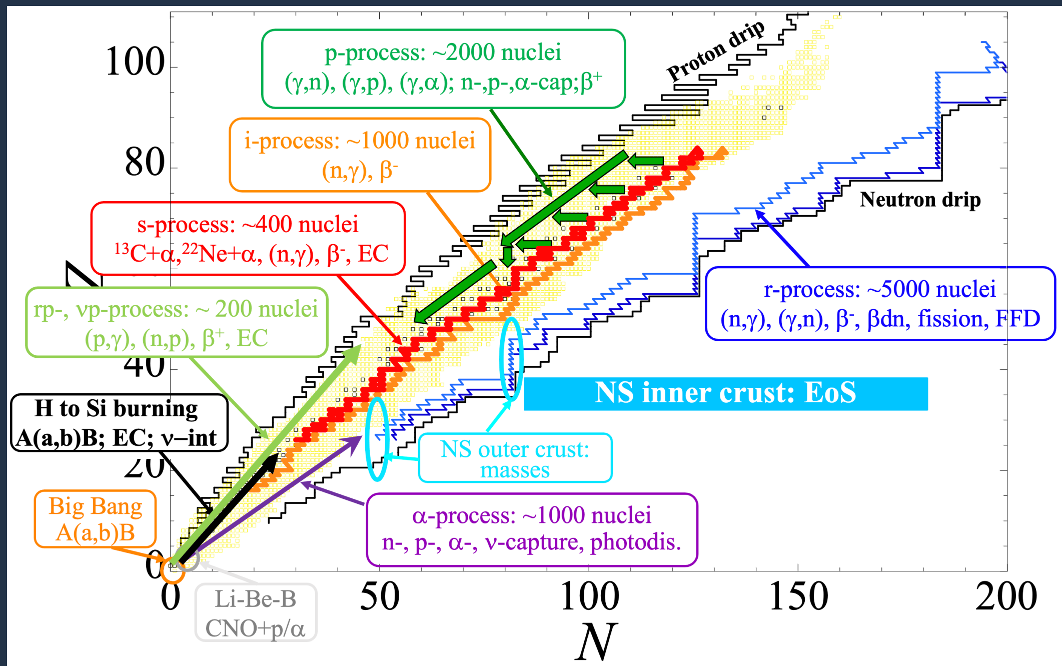
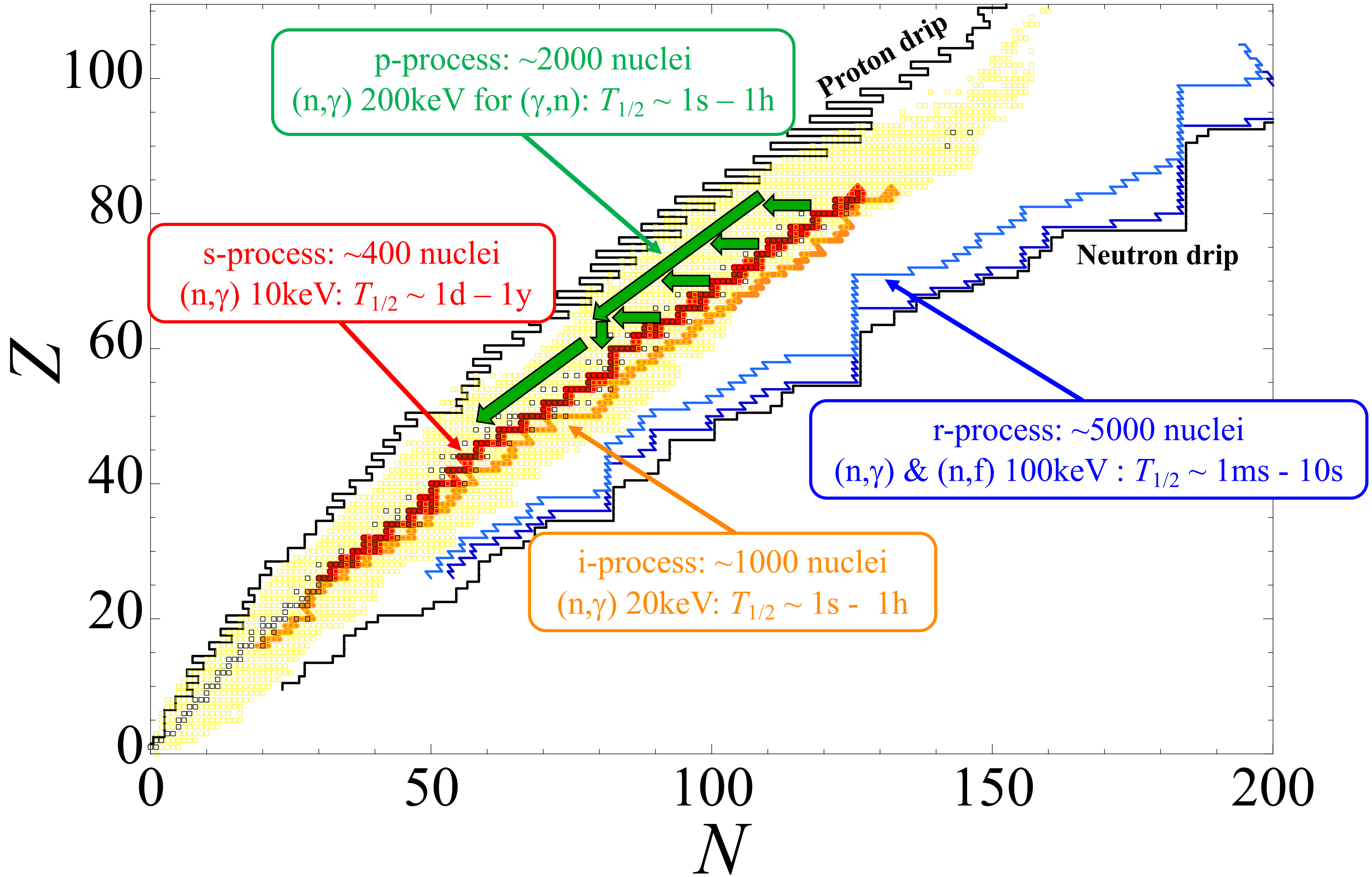
Predicting radiative neutron captures

S. Goriely (IAA-ULB)



In collaboration with
W. Ryssens, A. Sanchez, S. Martinet, A. Choplin, G. Grams, S. Hilaire, S. Péru, A Koning, D. Rochman

Neutron-induced reaction for nucleosynthesis applications

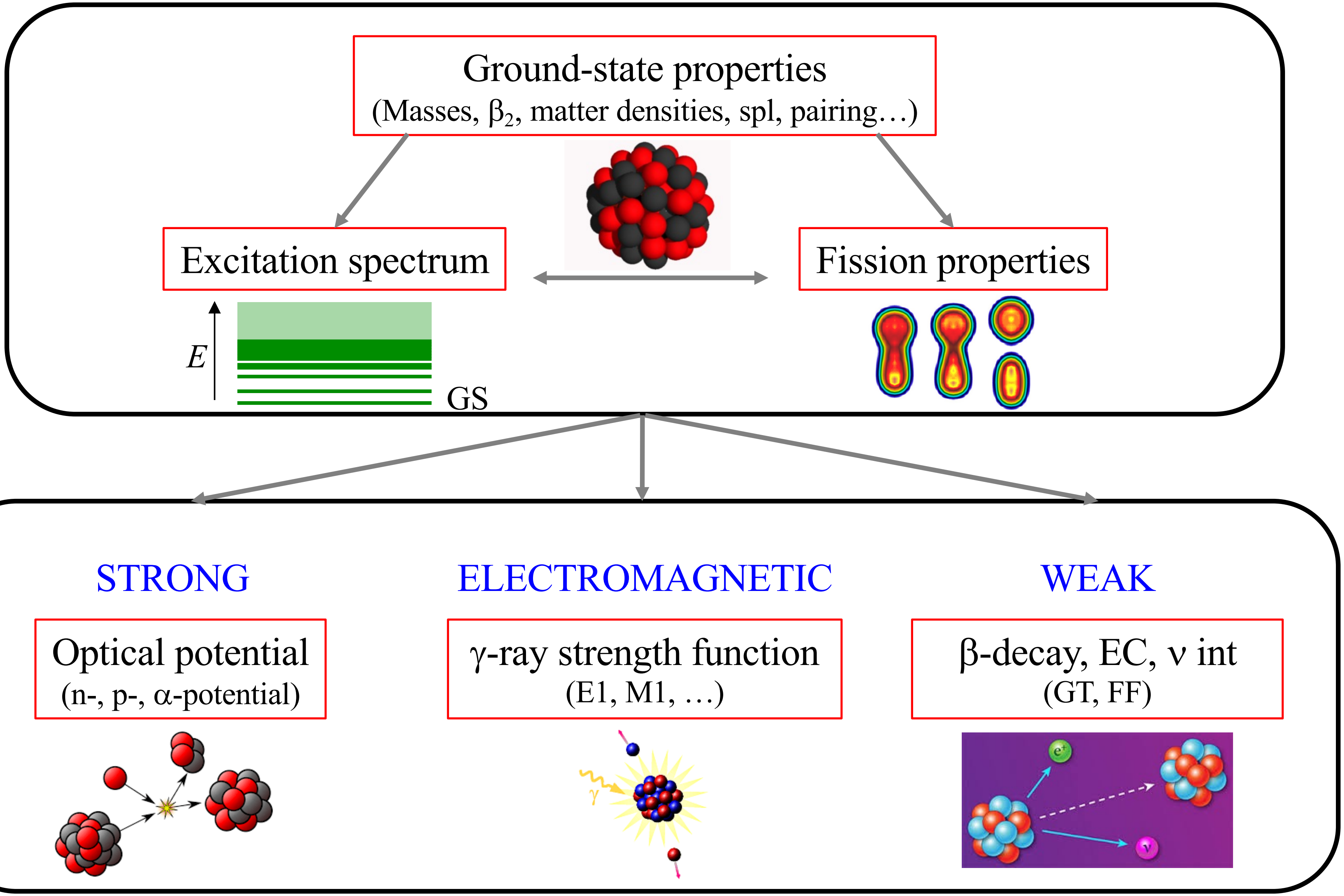


Only direct experimental data for the s-process → Theory needs to fill the gaps

Not everything is "crucial": How accurate should the predictions be ?

How do nuclear uncertainties affect astrophysics observables ?

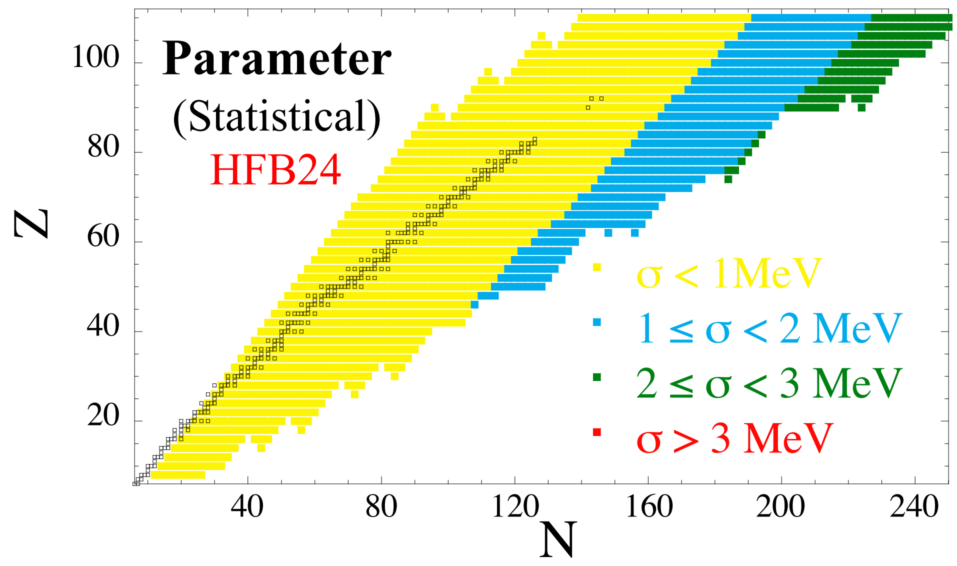
Nuclear inputs to nuclear reaction & decay calculations

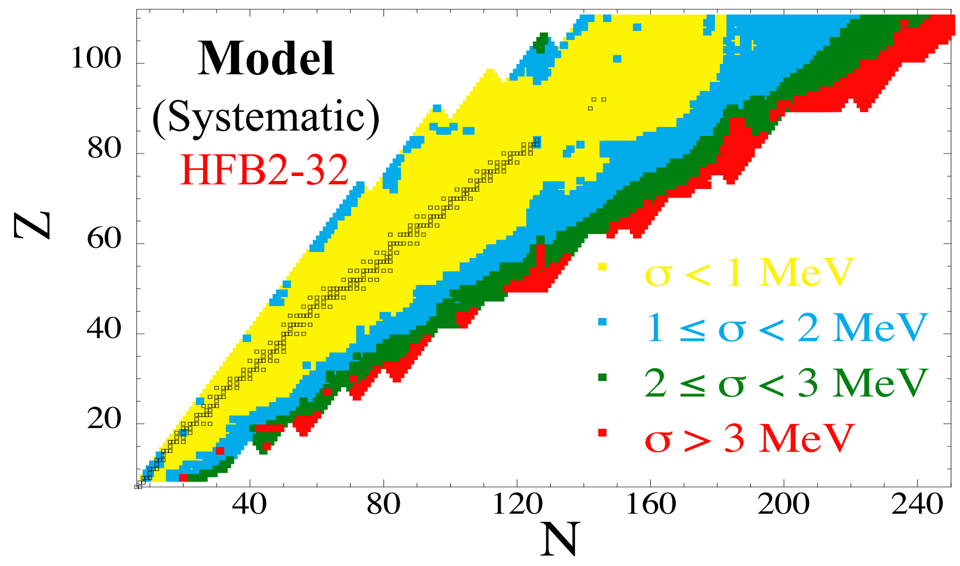


Quantification of nuclear uncertainties

Some progress in considering "theoretical nuclear uncertainties" in NA

Two types of uncertainties affecting theoretical inputs (e.g Masses)





Model or parameter variations must be constrained by experimental data

e.g Only *parameter* variations s.t. $\sigma_{rms} < 0.8$ MeV ⟺ Only mass *models* s.t. $\sigma_{rms} < 0.8$ MeV

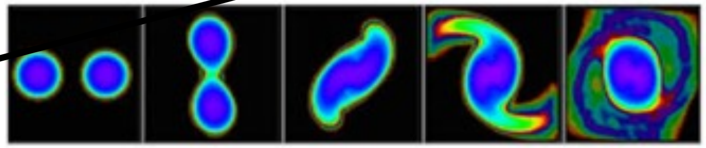
Only NLD/PSF *parameters* s.t. (n,γ) with $f_{rms} \leq 2$ ⟺ Only NLD/PSF *models* s.t. (n,γ) with $f_{rms} \leq 2$

Uncorrelated parameter variations

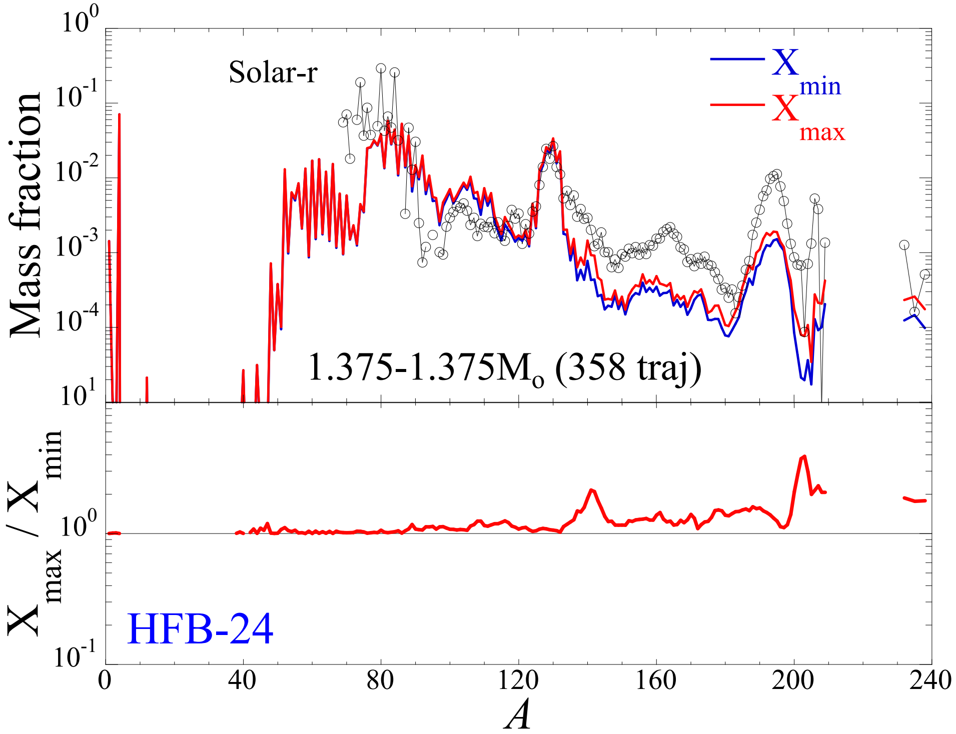
Masses/rates correlated by the model

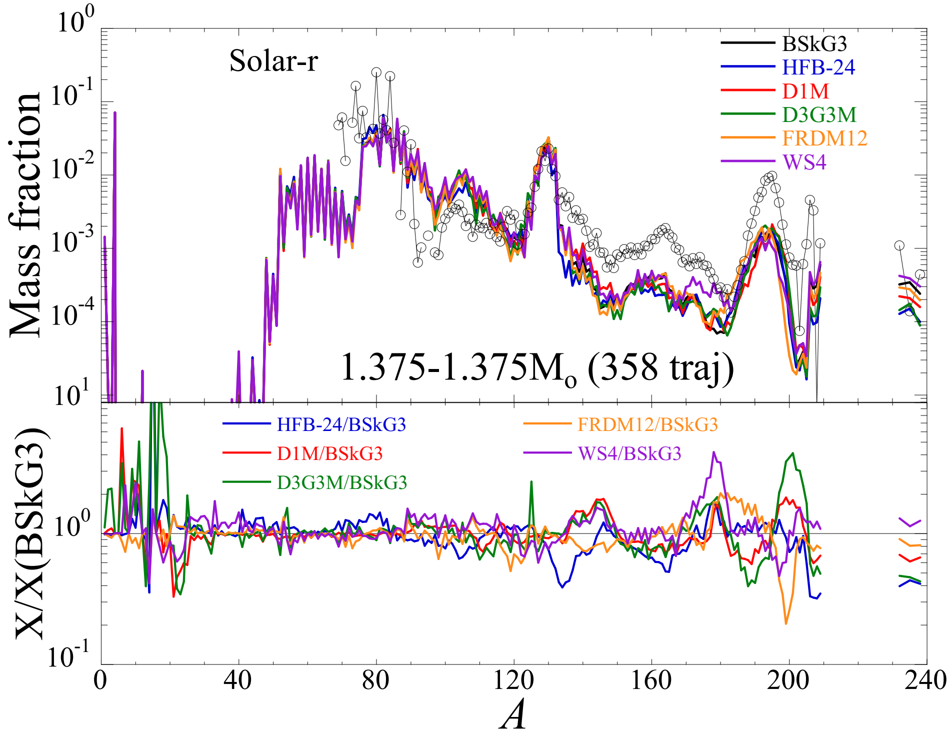
But what about their impact on astrophysical observables ?

Propagation of Mass uncertainties into NSM simulations



Uncorrelated *Parameter* uncertainties | Correlated *Model* uncertainties





- MC approach if uncorrelated uncertainties
- Additional correlations may exist, e.g S_n and M
- Parameters changes must be constrained by exp

- MC approach not correct
- Coherent model-correlated uncertainties
- Each model is affected by parameter unc.

S. Martinet et al. Astronomy and Astrophysics 694, A180 (2025)

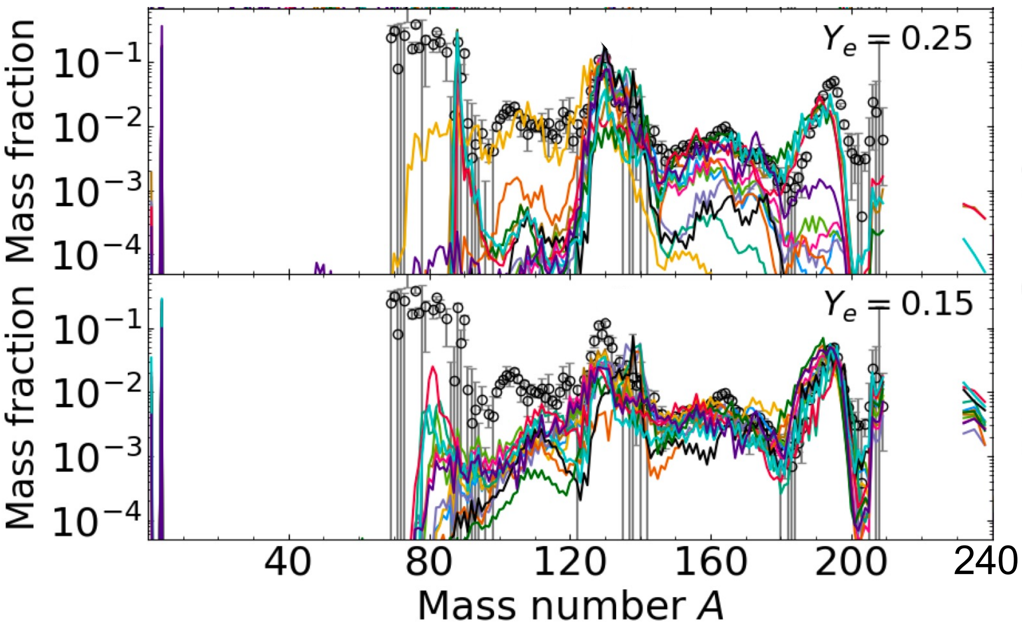
Impact of nuclear *model* uncertainties on the composition of NSM ejecta

15 different "acceptable" sets of nuclear inputs (masses, β-decay, n-capture, fission)

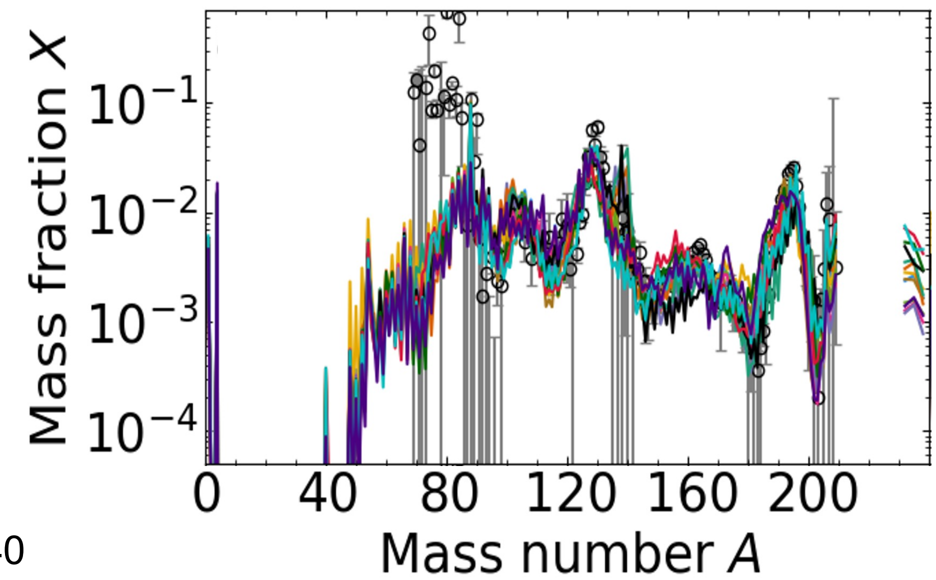
Kullmann et al. (2022)

Prompt dynamical ejecta: 1.35-1.35M_o (Bauswein 2022)

Single trajectory



Multiple trajectories



Global & Local discrepancies

Local (correlated) discrepancies

Astrophysical models evolve and may still not be robust

(what is "important" today may not be next year)

Uncertainty propagation must be applied to a *representative sample* of trajectories for a given astrophysical observable

Main uncertainties to (n,γ) reaction for *i*-process

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

γ-ray strength function
(E1, M1, def-dep, T-dep, PC)

Experimental data

- Photoabsorption data
- ARC/DRC data
- Oslo/NRF data
- MACS (though NLD dep)

Models

- Standard Lorentzian
- Modified Lorentzian
- Skyrme-HFB+QRPA
- Gogny-HFB+QRPA
- RMF+RRPA
- Beyond QRPA / Shell Model

Parameter adjustment

- Analytical: GR (E_0 Γ_0 σ_0), ...
- Tables: *etable, ftable, wtable*

Nuclear Level Densities
(E-, J-, π-dep., collective enh., …)

Experimental data

- Low-lying levels
- *s*/*p*-wave resonance spacings
- Oslo data
- MACS (though PSF dep)

Models

- Constant-T + BSFG
- BSFG
- HFBCS+statistical
- HFB+combinatorial
- Moments methods
- Shell model

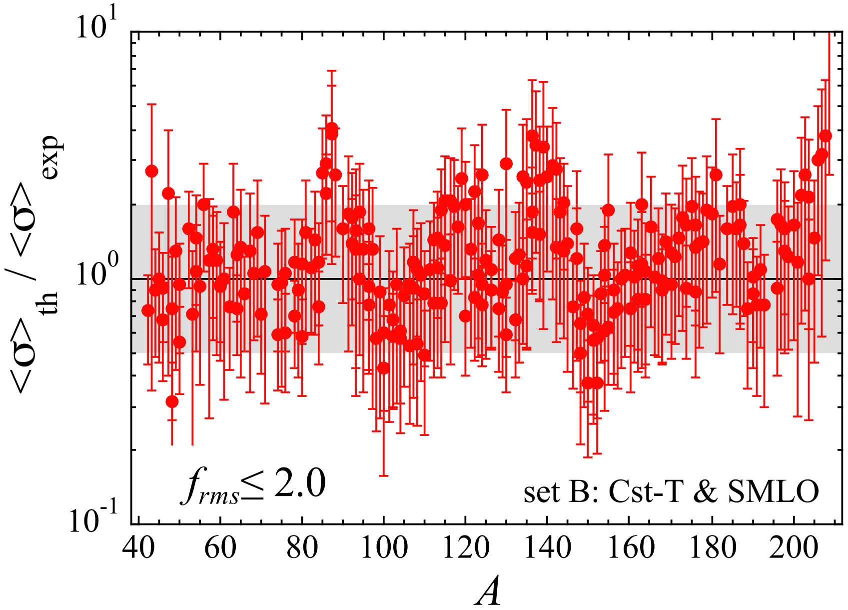
Parameter adjustment

- Analytical: a, Δ, T, δW, ...
- Tables: α and δ

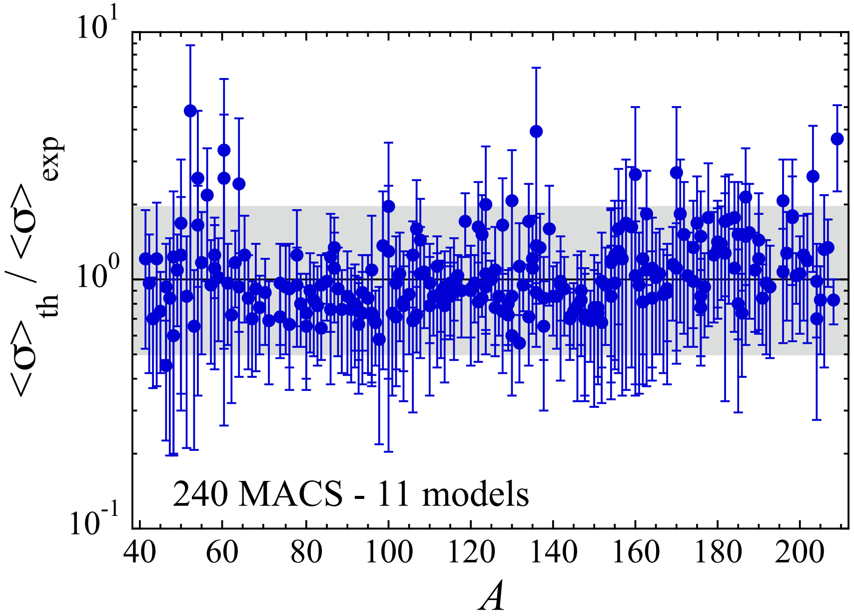
TALYS prediction of the 240 experimental MACS

$20 \leq Z \leq 83$

Uncorrelated parameter uncertainties



Correlated model uncertainties



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

  (Backward Monte Carlo)

- Experimental info on M, NLD, PSF
- 11 different models of NLD, PSF

  Inclusion or not of DC
- All with $f_{rms} \leq 1.4 - 2.0$

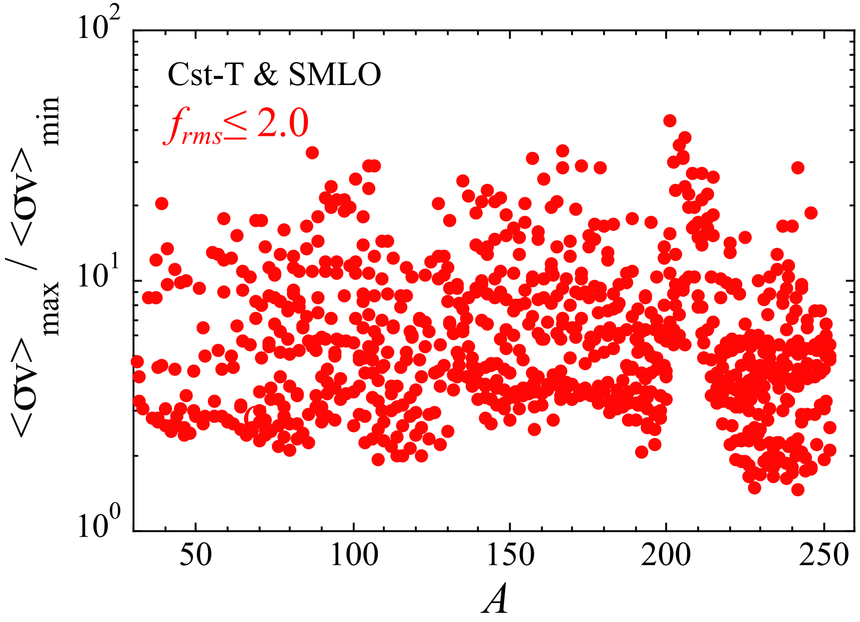
$$f_{rms} = \exp\left[\frac{1}{N_e}\sum_{i=1}^{N_e}\ln^2\frac{\langle\sigma\rangle_{th,i}}{\langle\sigma\rangle_{exp,i}}\right]^{1/2}$$

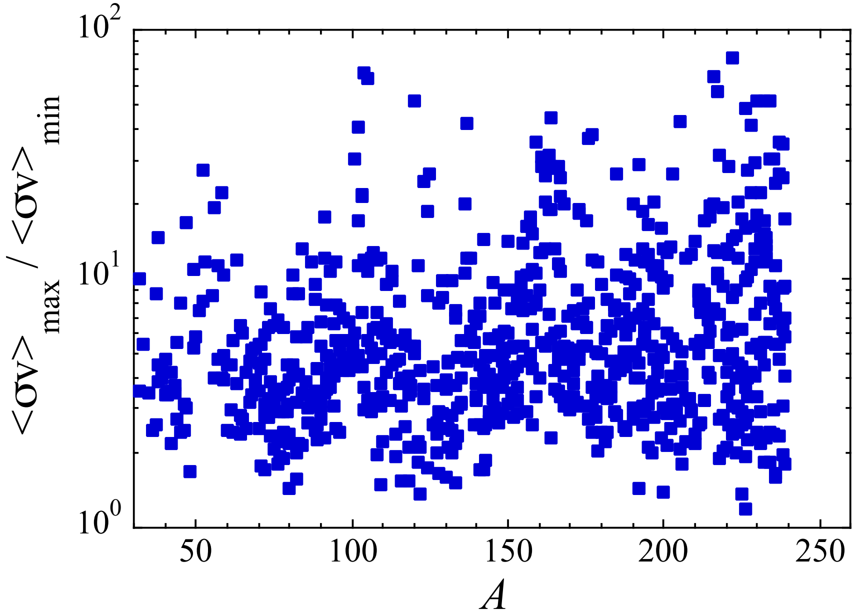
S. Martinet et al. Astronomy and Astrophysics 684, A8 (2024)

Propagation of uncertainties to 863 (n-rich) unknown MACS

$14 \leq Z \leq 98$

Uncorrelated parameter uncertainties	*Correlated model* uncertainties





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

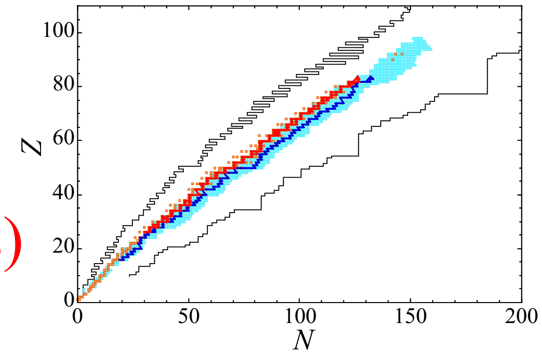
  (Forward Monte Carlo)

- Experimental info on M, NLD, PSF
- 11 different models of NLD, PSF

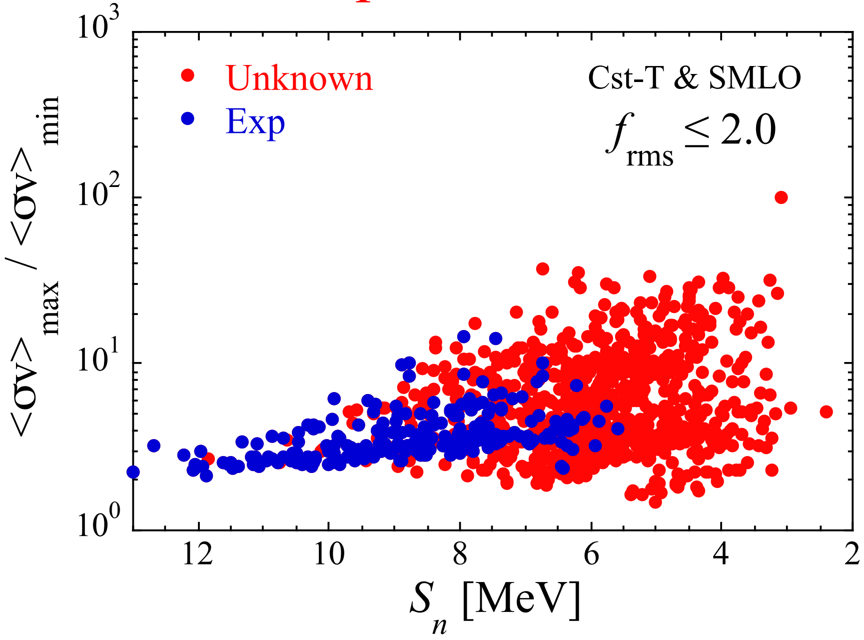
  Inclusion or not of DC
- All with $f_{rms} \leq 1.4 - 2.0$

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

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

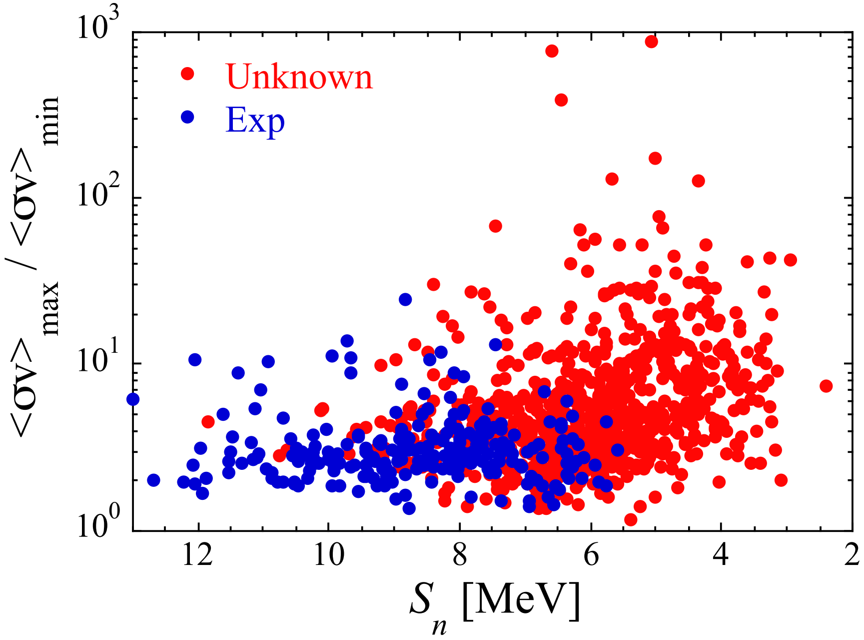


Uncorrelated parameter uncertainties



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

Correlated model uncertainties

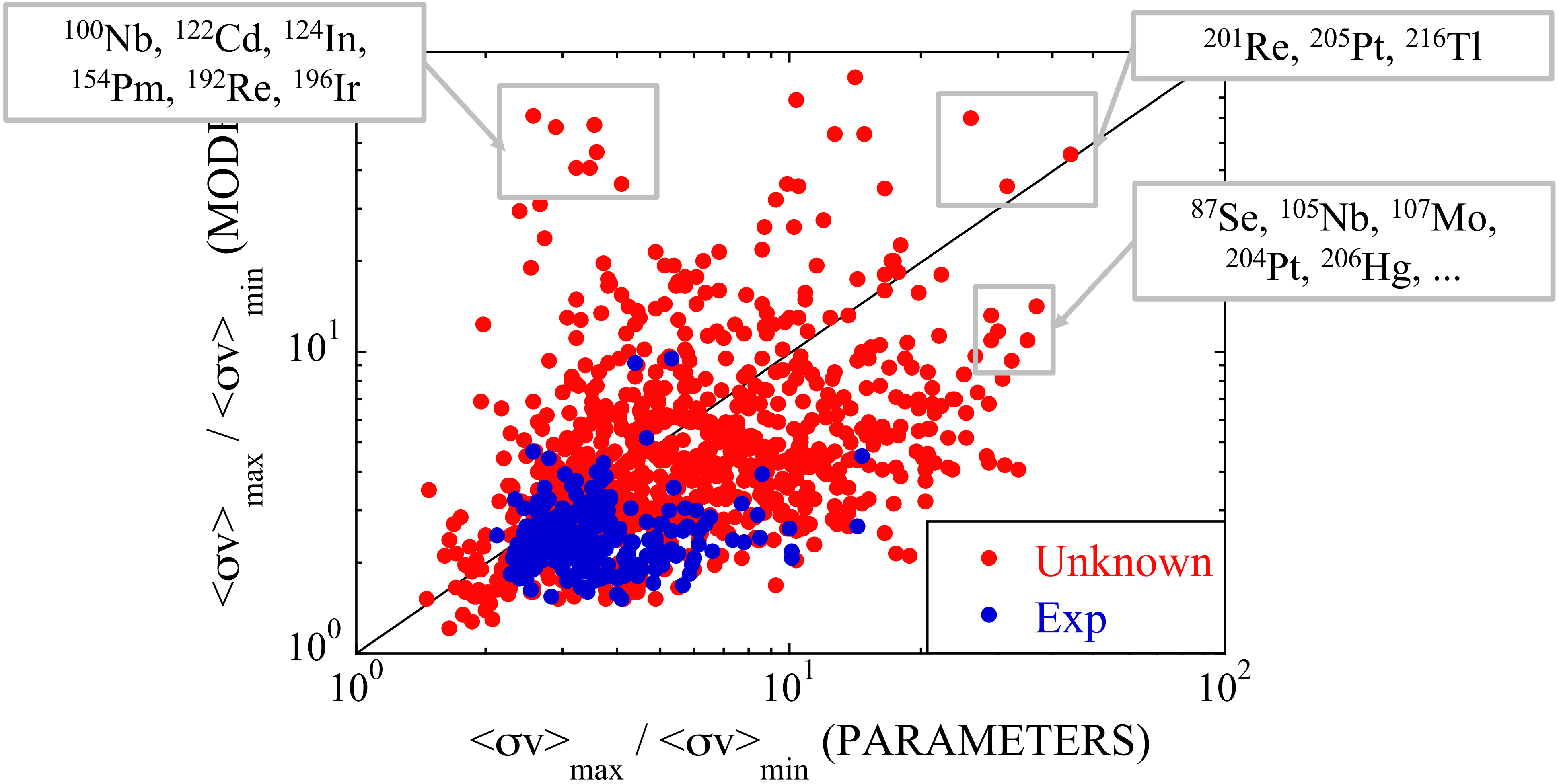


- Experimental info on M, NLD, PSF
- 11 different models of NLD, PSF
- All with $f_{rms} \leq 2.0$

Uncorrelated Parameter Uncertainties ~ Correlated Model Uncertainties

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

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



Uncorrelated Parameter Uncertainties ~ Correlated Model Uncertainties

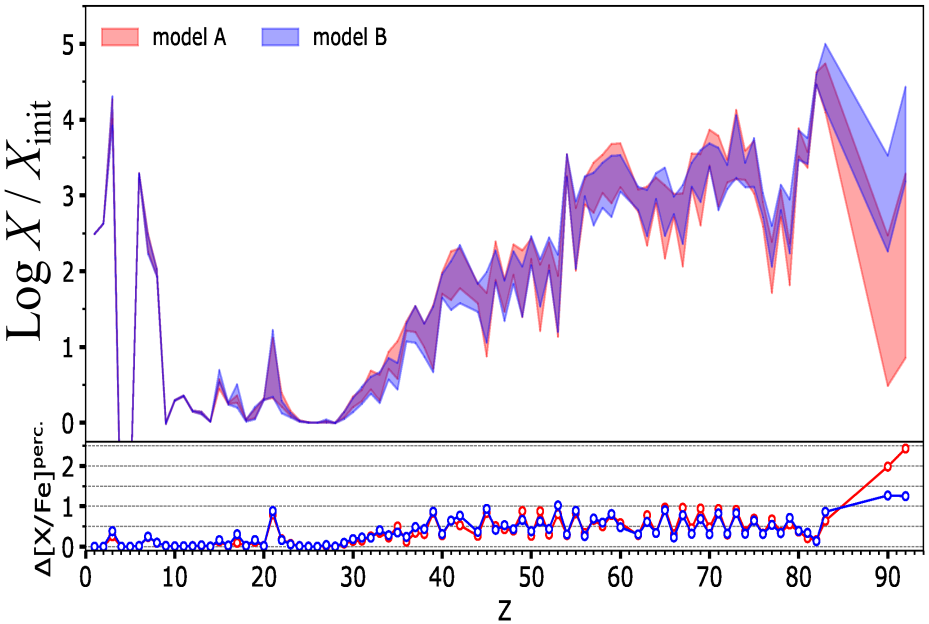
Same order of magnitude, BUT individually can be very different !!

Impact of on the i-process nucleosynthesis in low-Z low-M AGB stars

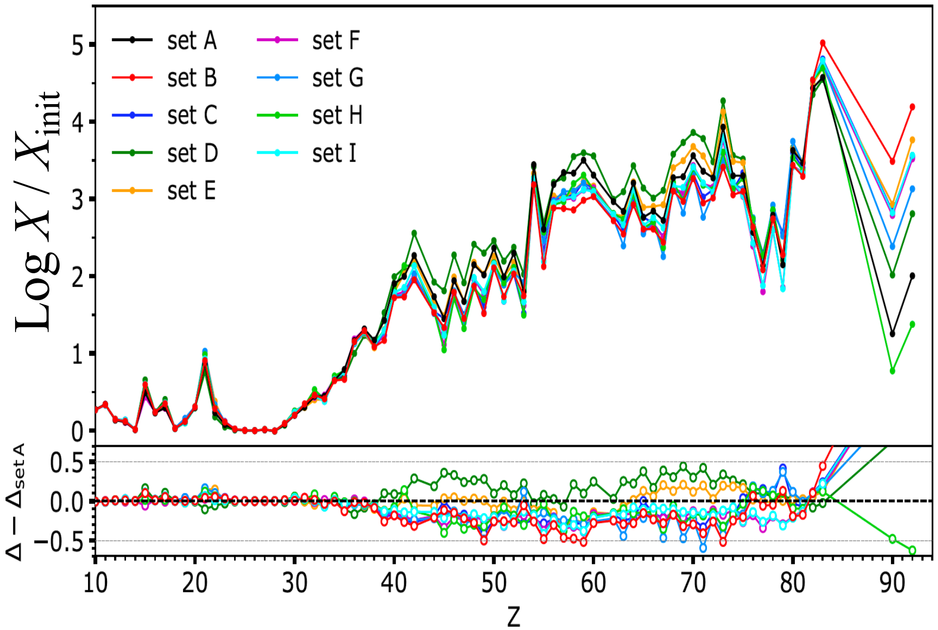
Surface abundances in a $1M_o$ [Fe/H]=-2.5 AGB star

(Martinet et al. 2024)

Uncorrelated *Parameter* uncertainties

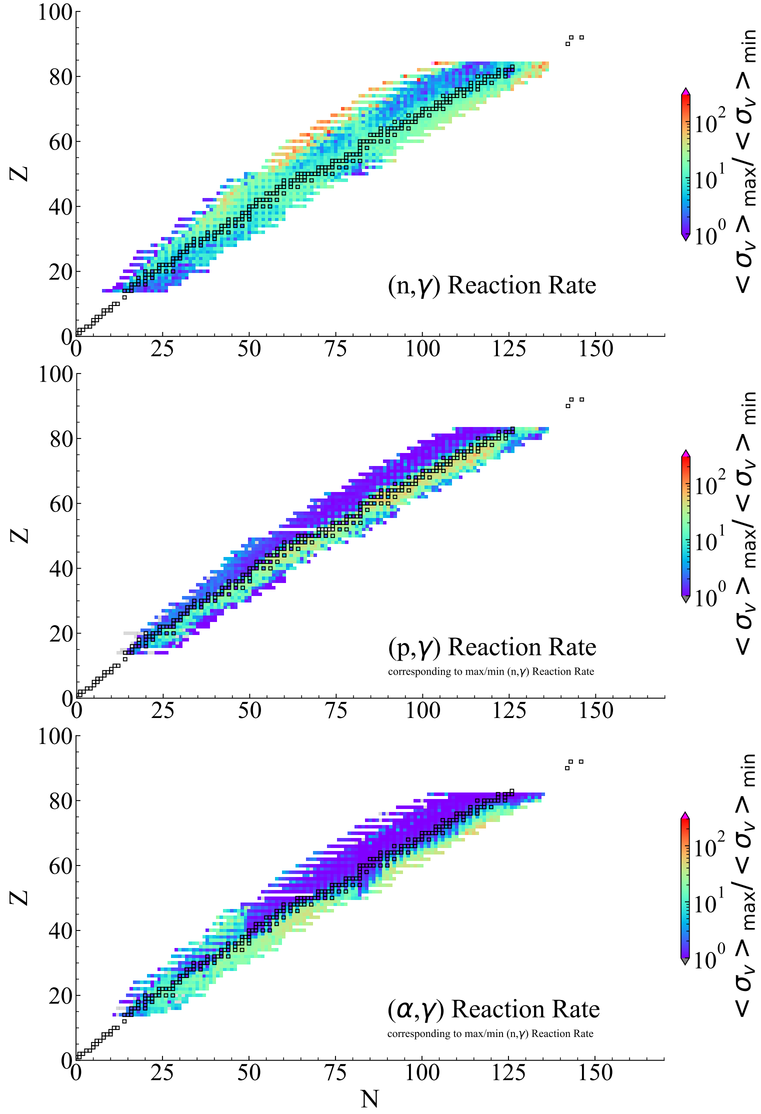


Correlated *Model* uncertainties

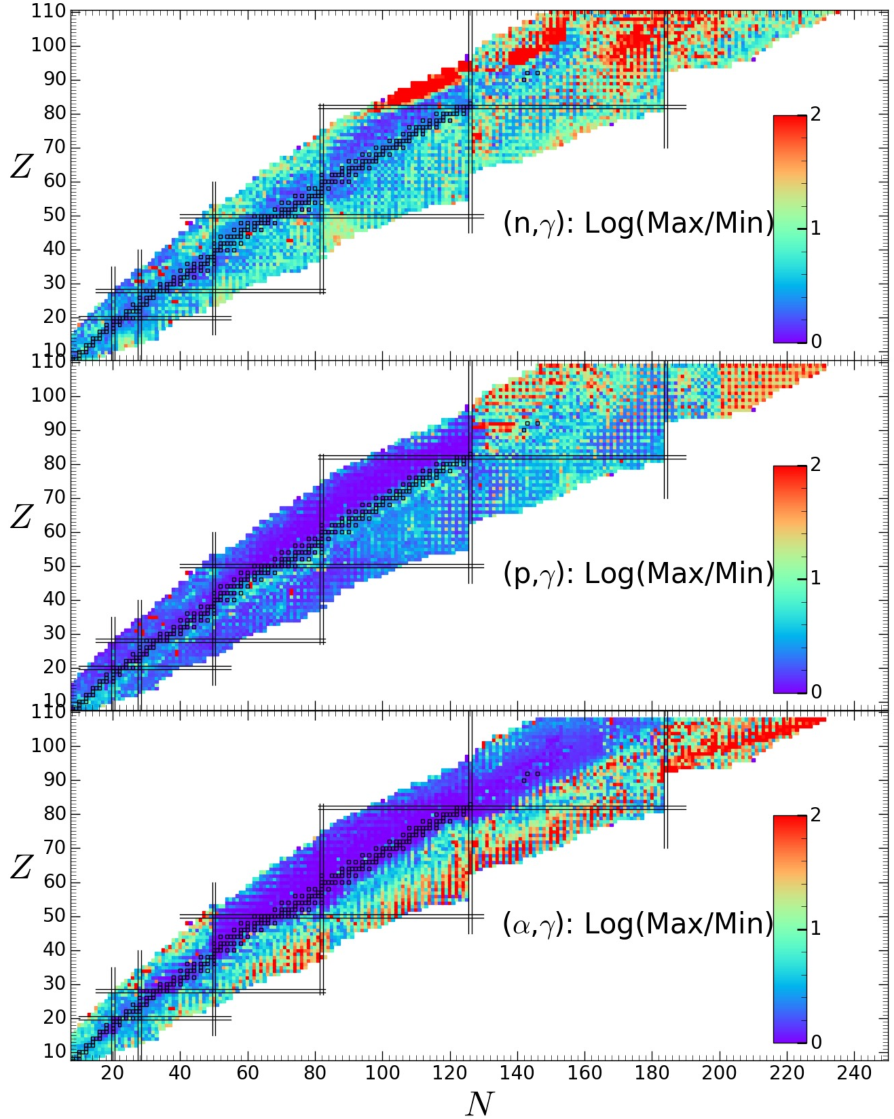


Impact of NLD/PSF uncertainties on the (n,γ), (p,γ), (α,γ) rates

Uncorrelated *Parameter* uncertainties



Correlated *Model* uncertainties



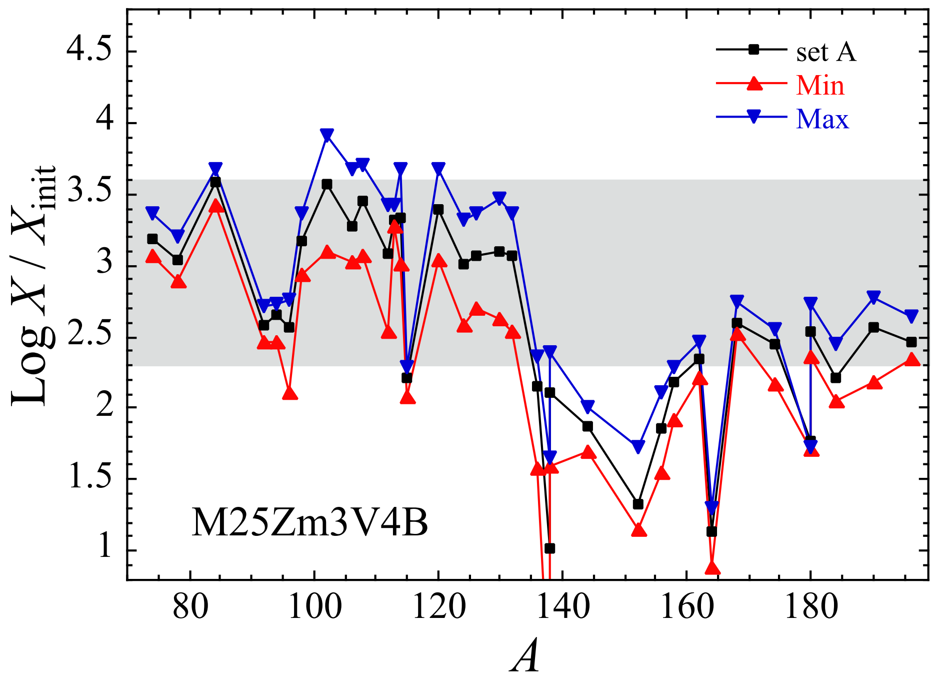
Impact of NLD/PSF uncertainties on the p-process nucleosynthesis

Overproduction of p-nuclei in the core of an exploding $25M_o$ Z=0.001 v/v_c=0.4 star

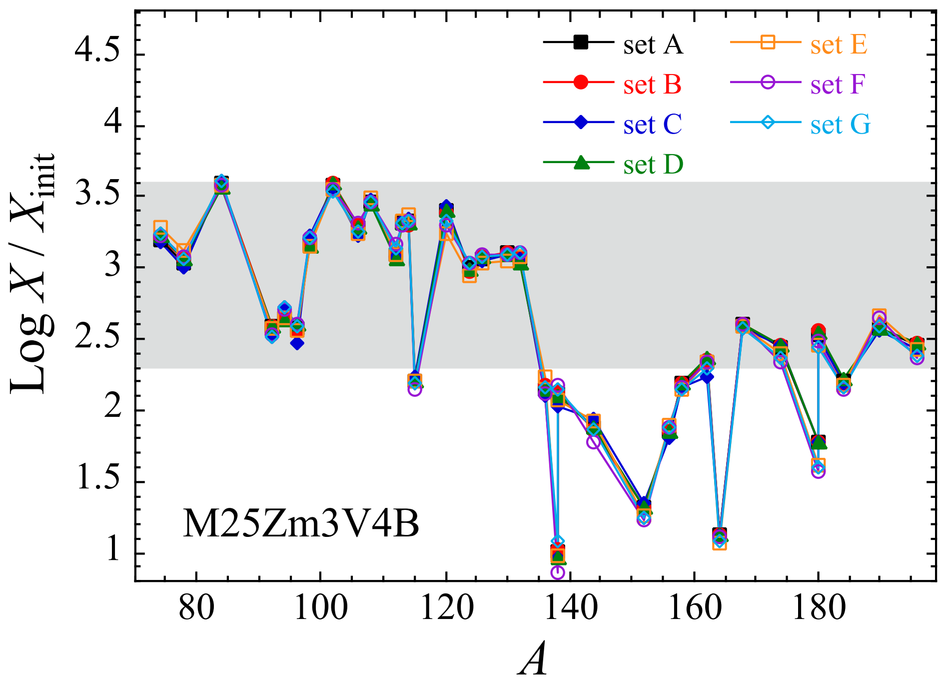
(Choplin et al. 2022)

Uncorrelated *Parameter* uncertainties

Highly dominated by (γ,n) parameter uncertainties



Correlated *Model* uncertainties

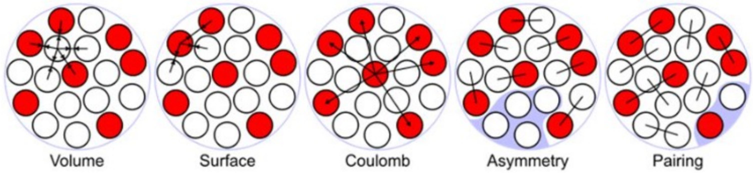


Reduction of the *model* & *parameter* uncertainties through

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

Improved nuclear models: towards microscopic predictions (at least for astrophysics applications)

MACROSCOPIC DESCRIPTION

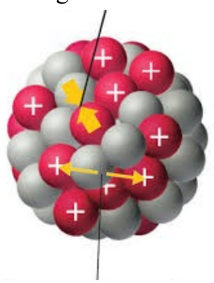


$$E_B = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \Delta(Z,N)$$

Mic-Mac models still widely used in many nuclear applications for Mass, NLD, PSF, OMP, Fission, β-decays, ...

GLOBAL MEAN-FIELD DESCRIPTION

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



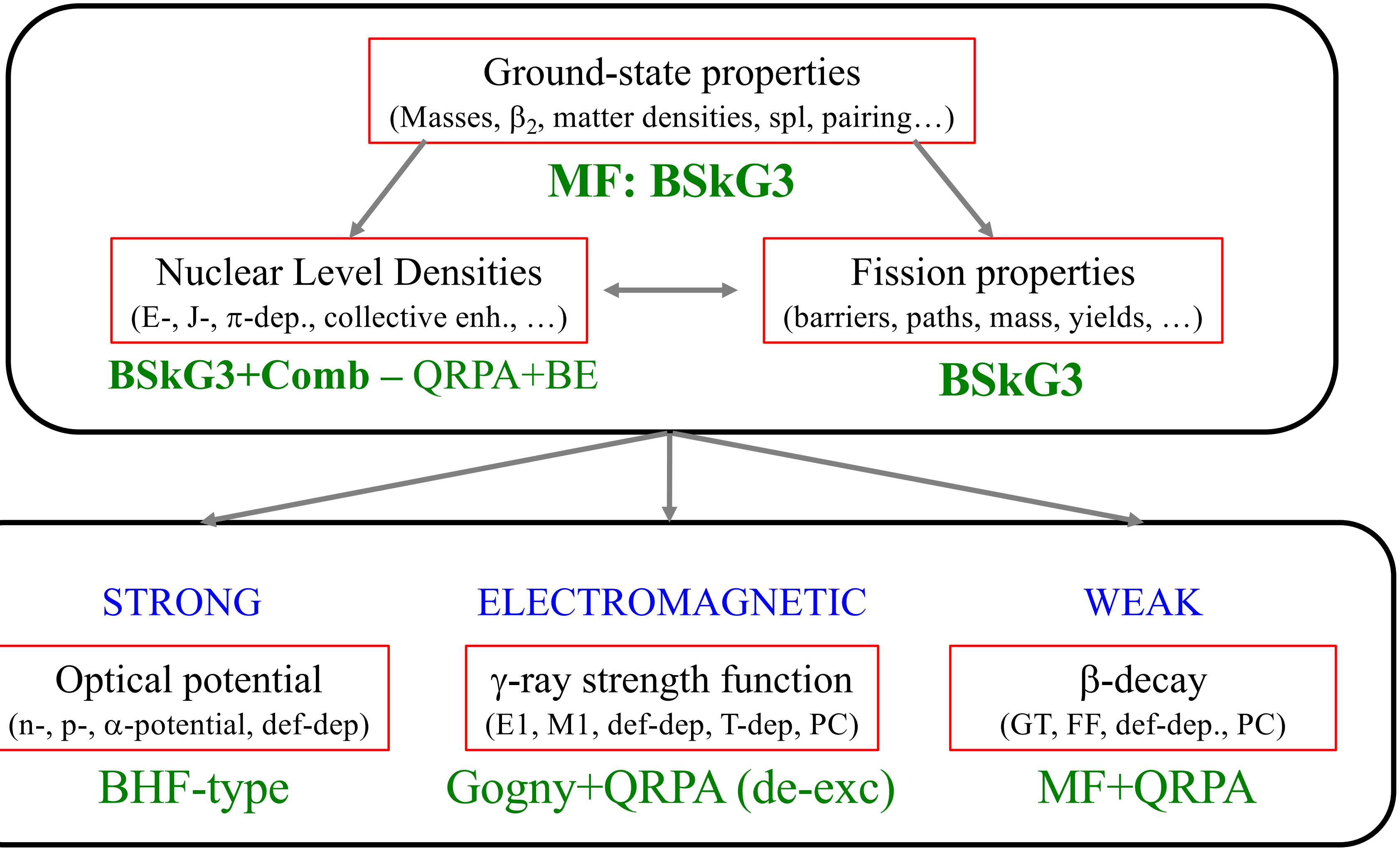
$$\begin{aligned}
\mathcal{E}_{\rm Sky} = & \sum_{q=n,p} \frac{\hbar^2}{2M_q}\tau_q + \frac{1}{2}t_0\left[\left(1+\frac{1}{2}x_0\right)\rho^2 - \left(\frac{1}{2}+x_0\right)\sum_{q=n,p}\rho_q^2\right] + \frac{1}{4}t_1\left[\left(1+\frac{1}{2}x_1\right)\left(\rho\tau+\frac{3}{4}(\nabla\rho)^2\right) -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

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

A challenge that will require 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 !

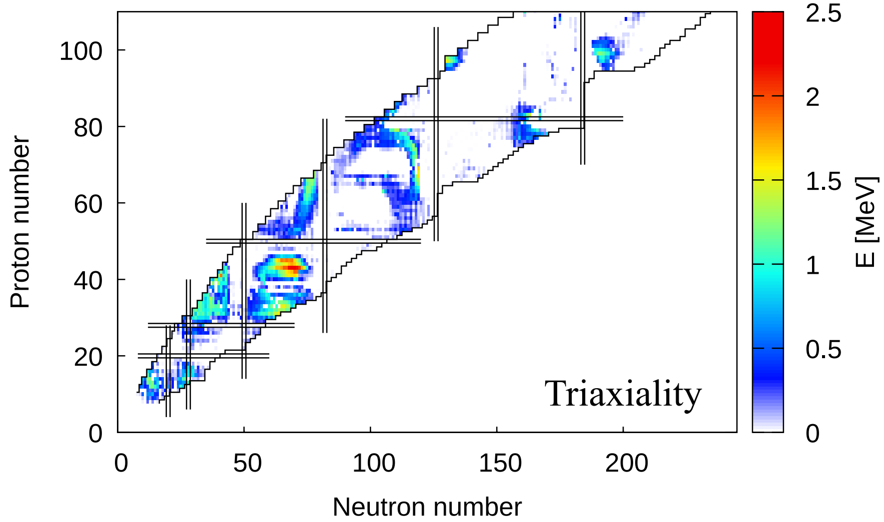
see also talk of S. Hilaire, G. Martinez-Pinedo

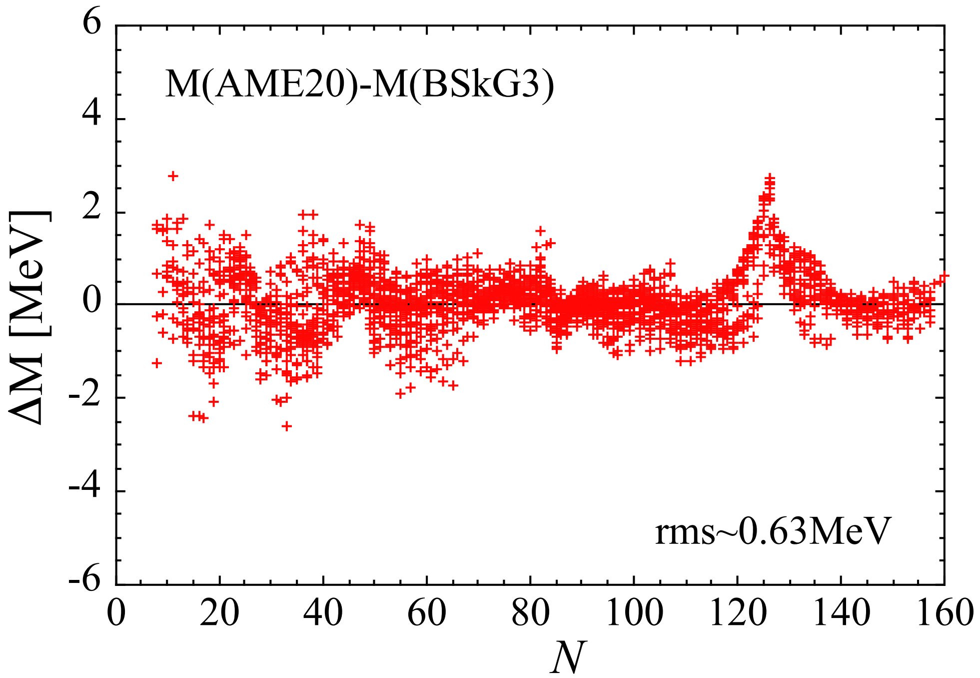
BSkG3 HFB nuclear mass models

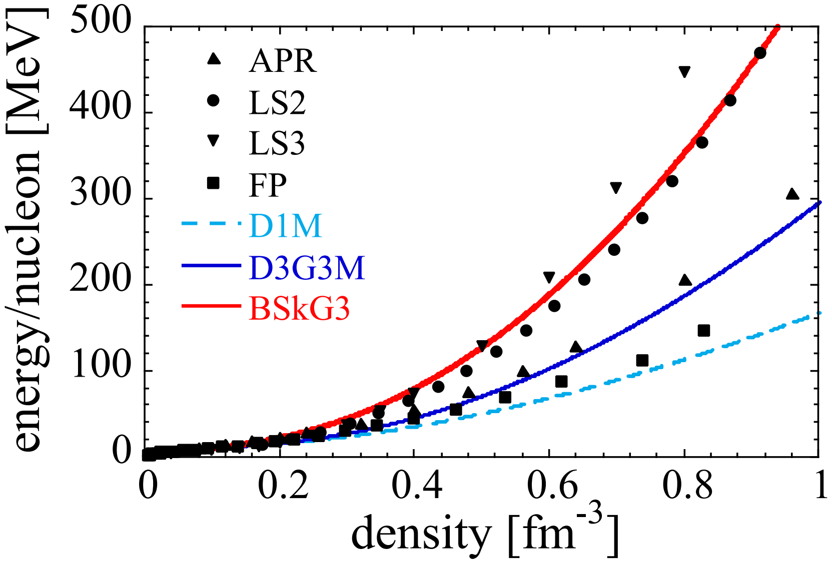
Grams, Ryssens et al. (EPJA 59, 270, 2023)

Recent Skyrme-HFB mass model: BSkG3

- Symmetry breaking: ***triaxiality***, octupolarity & time-reversal
- "Realistic" microscopic pairing
- Stiff EoS of pure neutron matter
- Accurate GS properties (M, R_{ch}, def, ...)
  $\sigma(2457M)$=0.63MeV



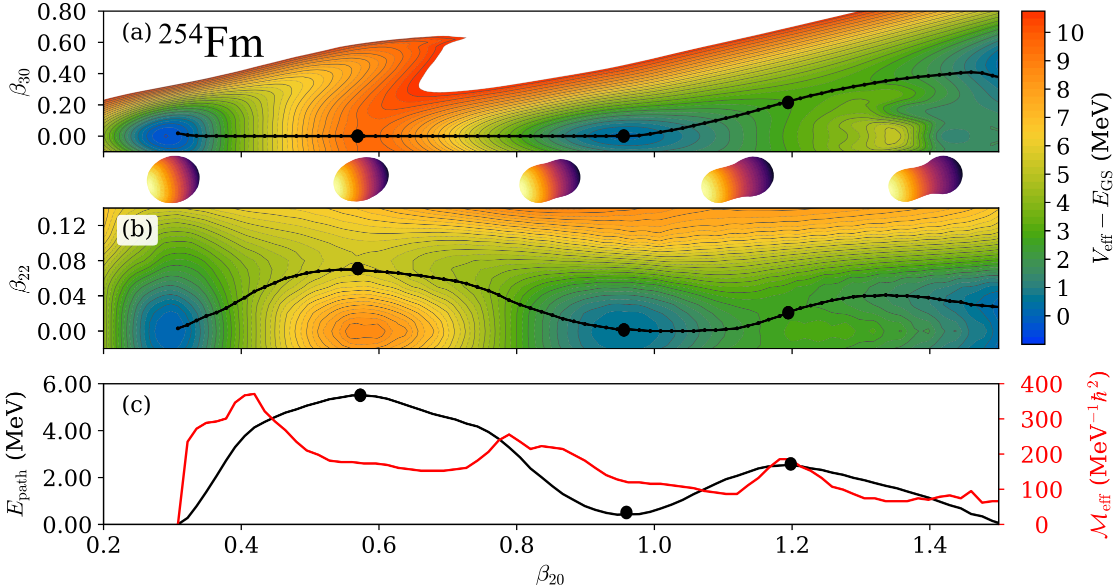




BSkG3: Remarkable description of fission properties

cf Sánchez Fernández et al. (2025)

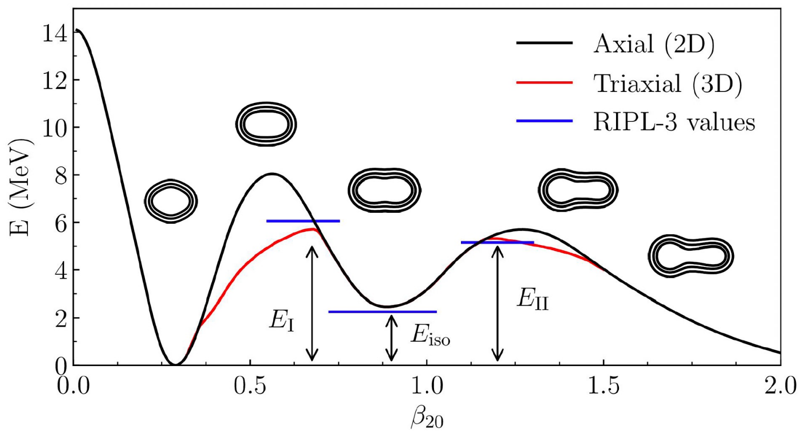
- Fission barriers



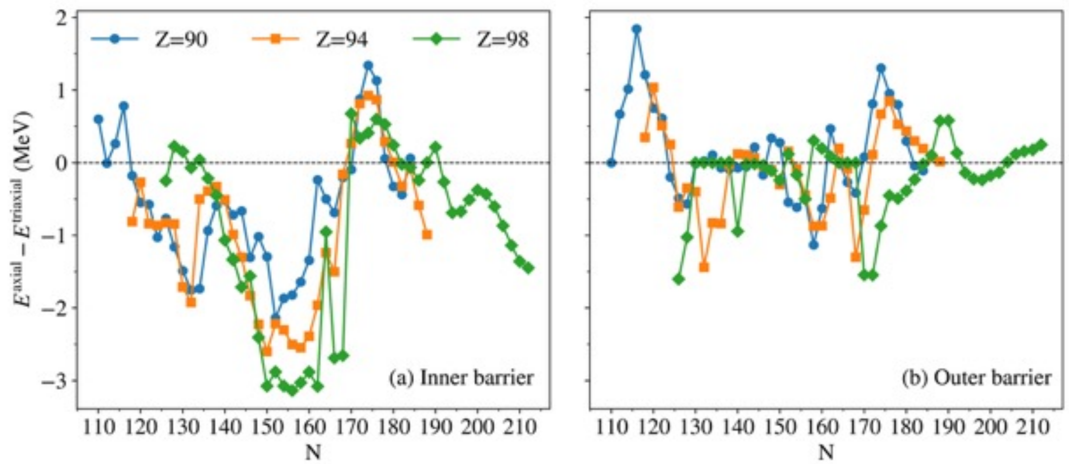
Deviations of the primary barrier wrt to RIPL-3 ones

rms (45 nuc)	σ(B_I) [MeV]
BSkG3	**0.33**
HFB-14	0.60
FRLDM	0.81
BCPM	1.48

Including both triaxial and octupole deformations coherently



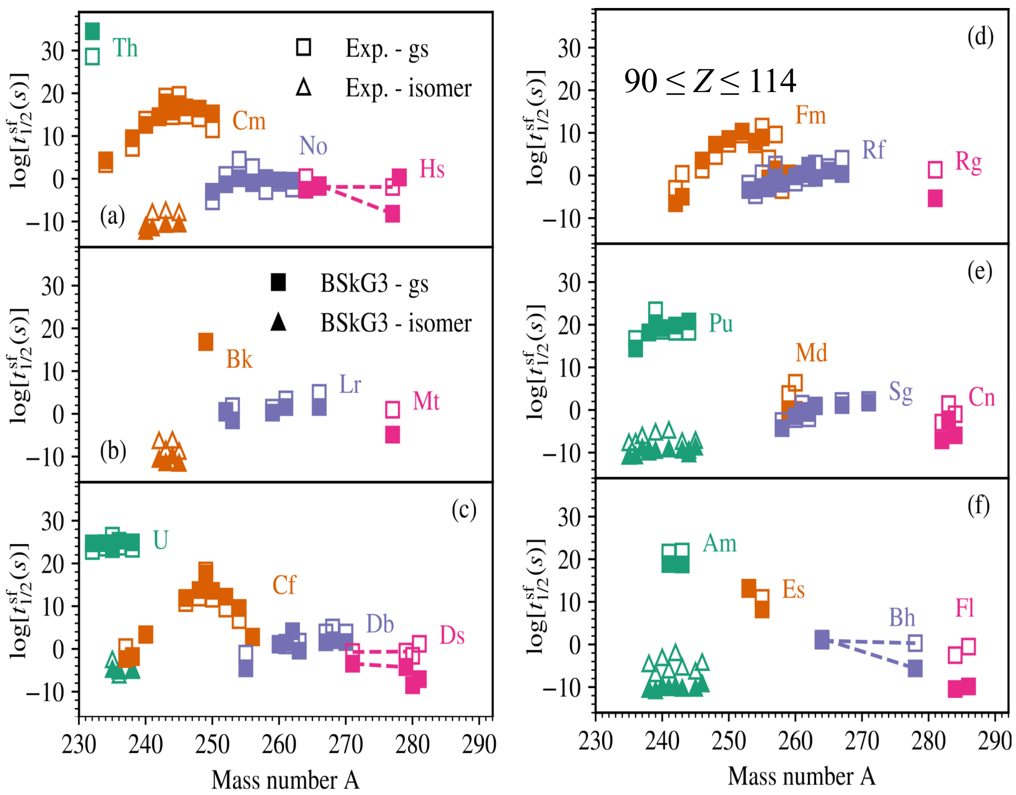
Impact of triaxiality on the barrier height



BSkG3: Remarkable description of fission properties

cf Sánchez Fernández et al. (2025)

- Spontaneous fission half-lives



For GS:

107 $t_{1/2}$: $f_{\rm rms}$=1.5 10^3

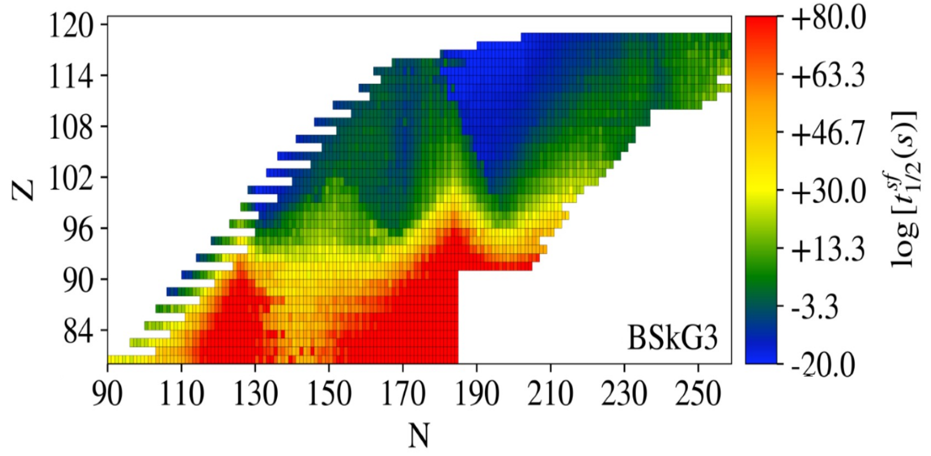
BCPM: $f_{\rm rms}$=4.7 10^4

For fission isomers:

29 $t_{1/2}$: $f_{\rm rms}$=5.3 10^3

$$f_{\rm rms} = \exp\left[\frac{1}{N}\sum_i^N (\ln r_i)^2\right]^{1/2}$$

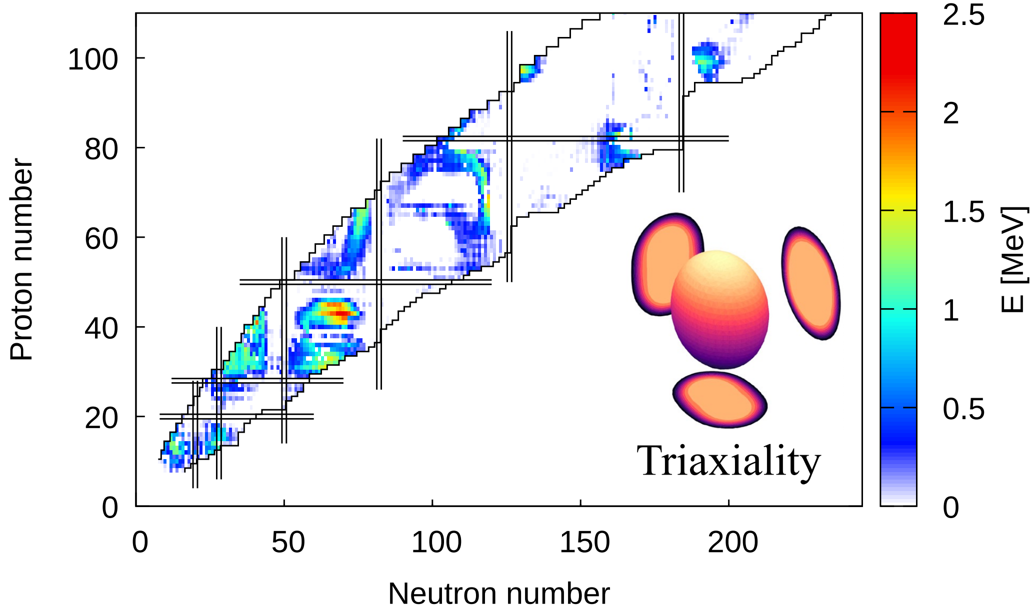
Fission PES (paths, barriers, SF) extended to ~3300 nuclei ($80 \leq Z \leq 118$) for r-process simulations ...



Nuclear Level densities

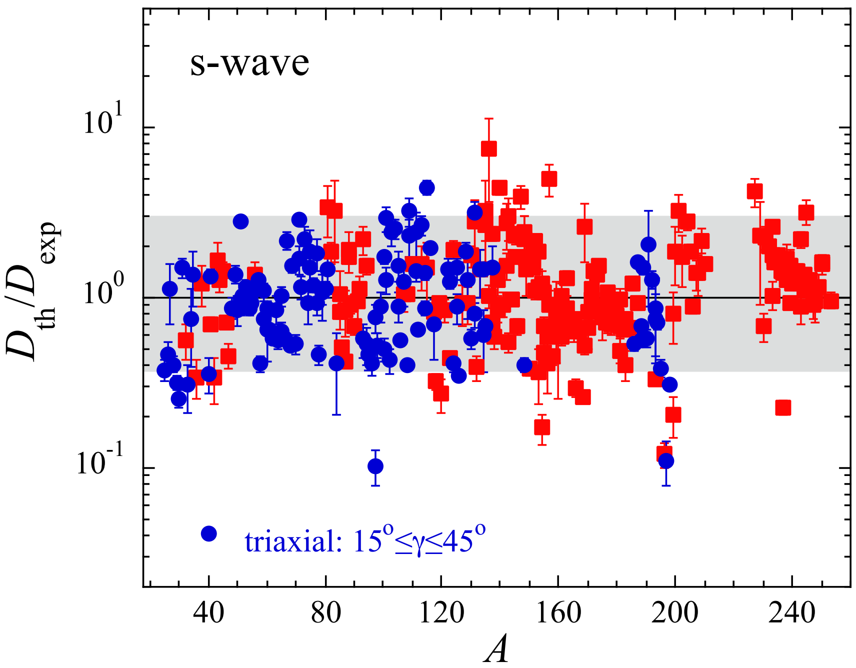
New *combinatorial* predictions based on the BSkG3 nuclear structure properties

- Improved nuclear structure properties
- Inclusion of triaxial degree of freedom



Comparison of BSkG3 combinatorial NLD with experimental data

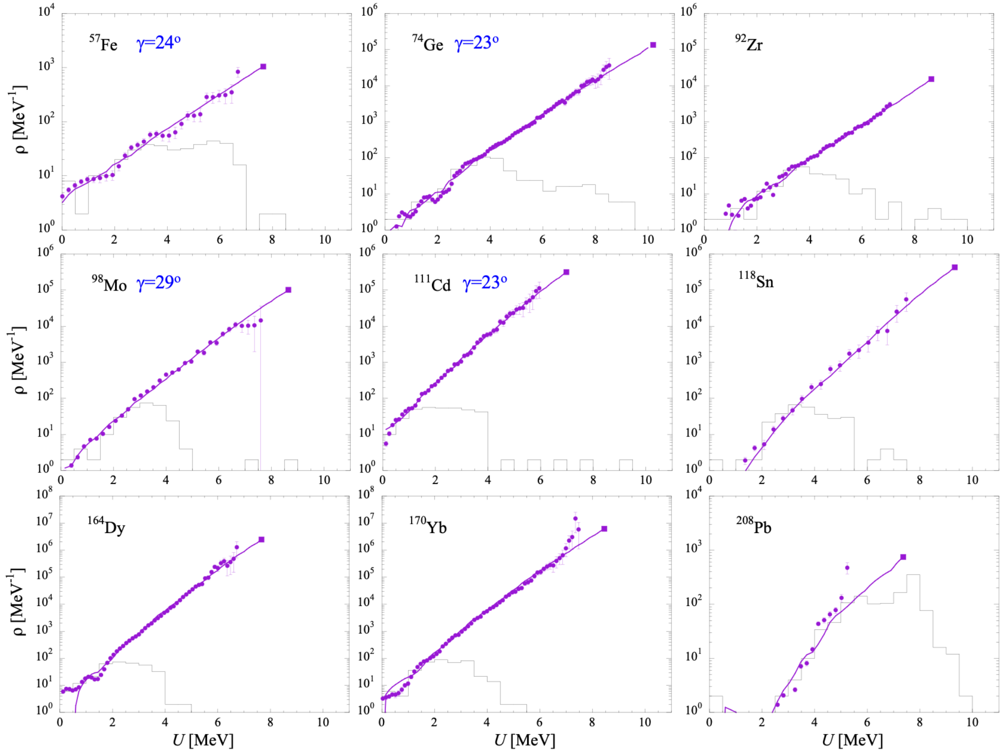
s-wave neutron resonance spacings at S_n



299 nuclei

D_0	f_{mean}	f_{rms}
BSkG3+Comb (2025)	**1.03**	**1.96**
BSk14+Comb (2008)	0.95	2.34
T-HFB+Comb (2012)	1.11	2.58

Oslo data



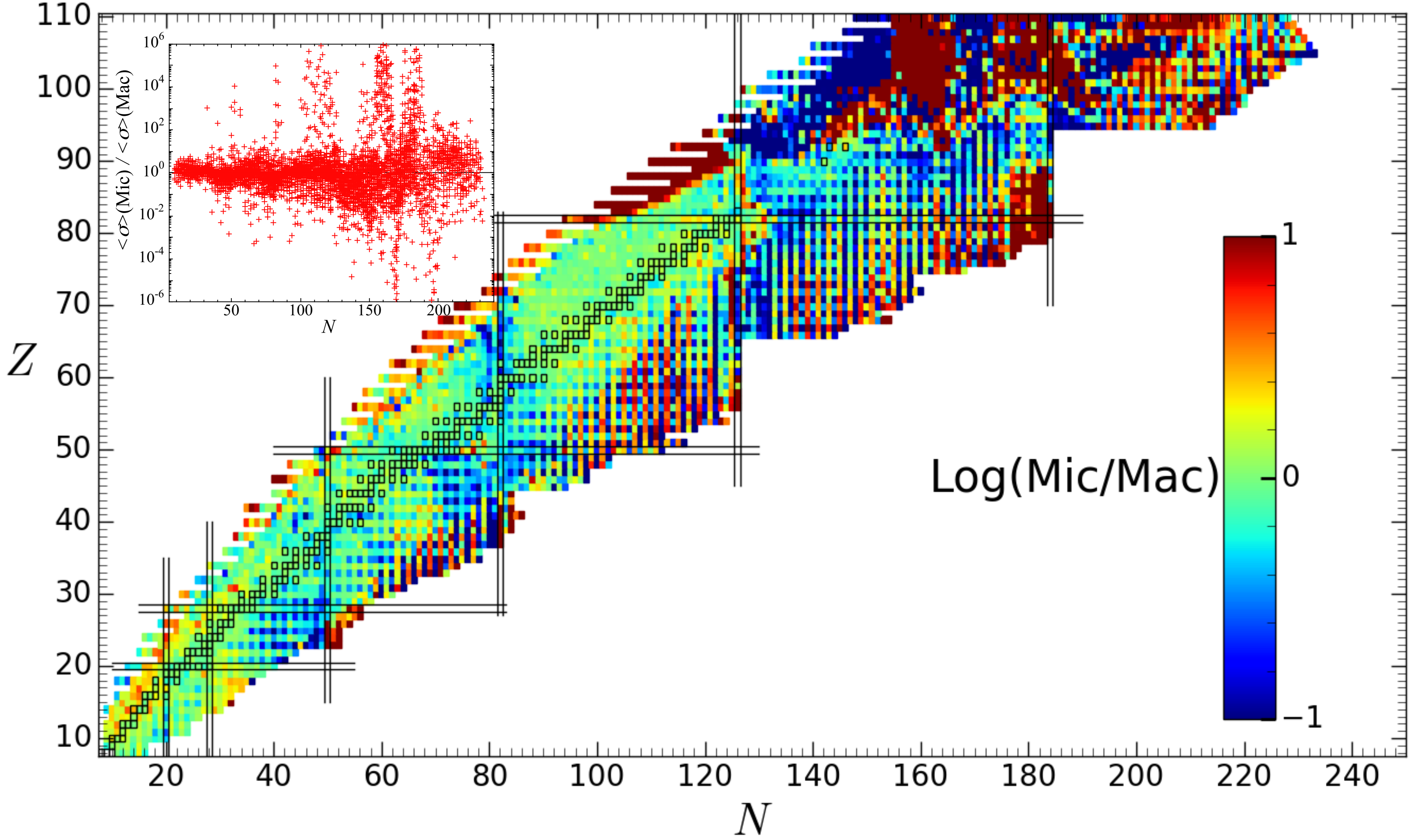
(after renormalisation on D_0)

cf Talk of S. Hilaire

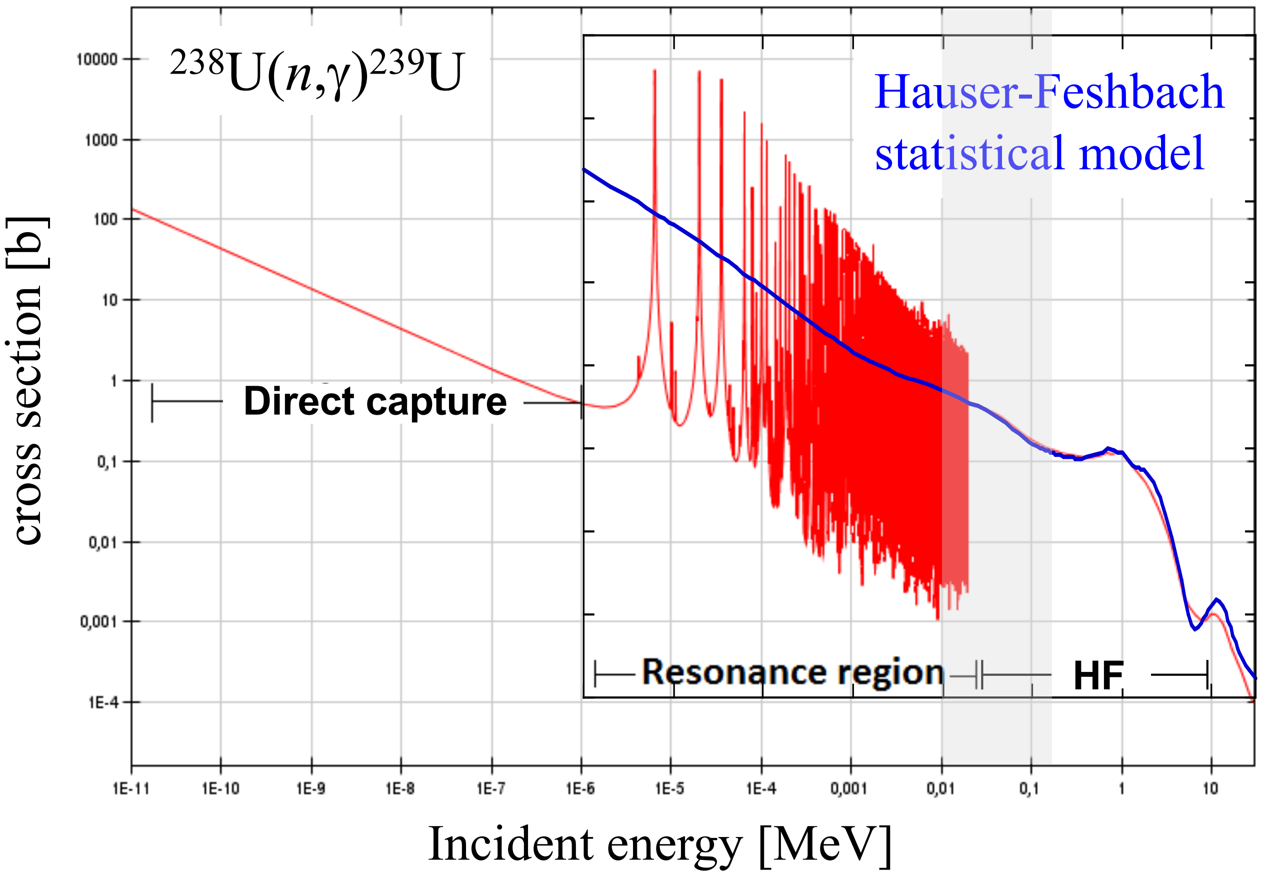
Comparison of (n,γ) reaction rates at T=10^9K: from Mac to Mic description

Mac = FRDM masses – Cst-T+FG NLD – SMLO PSF

Mic = BSkG3 masses – BSkG3+Comb NLD – D1M+QRPA PSF



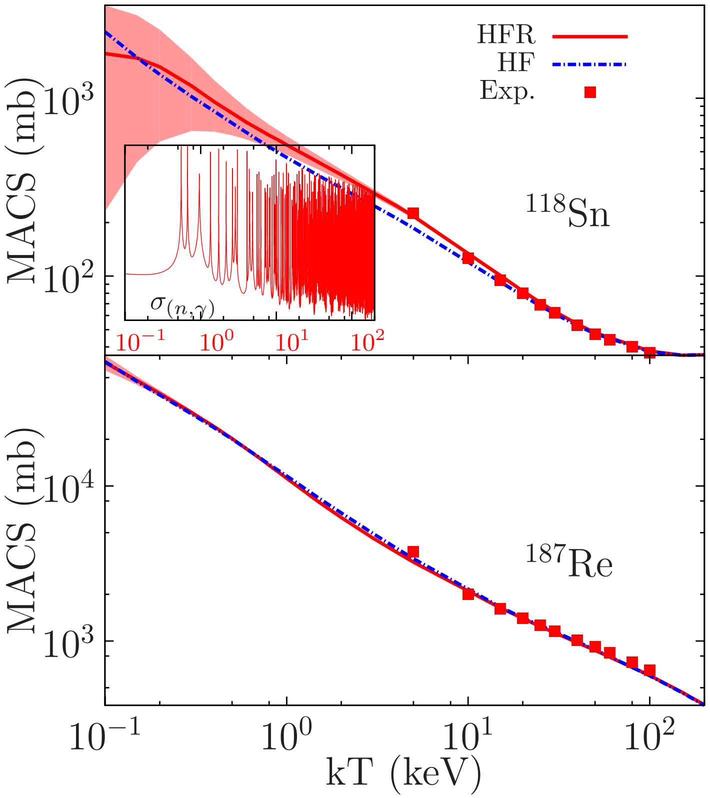
The High-Fidelity Resonance vs Hauser-Feshbach method to predict radiative n-capture cross section



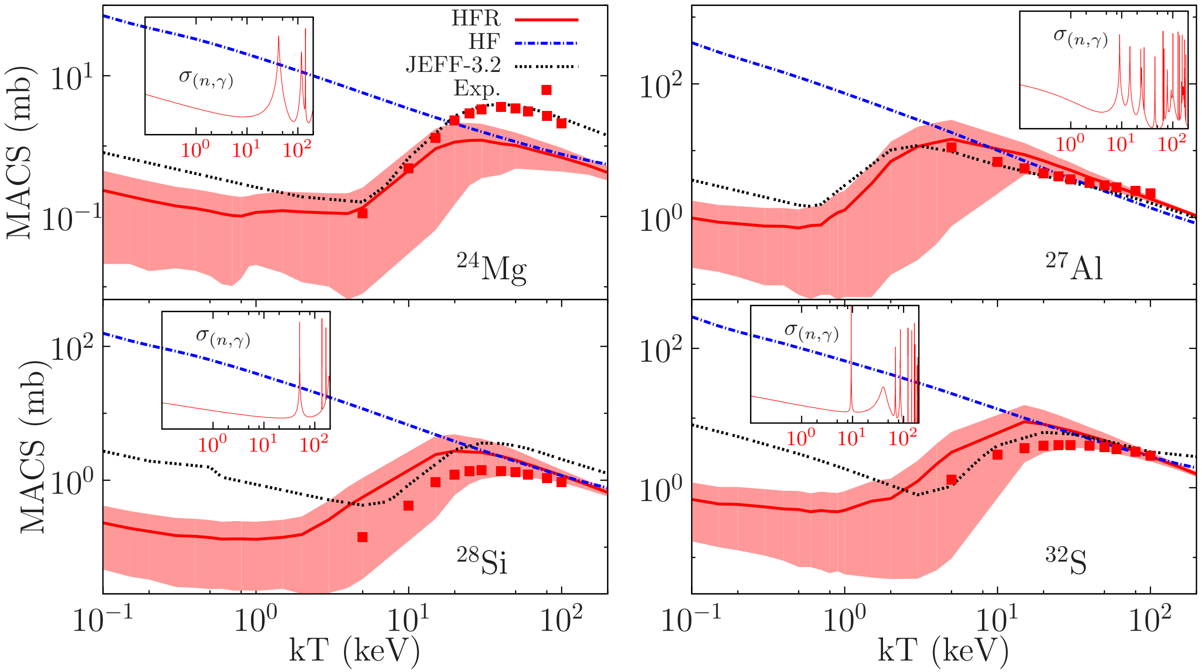
The High-Fidelity Resonance vs Hauser-Feshbach method to predict radiative n-capture cross section

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



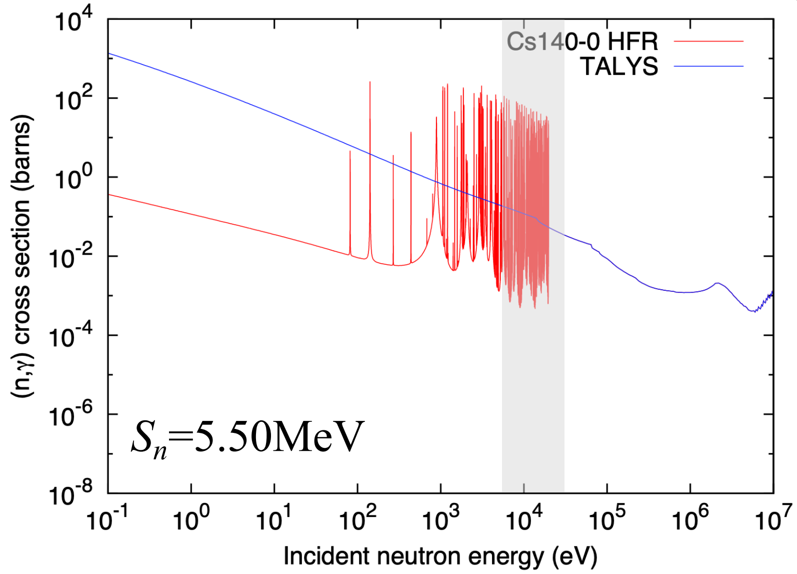
Improved description of MACS for light nuclei

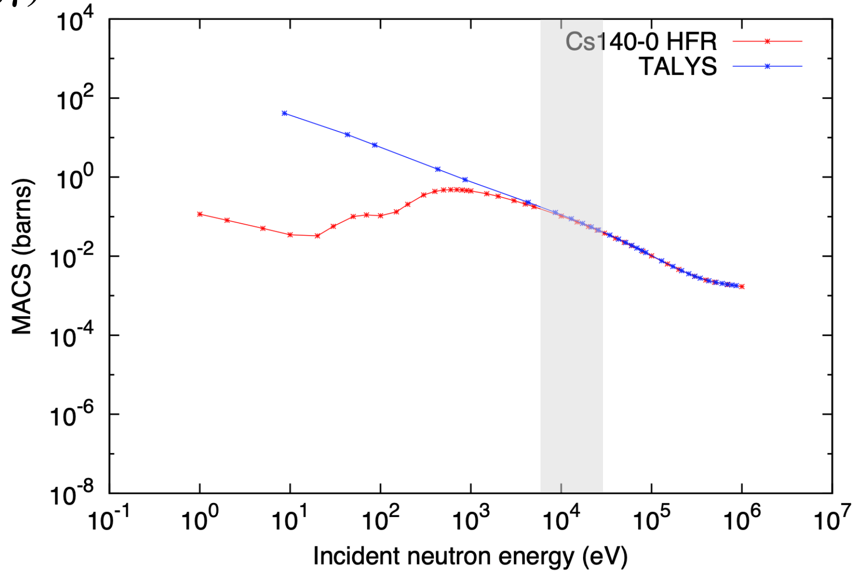


Rochman et al. PLB 764, 109 (2017)

HF is a good approximation for nuclei close to stability

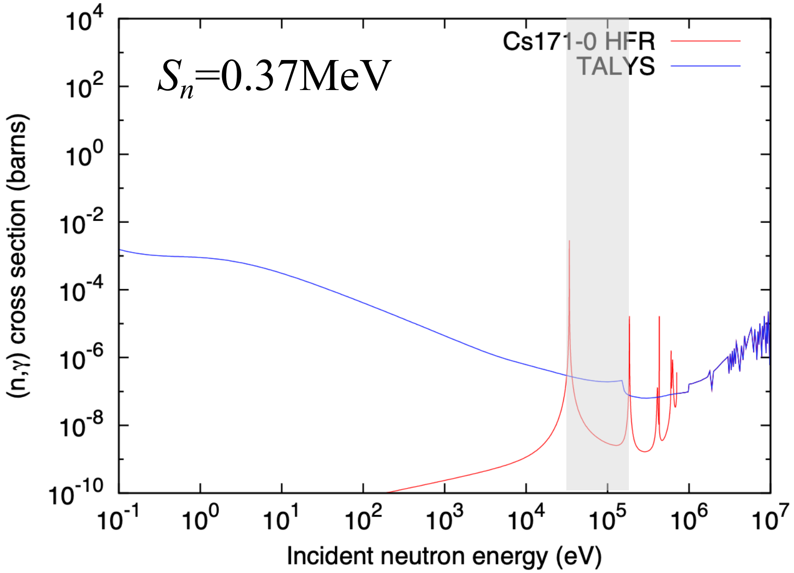
^{140}Cs(n,γ)^{141}Cs

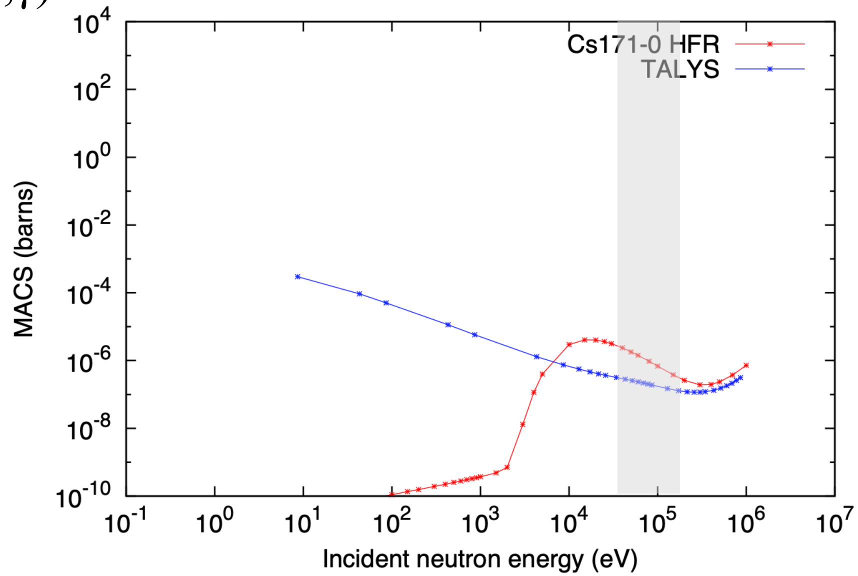




HF is not a good approximation for exotic n-rich nuclei

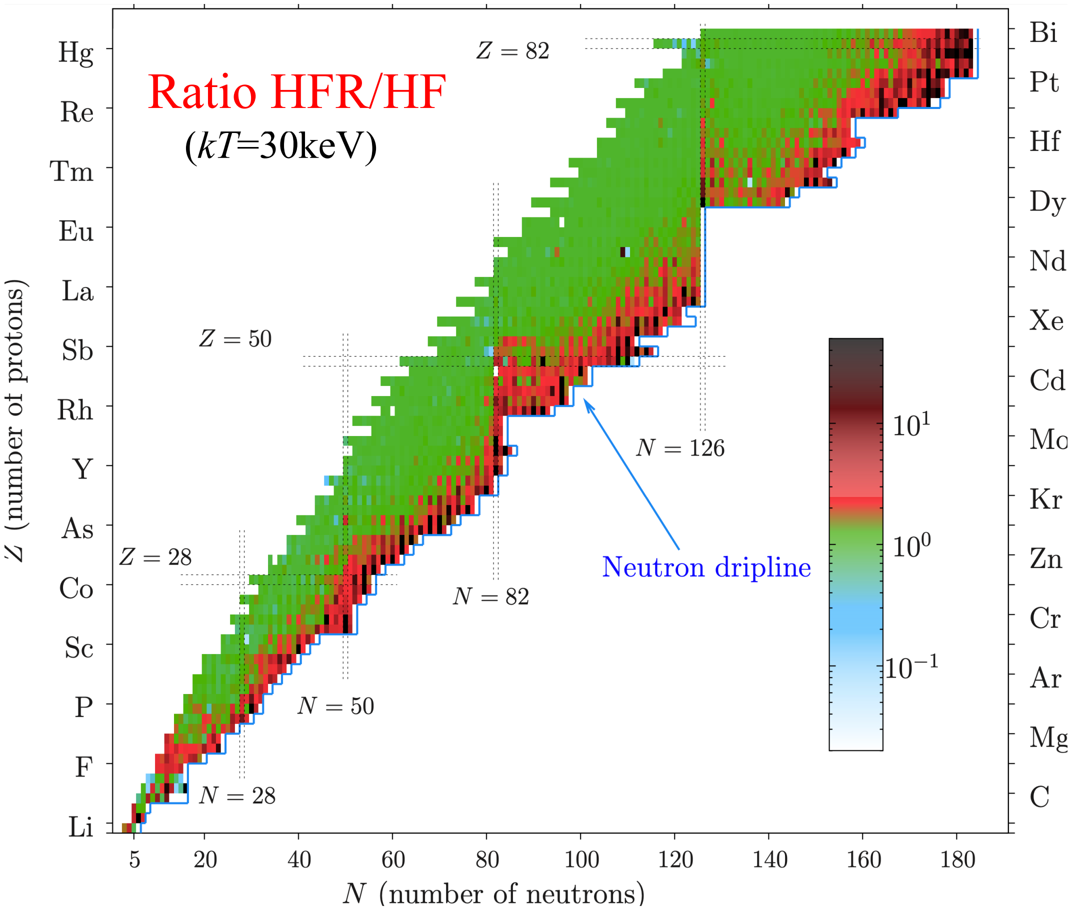
^{171}Cs(n,γ)^{172}Cs





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

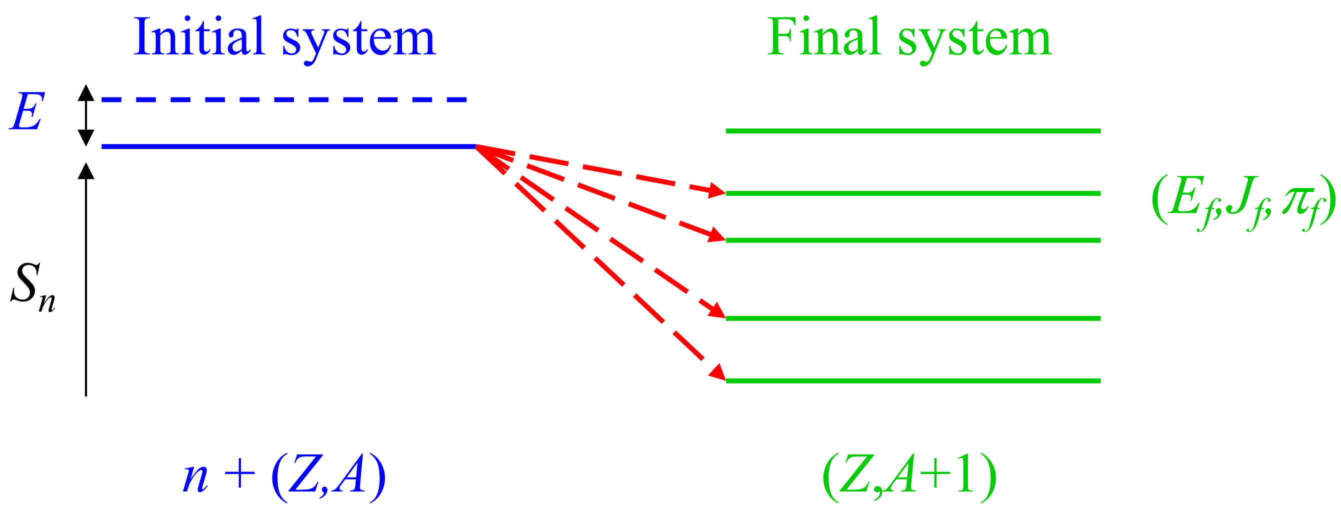
HFR method: average parameters (the scattering radius, level spacing, reduced neutron width and the radiative width) are used to create resolved resonances



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)

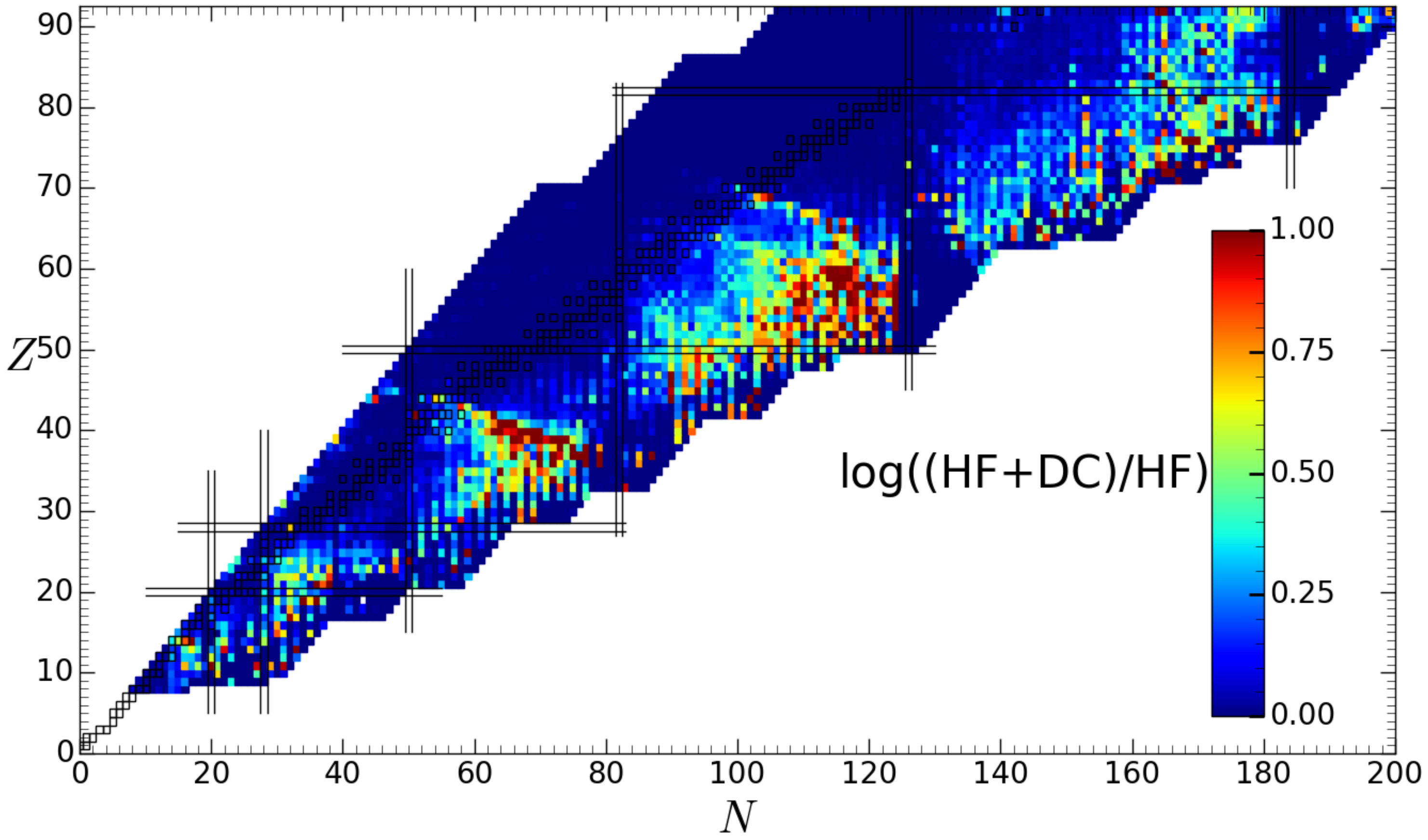


Different models exist (in particular the so-called potential model) but requires a detailed knowledge of

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

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

TALYS calculation



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

Conclusions

- **Major progress achieved and efforts ongoing**
  - Reaction model (e.g. TALYS) : still HF vs RR vs DC
  - MF, beyond MF, QRPA/FAM, SM, ab-initio
- **Selection of models for astrophysics application 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/SF/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/decay rates,
we are still far from being able to predict ***reliably***
n-, p- or α-captures, β-decay, and even less, fission of exotic nuclei
BUT progress is being made