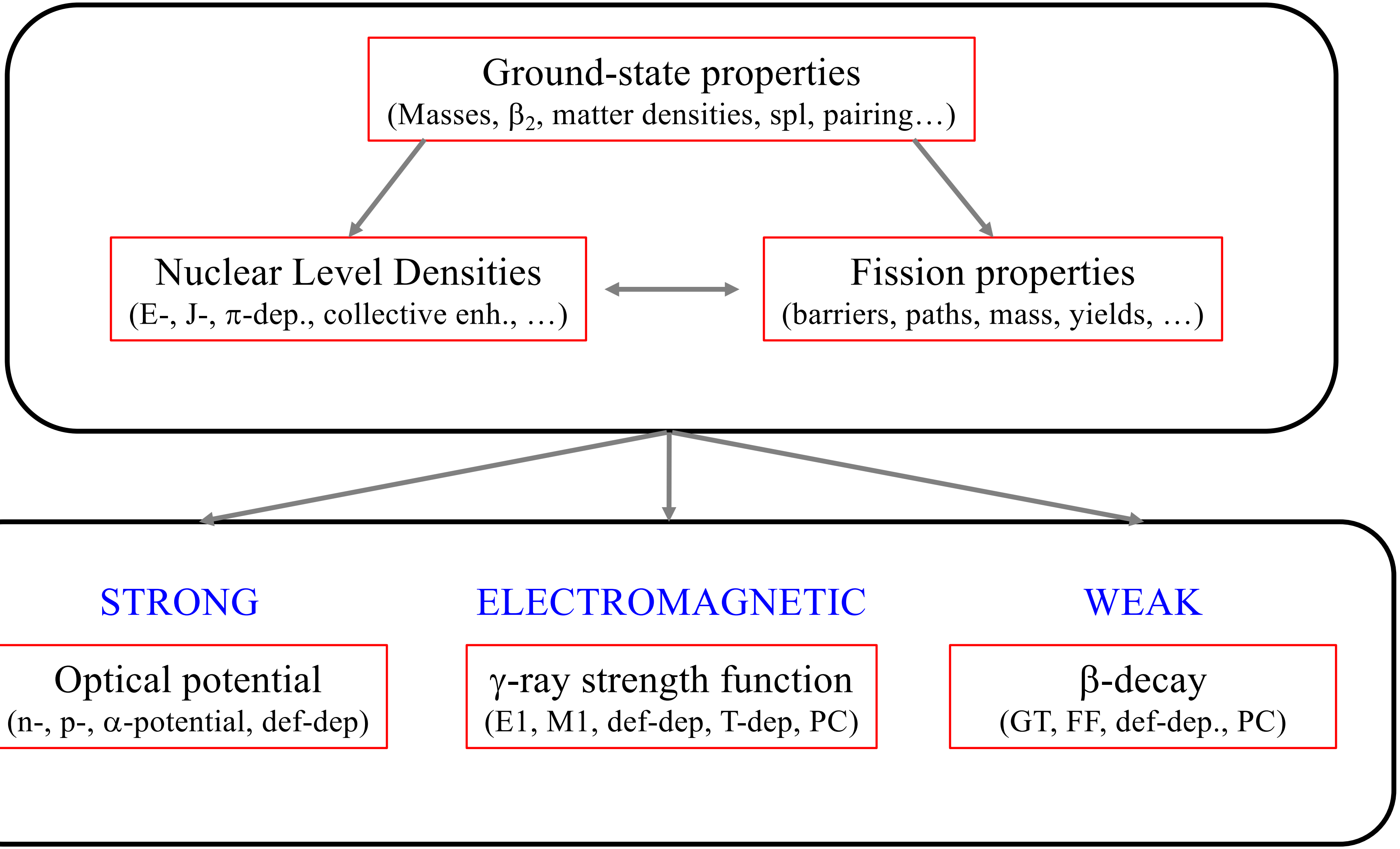




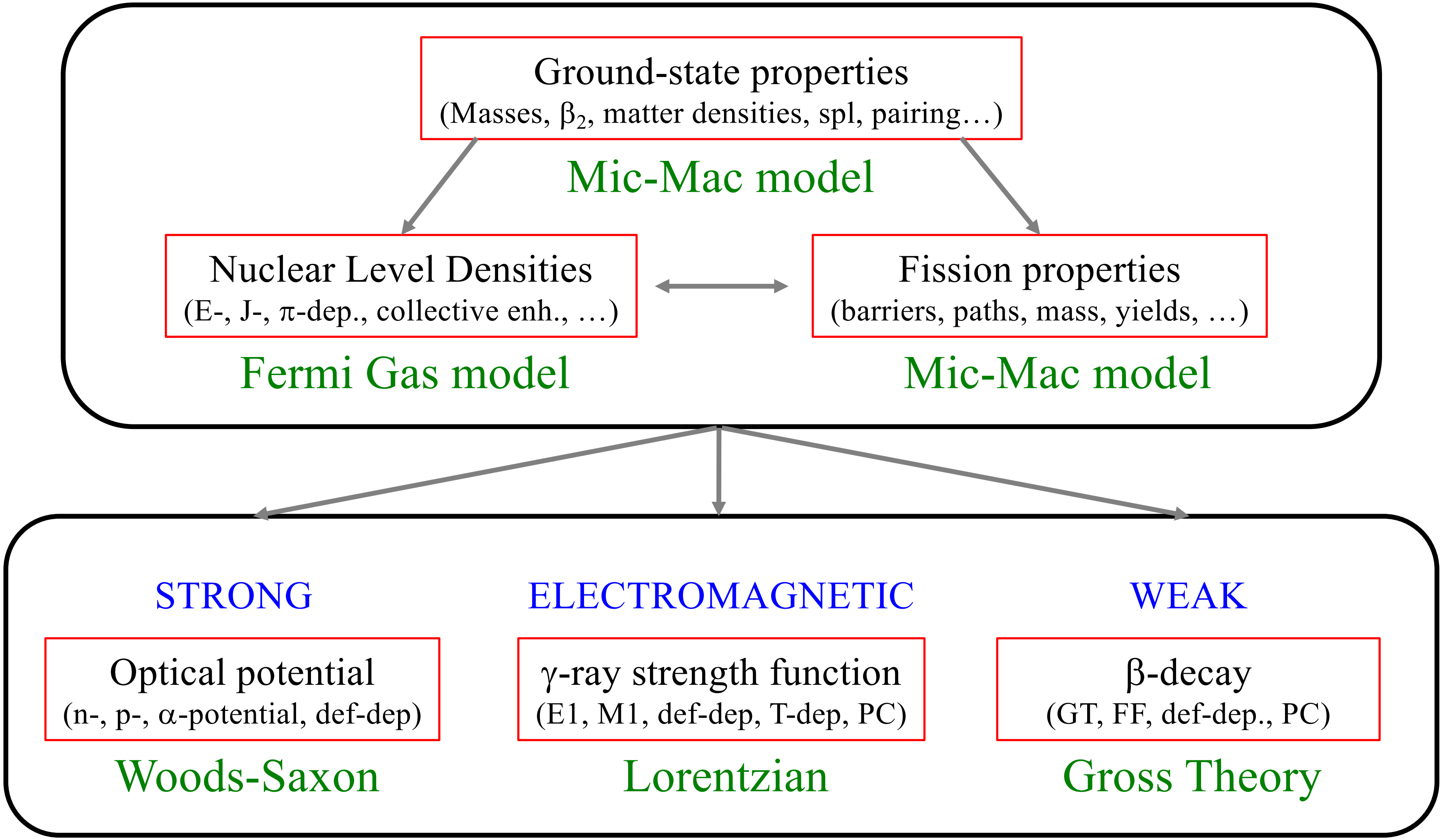


$$\langle \sigma \rangle = \frac{\langle \sigma v \rangle}{v_T}$$

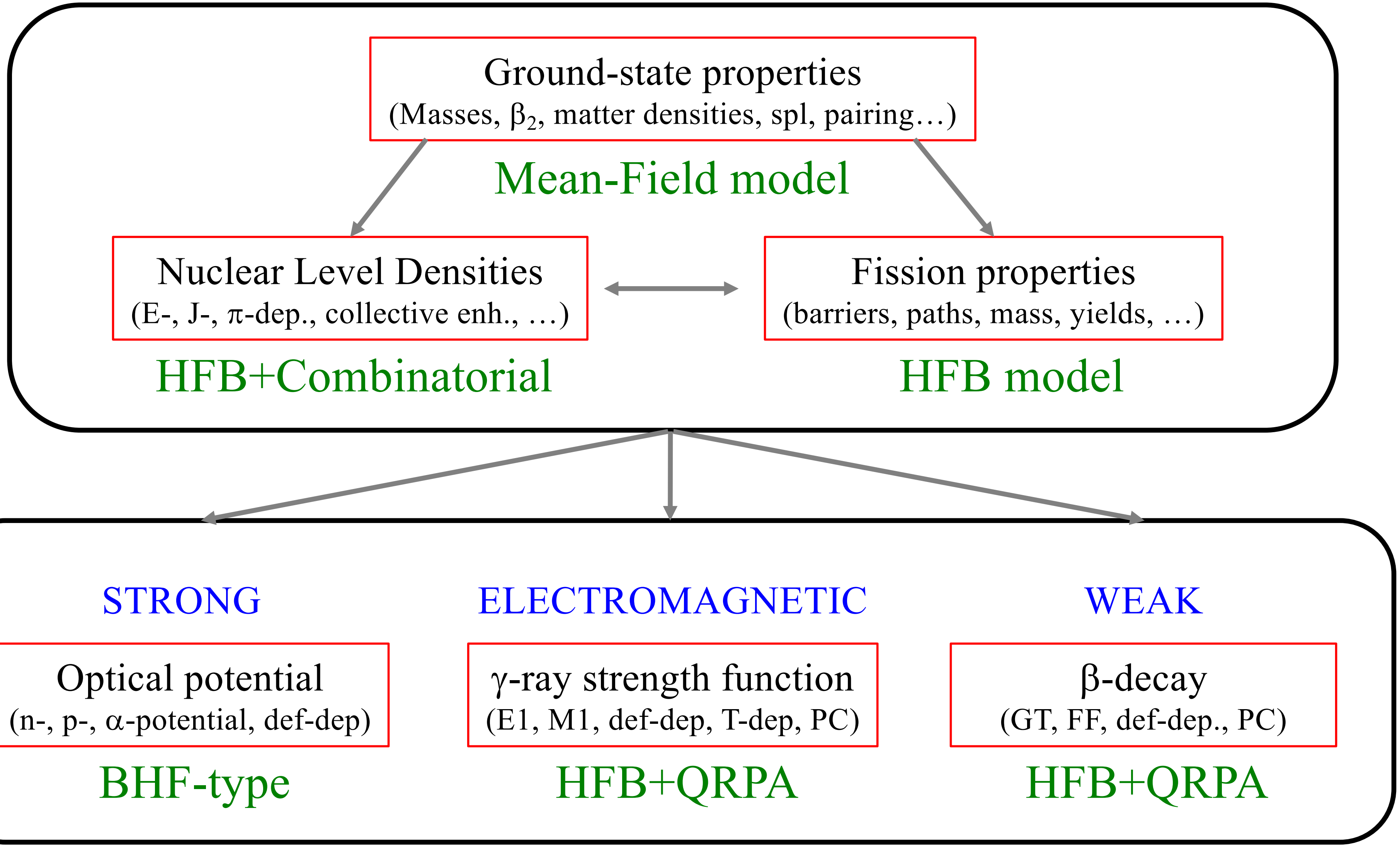
Nuclear inputs to nuclear reaction & decay calculations



Nuclear inputs to nuclear reaction & decay calculations



Nuclear inputs to nuclear reaction & decay calculations

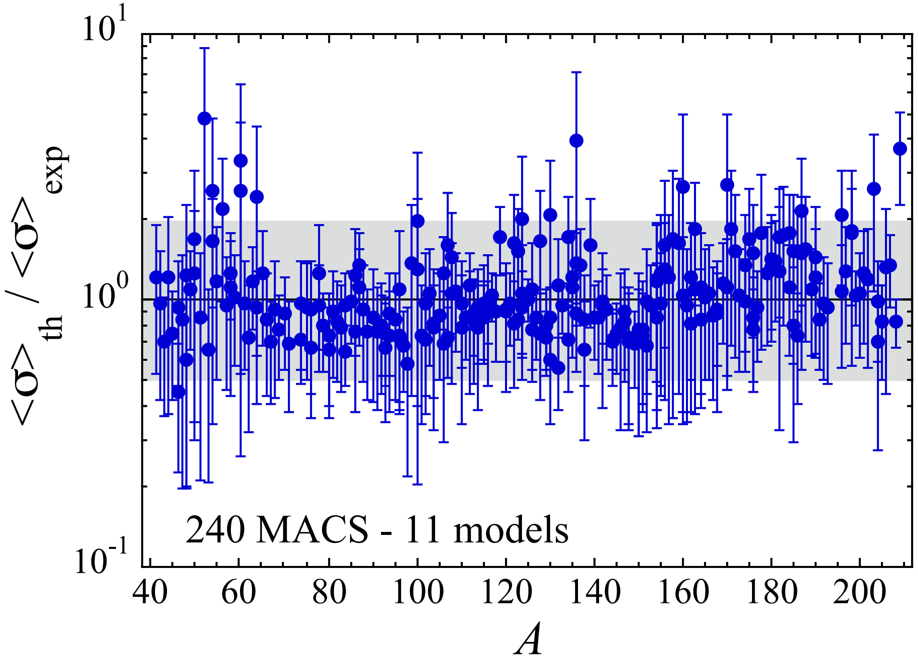


"Microscopic" approach is a necessary but not a sufficient condition !
"(Semi-)Microscopic" models must be competitive in reproducing exp. data !

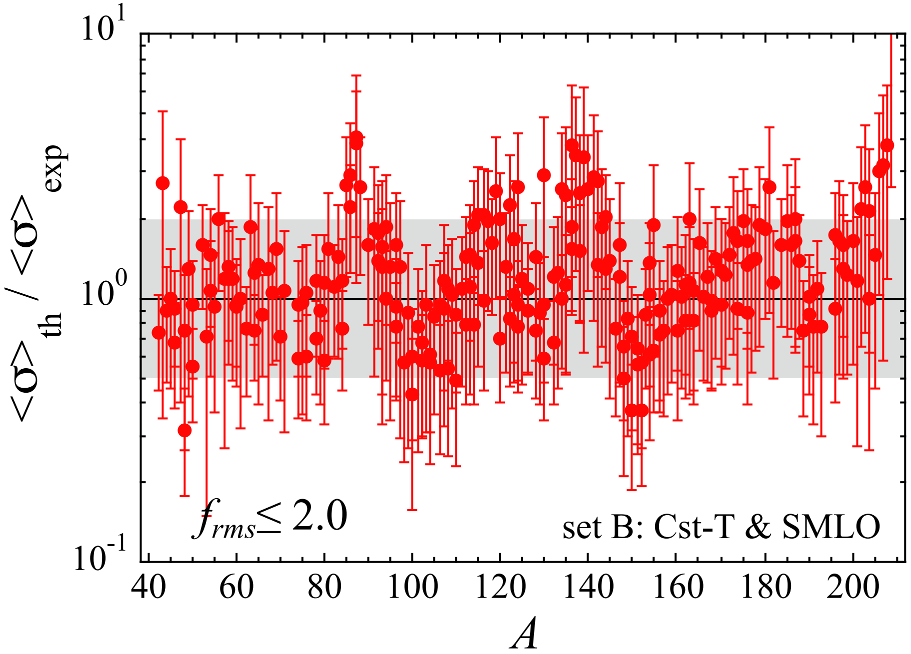
TALYS prediction of the 240 experimental MACS

$20 \leq Z \leq 83$

Correlated model uncertainties



Uncorrelated parameter uncertainties

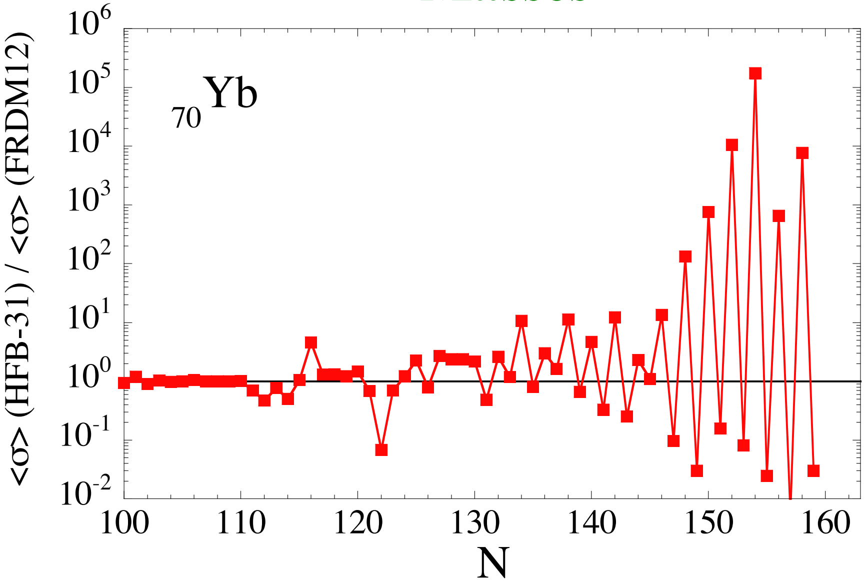


- Experimental info on *M*, NLD, PSF
- 11 different models of NLD, PSF
  Inclusion or not of DC
- All with $f_{rms} \leq 1.4 - 2.0$

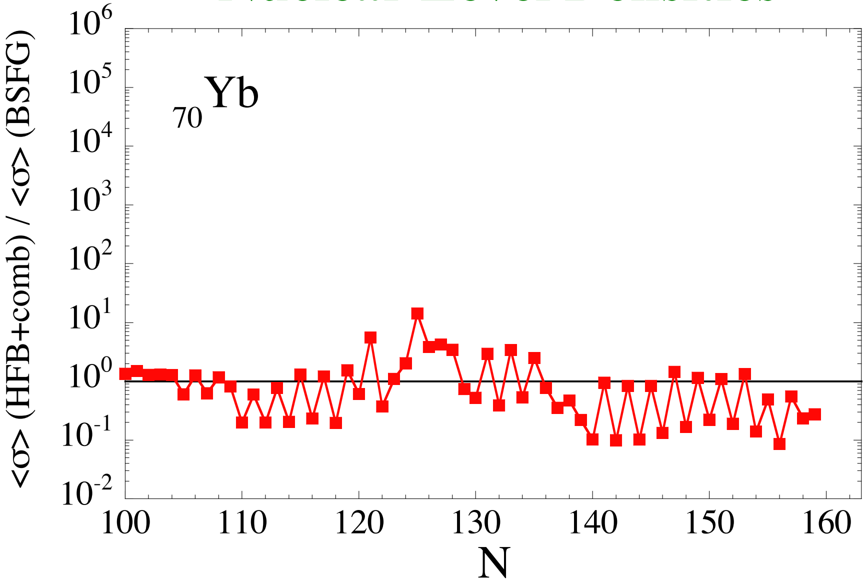
- Experimental masses
- NLD: Cst-T (E_0 & T)
- PSF: SMLO (Γ & ΔE)
- 4-parameter variation s.t. $f_{rms} \leq 2.0$

Impact of the various ingredients on the radiative neutron capture (T=10^9K, i.e E_n~100keV)

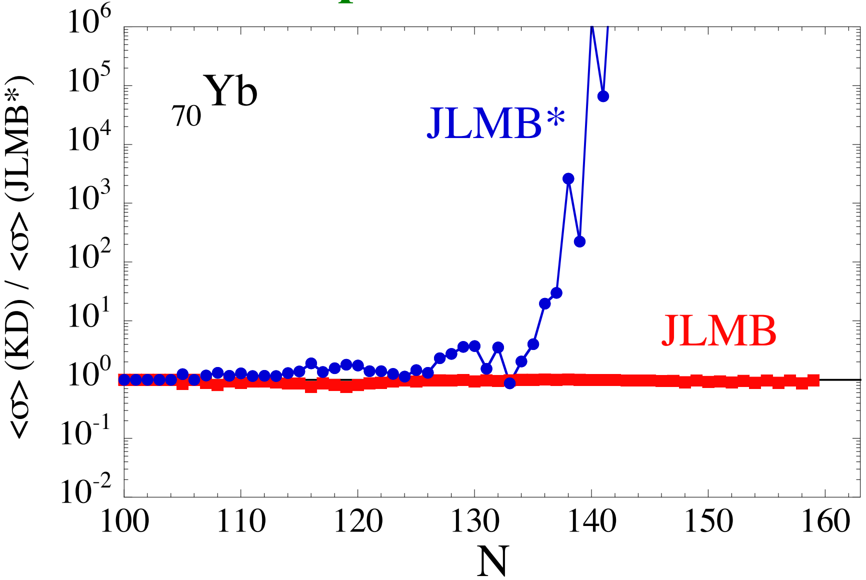
Masses



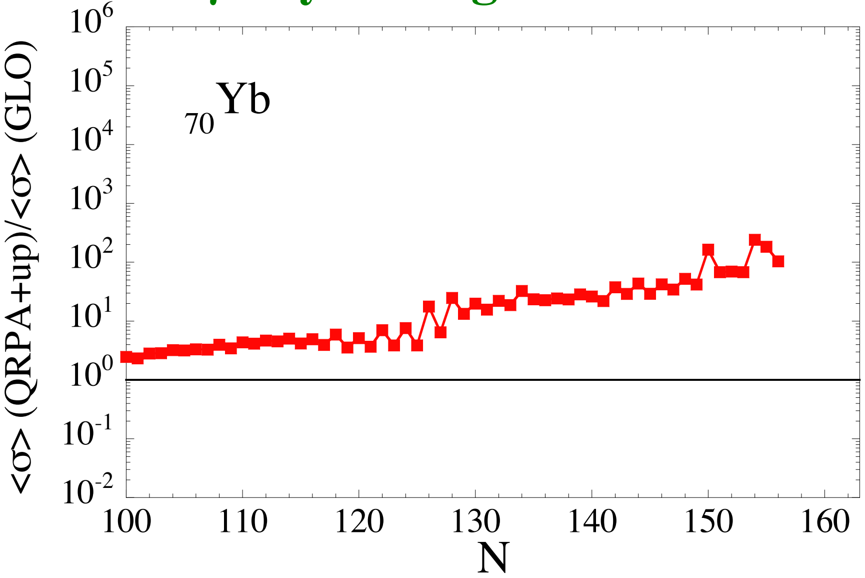
Nuclear Level Densities



Optical Potential

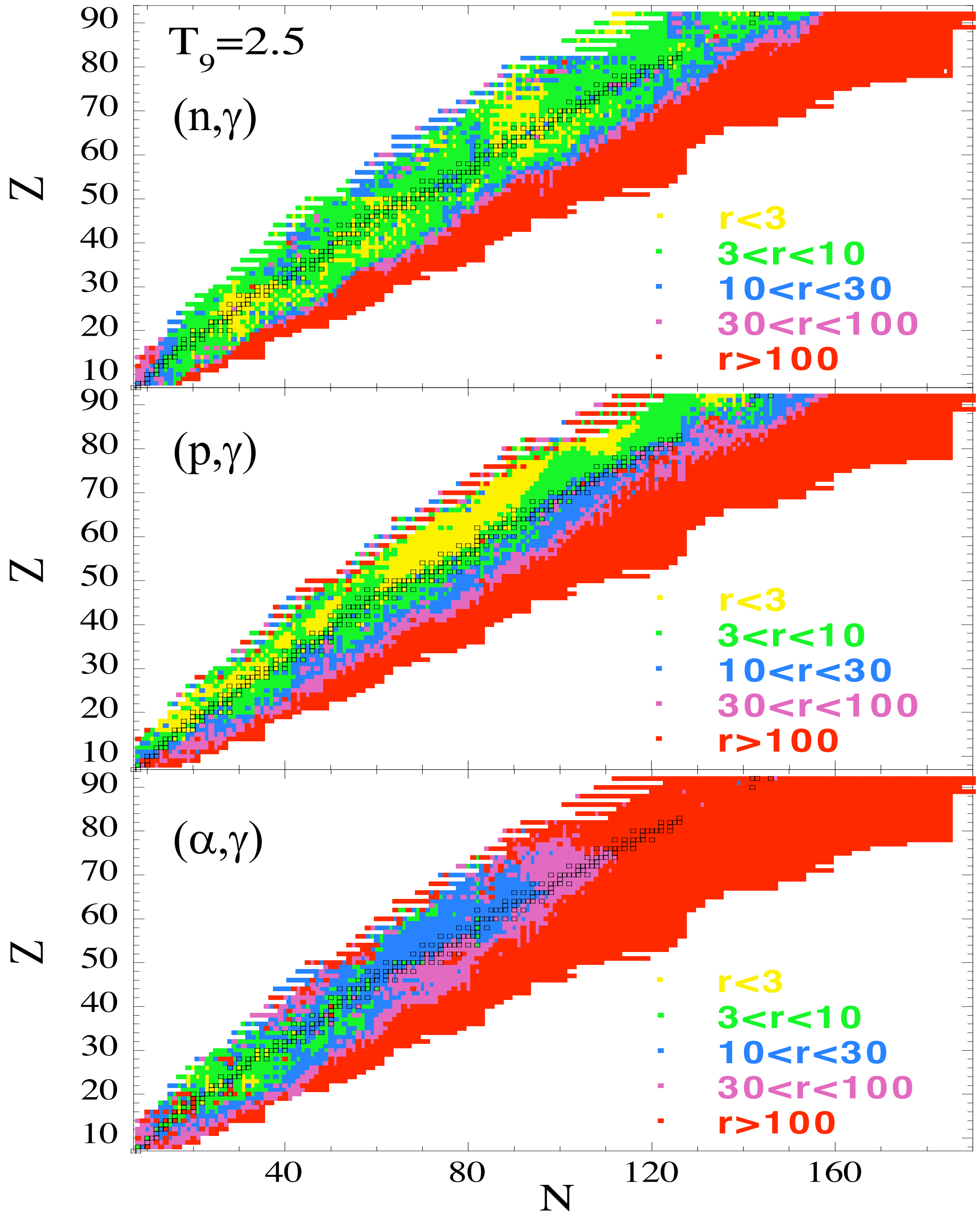


γ-ray Strength Function



Uncertainties in the prediction of the radiative capture rates

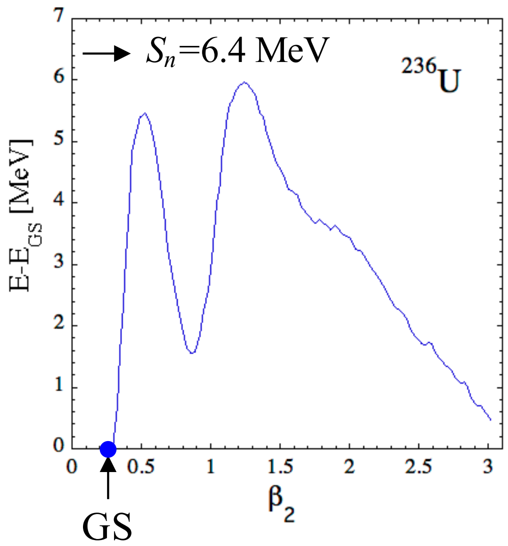
14 different combinations of Mass, NLD & PSF models in TALYS calculations

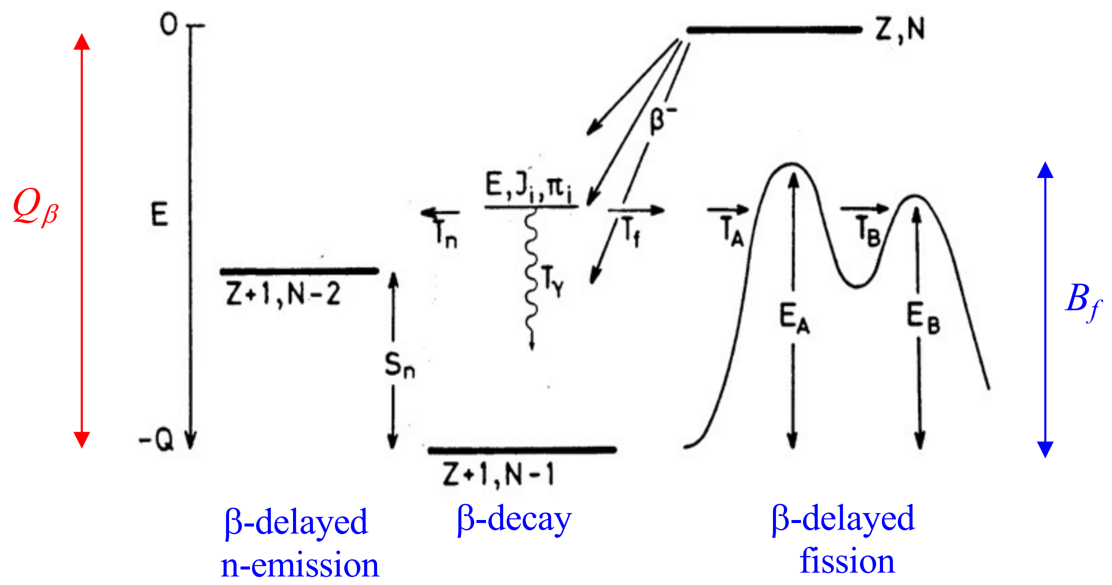


Fission probabilities and fragment distribution

Fission processes (**spontaneous, β-delayed, neutron-induced, photo**) and fission fragment distributions of relevance for estimating the

(in particular in sites like NSM)



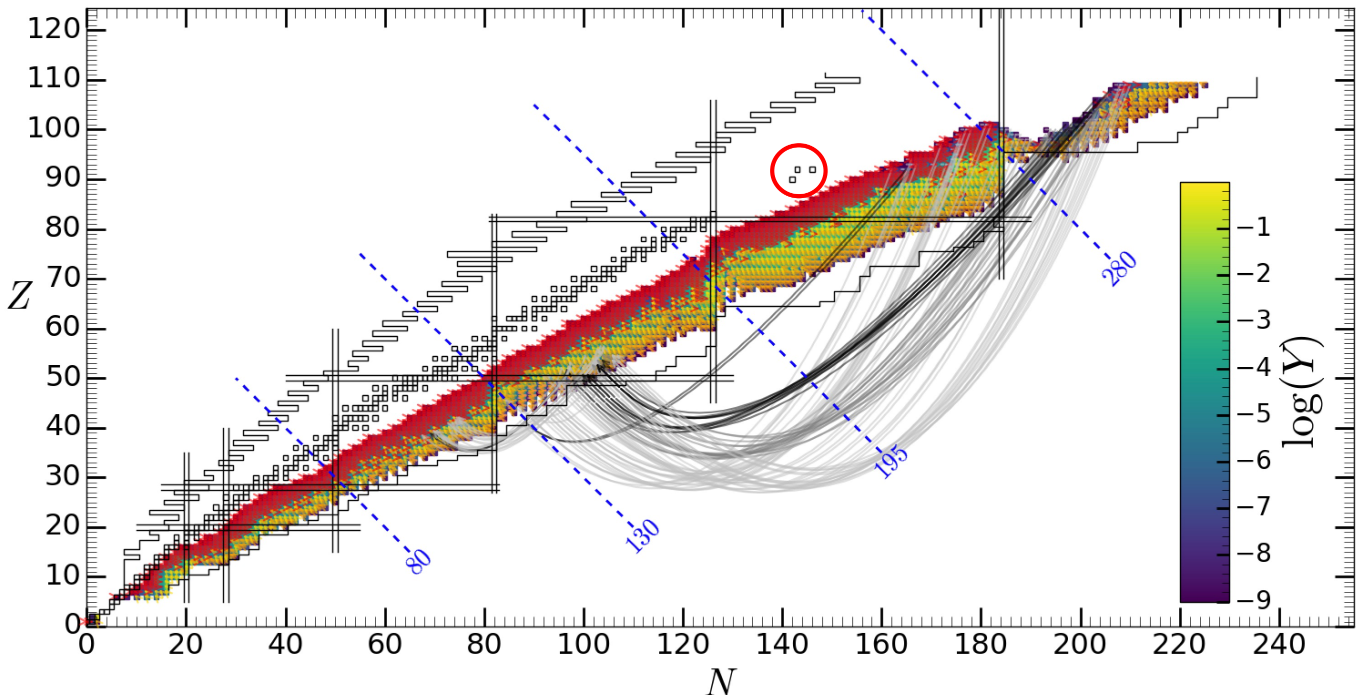


Fission probabilities and fragment distribution

Fission processes (**spontaneous, β-delayed, neutron-induced, photo**) and fission fragment distributions of relevance for estimating the

(in particular in sites like NSM)

- termination point of the r-process or production of SH
- production of light species (A~110-160) by fission recycling
- heating of the matter (affecting the light curve – large opacities)
- production of radiocosmochronometers (U, Th)



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Complicate nuclear physics associated with

- Full Potential Energy Surfaces (fission barriers/paths, collective mass, …)
- NLD at the saddle points (transition states) & in isomeric well (class-II states)
- Fission fragment distributions

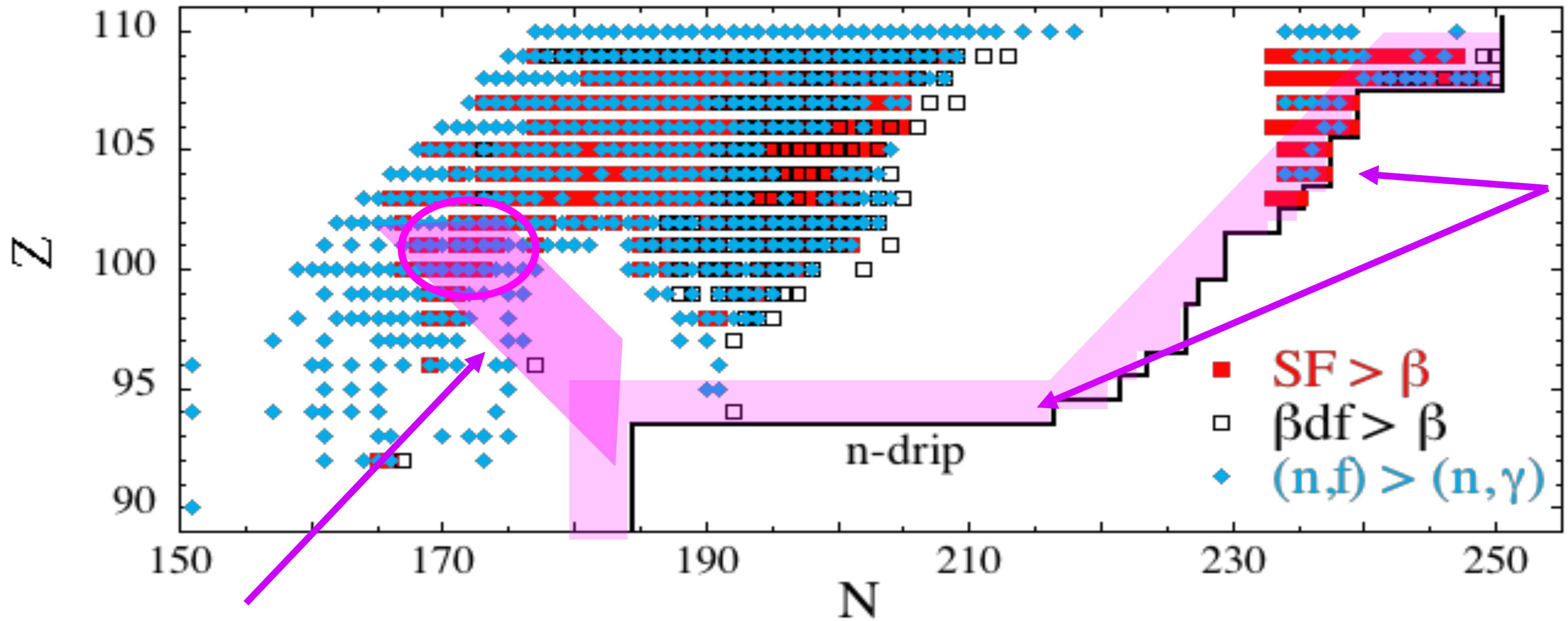
+ coupling with competitive n-, γ-, β-channels

for some 2000 heavy exotic n-rich nuclei with $90 \leq Z \leq 110$

→ Real effort needed to improve *predictions* of fission properties

(Still far from being achieved, even for U and Th !)

HFB-14 prediction of fission probabilities

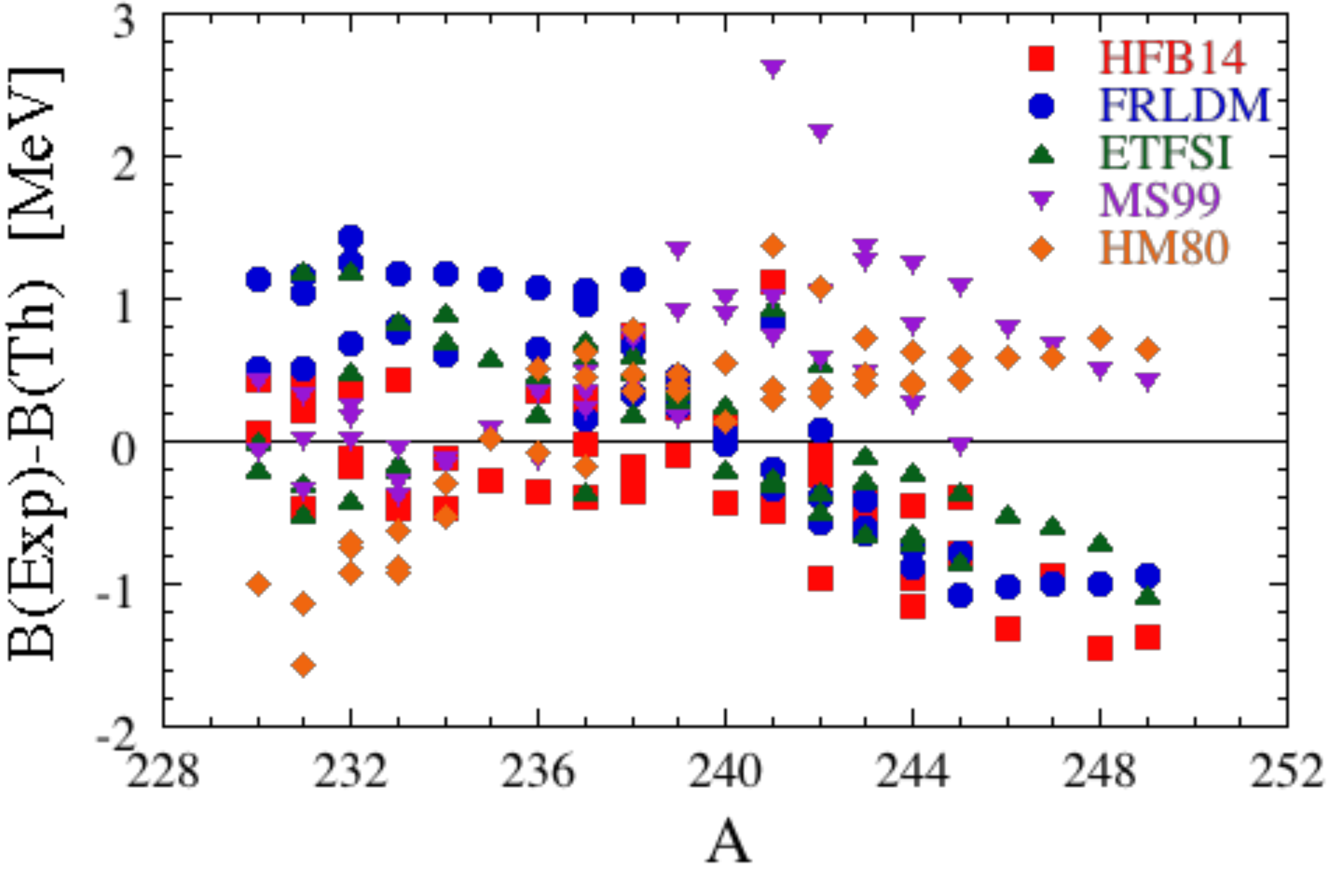


Region of interest
after n-irradiation
(A~276-280) ➡ Progenitors of A ~ 120 – 170 nuclei

Obviously, still many uncertainties affecting the prediction of the input physics necessary to estimate the (sf, βdf, nif) rates & fission fragment distribution

Description of the primary fission barriers by global models

45 « empirical » primary barriers 88 ≤ Z ≤ 96 (RIPL-3)



Model	σ [MeV]
HFB-14	0.60
FRLDM	0.81
ETFSI	0.57
MS99	0.82
HM80	0.66

Urgent need to improve the global prediction of barriers within « microscopic » models

e.g. mean-field model including l-r asymmetry & triaxial shape & long-range correlations

BSkG3: σ(M)=0.63MeV & σ(B_f)=0.33MeV Ryssens et al. (EPJA, 2023)

Fission Fragment Distribution

Fission fragment distribution plays a ***fundamental*** role, especially in scenarios where fission recycling is very efficient (NSM)

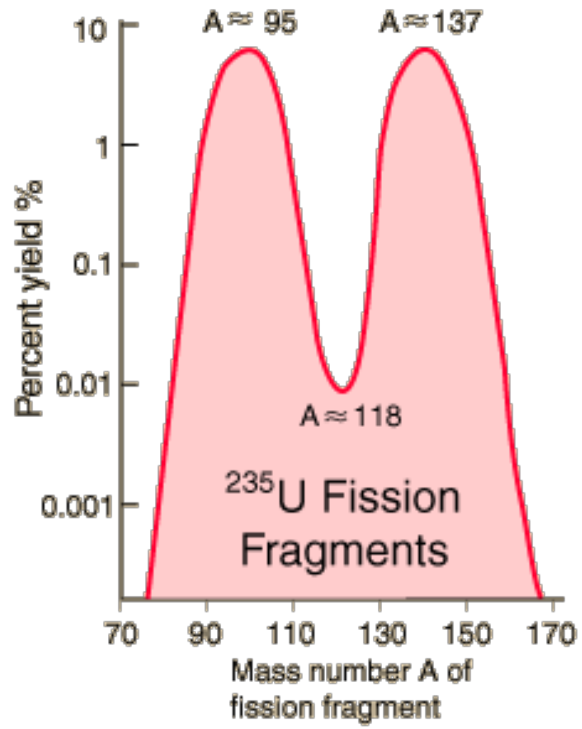
- Final r-abundance distribution ($110 \leq A \leq 170$) shaped by the FFD
- Emission of prompt neutrons that will be recaptured at late times

Many different phenomenological approaches exist, based on systematics, i.e highly-parametrized multi-Gaussian-type fits, with adjustement on available experimental FFD

→ Almost all kinds of FFD can be extrapolated for exotic nuclei !

→ Need for « serious » microscopic description of collective dynamics

(e.g time-dep. Schrödinger eq.)

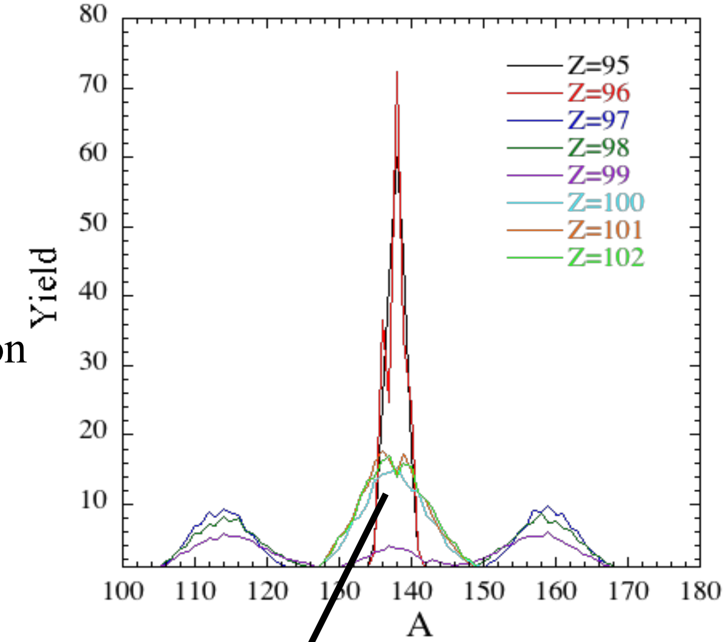


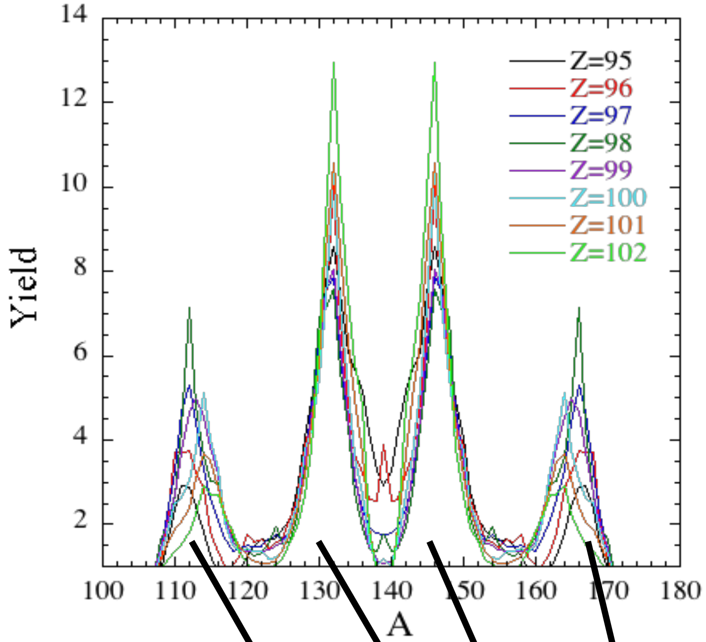
Sensitivity to the fission fragment distribution

along the *A*=278 isobar (from the *N*=184 closed shell)

GEF v1.4
K. Schmidt et al. (2013)

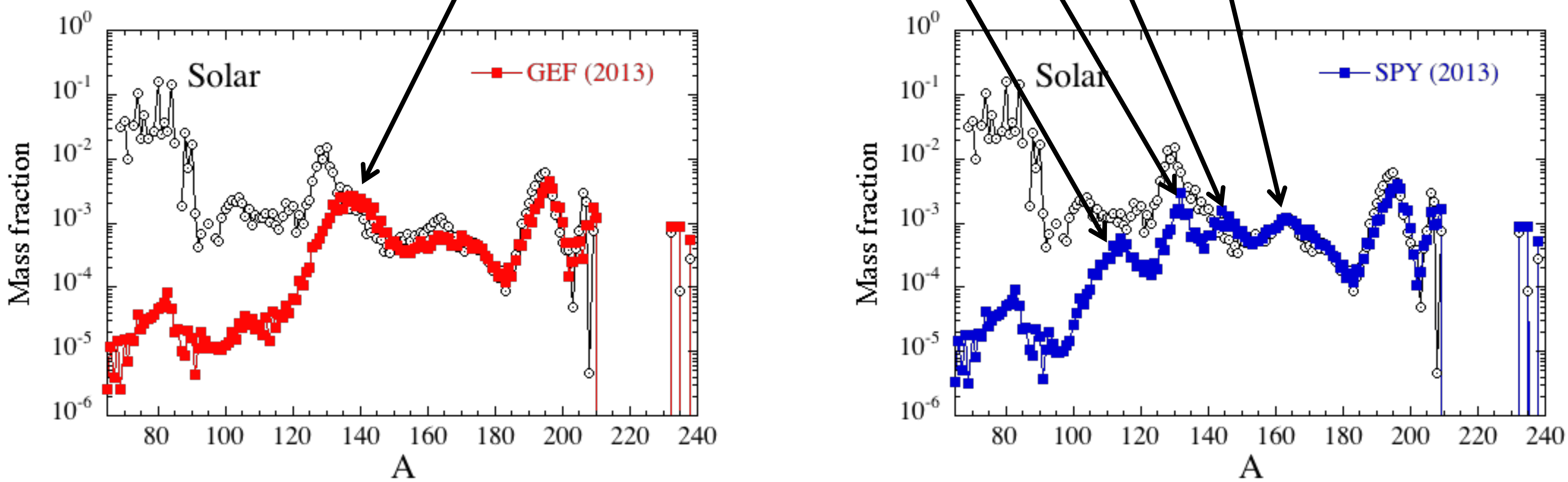
Semi-empirial mic-mac Scission Point model





SPY:
S. Panebianco et al. (2013)

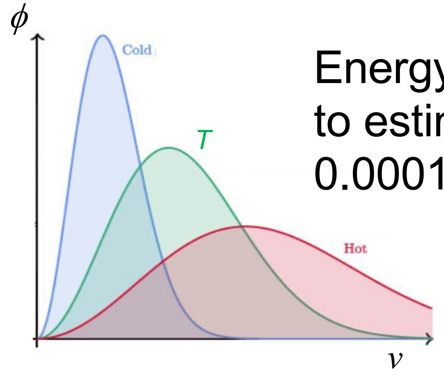
Parameter-free Scission Point model based on D1S potential energy surfaces



TALYS and the calculation of astrophysical rates

```
projectile n
element    u
mass       278
energy 1.
astro  y
astrogs n
ldmodel   5
fismodel 5
massmodel 2
strength 4
jlmomp y
radialmodel 1
alphaomp 5

racap y
```



Energy grid automatically built to estimate MA distributions for $0.0001 \le T[10^9\text{K}] \le 10$

Calculate astrophysical rates $N_A<\sigma v>^*$ and MACS for (n,γ) (→ files astrorate.tot, astrorate.g, …) on the defined *T*-grid (30 *T*: 1e5K → 1e10K)

astrogs = y → assume targets in GS only
estimate $N_A<\sigma v>$ (not $N_A<\sigma v>^*$)
(by default astrogs=n)

Microscopic inputs based on the **Skyrme** HFB models

Possible inclusion of Direct Capture component

TALYS and the calculation of astrophysical rates

```
projectile n
element    u
mass       278
energy 1.
astro  y
astrogs n
ldmodel  6
fismodel 5
massmodel 3
strength 8
strengthM1 8
jlmomp y
radialmodel 2
alphaomp 5

racap y
```

astro y → Calculate astrophysical rates $N_A<\sigma v>^*$ and MACS for (n,γ) (→ files astrorate.tot, astrorate.g, …) on a defined *T*-grid (30 T: 1e5K → 1e10K)

astrogs = y → assume targets in GS only
estimate $N_A<\sigma v>$ (not $N_A<\sigma v>^*$)
(by default astrogs=n)

ldmodel, massmodel, strength, strengthM1, jlmomp, radialmodel, alphaomp → Microscopic inputs based on the Gogny-HFB models

racap y → inclusion of Direct Capture component

Conclusions

Nuclear physics is a necessary but a not sufficient condition for Nuclear Astrophysics

Still many open nuclear physics questions

The exact role of nuclear physics in Astrophysics will remain unclear as long as the astrophysics sites and the exact nuclear mechanisms of relevance are not fully under control

Conclusions : still many open Nuclear Physics questions for Astrophysics

- **Fundamental role of experiments** (masses, β-decays, cross sections, nuclear ingredients, ...) though *mainly to adjust/guide models*
- **Nuclear inputs to the reaction model**
  - GS properties: masses (correlations - GCM, odd-nuclei)
  - Fission: fission paths, NLD at the saddle points, FFD
  - E1/M1-strength function: GDR tail, PR, $\varepsilon_\gamma=0$ limit, T-dep, PC
  - Nuclear level Densities: pairing, shell and collective effects
  - Optical potential: the low-E isovector imaginary component, the α-nucleus potential far below the Coulomb barrier
- **The reaction model**
  - CN vs Direct capture for low-S_n nuclei
- **The β-decay rates**
  - Forbidden transitions, deformation effects, odd-nuclei, PC

We are still far from being capable of estimating ***reliably*** the neutron capture, β-decay and fission properties of exotic nuclei

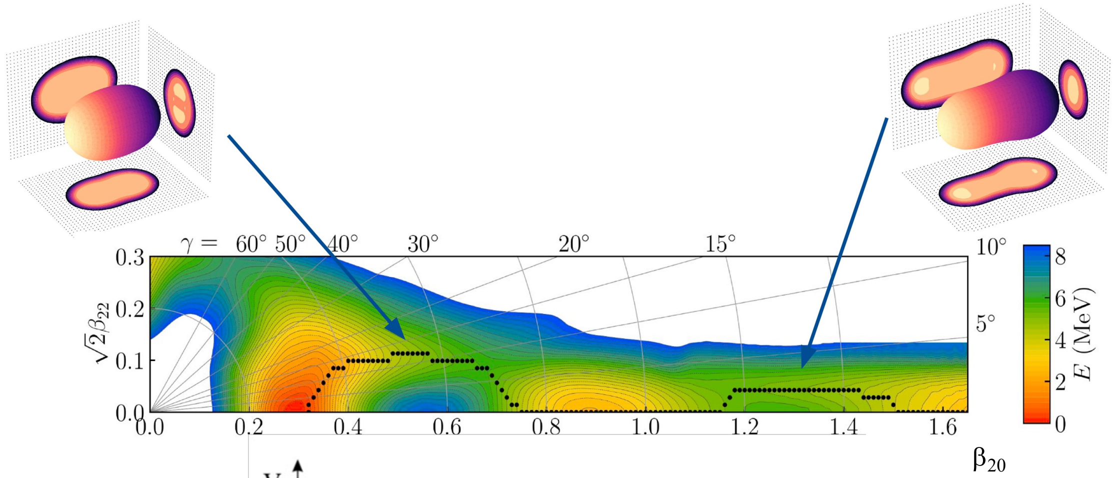
Open POST-DOC Position (2y) at IAA – ULB on Fission

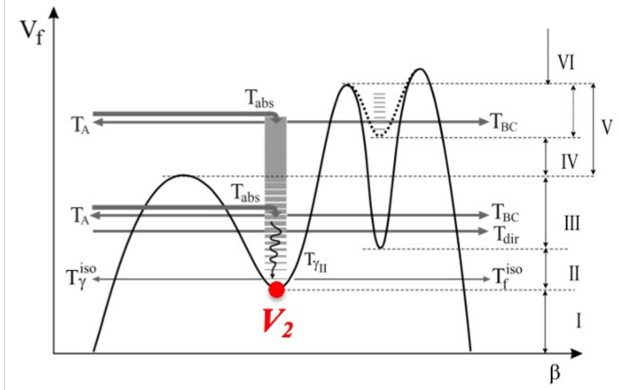
- Analysis of BSkG3 PES
  → fission path, collective mass, NLD at saddle points, ..

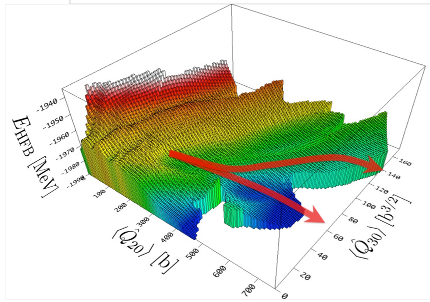
- Calculation of sf, nif, βdf
  → TALYS calculation of the fission transmission

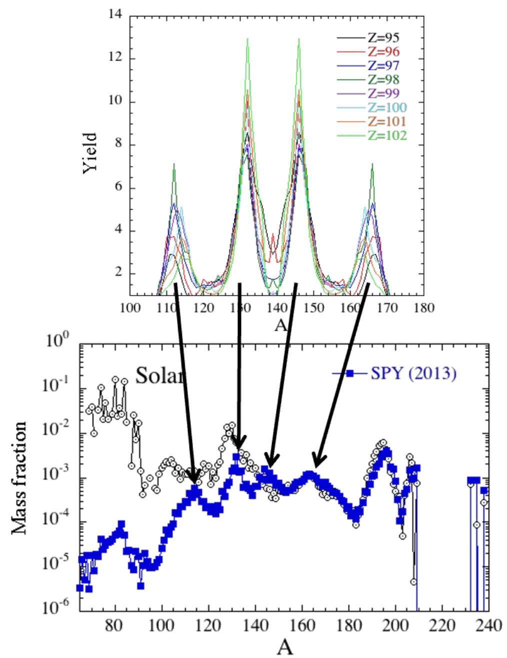
- Calculation of fission yields
  → TALYS calculation of the fission transmission

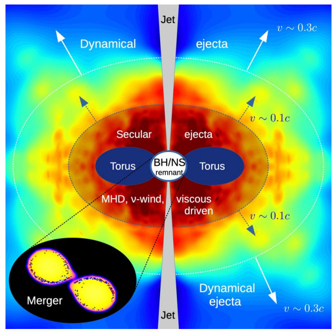
- Application to the r-process in state-of-the-art NSM models











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