Predicting neutron-induced reactions on short-lived nuclei

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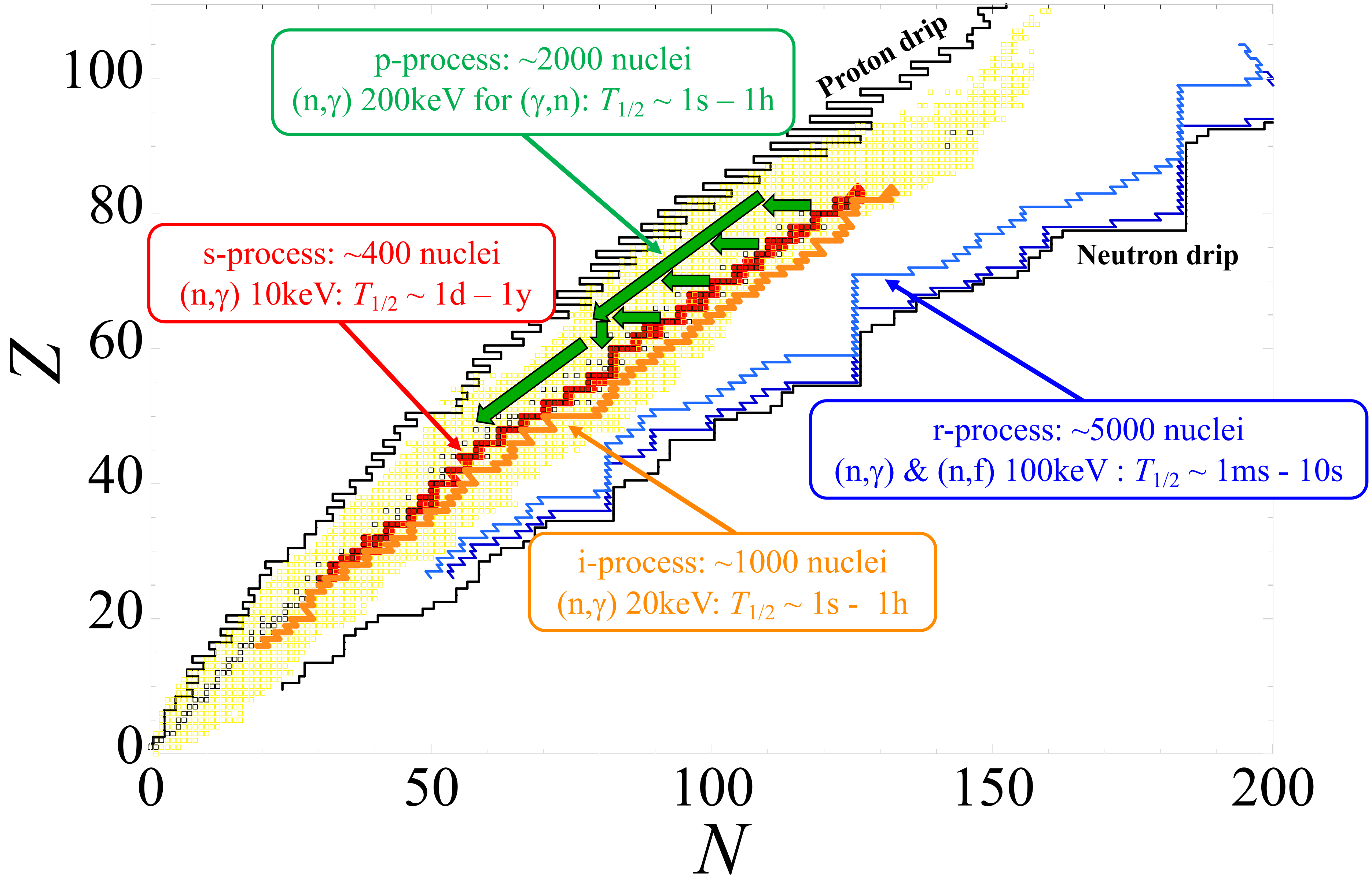
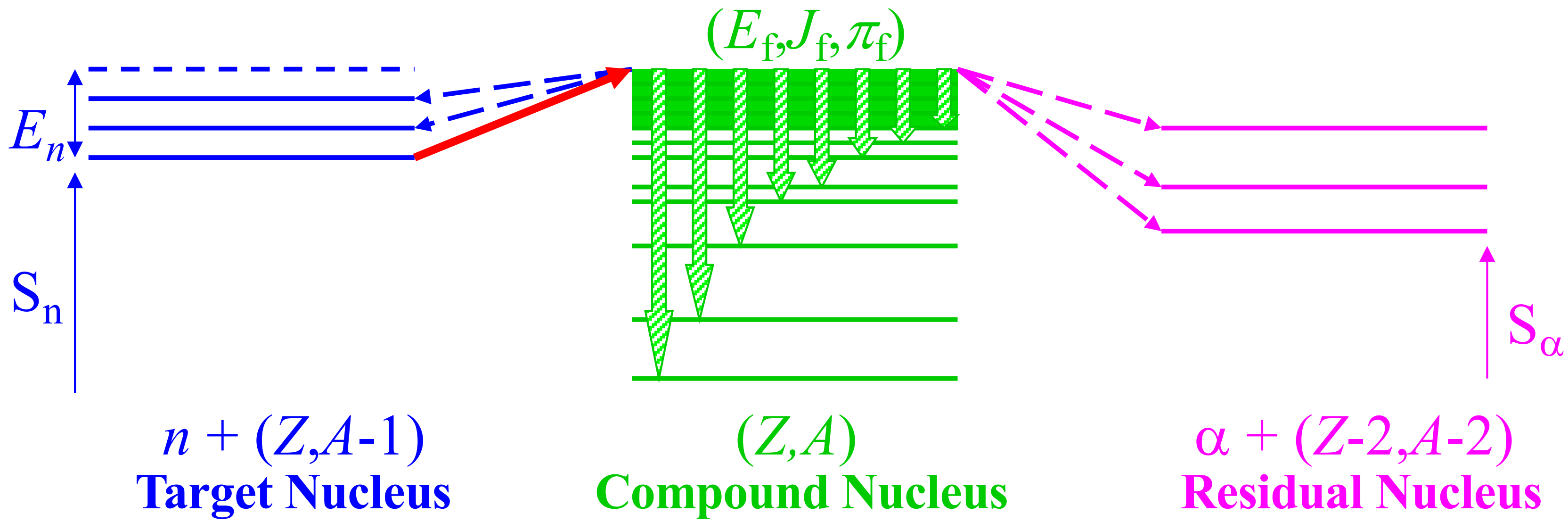
Neutron-induced reaction on short-lived nuclei for nucleosynthesis



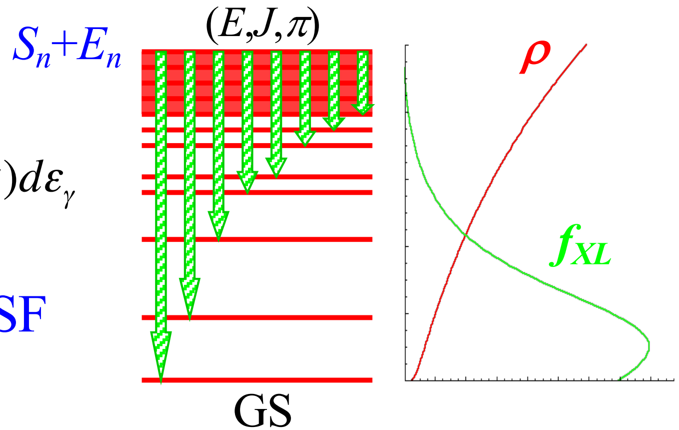
Almost no direct experimental data → Theory needs to fill the gaps

Hauser-Feshbach model for radiative neutron capture reactions



$$\sigma_{(n,\gamma)} \propto \sum_{J,\pi} \frac{T_n(J^\pi)T_\gamma(J^\pi)}{T_n(J^\pi)+T_\gamma(J^\pi)} \approx \sum_{J,\pi} T_\gamma(J^\pi) \quad \text{since } T_n(J^\pi) >> T_\gamma(J^\pi)\text{: } E_n \sim \text{keV}$$

$$T_\gamma = \sum_{J^\pi XL} \int_0^{S_n+E_n} 2\pi\varepsilon_\gamma^{2L+1} f_{XL}(\varepsilon_\gamma)\rho(S_n+E_n-\varepsilon_\gamma, J, \pi)d\varepsilon_\gamma$$

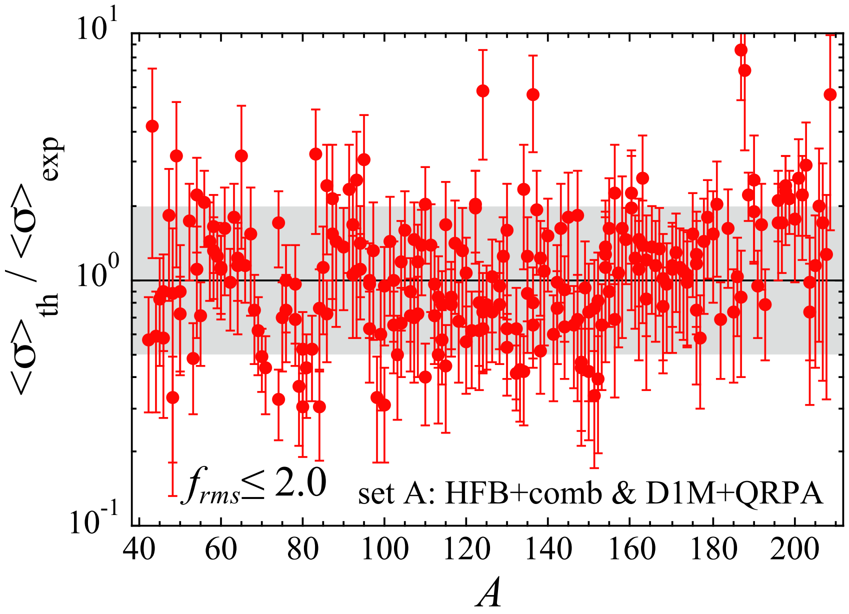


Nuclear astrophysics apps require NLDs & GSF for ~ 8000 nuclei

TALYS prediction of the 240 experimental MACS

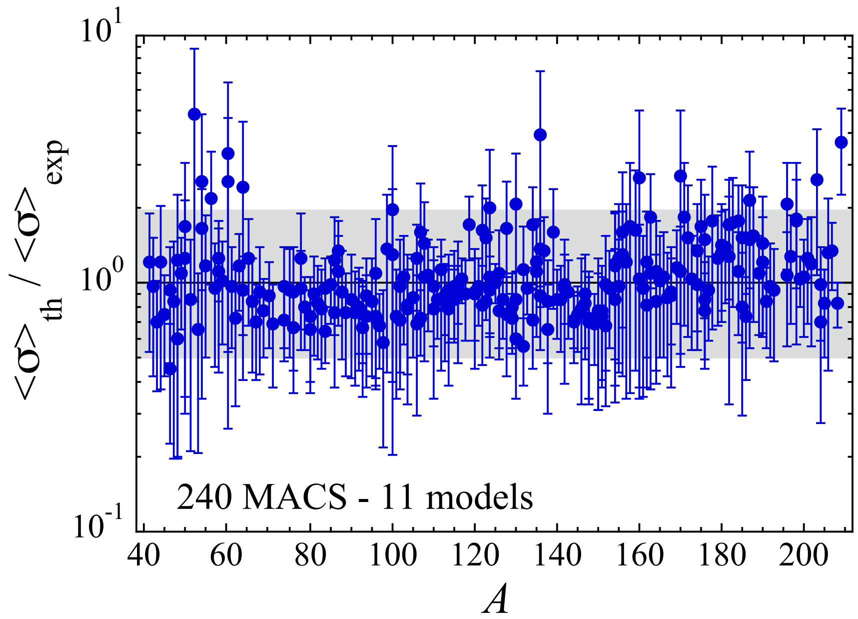
$20 \leq Z \leq 83$

Uncorrelated parameter uncertainties



- Experimental masses
- NLD: HFB+Comb (α & δ)
- PSF: D1M+QRPA ($\Delta\Gamma$ & ΔE)
- BFMC: 4-parameter var. s.t. $f_{rms} \leq 2.0$

Correlated model uncertainties



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

$$f_{rms} = \exp\left[\frac{1}{N_e}\sum_{i=1}^{N_e}\ln^2\frac{\langle\sigma\rangle_{th,i}}{\langle\sigma\rangle_{exp,i}}\right]^{1/2}$$

S. Martinet et al. Astronomy and Astrophysics 684, A8 (2024)

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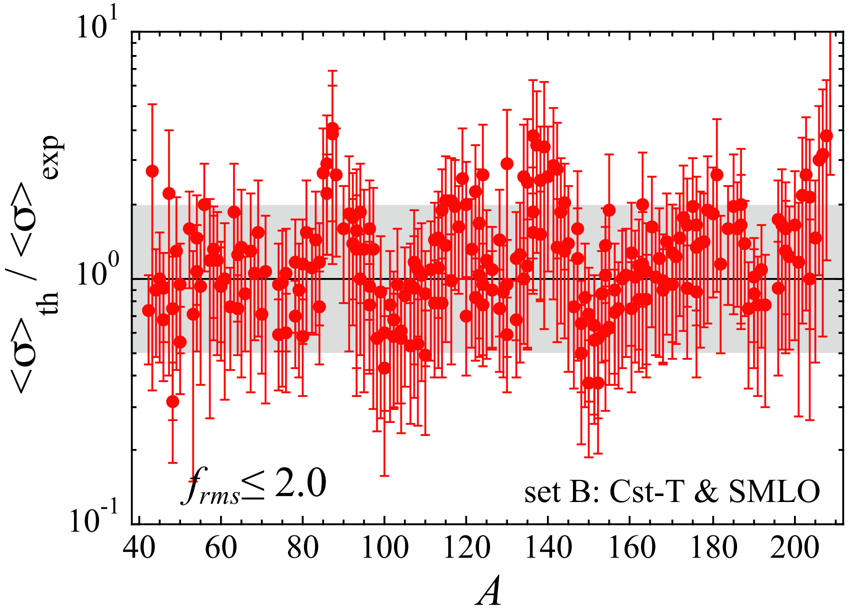

- Experimental masses
- NLD: Cst-T (E_0 & T)
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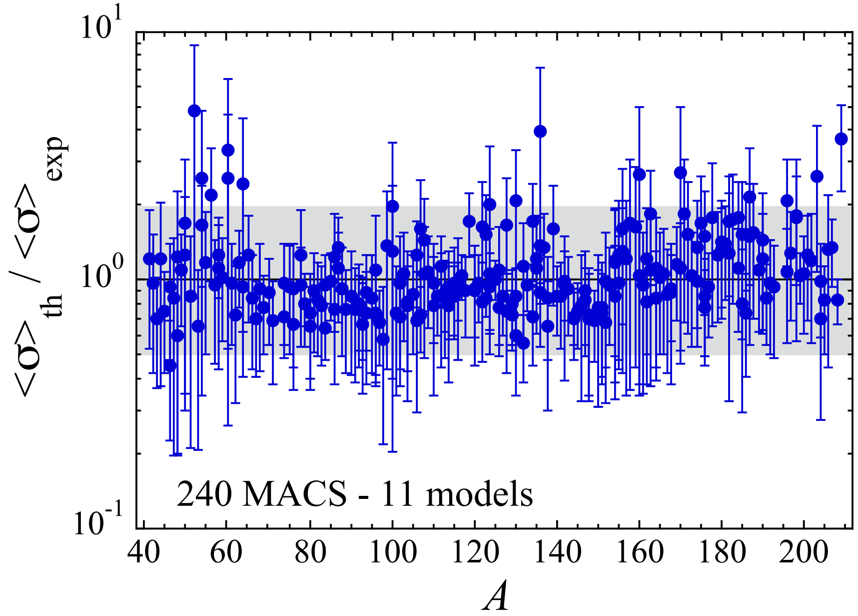

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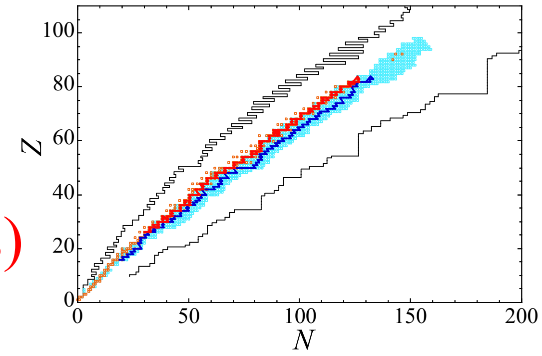
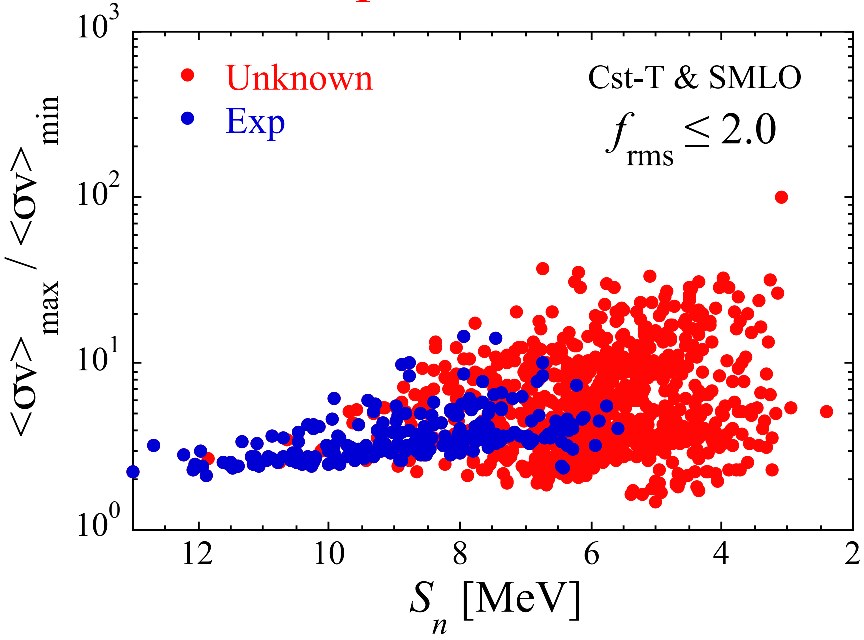
Impact of NLD/PSF uncertainties on (n,γ) MACS

$14 \leq Z \leq 98$: 240 exp + 868 unknows ($T_{1/2}$>1s)



Uncorrelated parameter uncertainties



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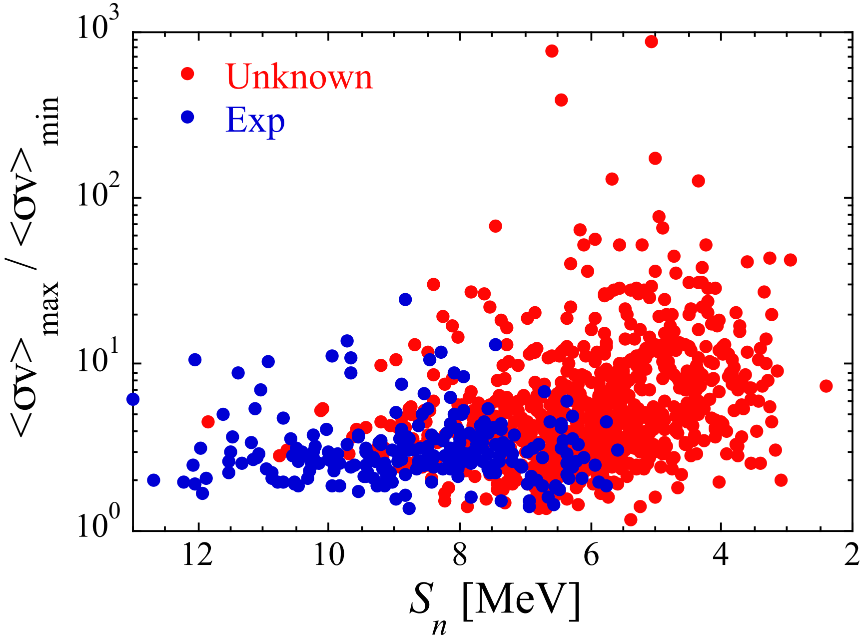

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Uncorrelated Parameter Uncertainties ~ Correlated Model Uncertainties

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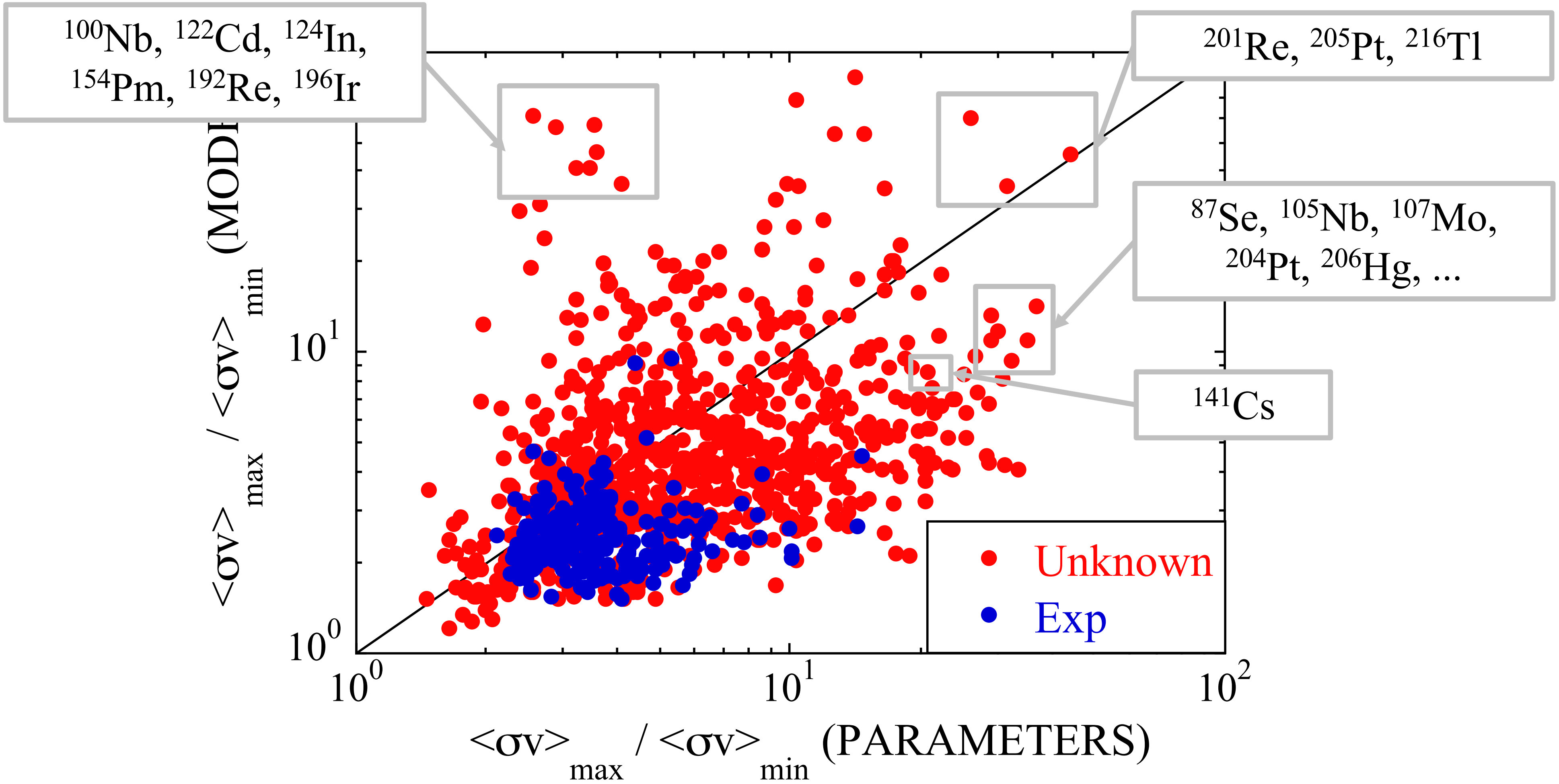

Uncorrelated Parameter Uncertainties ~ Correlated Model Uncertainties

Same order of magnitude, BUT individually can be very different !!

Impact of NLD/PSF uncertainties on the (n,γ) MACS

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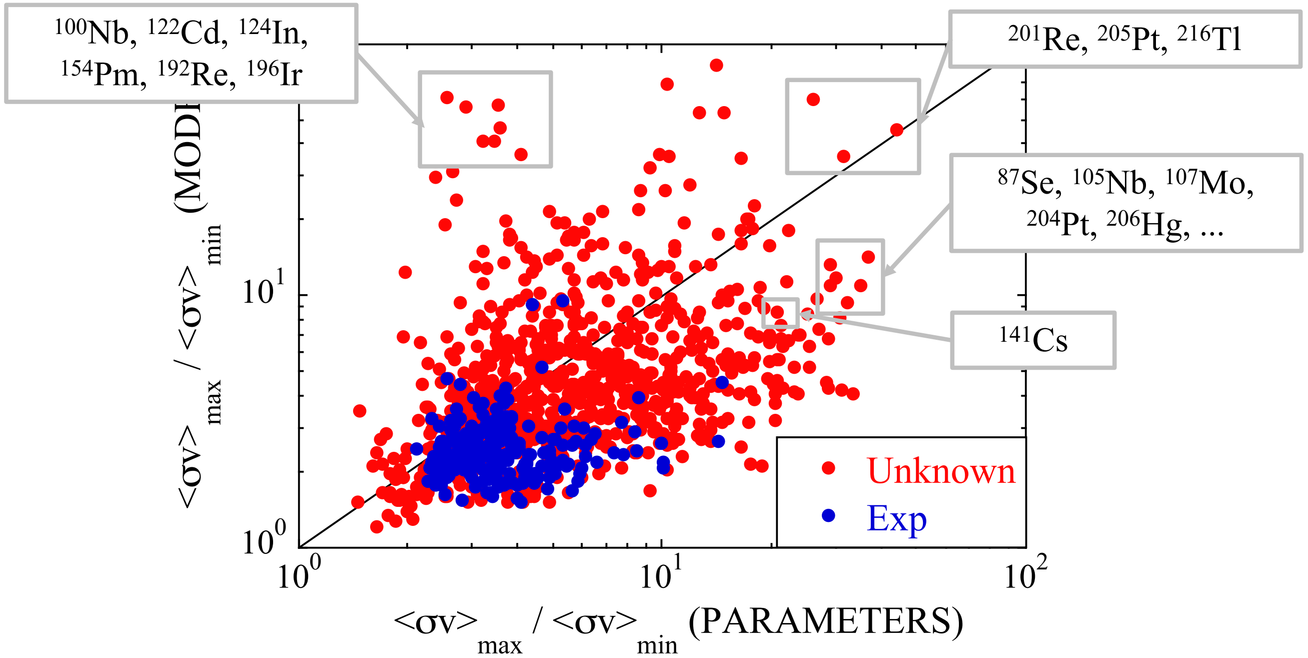
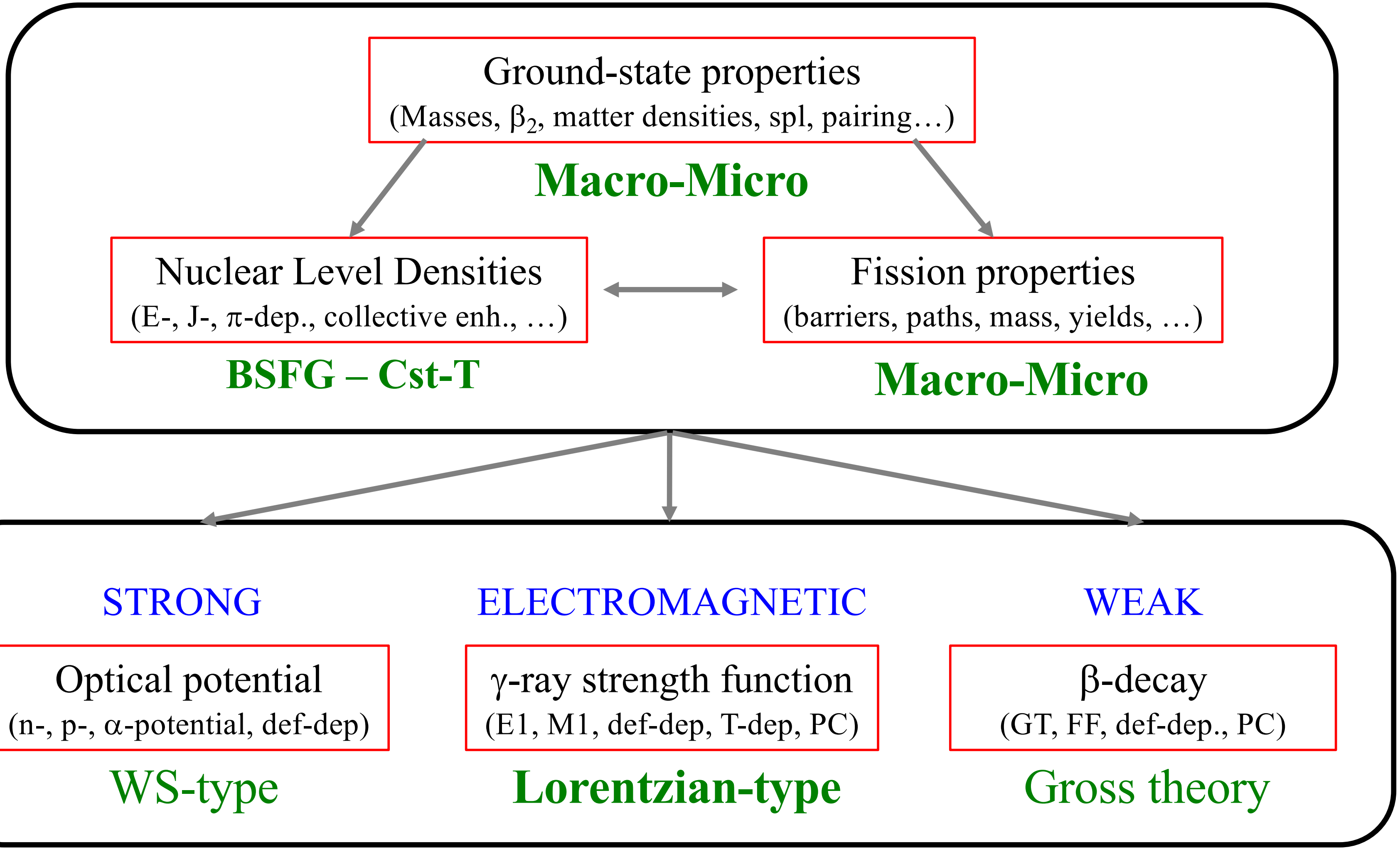


Reduction of the model & parameter uncertainties through

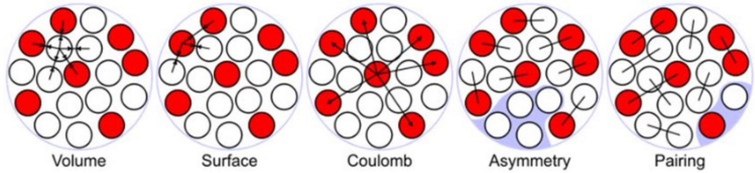
- More experimental constraints (in particular for unstable nuclei)
- **Improved nuclear models**
  - ➢ Their **reliability**, *i.e.* their physical robustness
  - ➢ Their **accuracy**, *i.e.* their capacity to reproduce experimental data

Nuclear inputs to nuclear reaction (HF) & decay calculations



Challenge in theoretical nuclear physics (at least for astrophysics applications)

MACROSCOPIC DESCRIPTION

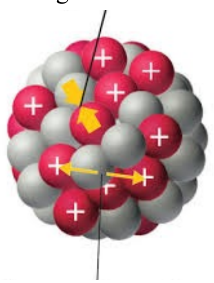


$$E_B = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \Delta(Z,N)$$

Macro-Micro models still widely used in most of nuclear applications

GLOBAL MEAN-FIELD DESCRIPTION

$$E_{MF} = \int \mathcal{E}_{nuc}(\mathbf{r}) d^3\mathbf{r} + \int \mathcal{E}_{coul}(\mathbf{r}) d^3\mathbf{r}$$



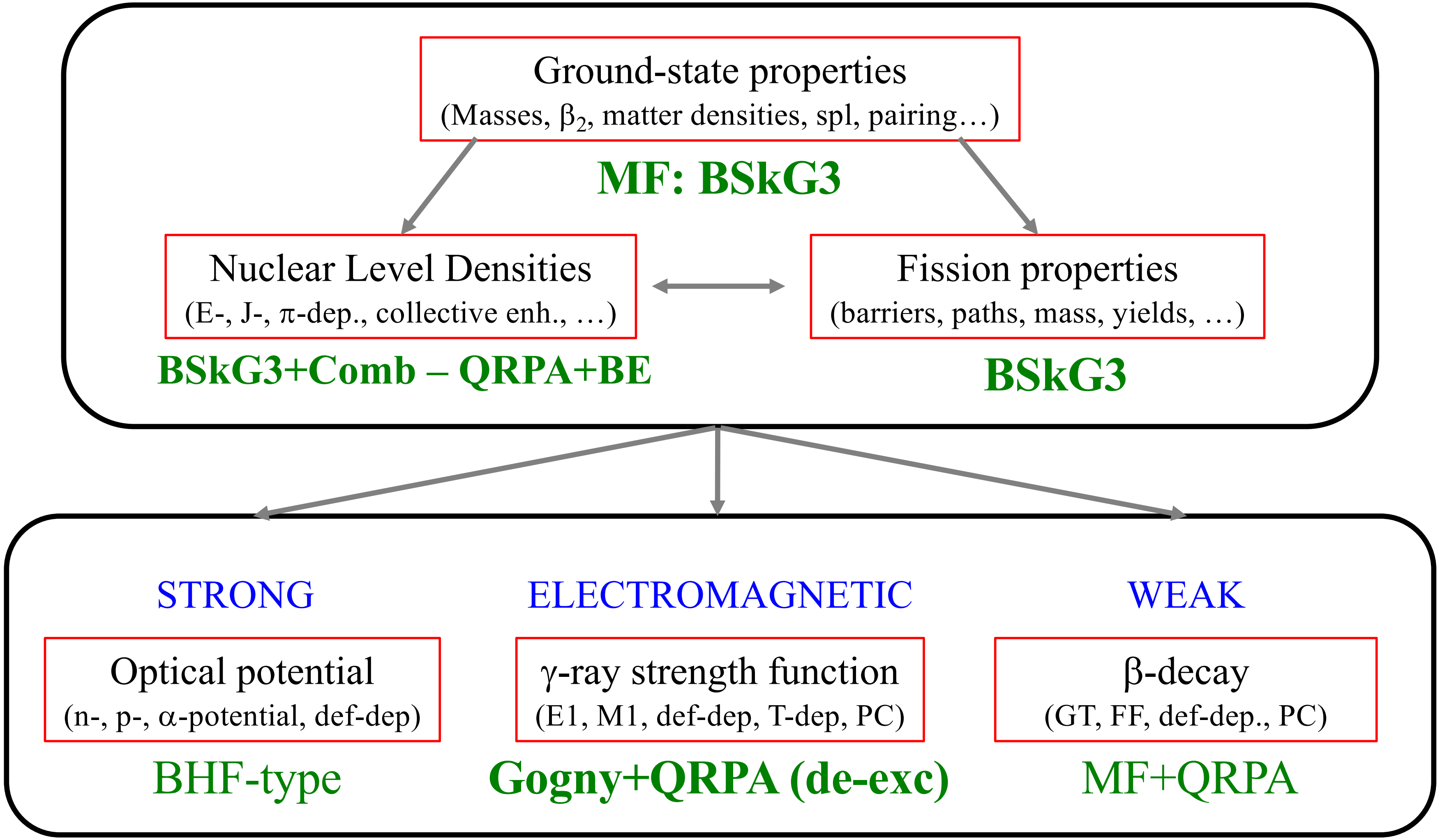
$$\begin{aligned}
\mathcal{E}_{\rm Sky} = & \sum_{q=n,p} \frac{\hbar^2}{2M_q}\tau_q + \frac{1}{2}t_0\left[\left(1+\frac{1}{2}x_0\right)\rho^2 - \left(\frac{1}{2}+x_0\right)\sum_{q=n,p}\rho_q^2\right] + \frac{1}{4}t_1\left[\left(1+\frac{1}{2}x_1\right)\left(\rho\tau+\frac{3}{4}(\nabla\rho)^2\right) - \left(\frac{1}{2}+x_1\right)\sum_{q=n,p}\left(\rho_q\tau_q+\frac{3}{4}(\nabla\rho_q)^2\right)\right] \\
& + \frac{1}{4}t_2\left[\left(1+\frac{1}{2}x_2\right)\left(\rho\tau-\frac{1}{4}(\nabla\rho)^2\right) + \left(\frac{1}{2}+x_2\right)\sum_{q=n,p}\left(\rho_q\tau_q-\frac{1}{4}(\nabla\rho_q)^2\right)\right] + \frac{1}{12}t_3\rho^\alpha\left[\left(1+\frac{1}{2}x_3\right)\rho^2 - \left(\frac{1}{2}+x_3\right)\sum_{q=n,p}\rho_q^2\right] \\
& + \frac{1}{4}t_4\left[\left(1+\frac{1}{2}x_4\right)\left(\rho\tau+\frac{3}{4}(\nabla\rho)^2\right) - \left(\frac{1}{2}+x_4\right)\sum_{q=n,p}\left(\rho_q\tau_q+\frac{3}{4}(\nabla\rho_q)^2\right)\right]\rho^\beta + \frac{\beta}{8}t_4\left[\left(1+\frac{1}{2}x_4\right)\rho(\boldsymbol{\nabla}\rho)^2 - \left(\frac{1}{2}+x_4\right)\boldsymbol{\nabla}\rho\cdot\sum_{q=n,p}\rho_q\boldsymbol{\nabla}\rho_q\right]\rho^{\beta-1} \\
& + \frac{1}{4}t_5\left[\left(1+\frac{1}{2}x_5\right)\left(\rho\tau-\frac{1}{4}(\nabla\rho)^2\right) + \left(\frac{1}{2}+x_5\right)\sum_{q=n,p}\left(\rho_q\tau_q-\frac{1}{4}(\nabla\rho_q)^2\right)\right]\rho^\gamma - \frac{1}{16}\left(t_1x_1+t_2x_2\right)J^2 + \frac{1}{16}\left(t_1-t_2\right)\sum_{q=n,p}J_q^2 \\
& - \frac{1}{16}\left(t_4x_4\rho^\beta+t_5x_5\rho^\gamma\right)J^2 + \frac{1}{16}\left(t_4\rho^\beta-t_5\rho^\gamma\right)\sum_{q=n,p}J_q^2 + \frac{1}{2}W_0\left(\boldsymbol{J}\cdot\boldsymbol{\nabla}\rho + \sum_{q=n,p}\boldsymbol{J_q}\cdot\boldsymbol{\nabla}\rho_q\right)
\end{aligned}$$

- Still *phenomenological*, but at the level of the effective *n-n* interaction
- More complex, but models have reached stability and **accuracy** !

A challenge that requires a continued effort…

Some new efforts to improve the nuclear predictions for astrophysical applications

Nuclear inputs to nuclear reaction & decay calculations



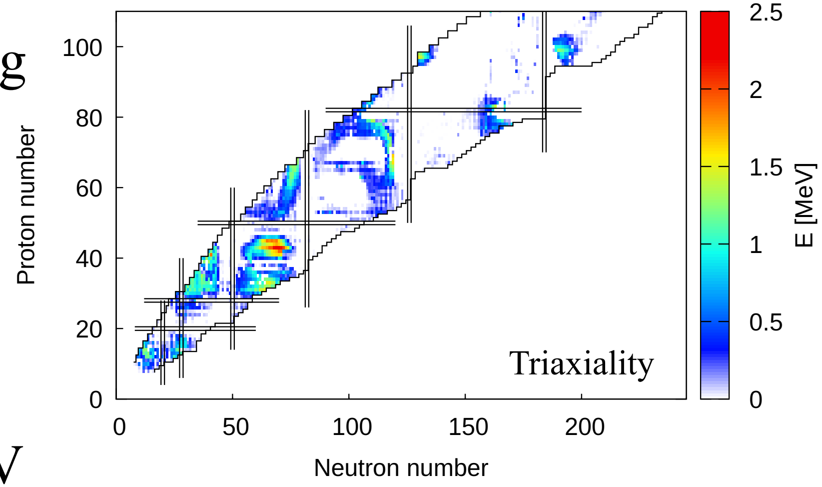
"Microscopic" approach is a necessary but not a sufficient condition !
"(Semi-)Microscopic" models must be competitive in reproducing exp. data !

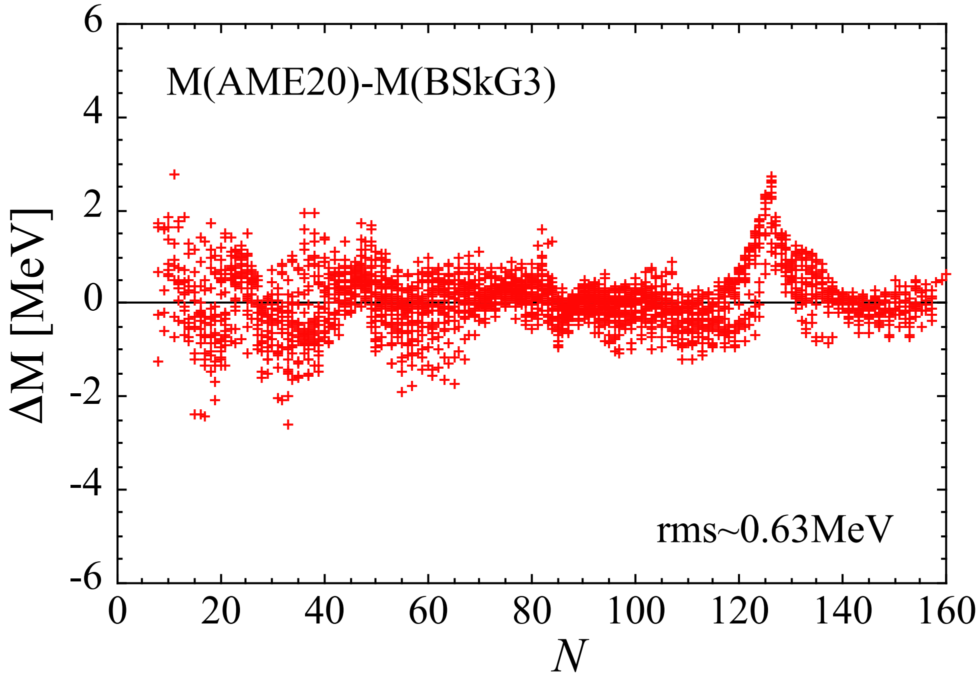
BSkG3 HFB nuclear mass models

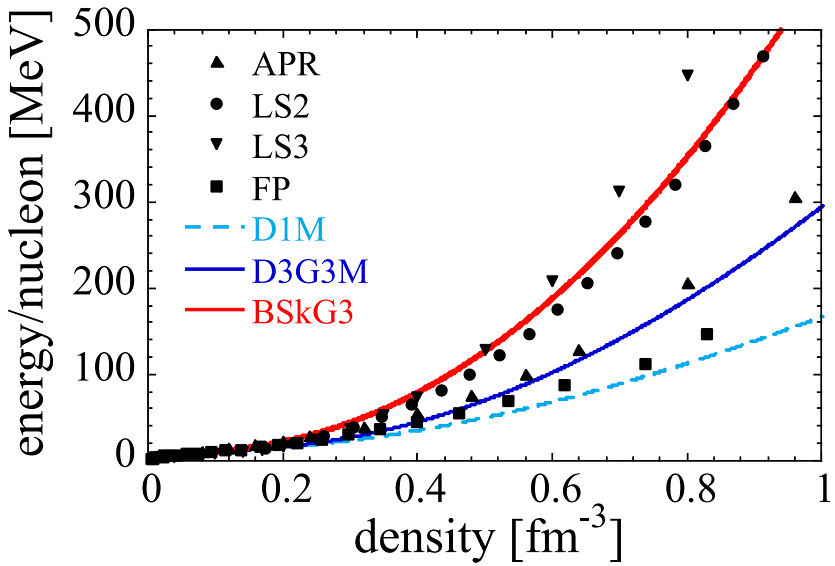
Grams, Ryssens et al. (EPJA 59, 270, 2023)

Recent Skyrme-HFB mass model: BSkG3

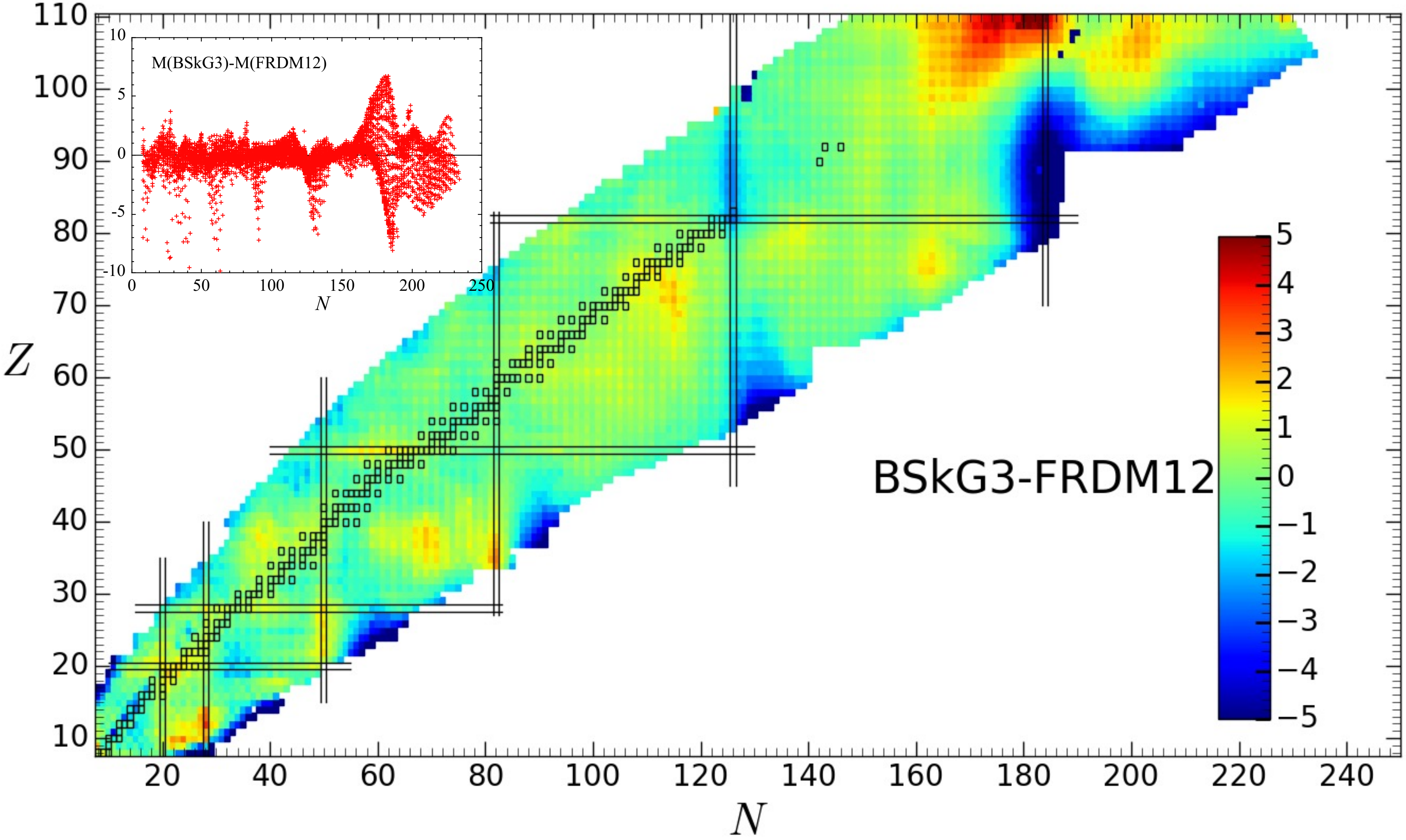
- Triaxiality, time-reversal symmetry breaking & octupole GS deformation
- Microscopic pairing from "realistic" calculations
- Stiff EoS
- Accurate masses: σ(2457*M*)=0.63MeV
- Accurate fission barriers: σ(45B_I)=0.33MeV



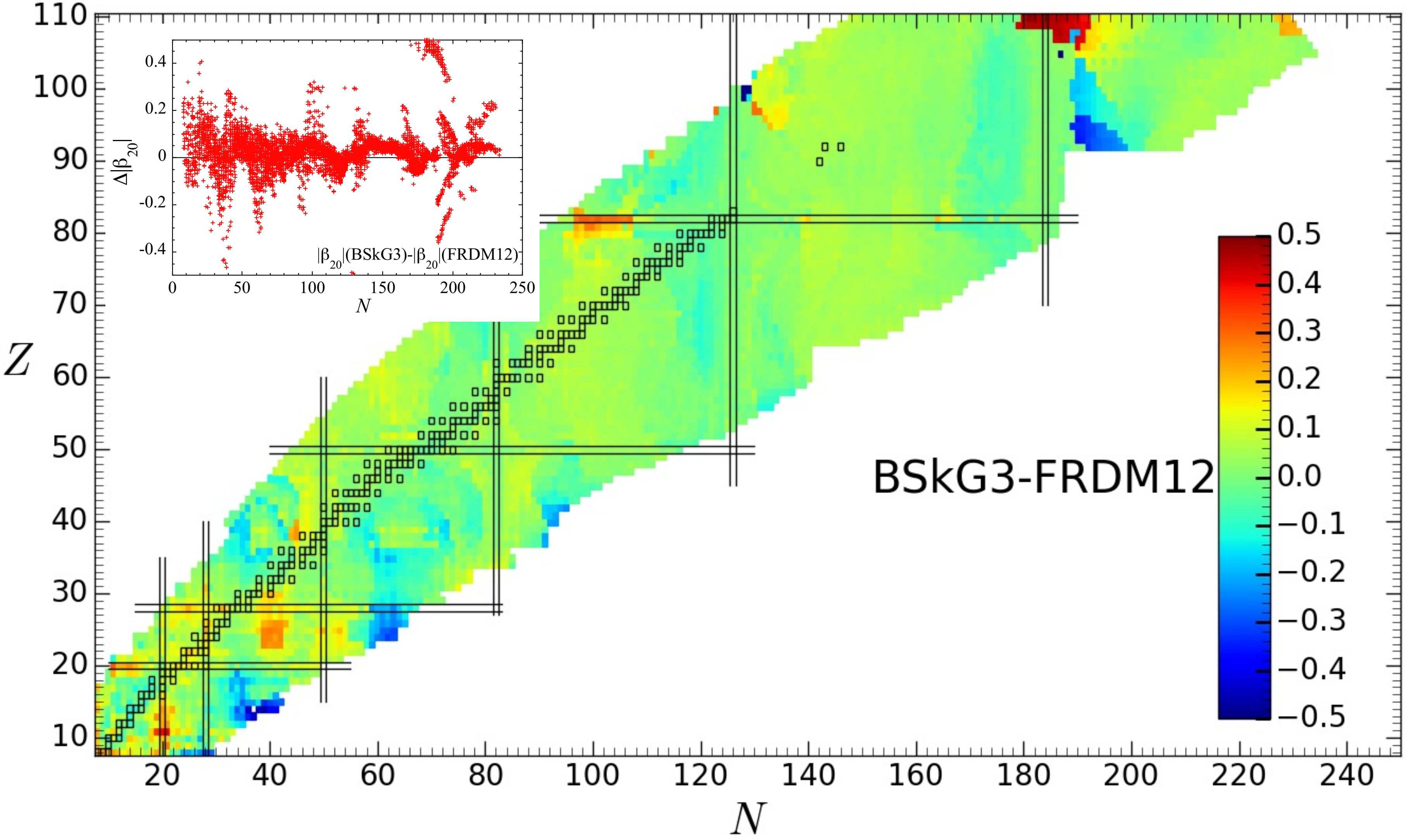




Differences in the *mass predictions* between BSkG3 and FRDM12



Differences in the deformations $|\beta_{20}|$ predicted by BSkG3 and FRDM12



New developments in Nuclear Level Density models

1. BSkG3 + Combinatorial model including triaxiality

   (S. Goriely, W. Ryssens, S. Hilaire, A. Koning)

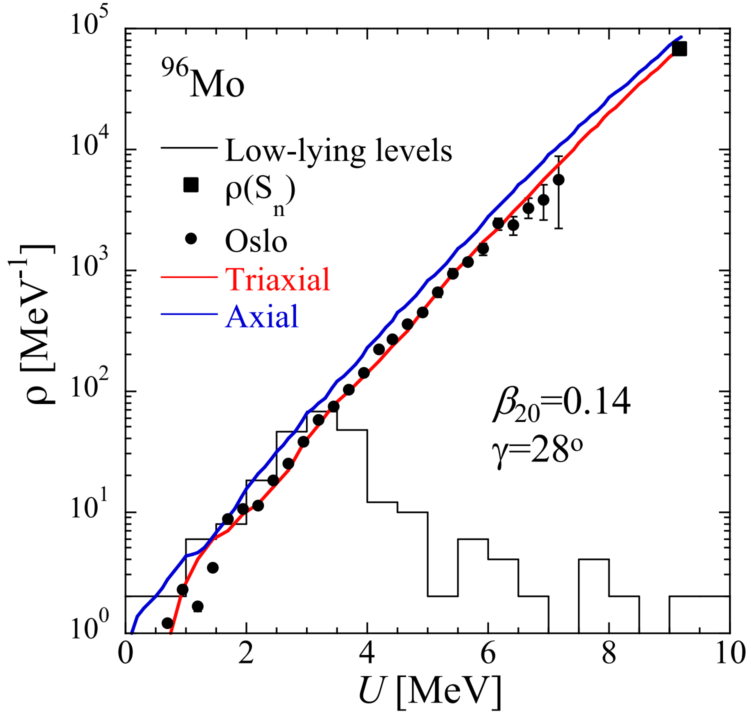
2. QRPA + Boson Expansion model

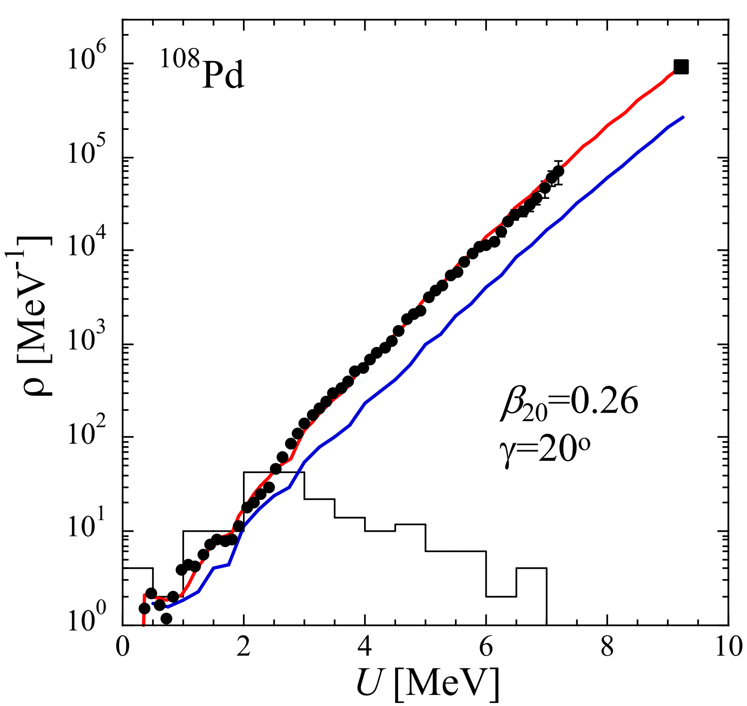
   (S. Hilaire, S. Péru, S. Goriely)

Effects of triaxality on BSkG3+Combinatorial NLD

Main impact of the triaxiality on the NLD:

- Reduction of the spl density → Lower intrinsic NLD
- Additional collective enhancement → Increase total NLD



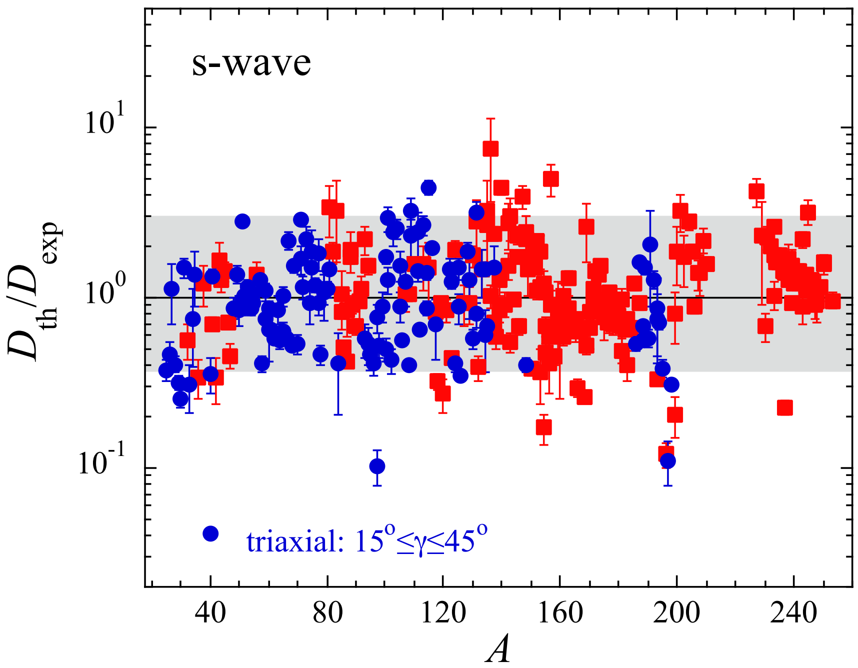


For modestly deformed nuclei:
Decrease of NLD

For well deformed nuclei:
Increase of NLD

Comparison with RIPL-3 resonance spacings

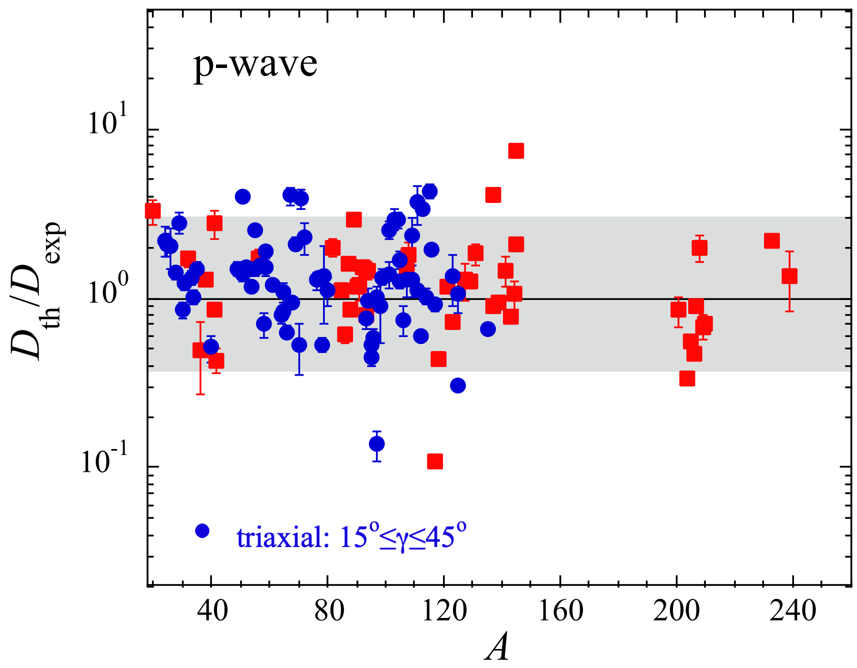
D_0 = *s*-wave neutron resonance spacings



300 nuclei

D_0	f_{mean}	f_{rms}
BSkG3 (2025)	1.03	1.96
HFB+Comb (2008)	0.95	2.34
T-HFB+Comb (2012)	1.11	2.58
QRPA+BE (2025)	1.12	2.20

D_1 = *p*-wave neutron resonance spacings

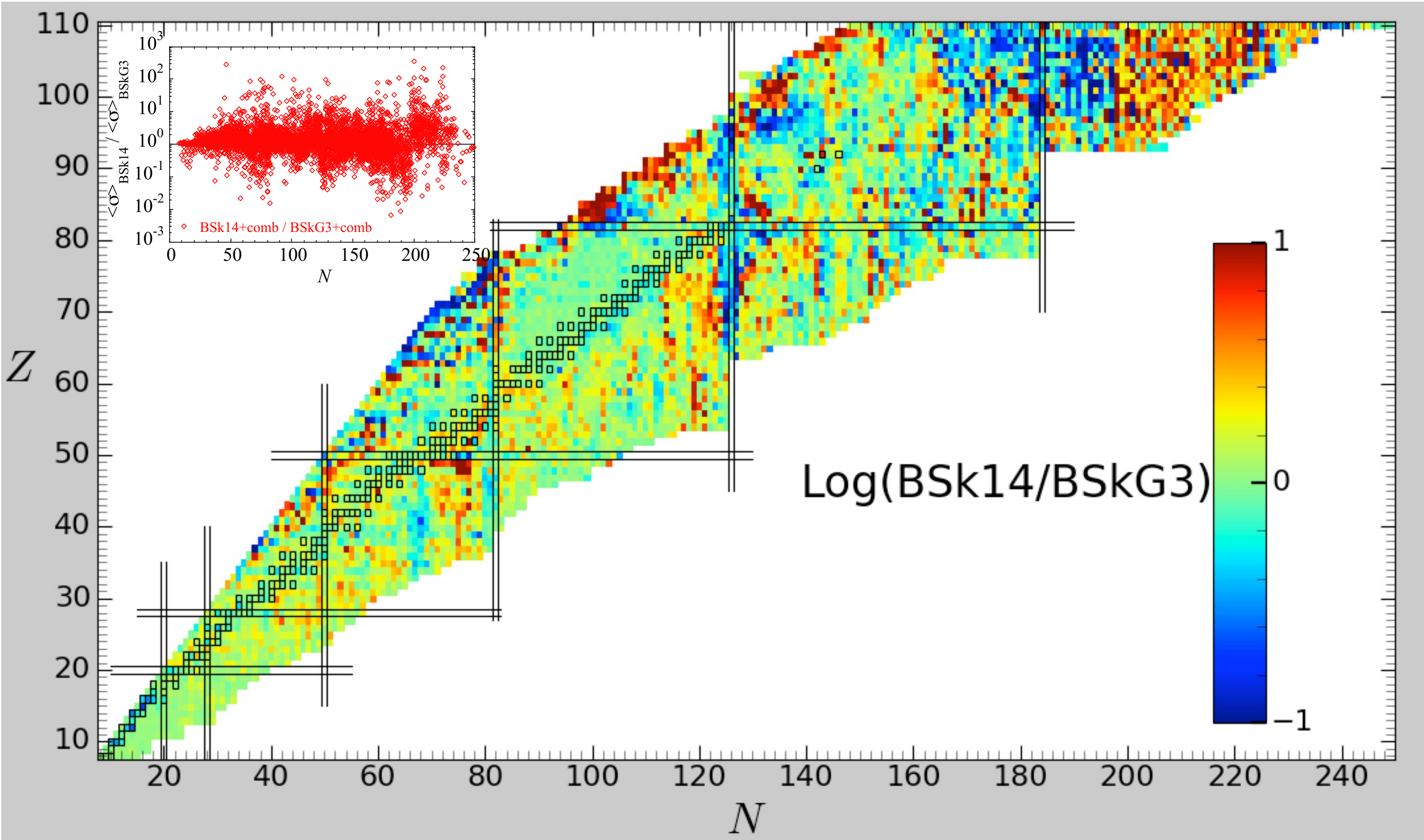


116 nuclei

D_1	f_{mean}	f_{rms}
BSkG3	1.21	1.99
HFB+Comb	1.01	2.24
T-HFB+Comb	1.62	4.38
QRPA+BE	1.72	3.75

Impact of the BSkG3+combinatorial on HF (n,γ) reaction rates (T_9=1)

Comparison of BSk14+comb (2008) vs BSkG3+comb (2024) impact on N_a<σv>



Energy-, spin- and parity-depencent NLD tables ready for use for 7677 nuclei ($8 \leq Z \leq 110$) including renormalisation coefficients (α,δ) on experimental D_{exp} & LLL (when available)

QRPA + Boson Expansion Method: a conceptually new approach:

- **deformed QRPA calculations** => collective levels (***Bosons***) for various given multipolarities and parities: K^{π} [illegible] up to $9^{+/-}$ for even-even nuclei (Gogny D1M+QRPA) with a [illegible]-off ε_c=200MeV

- **Boson Expansion** : Coupling Boso[illegible] [illegible]neralized boson partition function

$$\mathcal{Z}_{\text{boson}} = \ldots y^{\varepsilon_{\lambda\mu}} t^{\mu} p_{\lambda}]^{N_{\text{boson}}}$$

- **Construction of spin- a[illegible] [illegible]ndent NLD**

spherical nuclei: $\ldots_{\text{tot}}(U, M = J, \pi) - \omega_{\text{tot}}(U, M = J+1, \pi)$

well deformed n[illegible] $\ldots = \frac{1}{2}\left[\sum_{K=-J, K\neq 0}^{J} \omega_{\text{tot}}(U - E_{rot}^{J,K}, K, \pi)\right] + \omega_{\text{tot}}(U - E_{rot}^{J,0}, 0, \pi)$

No independent-particle approximation

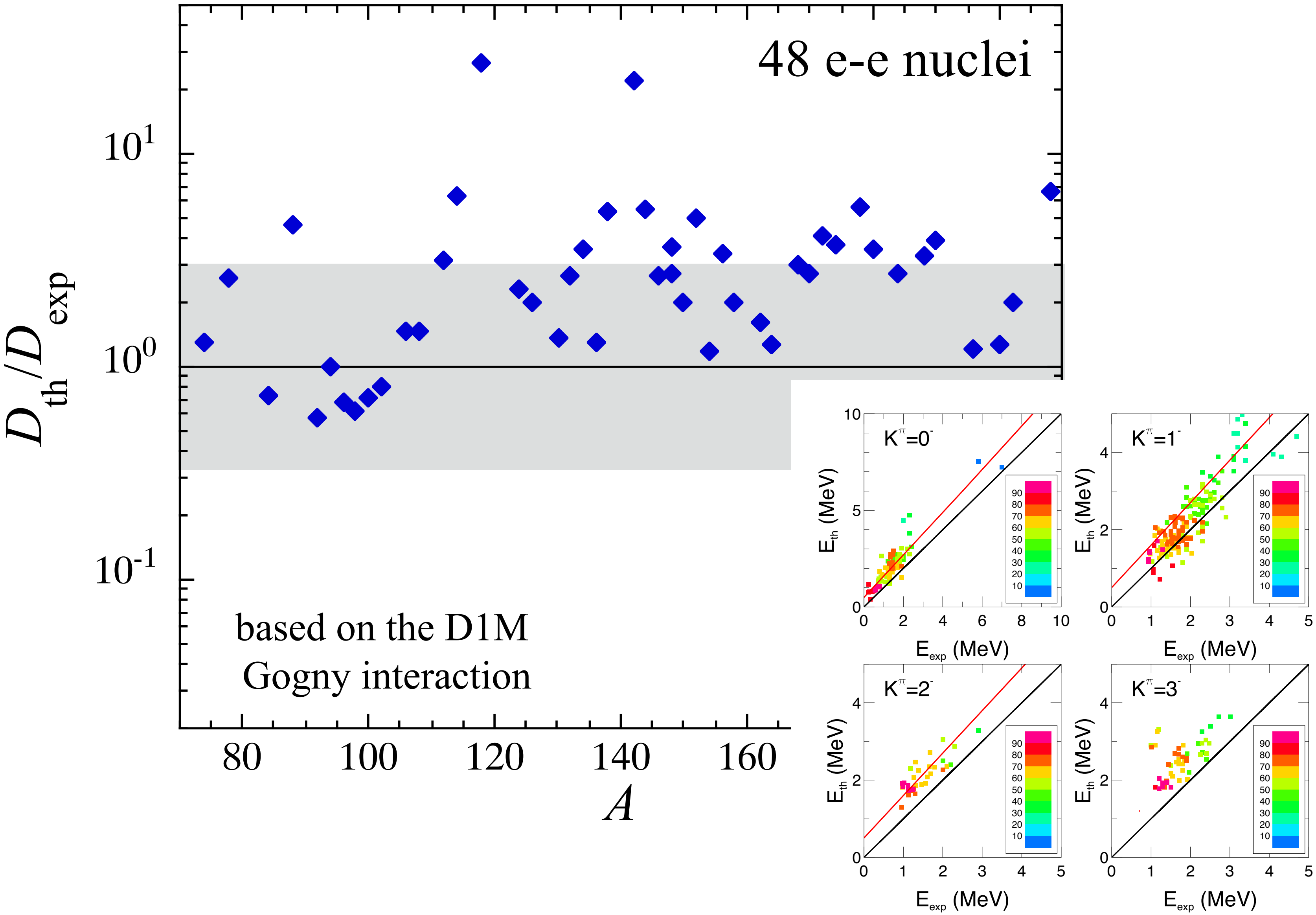
- **Phenomenologi[illegible] [illegible]ng** between spherical and well deformed nuclei

$$\rho(U, J, \pi) = \left[1 - \mathcal{F}\right]\rho_s(U, J, \pi) + \mathcal{F}\rho_d(U, J, \pi) \qquad \text{where} \quad \mathcal{F} = 1 - \left[1 + e^{(r_{42} - 2.90)/0.35}\right]^{-1}$$

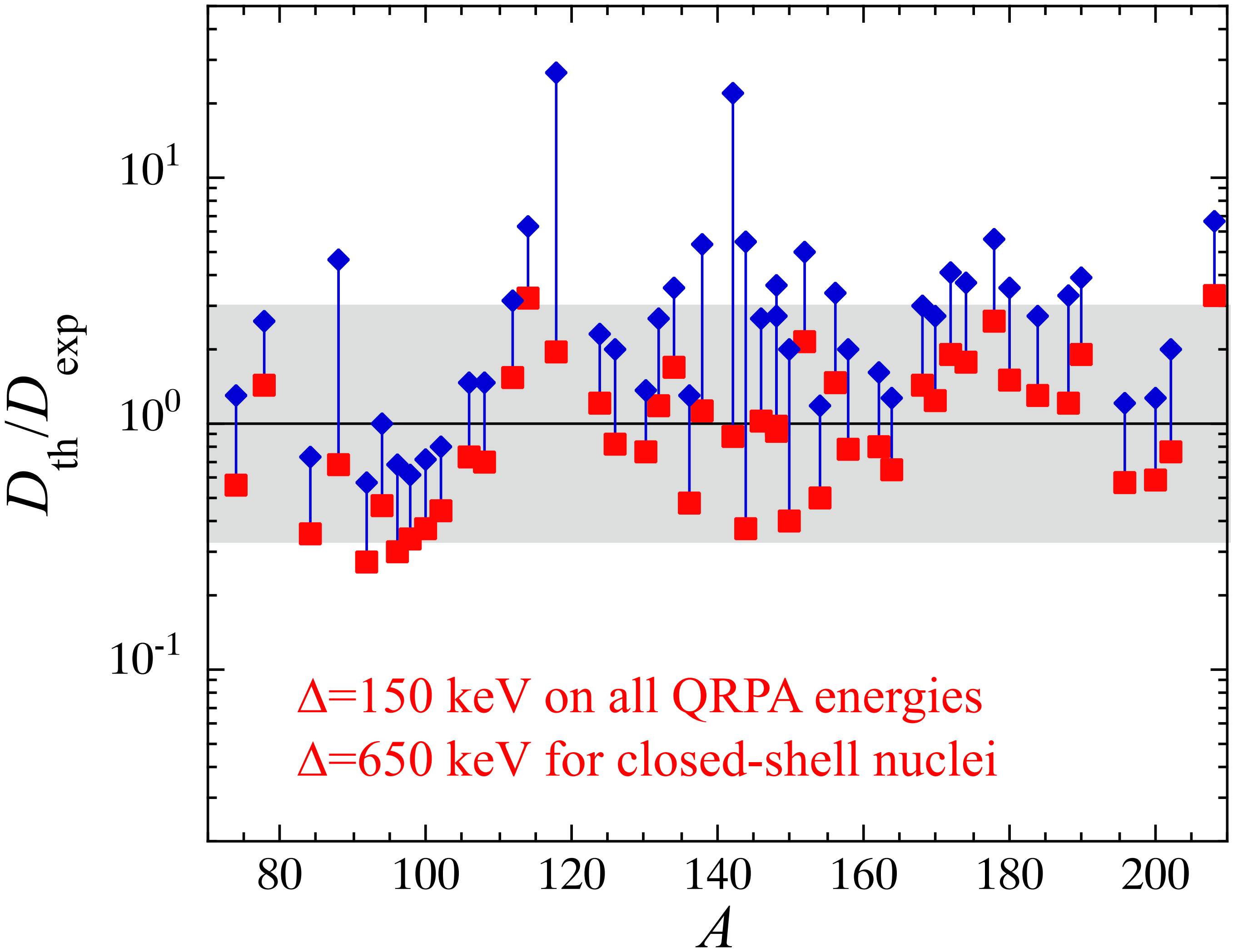
$r_{42}=E(J=4)/E(J=2)$=3.3 rotator
2.0 vibrator

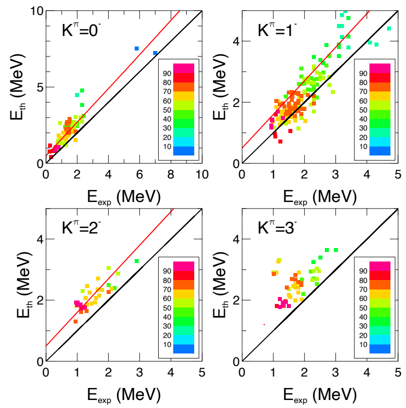
The QRPA + Boson Expansion Method

Relatively satisfactory description of D_0, but overall overestimation (*i.e.* underestimation of ρ)



The QRPA + Boson Expansion Method

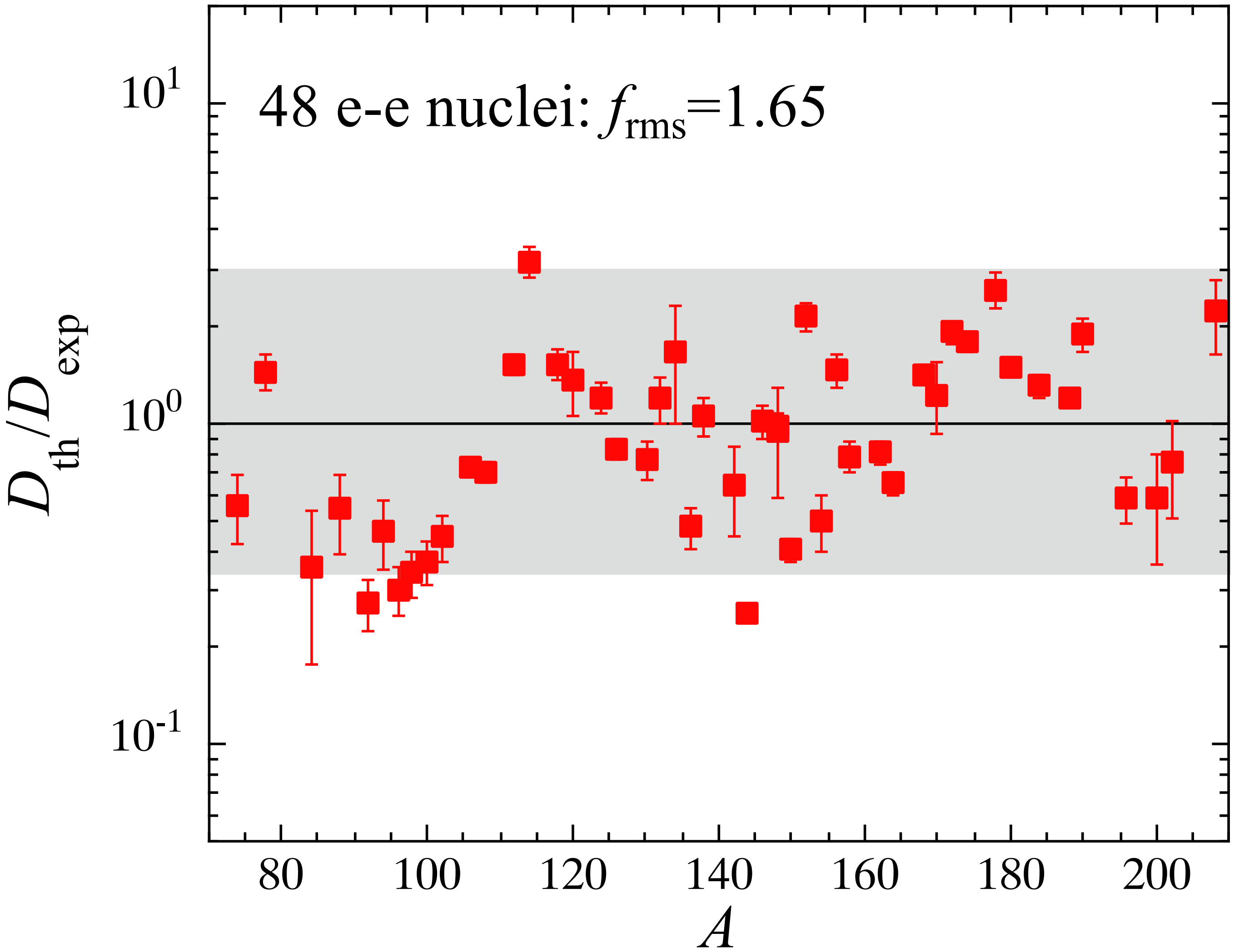




→ Need for an accurate estimate of the lowest QRPA exitations energies

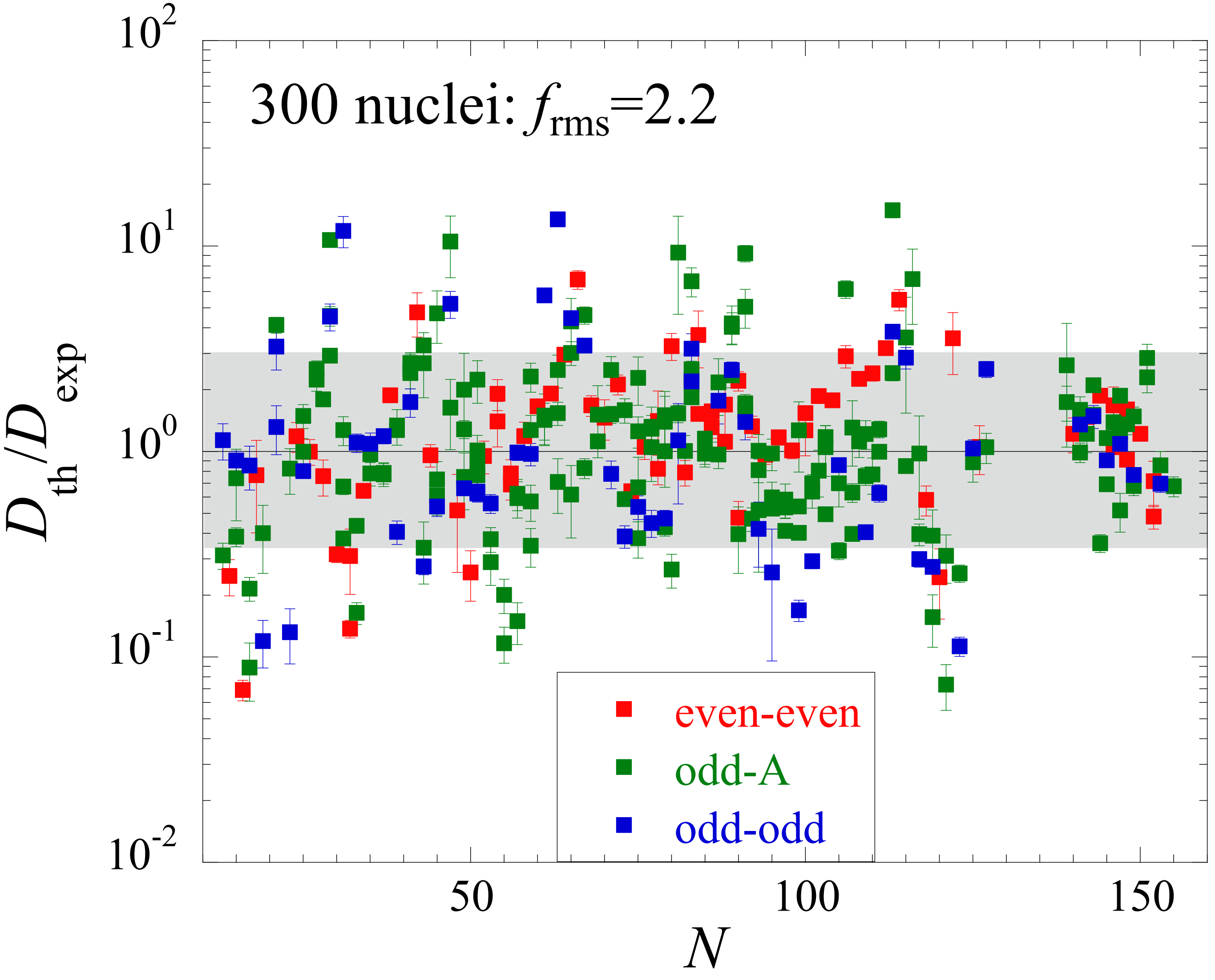
The QRPA + Boson Expansion Method

Finally, including experimental uncertainties

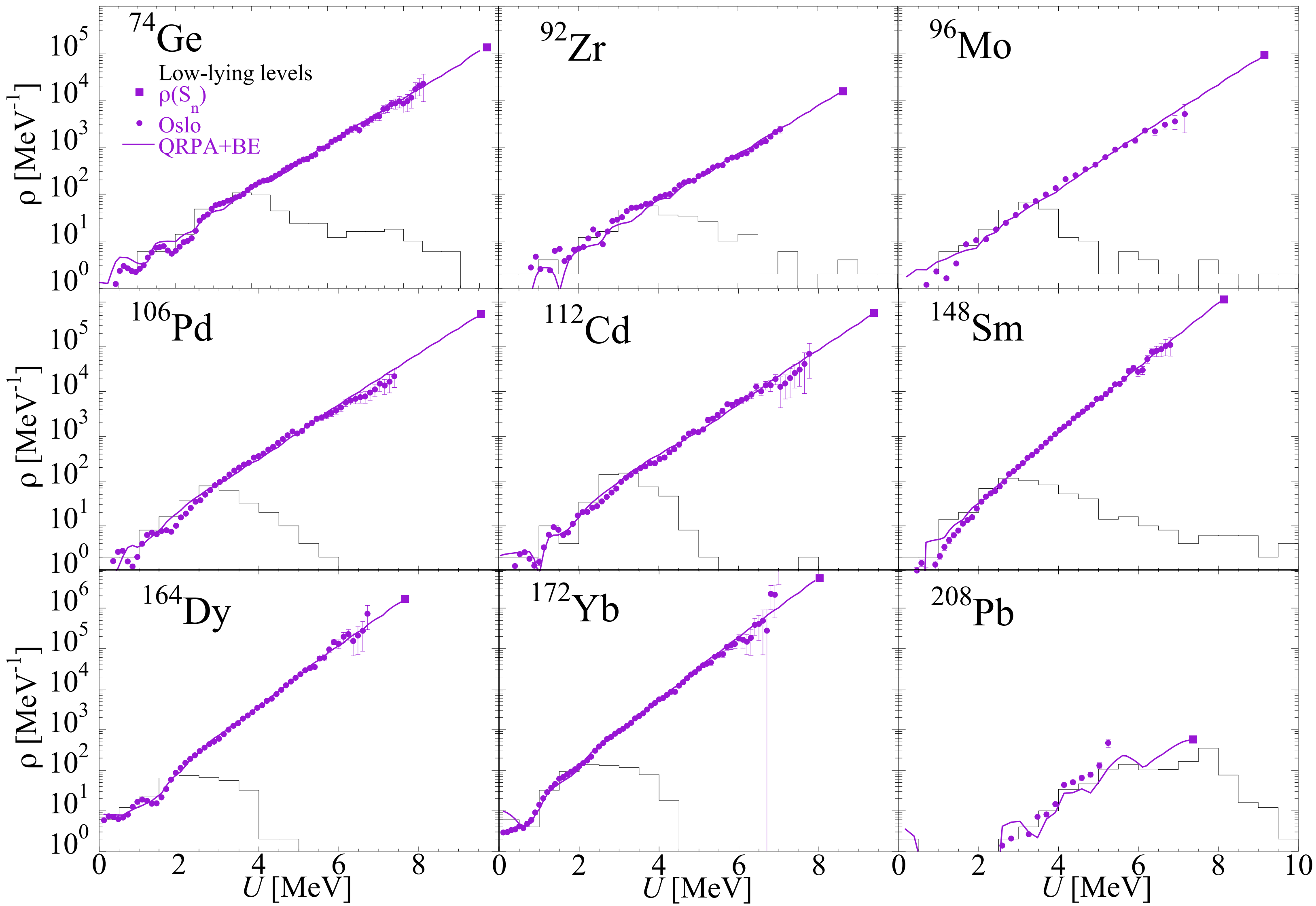


On the same data set: Cst-T: f_{rms}=1.5 - HFB+Comb: f_{rms}=2.4

The QRPA + Boson Expansion Method

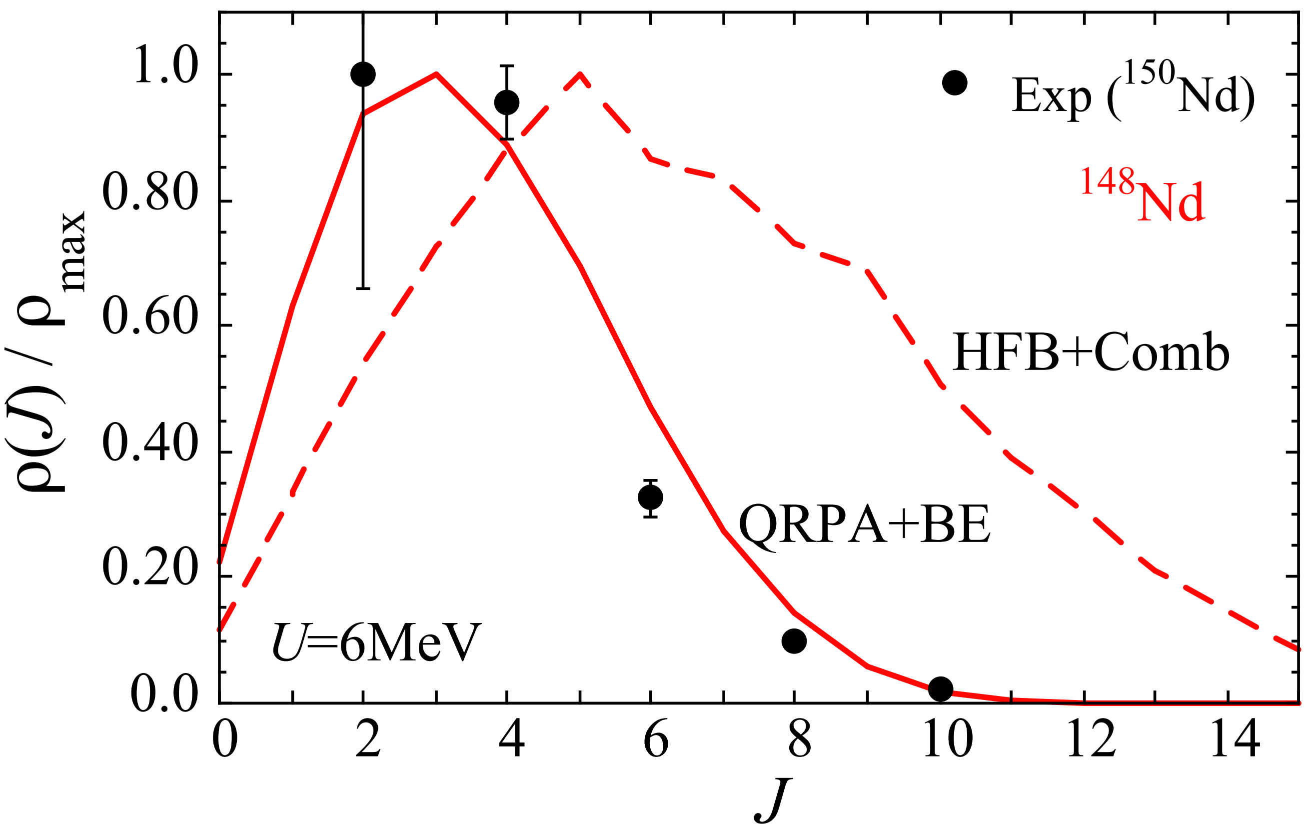


The QRPA + Boson Expansion Method



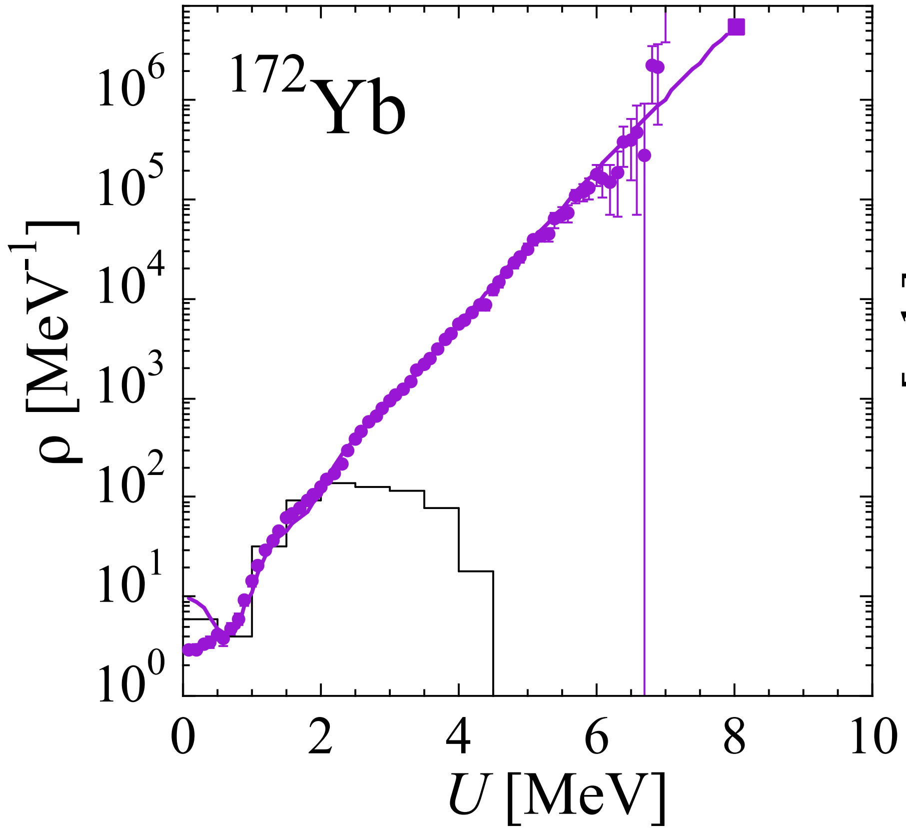
Following the normalisation procedure of Oslo data (SG, Larsen, Mücher, PRC106, 044315, 2022)

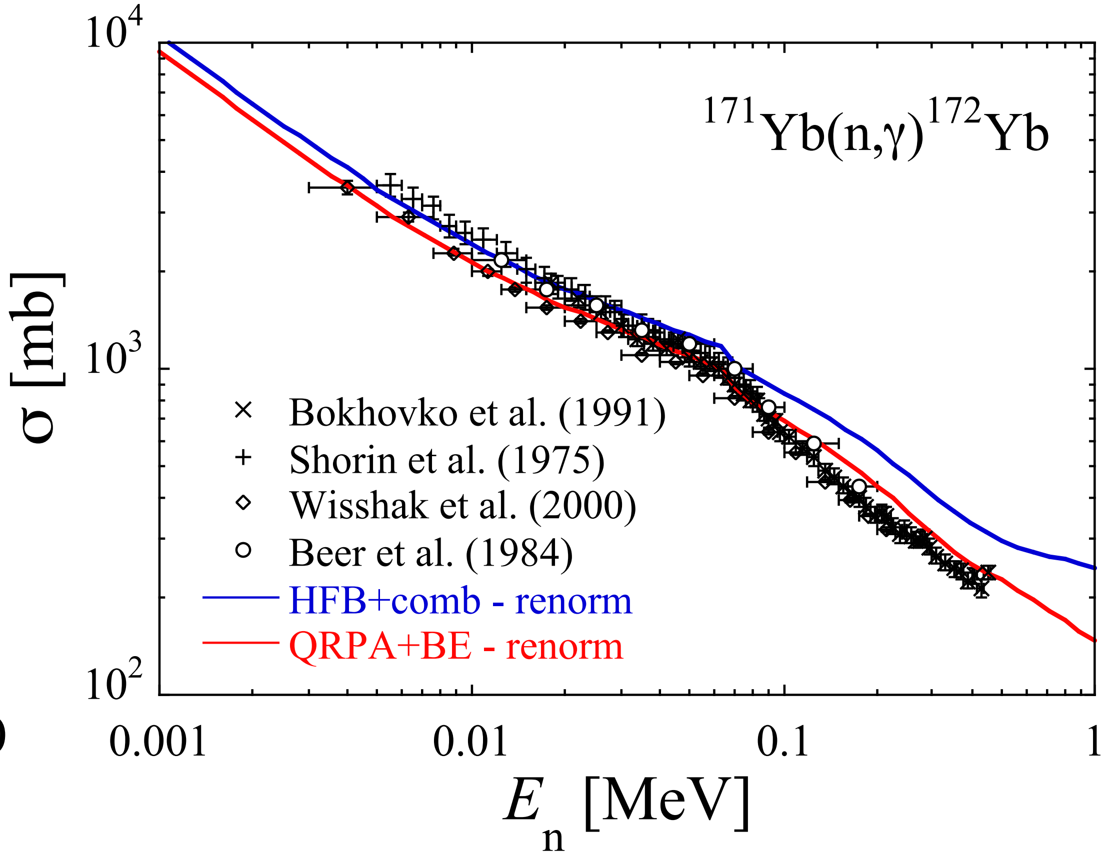
The QRPA + Boson Expansion Method



Experimental spin distribution from (p,p') reaction: σ=2.9 ± 0.2
(Guttormsen et al., 2022)

The QRPA + Boson Expansion Method



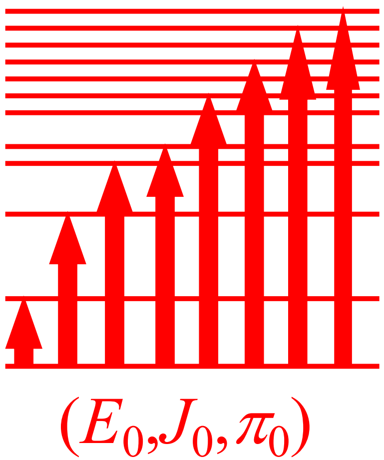


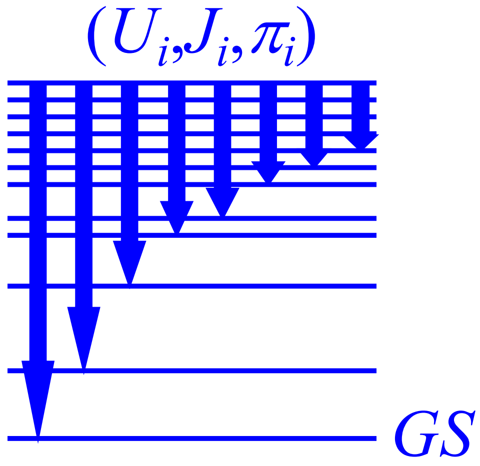
NLD renormalized on known D_0

Photon Strength Function

New calculations of the **de-excitation** PSF

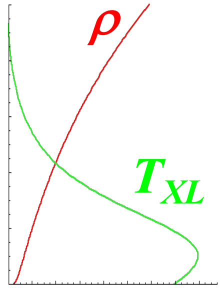
In particular: (γ,n), (γ,p), (γ,α)   (n,γ), (p,γ), (α,γ)

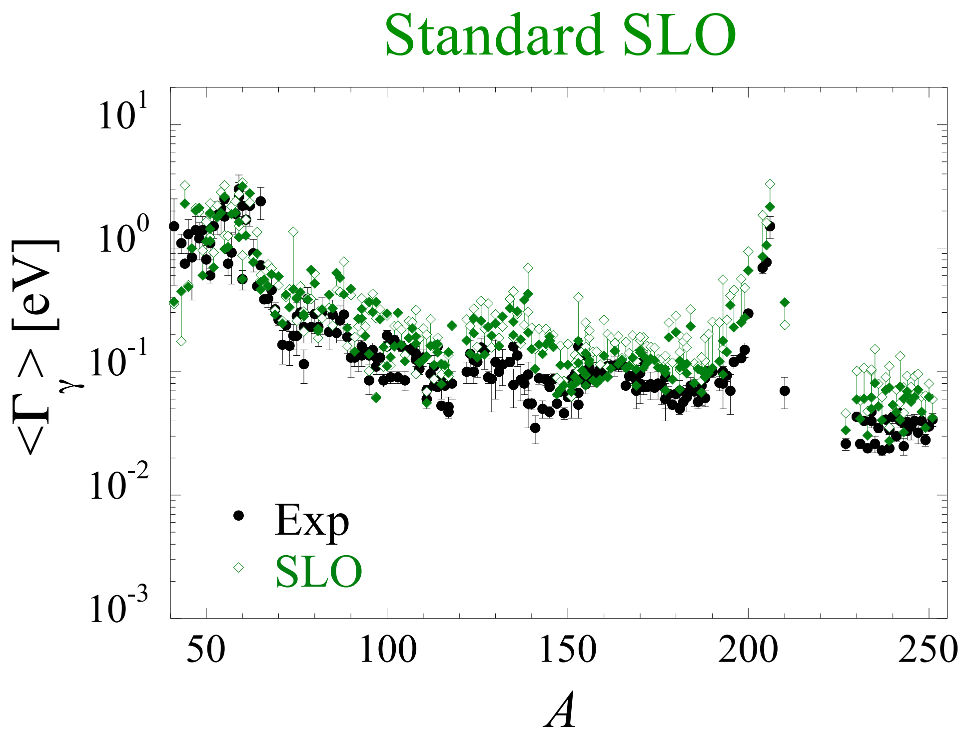


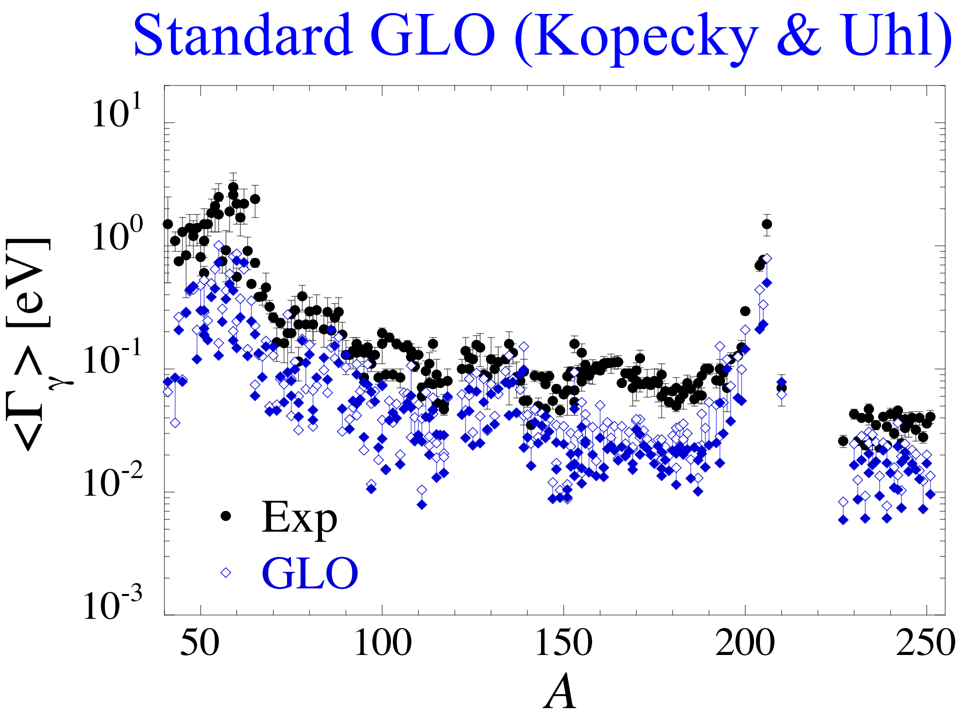


The long-standing problem of the average radiative width $<\Gamma_\gamma>$

$$\langle \Gamma_\gamma \rangle = \frac{D_0}{2\pi} \sum_{X,L,J,\pi} \int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma) \times \rho(S_n + E_n - \varepsilon_\gamma, J, \pi) d\varepsilon_\gamma$$







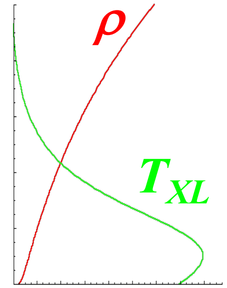
230 nuclei

Full diamonds = CT + BSFG

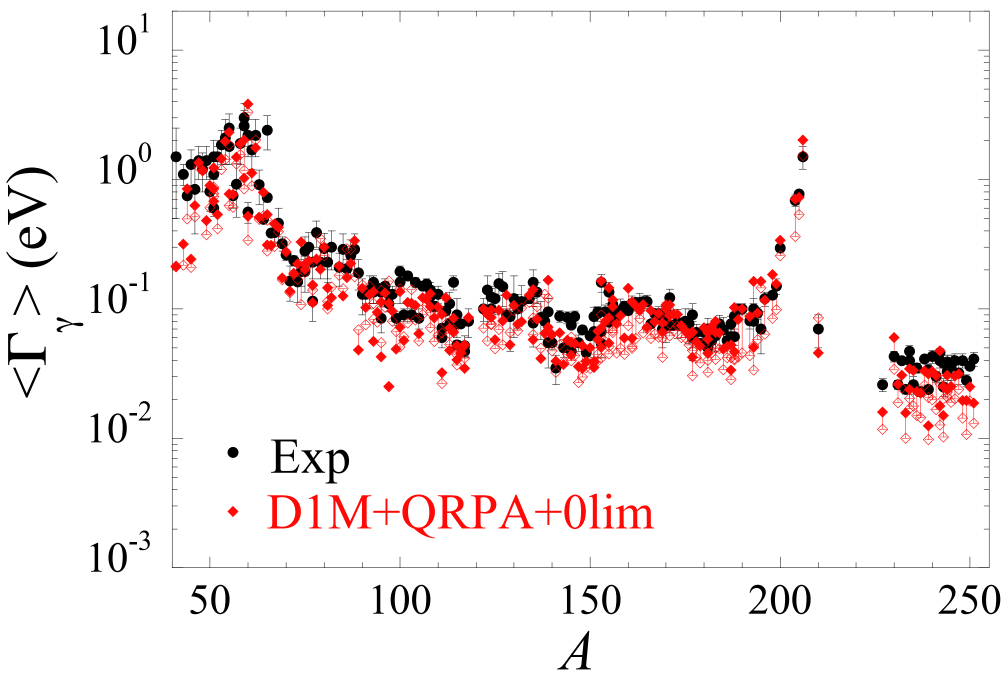
Open diamonds = HFB + Combinatorial

Comparison of D1M+QRPA+0lim and SMLO with <Γ$_\gamma$> data

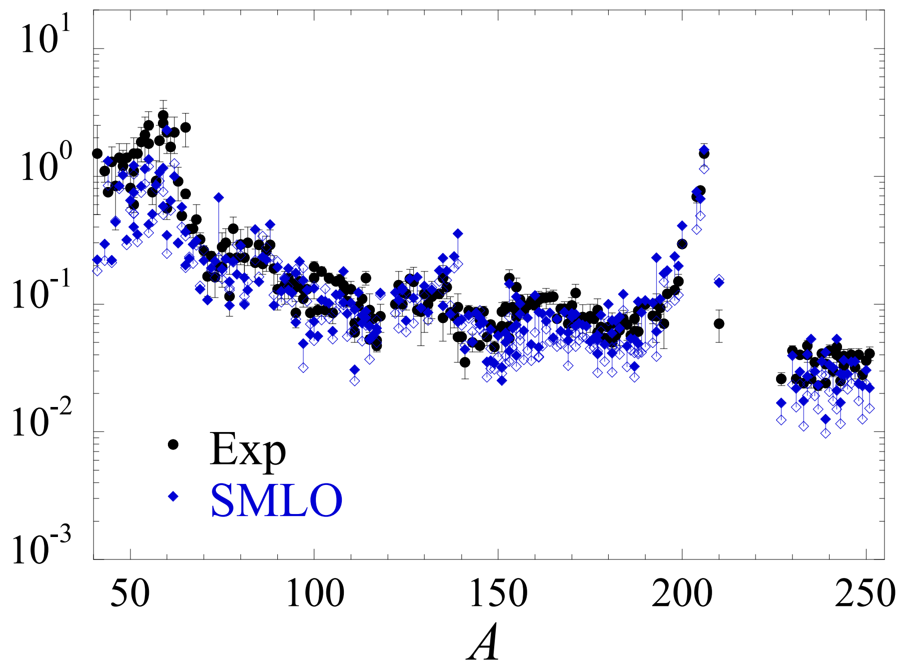
$$\langle\Gamma_\gamma\rangle = \frac{D_0}{2\pi}\sum_{X,L,J,\pi}\int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma)\times\rho(S_n+E_n-\varepsilon_\gamma,J,\pi)d\varepsilon_\gamma$$



D1M+QRPA+0lim



SMLO



Open diamonds = CT + BSFG

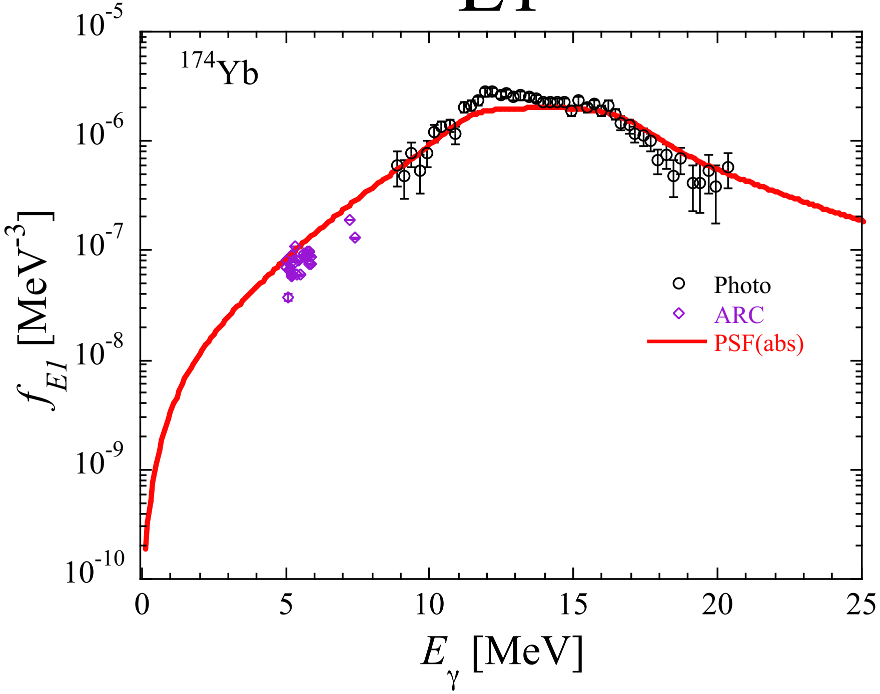
Full diamonds = HFB + Combinatorial

Both PSF models reproduce ~230 <Γ$_\gamma$> within ~ 30-50%

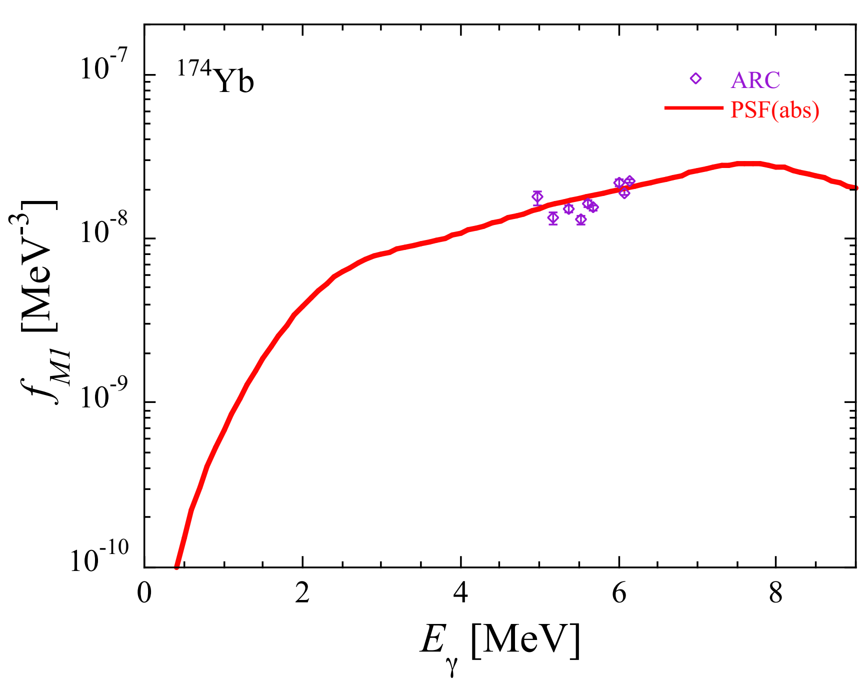
QRPA photoabsorption PSF from the GS

Gogny-HFB+QRPA

E1



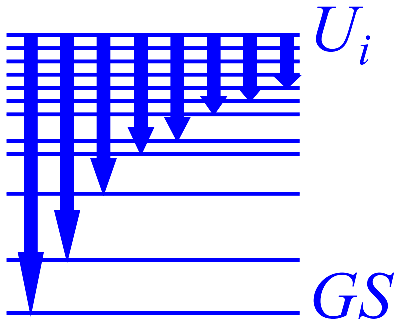
M1



Successful in describing photo, Oslo, ARC, NRF, $\langle\Gamma_\gamma\rangle$, MSC, MD,... data provided some phenomenological corrections and inclusion of an upbend

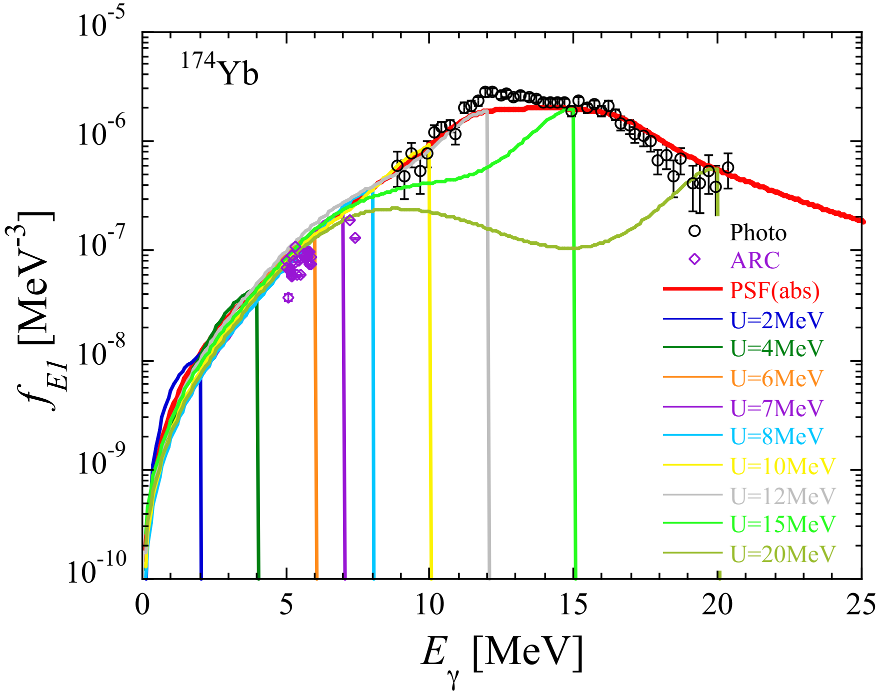
QRPA de-excitation PSF at an initial energy U_i

deformed ^{174}Yb



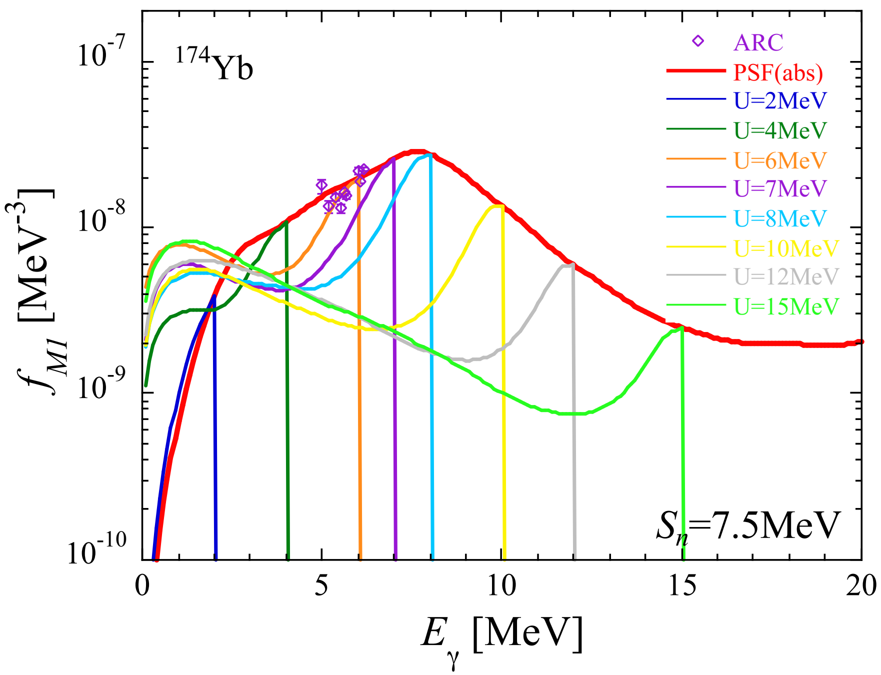
Gogny-HFB+QRPA

E1



Negligible low-energy E1 enhancement

M1

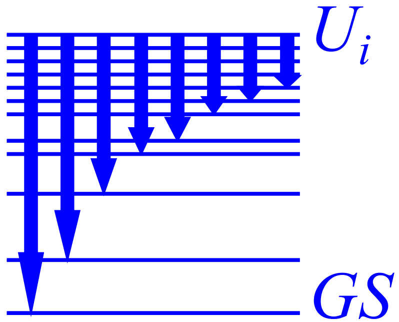


Significant low-energy M1 enhancement ("upbend") but also reduction at higher E_γ

2 billions CPU hours for about 160 even-even Z<80 nuclei

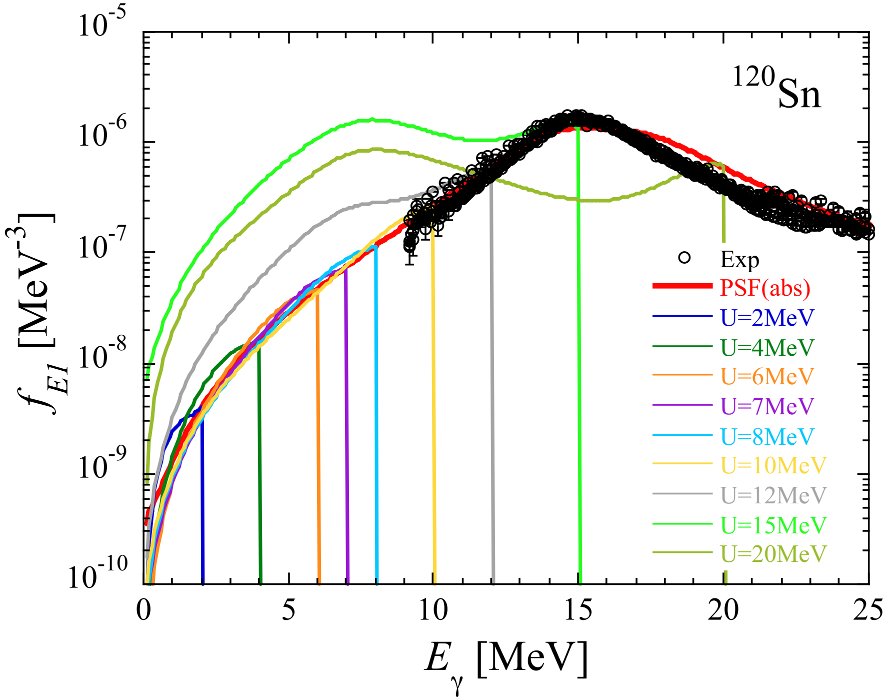
QRPA de-excitation PSF at an initial energy U_i

spherical ^{120}Sn



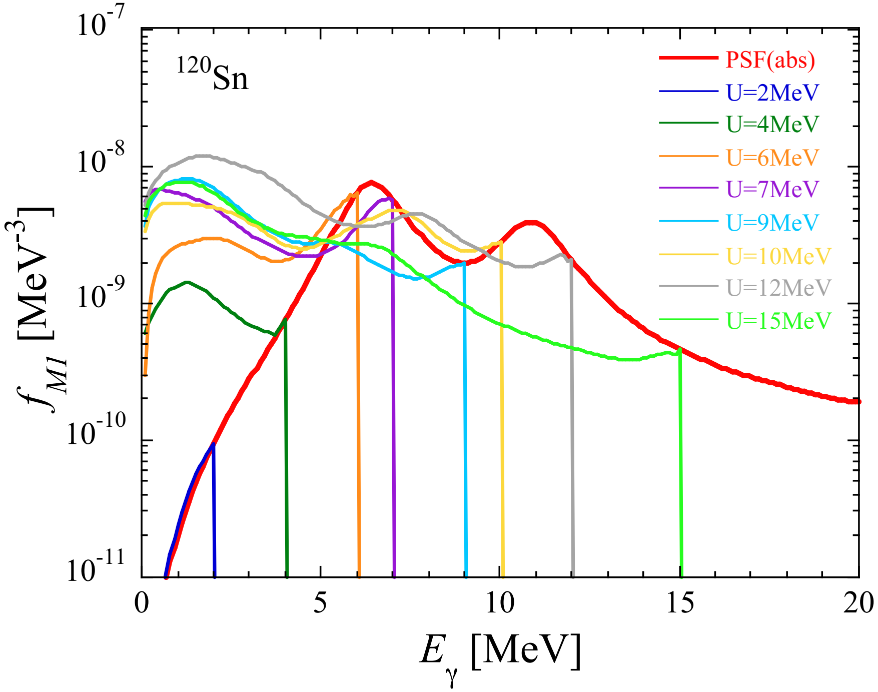
Gogny-HFB+QRPA

E1



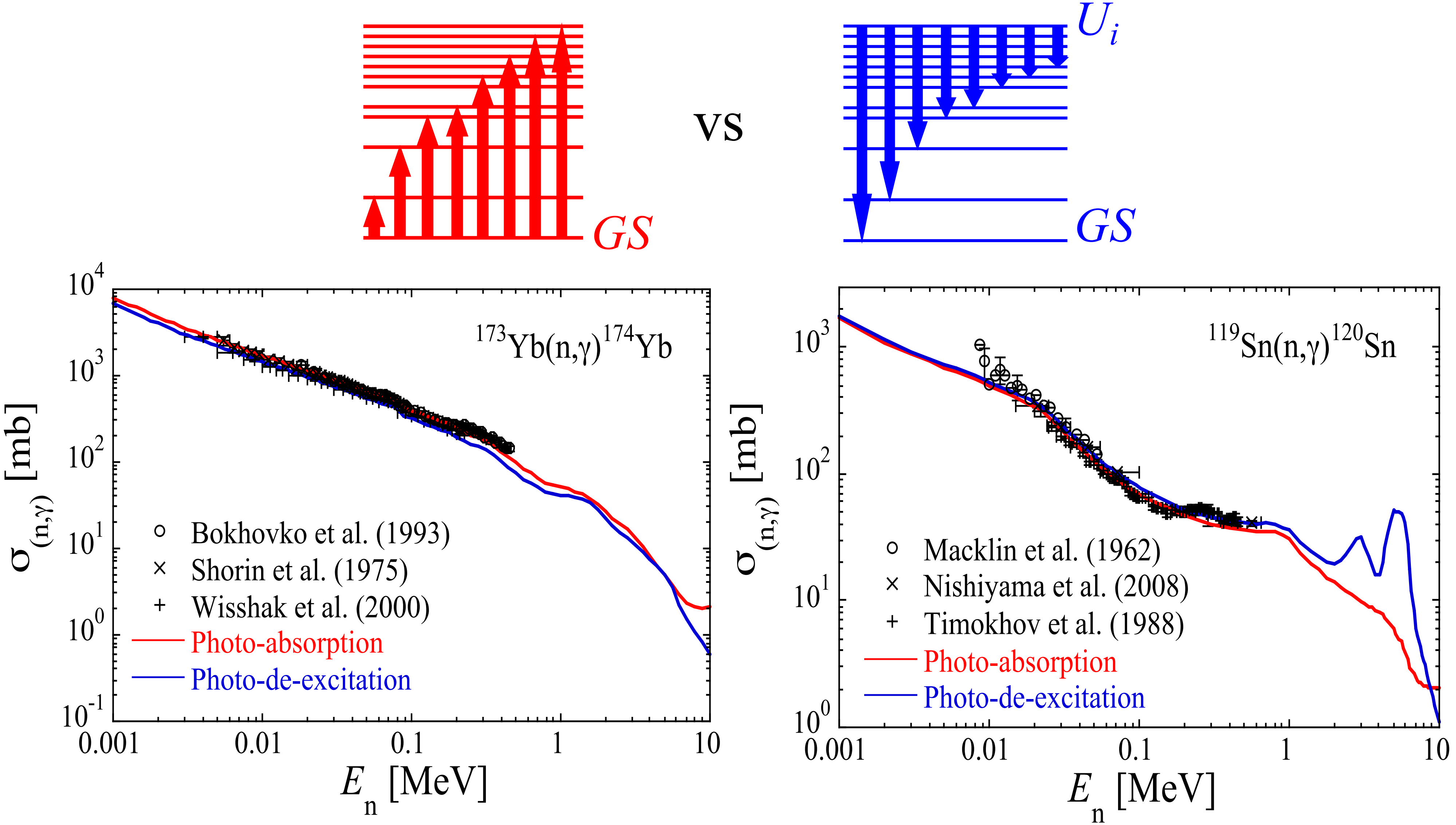
Non-negligible low-energy E1 enhancement at E_γ>10MeV

M1



Significant low-energy M1 enhancement ("upbend") but also reduction at higher E_γ

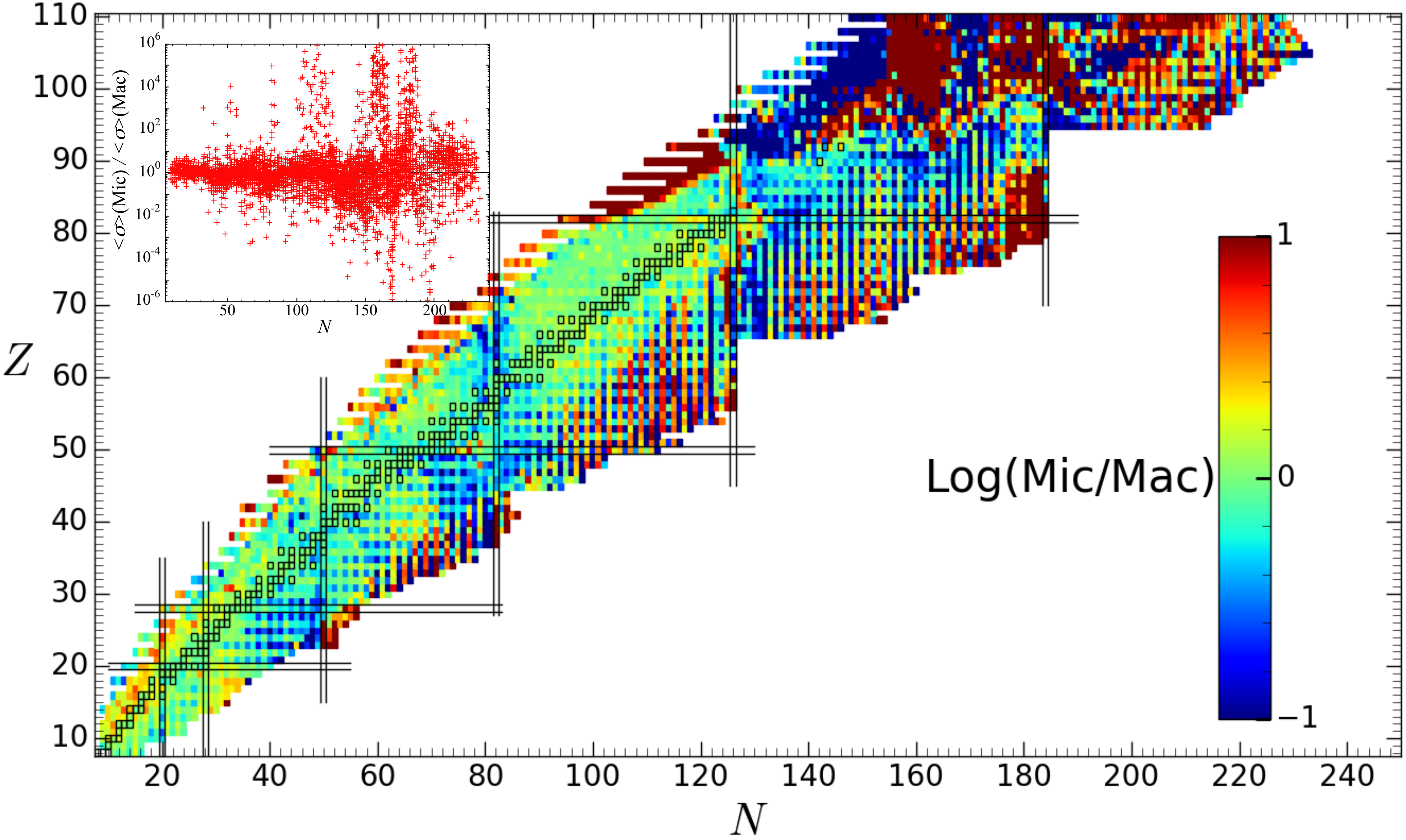
QRPA de-excitation PSF at an initial energy U_i



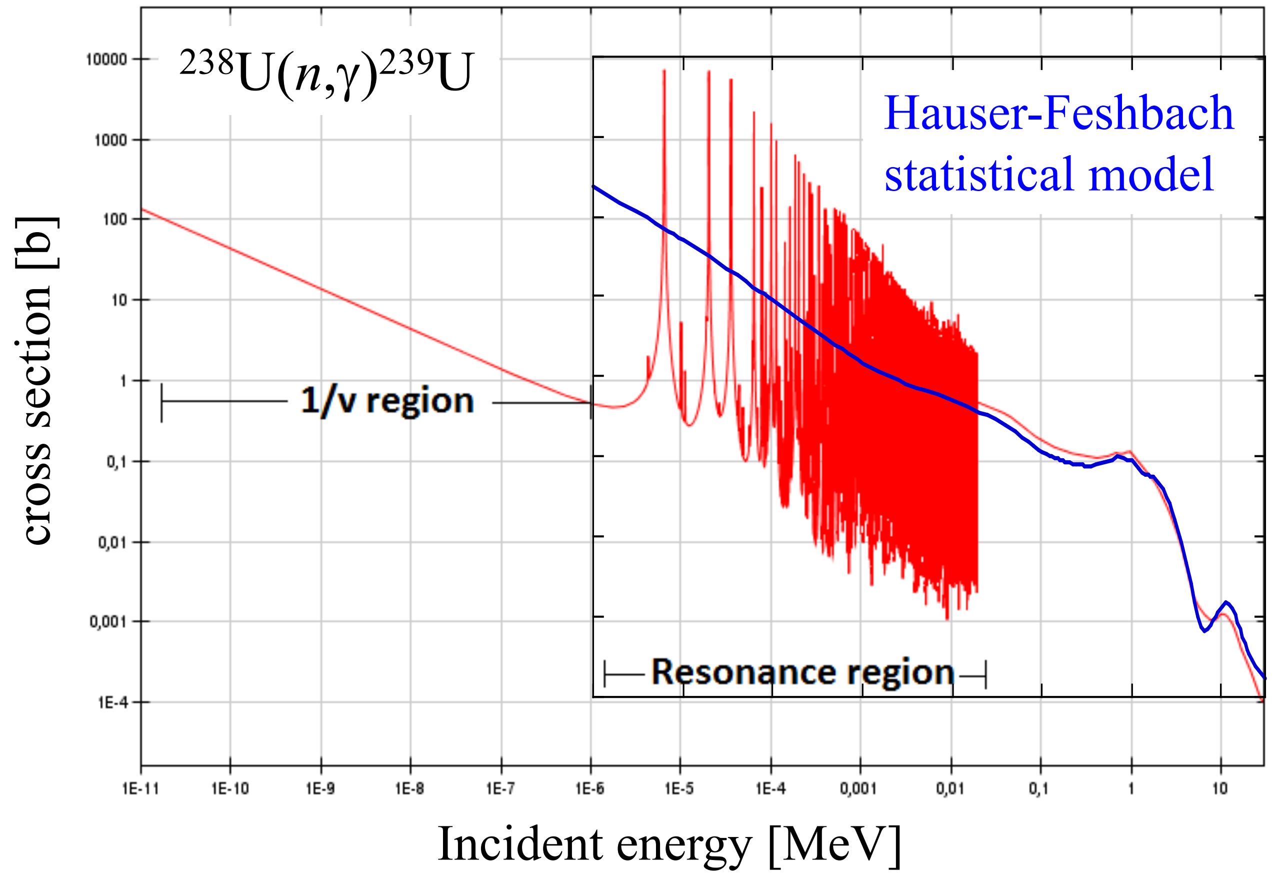
Application to cross section calculations still ongoing

Comparison of (n,γ) reaction rates at T=10^9K

Mic = BSkG3 masses – BSkG3+Comb NLD – D1M+QRPA PSF
Mac = FRDM masses – Cst-T+FG NLD – SMLO PSF



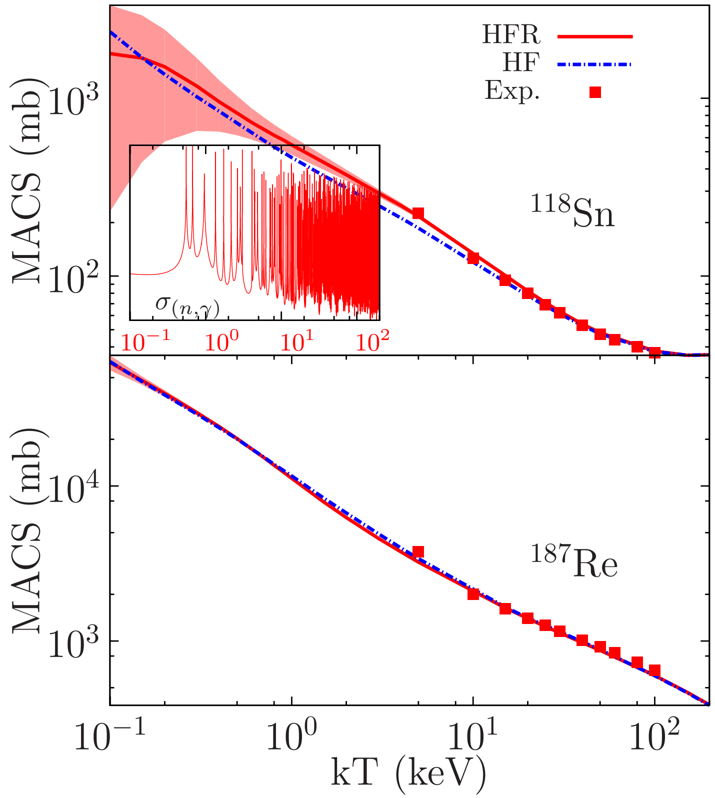
The High-Fidelity Resonance vs Hauser-Feshbach method to predict radiative n-capture cross section



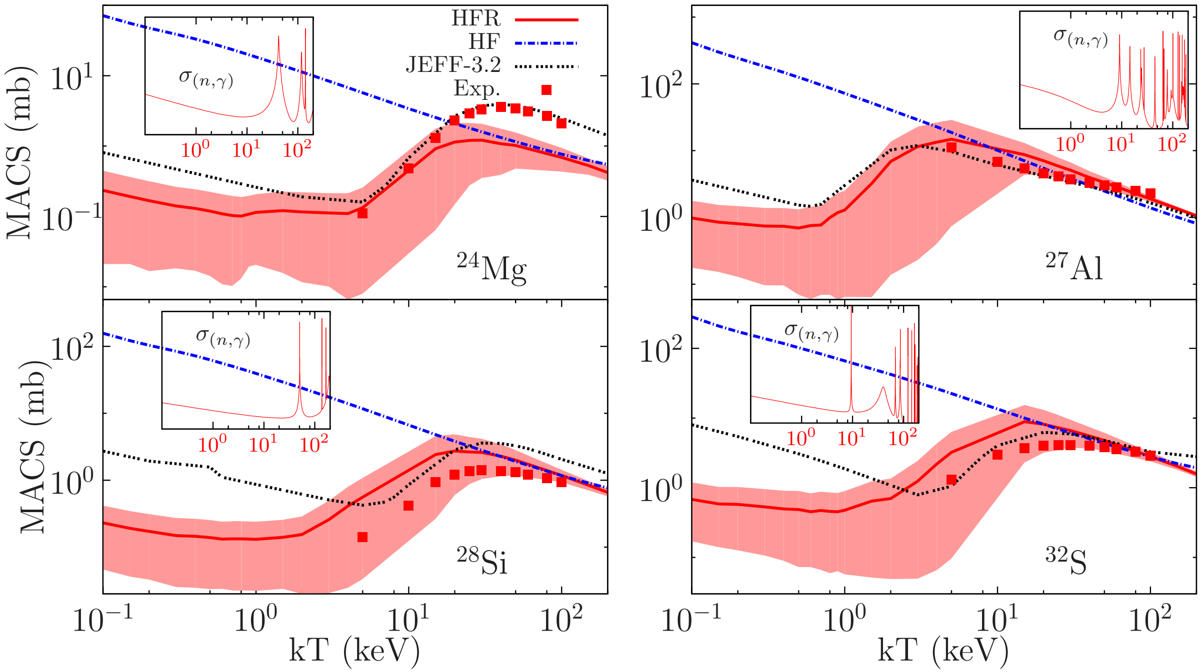
The High-Fidelity Resonance vs Hauser-Feshbach method to predict radiative n-capture cross section

HFR method: average parameters (the scattering radius, level spacing, reduced neutron width and the radiative width) are used to generate resolved resonances

Similar to HF for heavy nuclei



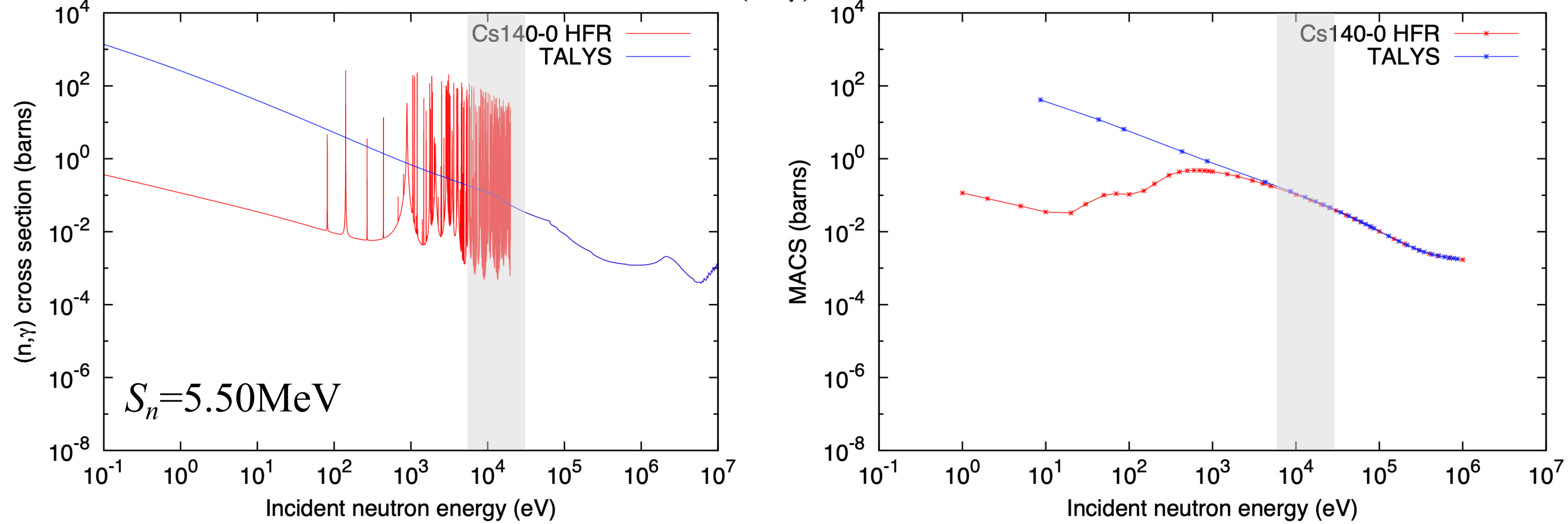
Improved description of MACS for light nuclei



Rochman et al. PLB 764, 109 (2017)

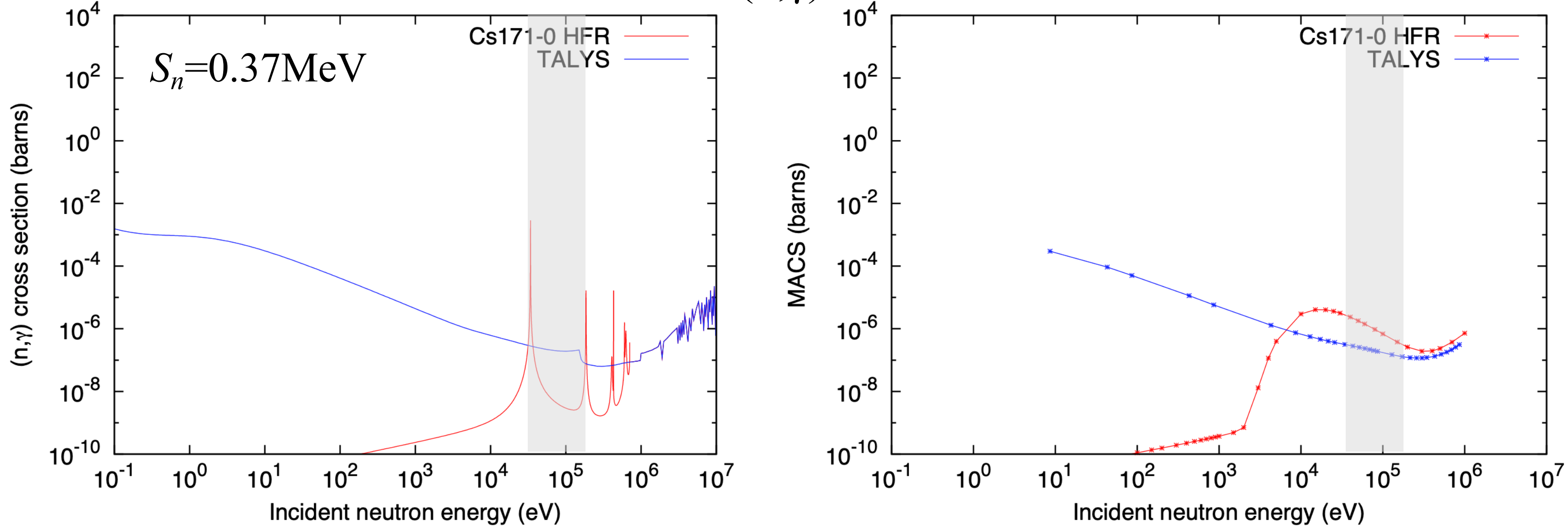
HF is a good approximation for nuclei close to stability

$^{140}Cs(n,\gamma)^{141}Cs$

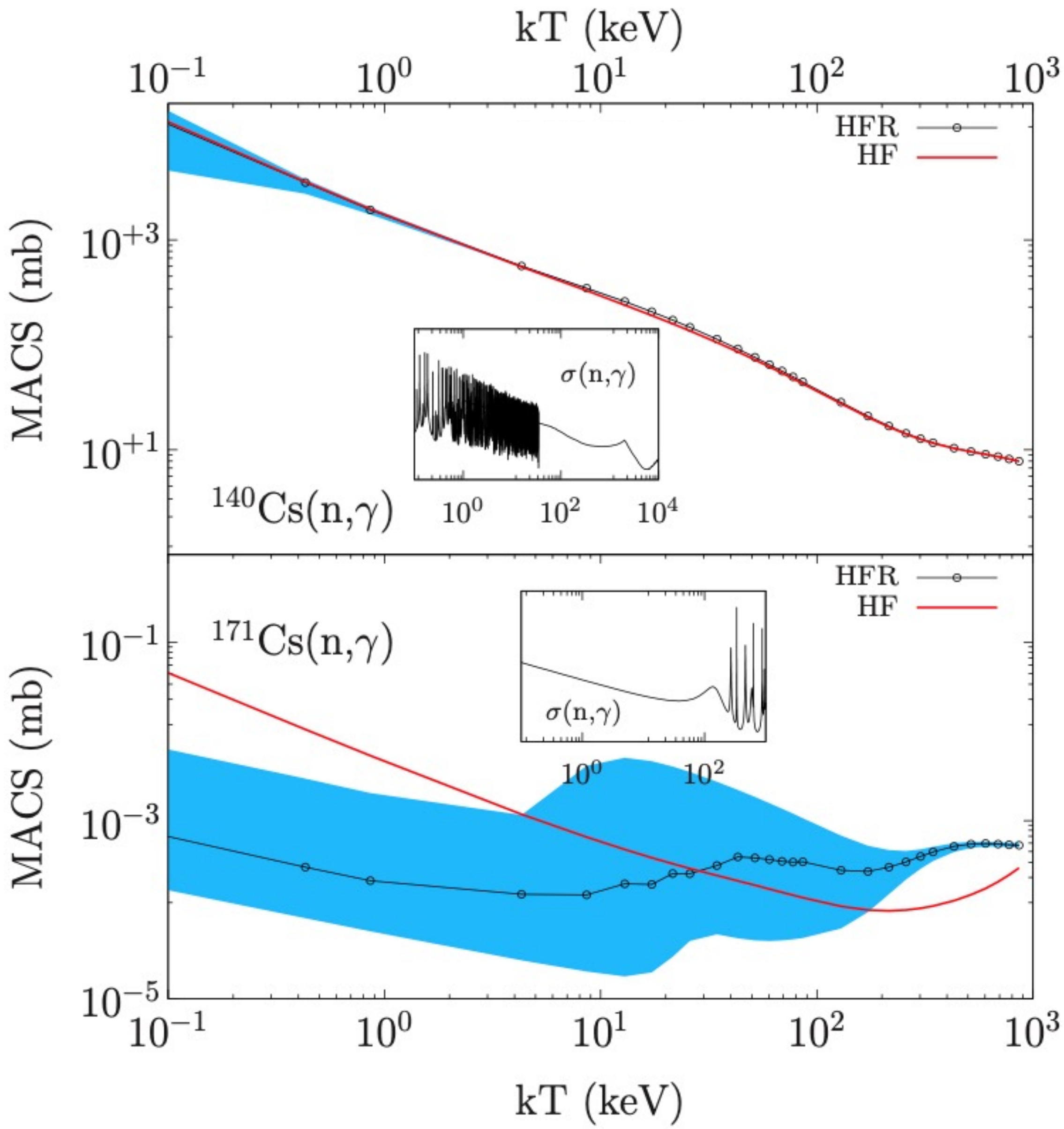


HF is not a good approximation for exotic n-rich nuclei

$^{171}Cs(n,\gamma)^{172}Cs$

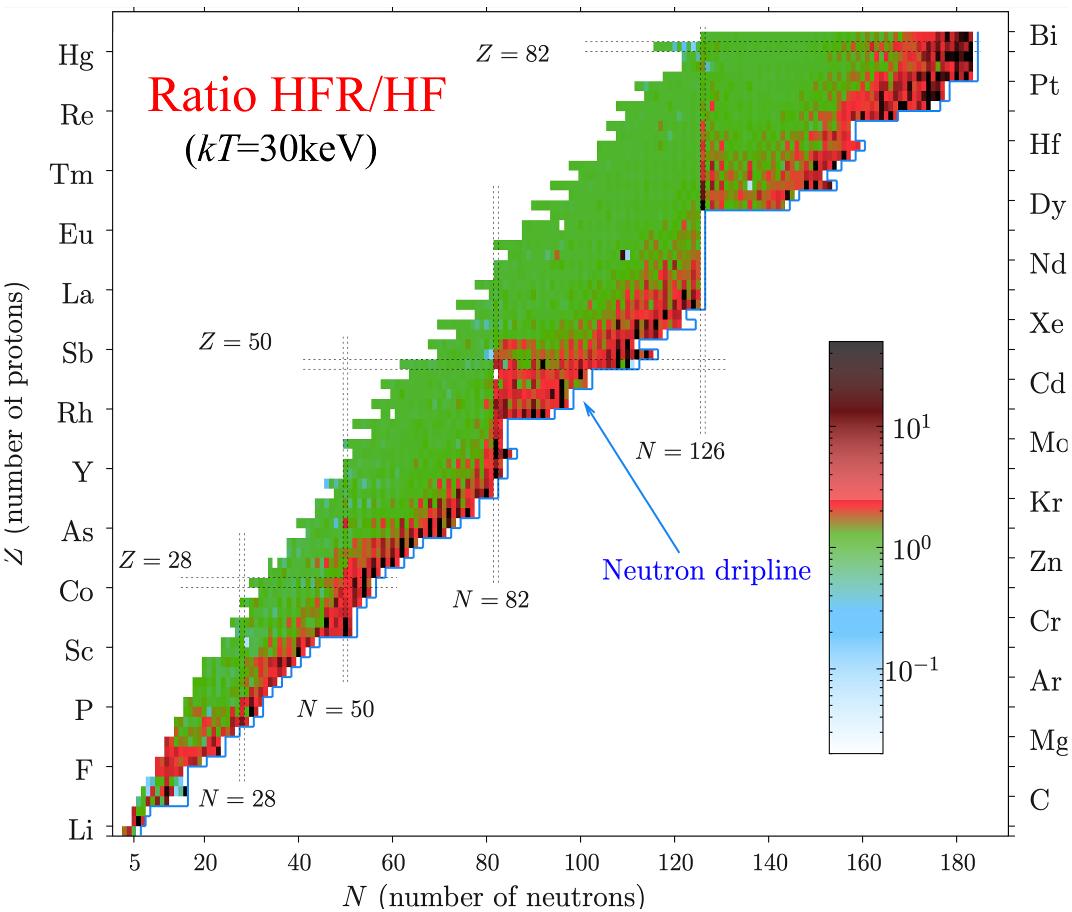


Uncertainty in the location of the resolved resonances



The High-Fidelity Resonance vs Hauser-Feshbach method to predict radiative n-capture cross section

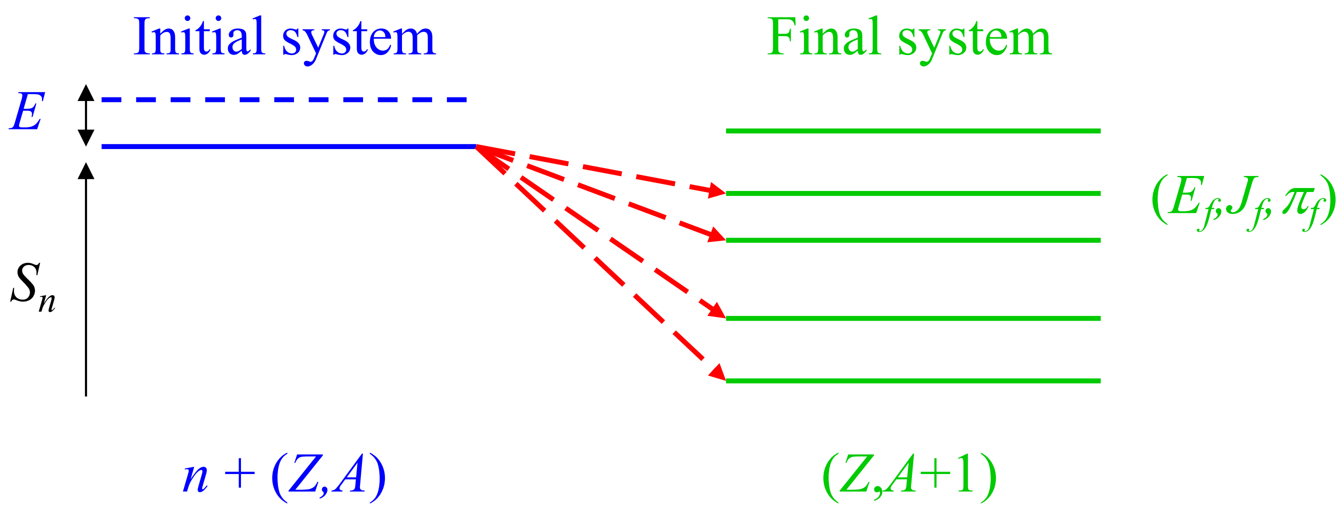
HFR method: average parameters (the scattering radius, level spacing, reduced neutron width and the radiative width) are used to create resolved resonances



HFR > HF for n-rich nuclei (up to ~ 1000)

Direct captures

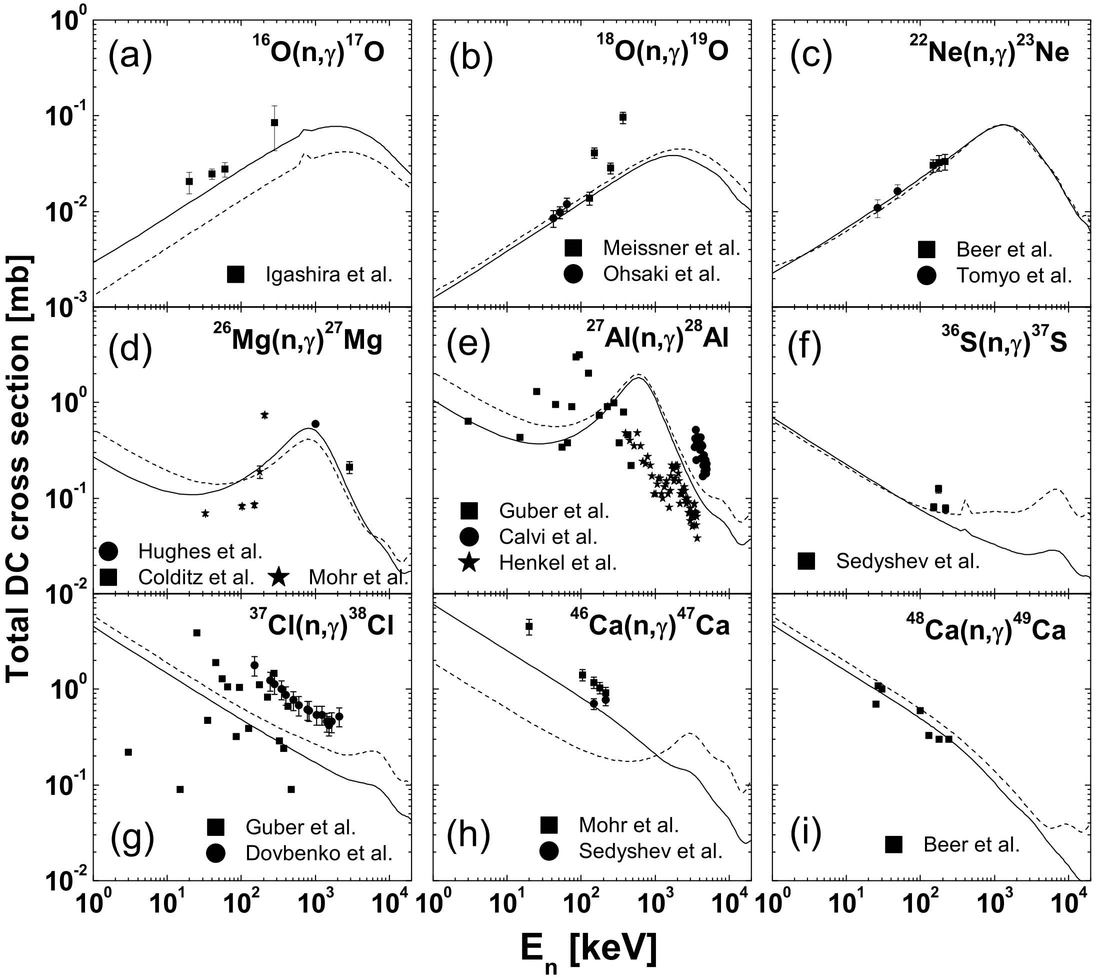
Direct scatter of incoming neutrons into a bound state without formation of a Compound Nucleus (particularly important for light and low-S_n n-rich nuclei)



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

- spectroscopy of low-excited states (E_f, J_f, π_f), including the spectroscopic factor of each excited state, n-nucleus interaction potential

TALYS calculation of Direct Captures



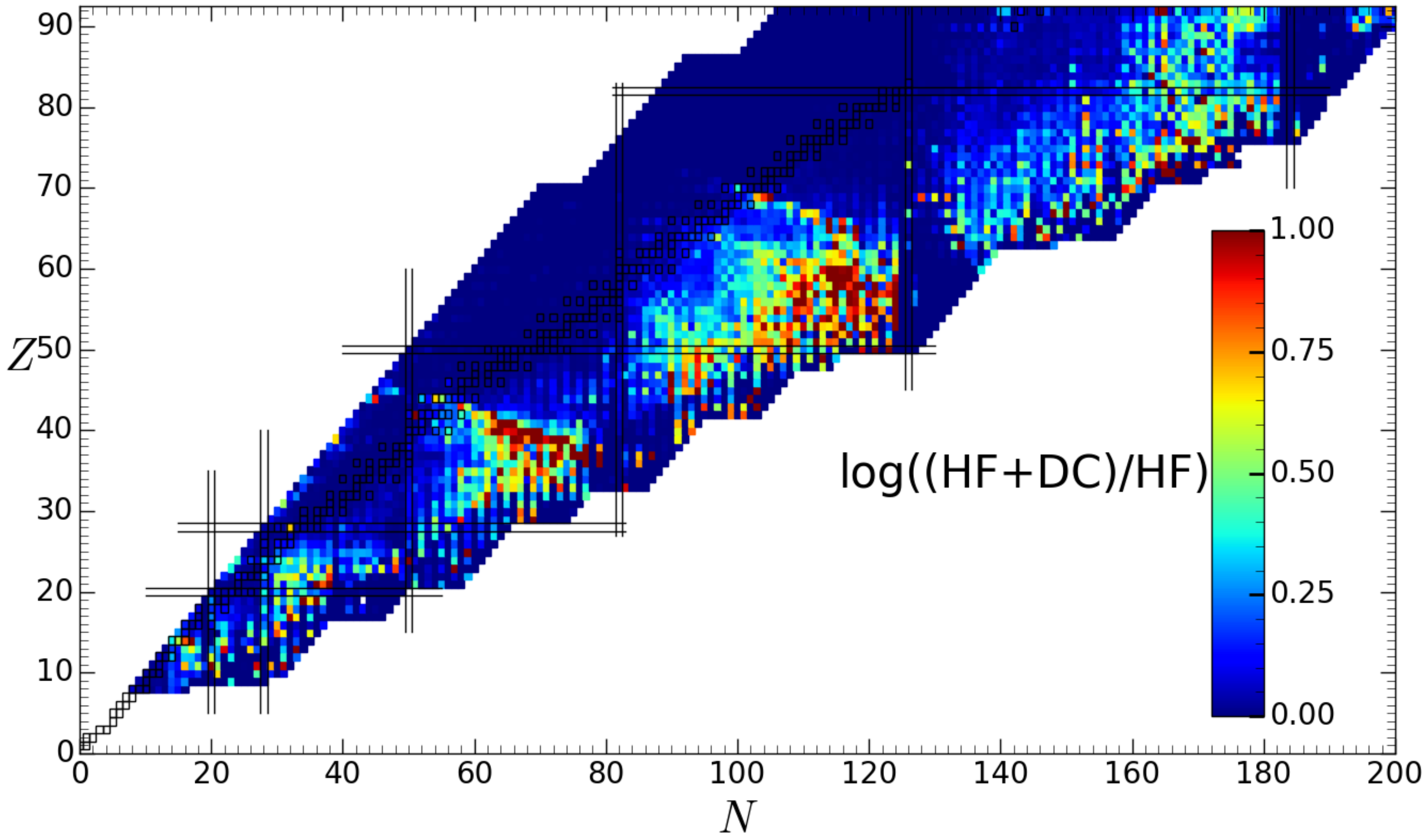
——— including experimental level and known S_f

- - - - theoretical predictions: 1p-1h NLD and $<S_f>=1$

Y. Xu & SG, PRC86, 045801 (2012)
K. Sieja & SG, EPJA57, 110 (2021)

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

TALYS calculation

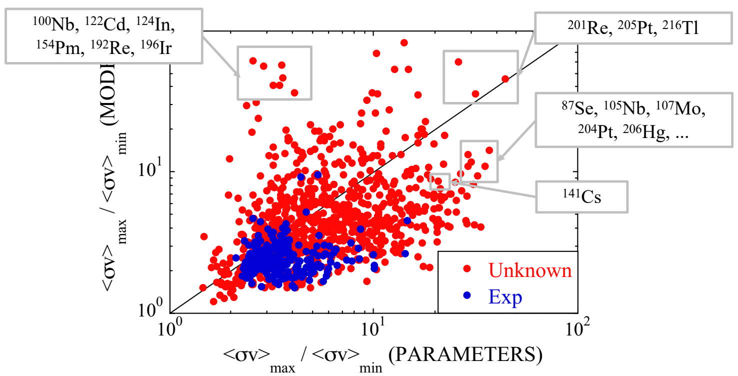


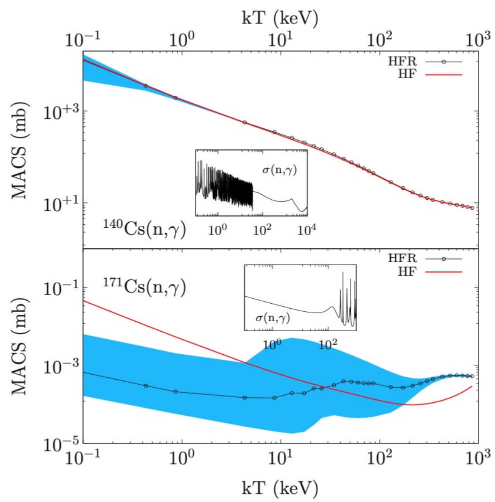
Still many uncertainties in DC estimates (level scheme, SF, OMP…)

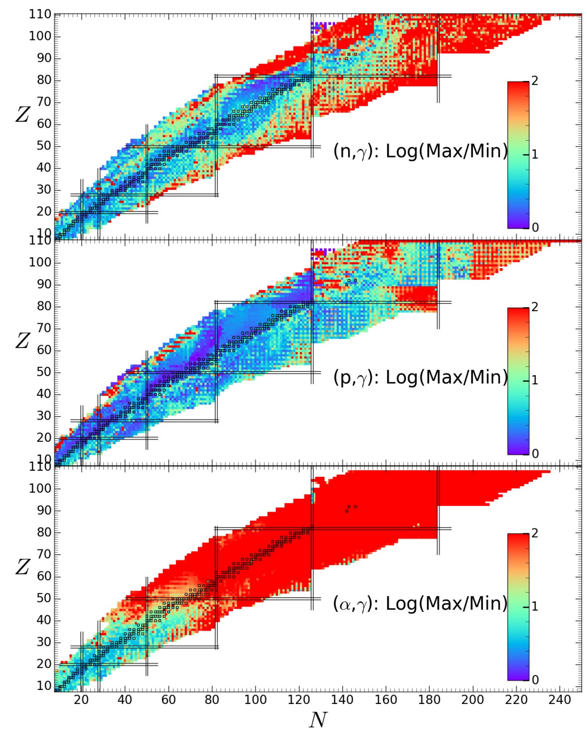
Still many uncertainties associated with NP inputs

- **Improved MF models for nuclear inputs to the reaction model**
  - GS properties: correlations, odd-A, triaxiality
  - Fission: 3D fission paths, NLD at the saddle points, FFD
  - E1/M1-strength functions: PR, ε_γ=0 limit, T-dep, PC, J^π-dep
  - Nuclear level Densities: low-E, correlations, pairing, vib-rot
  - Optical potential: low-E isovector imaginary n-OMP, α-OMP below Coulomb barrier

- **Reaction model**
  - HF vs RR vs Direct capture







Conclusions

- **Major progress achieved and efforts ongoing**
  - Reaction model (e.g. TALYS)
  - inputs from MF, beyond MF, QRPA/FAM, SM, ab-initio
- **Selection of models for n-captures on short-lived nuclei according to**
  - Their reliability, *i.e.* their physical robustness

    e.g. avoid extrapolation with "macroscopic" models (or ML algorithms)
  - Their accuracy, *i.e.* capacity to reproduce experimental data

    e.g. SLO, GLO models of PSF should not be used

- **Updated experimental libraries to reduce parameter uncertainties**

  → A regularly-updated library of cross sections / rates

  in particular: n-, p-, α-captures, $\beta^{\pm}$/EC/α decay

  → A regularly-updated library of evaluated input parameters

  in particular: M, R_c, β_2, J^{π}, B_f, D_0, S_0, $<\Gamma_{\gamma}>$, PSF, NLD, OMP, ...

If we can describe relatively accurately known reaction rates,
we are still far from being able to predict ***reliably***
n-captures, and even less fission, of exotic short-lived nuclei
BUT progress is being made

THANK YOU
FOR
YOUR ATTENTION