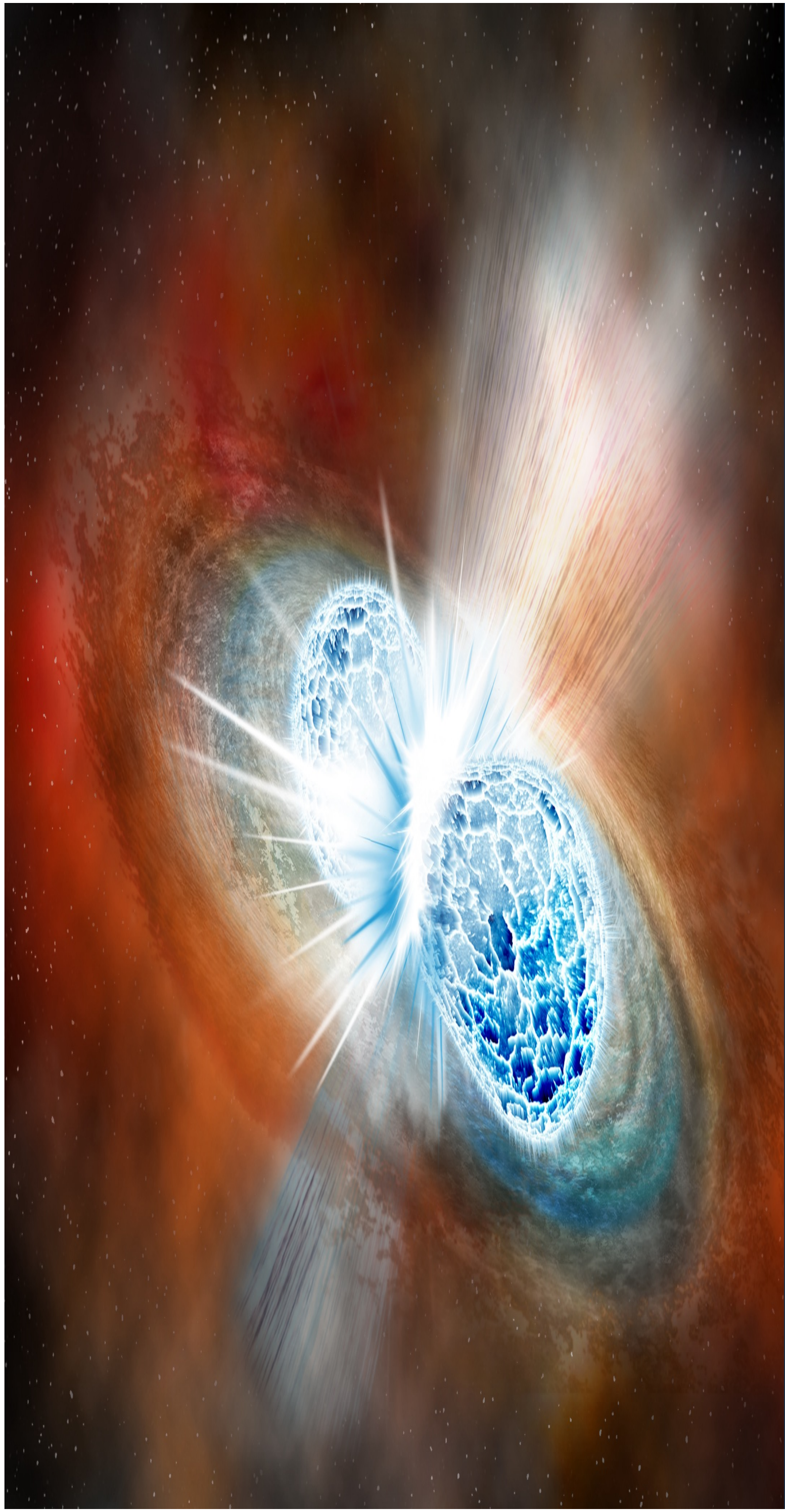
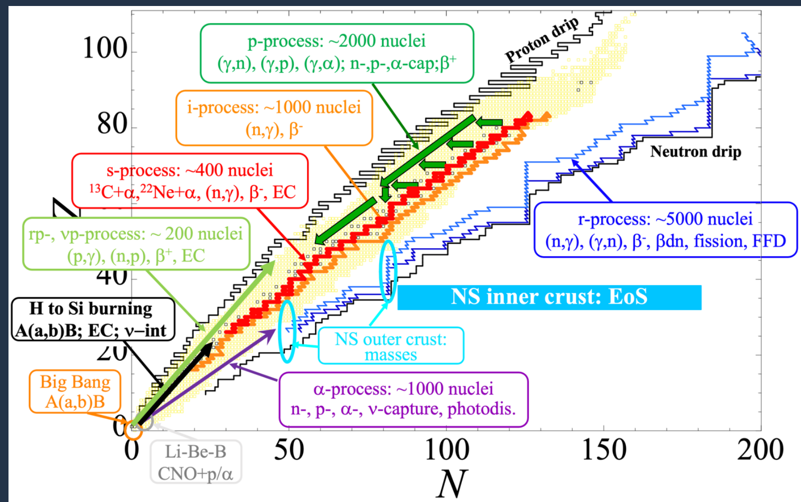


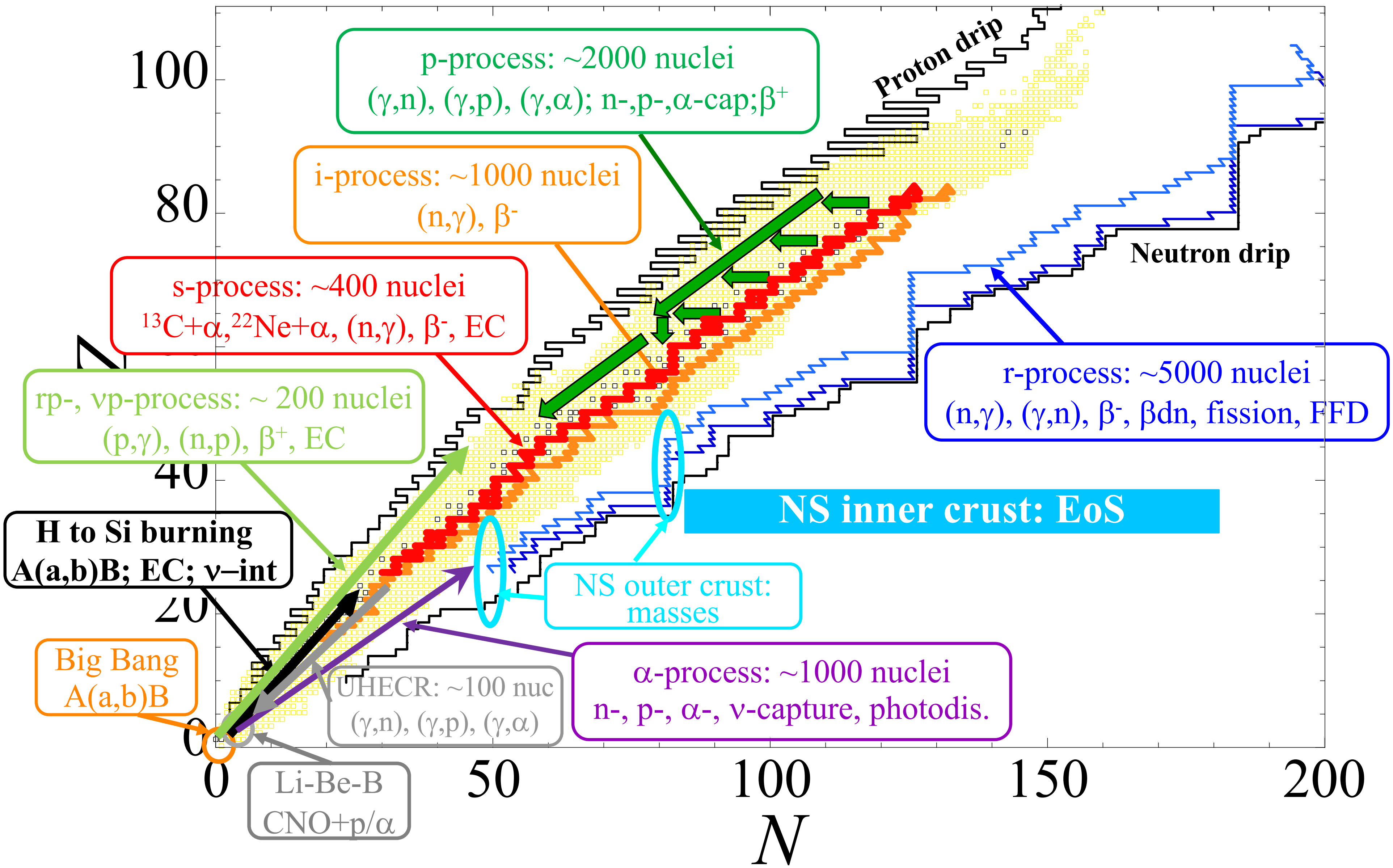
Progress in the development of nuclear models for astrophysical applications



S. Goriely (IAA-ULB)

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

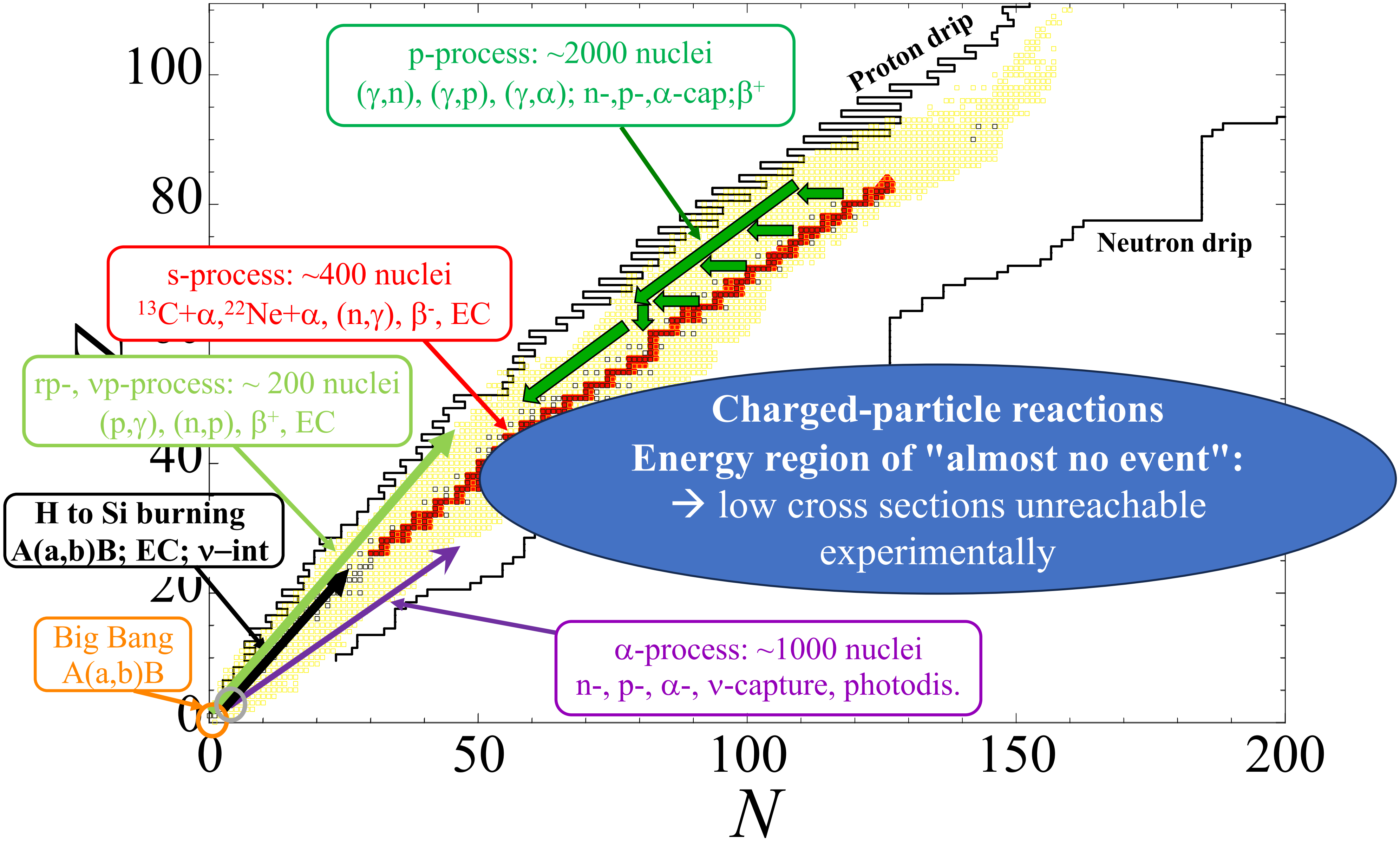
Nuclear Astrophysics: a field with high NP demands



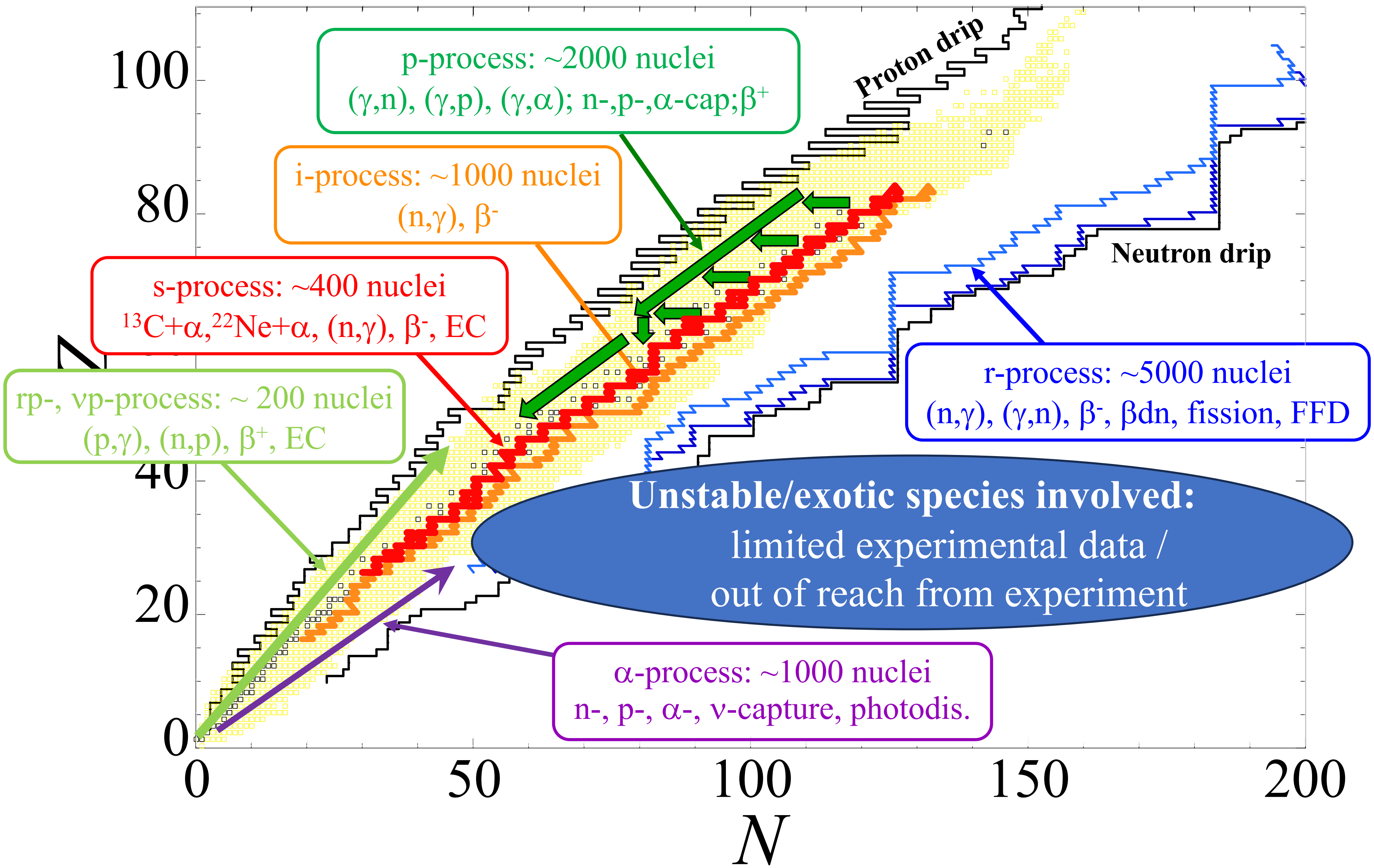
Note: Essentially thermonuclear processes

For spallation reactions (CR, jets, ...), see talks from Kampert, Farrar, Tatischeff

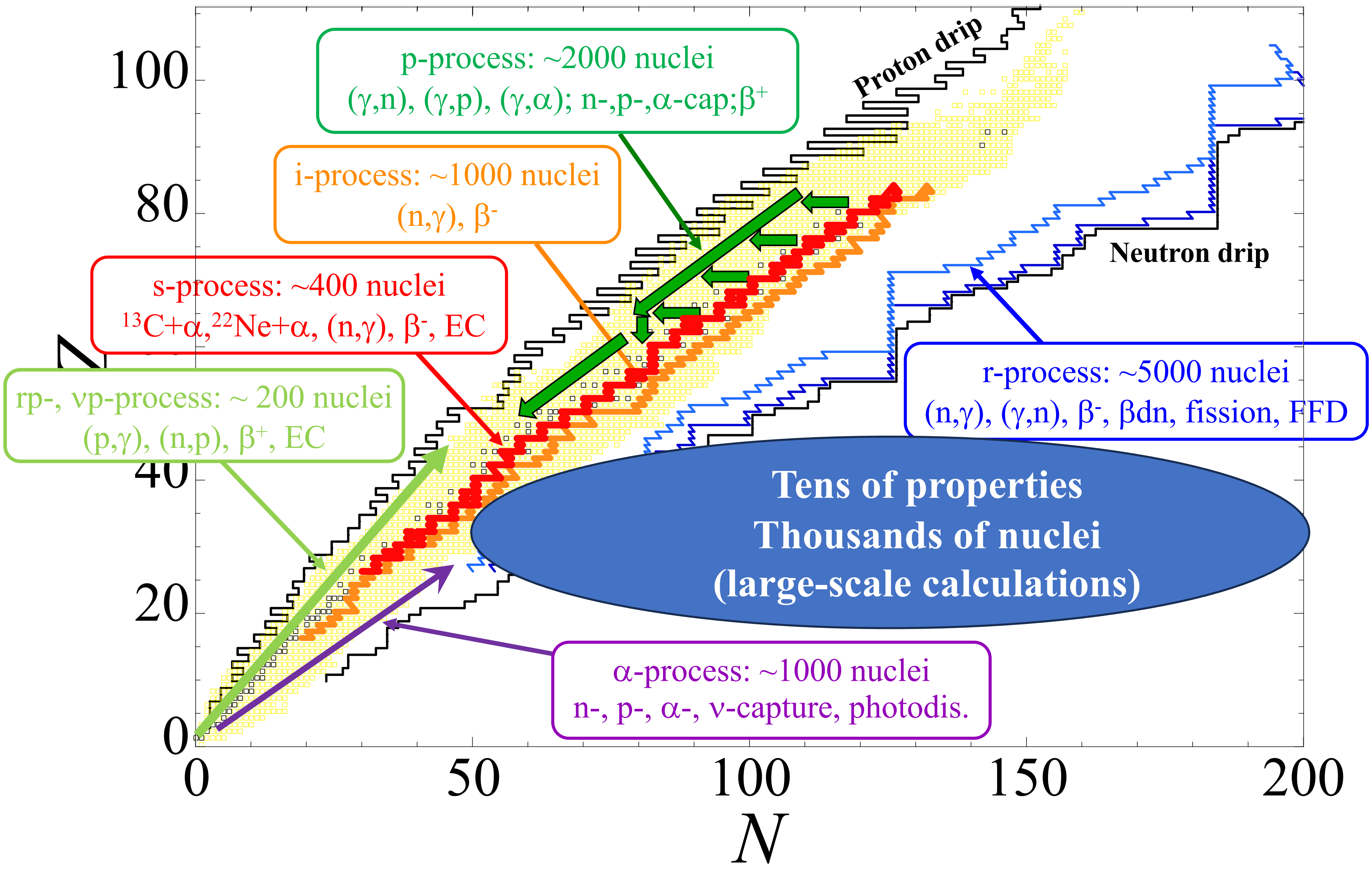
Some specific features of the astrophysical plasma



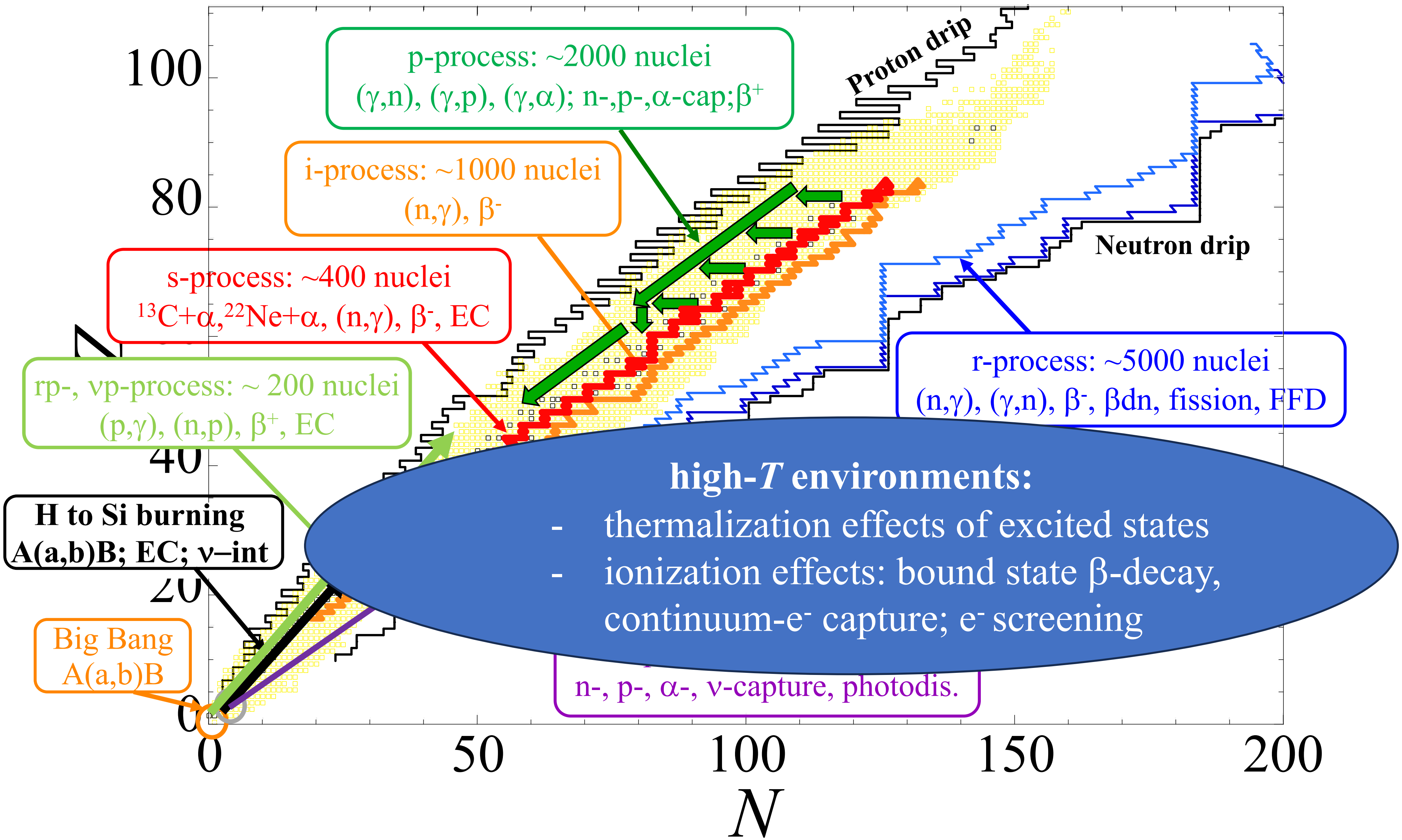
Some specific features of the astrophysical plasma



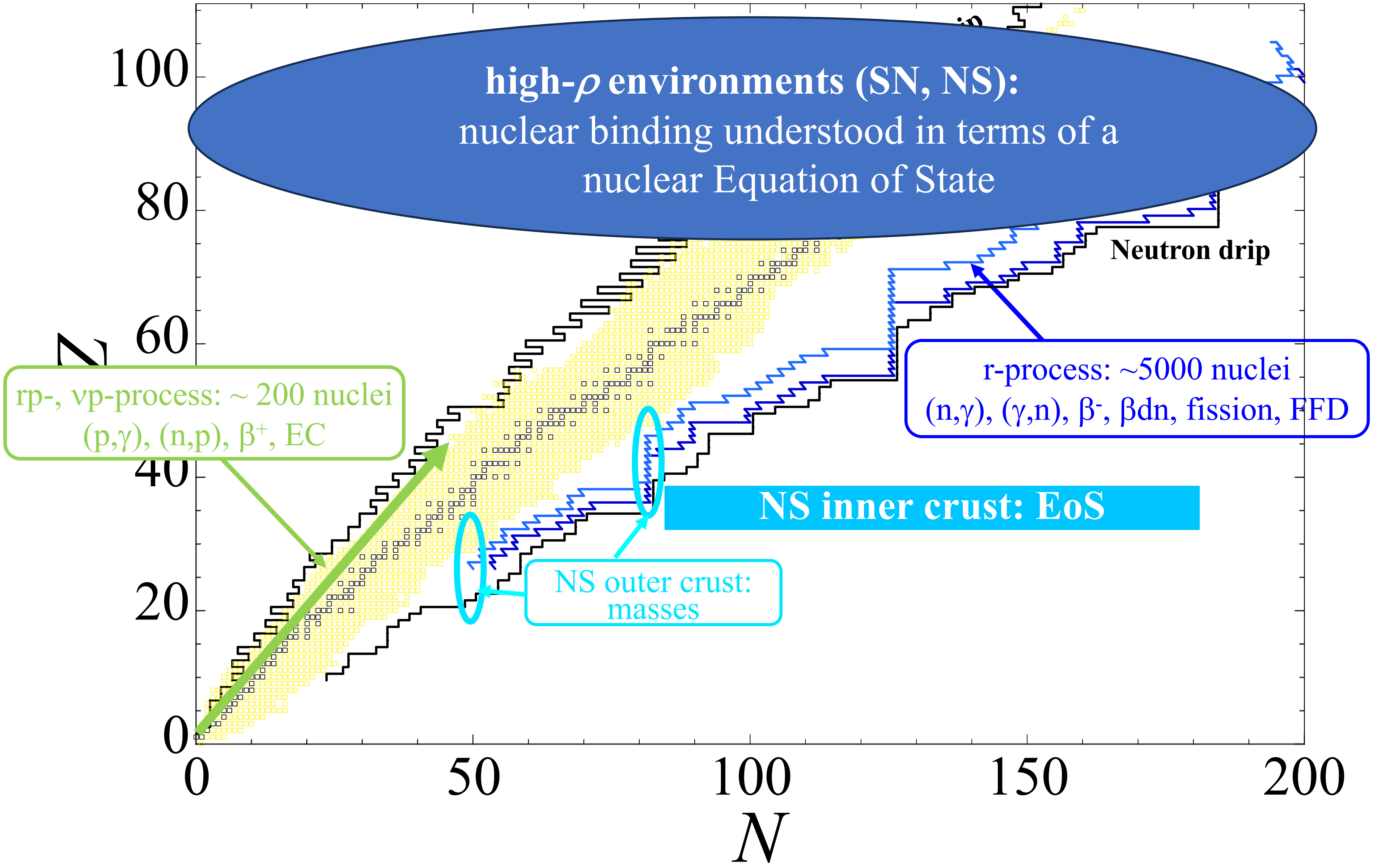
Some specific features of the astrophysical plasma



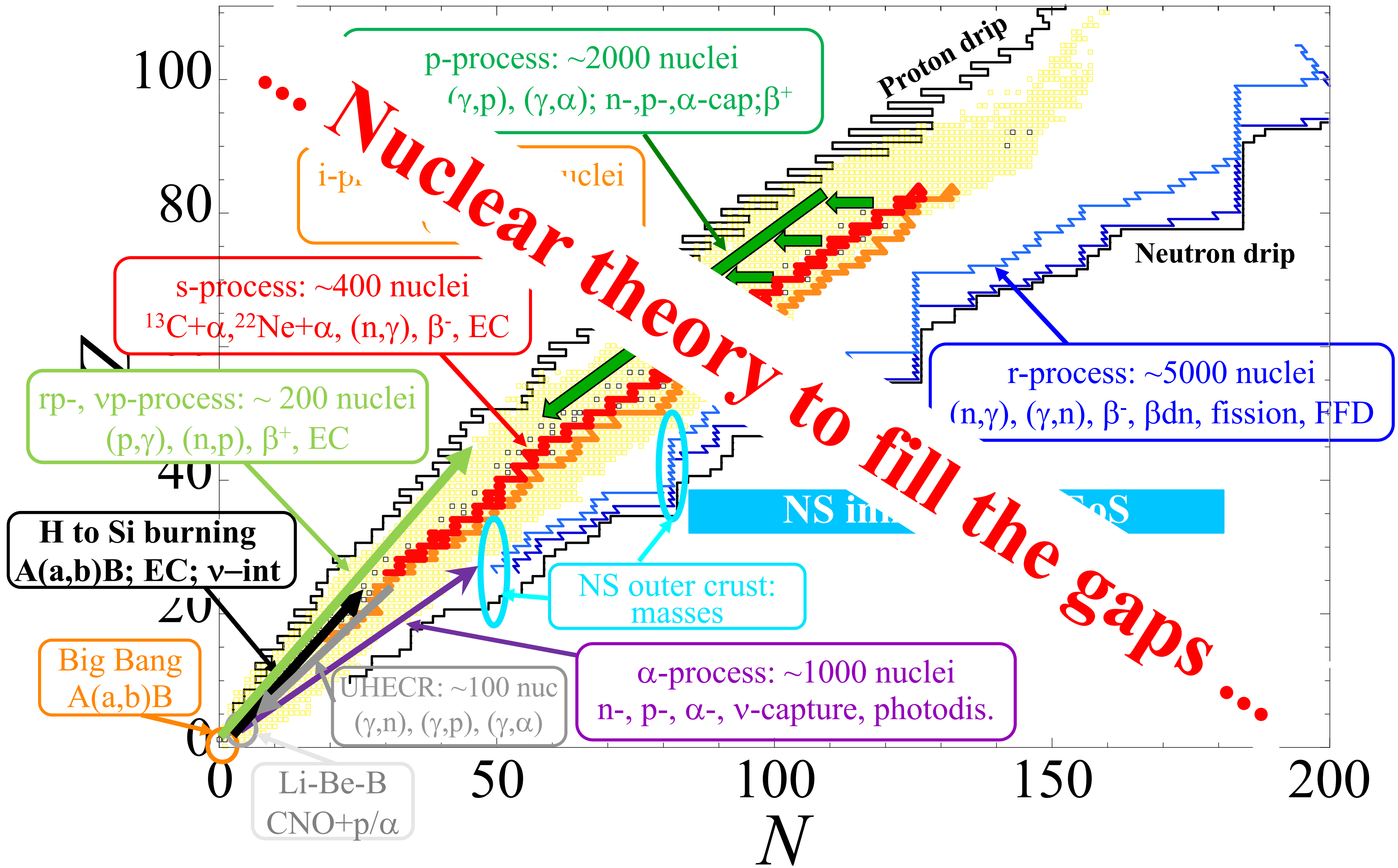
Some specific features of the astrophysical plasma



Some specific features of the astrophysical plasma



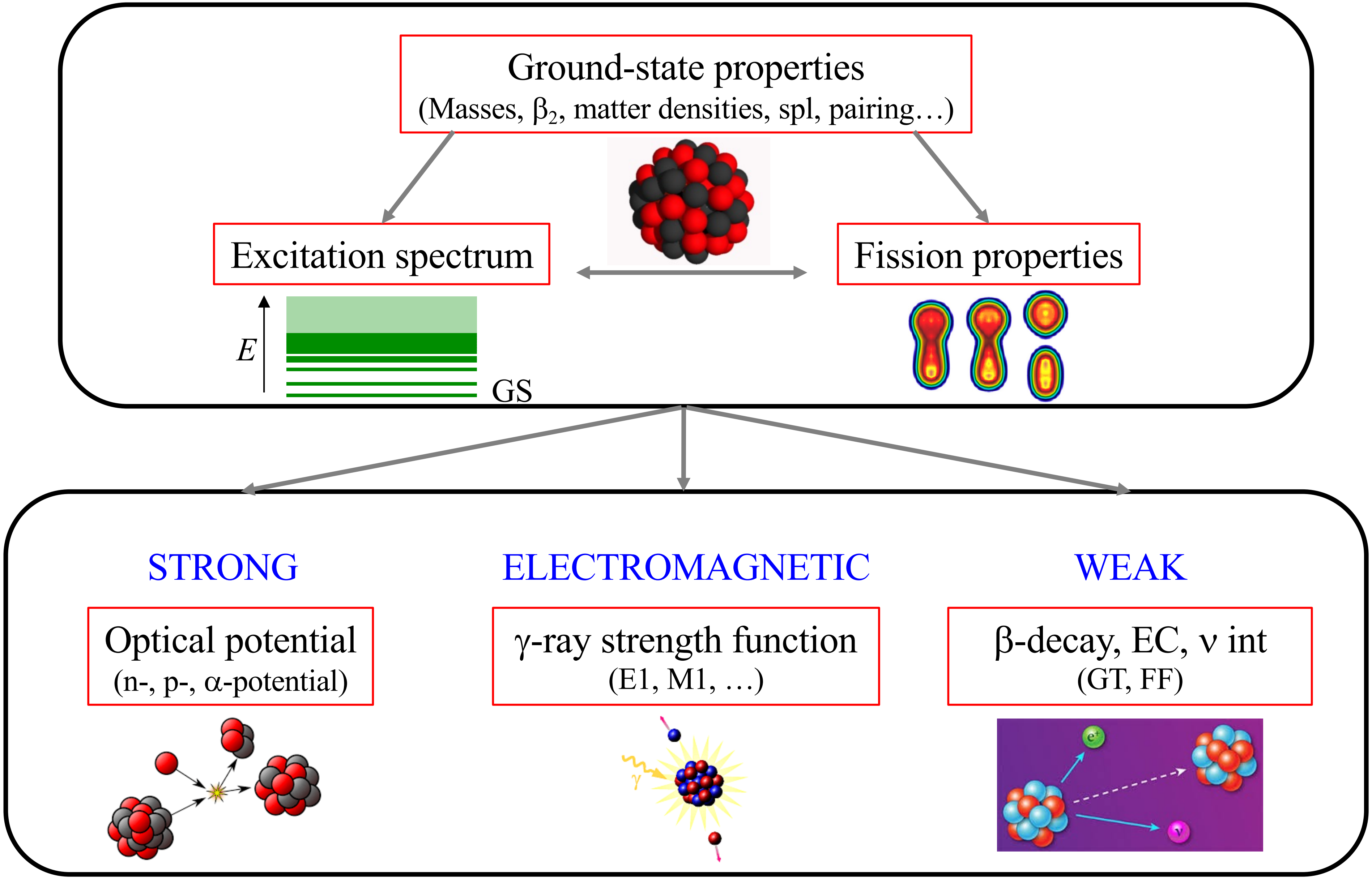
Nuclear Astrophysics: a field with high NP demands



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

How do nuclear uncertainties affect astrophysics observables ?

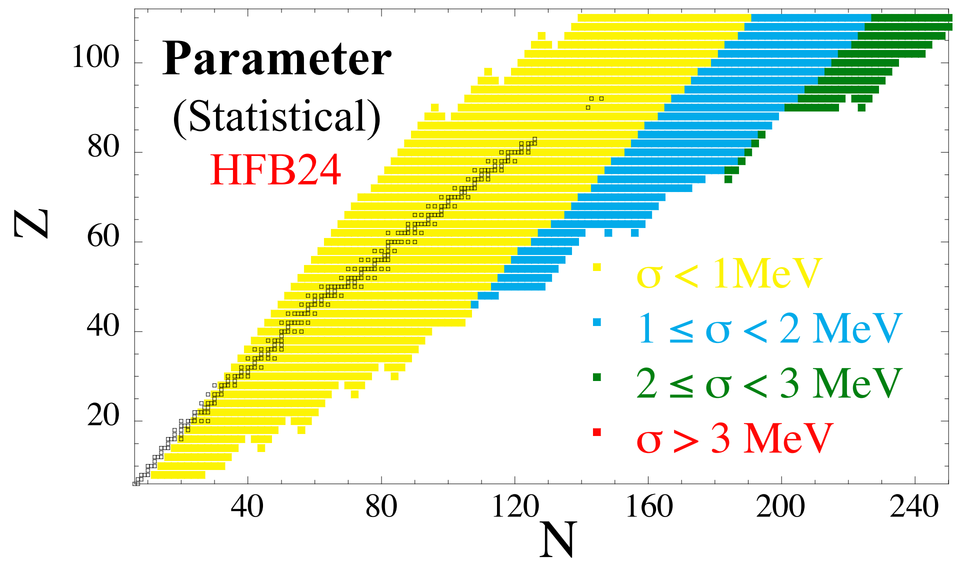
Nuclear inputs to nuclear reaction & decay calculations

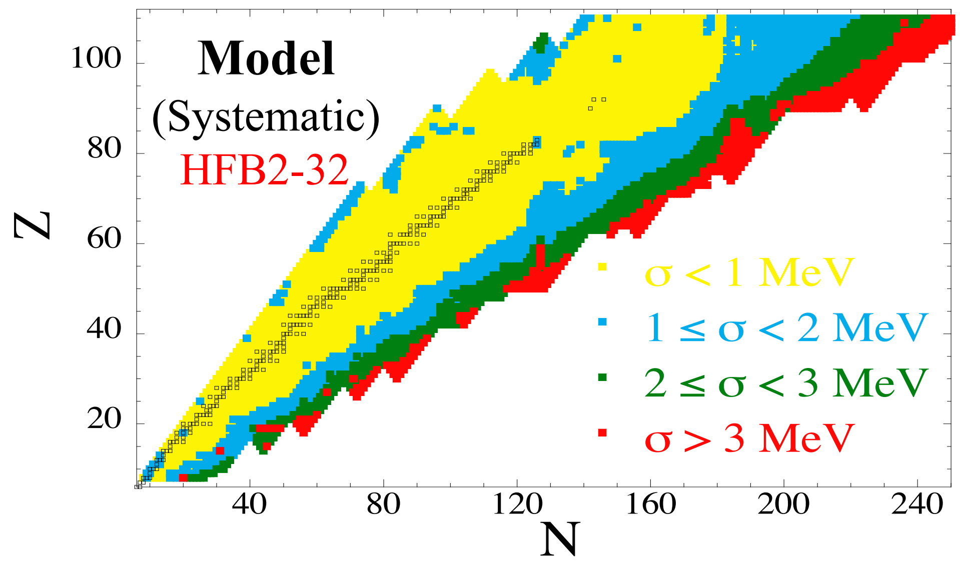


Quantification of nuclear uncertainties

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

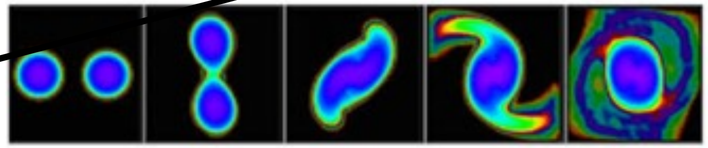
Only NLD/PSF *parameters* s.t. (n,γ) with $f_{rms} \leq 2$ ⟺ Only NLD/PSF *models* s.t. (n,γ) with $f_{rms} \leq 2$

Uncorrelated parameter variations

Masses/rates correlated by the model

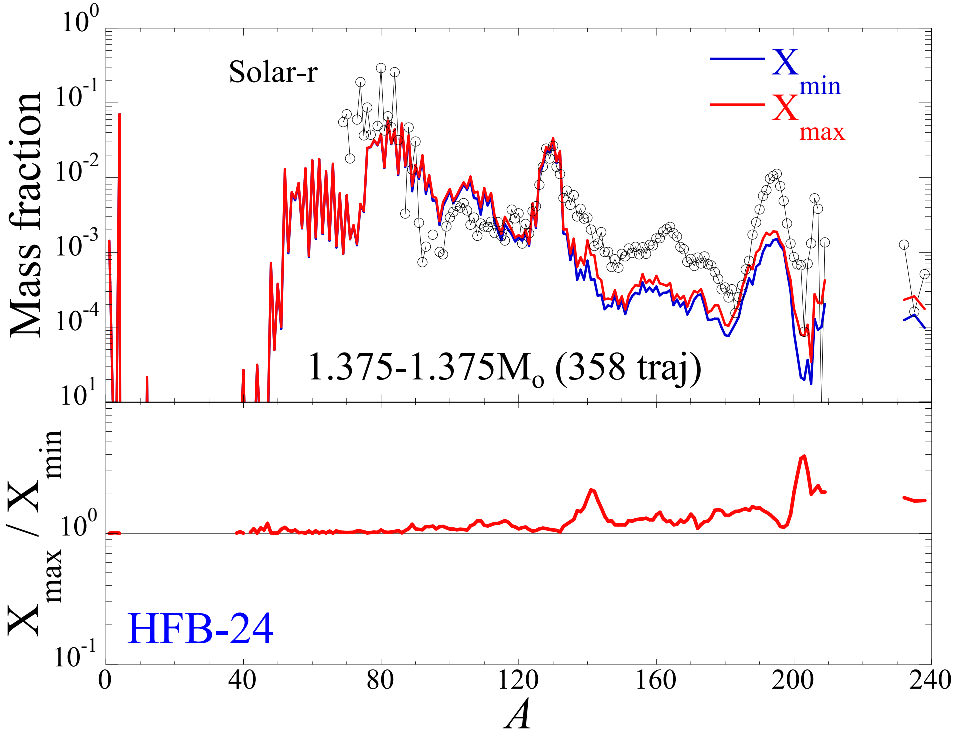
But what about their impact on astrophysical observables ?

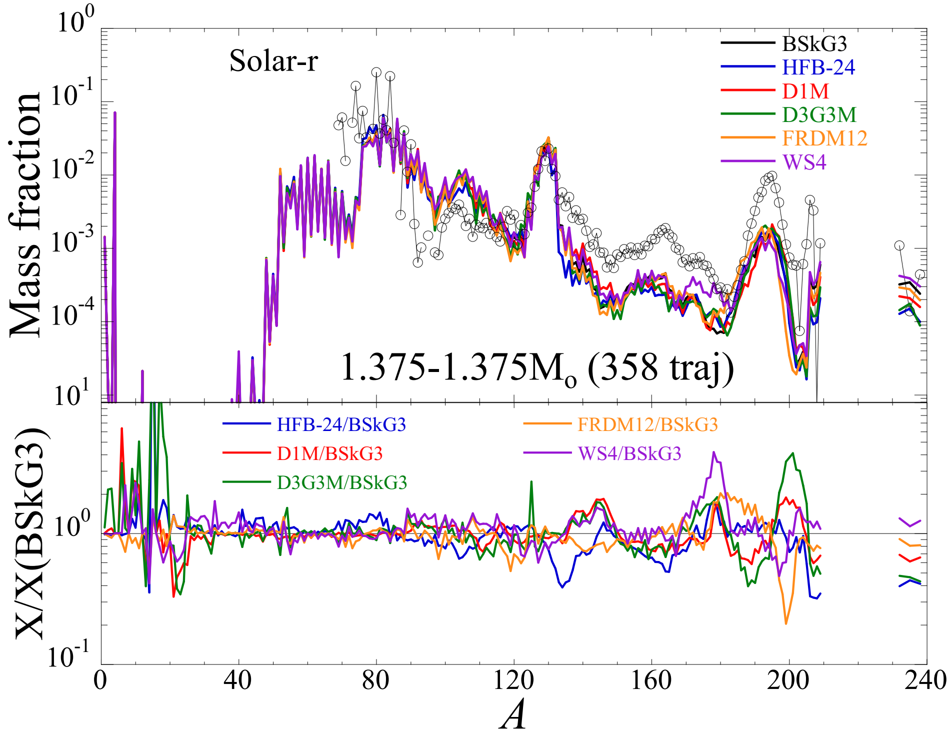
Propagation of Mass uncertainties into NSM simulations



Uncorrelated *Parameter* uncertainties

Correlated *Model* uncertainties



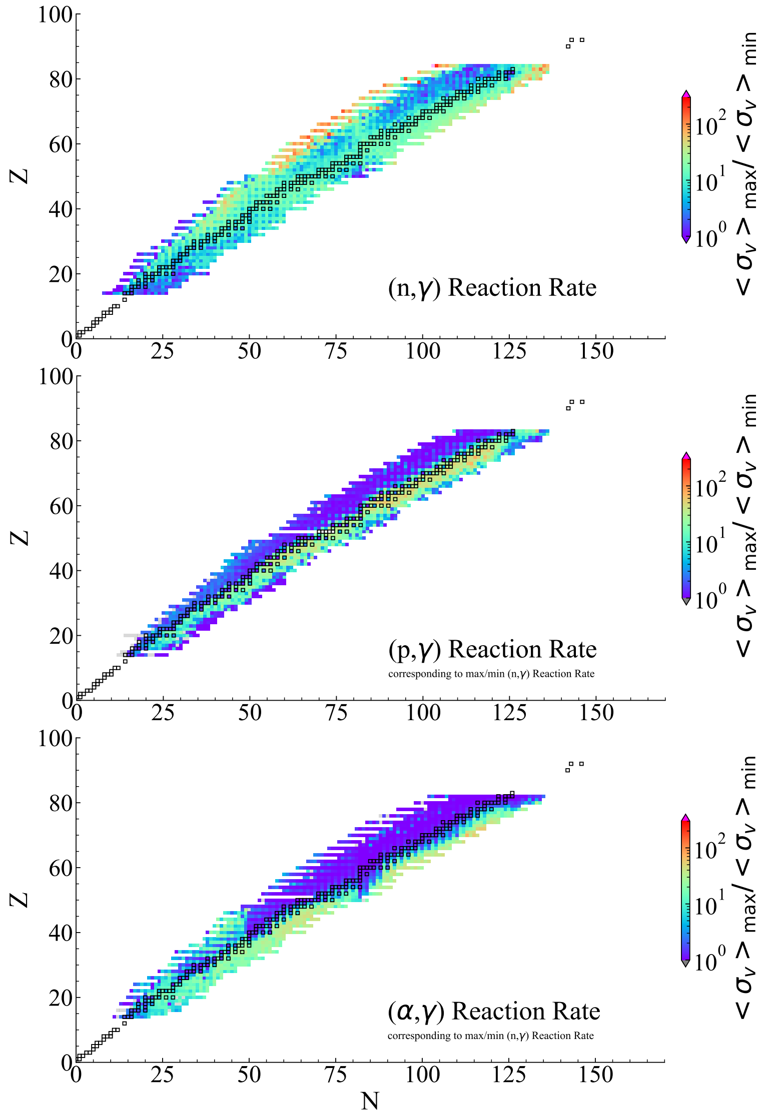


- MC approach if uncorrelated uncertainties
- Additional correlations may exist, e.g S_n and *M*
- Parameters changes must be constrained by exp

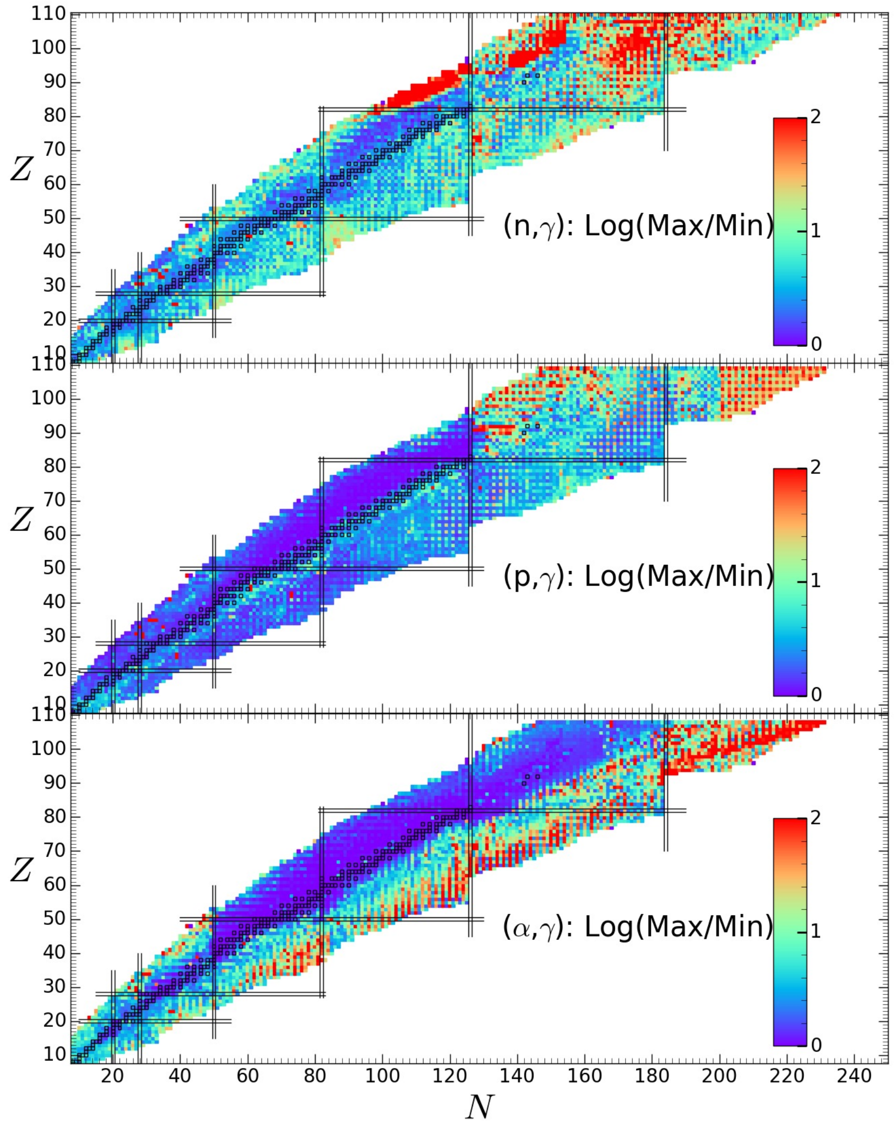
- MC approach not correct
- Coherent model-correlated uncertainties
- Each model is affected by parameter unc.

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

Uncorrelated *Parameter* uncertainties



Correlated *Model* uncertainties

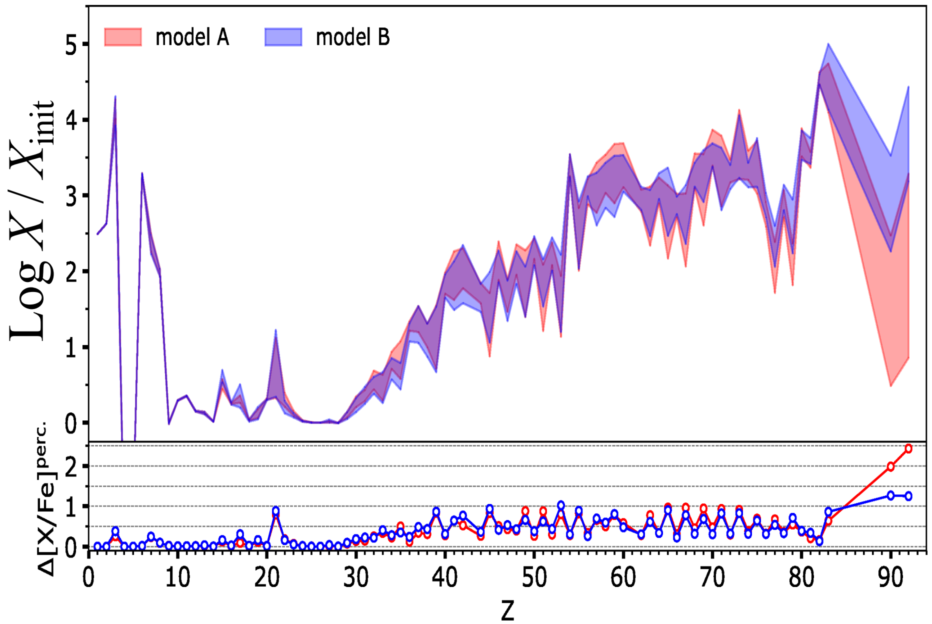


Impact of on the i-process nucleosynthesis in low-*Z* low-*M* AGB stars

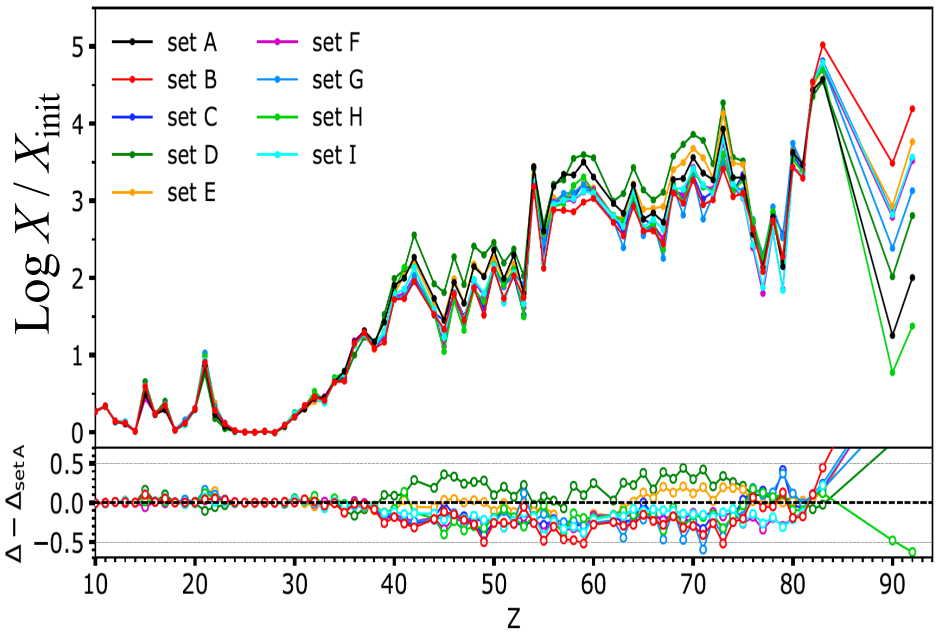
Surface abundances in a $1M_{o}$ [Fe/H]=-2.5 AGB star

(Martinet et al. 2023)

Uncorrelated *Parameter* uncertainties



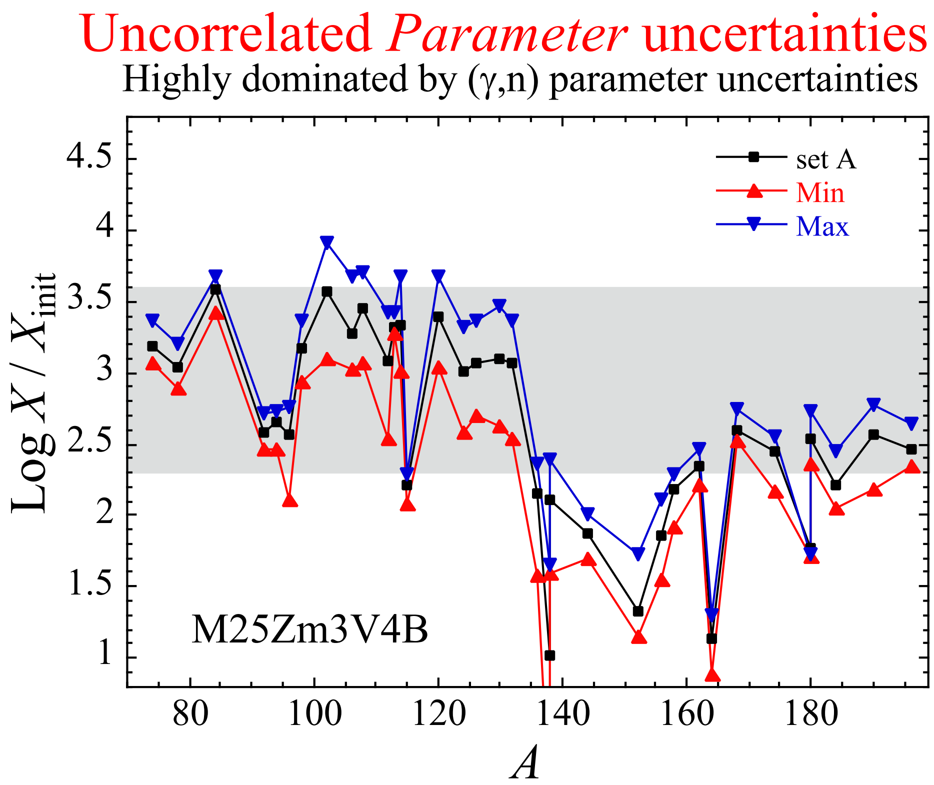
Correlated *Model* uncertainties

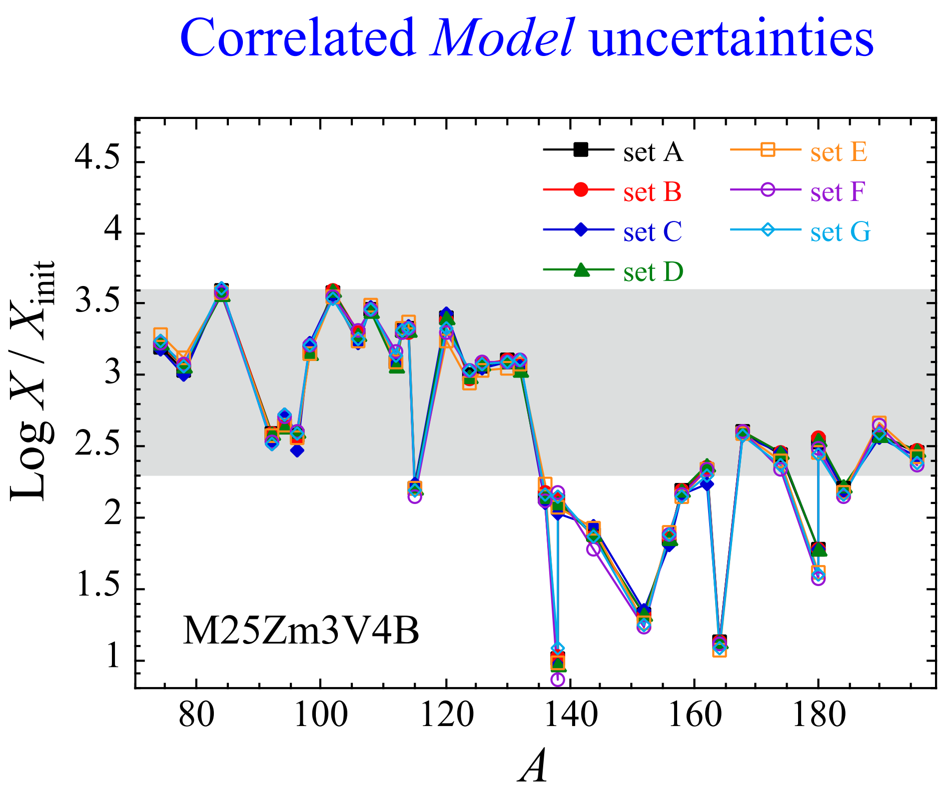


Impact of NLD/PSF uncertainties on the p-process nucleosynthesis

Overproduction of p-nuclei in the core of an exploding $25M_{\odot}$ Z=0.001 v/v_c=0.4 star

(Choplin et al. 2022)





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

- More experimental constraints
- **Improved nuclear models**
  - Their **accuracy**, *i.e.* their capacity to reproduce experimental data
  - Their **reliability**, *i.e.* their physical robustness

Nuclear Applications

Different possible "global" approaches depending on the nuclear applications

(valid for all NP ingredients: Masses, Fission, NLD, PSF, OMP, EoS...)

PHENOMENOLOGICAL DESCRIPTIONS

ACCURACY
(reproduce exp.data)

Concern of
Nuclear applications

Concern of
nuclear astrophysics

Phenomenological models
(Parametrized formulas, Empirical Fits)
Classical models
(e.g Liquid drop, Droplet)
Semi-classical models
(e.g Thomas - Fermi)
mic-mac models
(e.g Classical with micro corrections)
semi-microscopic
(e.g MF models with phenomenological corrections)
microscopic
(e.g mean field, beyond-MF)
fully microscopic (not global yet)
(e.g shell model, ab-initio, ...)

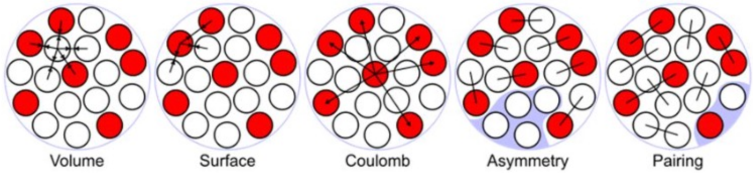
RELIABILITY
(Sound physics)

Concern of
fundamental physics

« MICROSCOPIC » DESCRIPTIONS

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

MACROSCOPIC DESCRIPTION

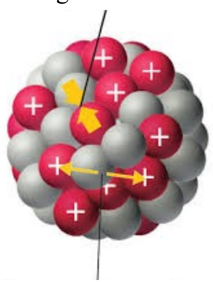


$$E_B = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \Delta(Z,N)$$

Mic-Mac models still widely used in many nuclear applications

GLOBAL MEAN-FIELD DESCRIPTION

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



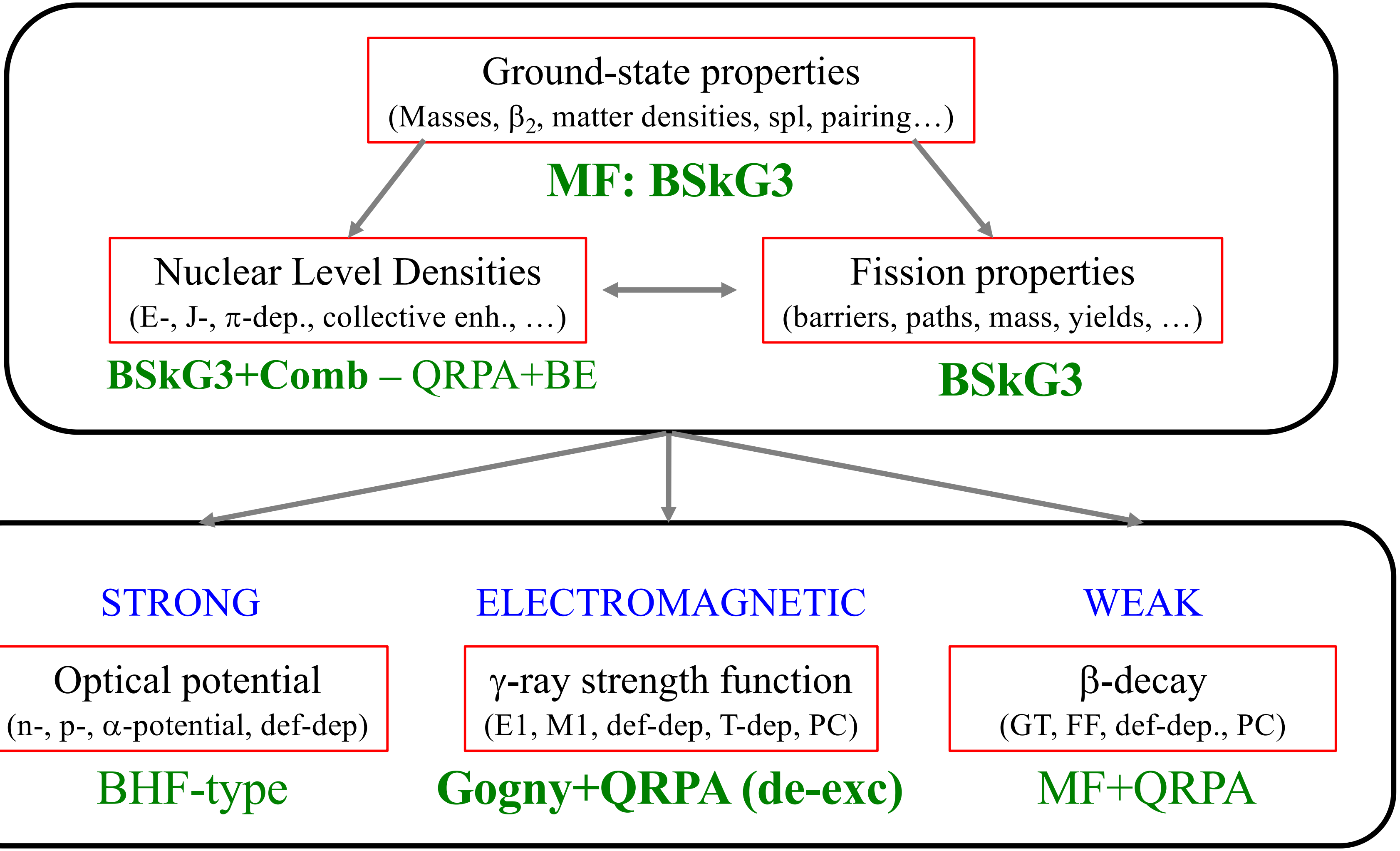
$$\begin{aligned}
\mathcal{E}_{\rm Sky} = & \sum_{q=n,p} \frac{\hbar^2}{2M_q}\tau_q + \frac{1}{2}t_0\left[\left(1+\frac{1}{2}x_0\right)\rho^2 - \left(\frac{1}{2}+x_0\right)\sum_{q=n,p}\rho_q^2\right] + \frac{1}{4}t_1\left[\left(1+\frac{1}{2}x_1\right)\left(\rho\tau+\frac{3}{4}(\nabla\rho)^2\right) -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

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

A challenge that will require a continued effort…

Some new efforts to improve the nuclear predictions for astrophysical applications

Nuclear inputs to nuclear reaction & decay calculations



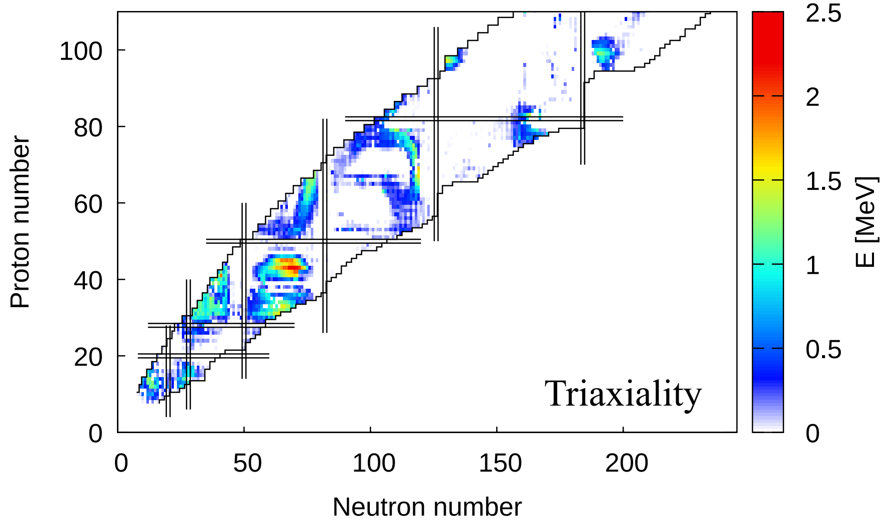
"Microscopic" approach is a necessary but not a sufficient condition !
"(Semi-)Microscopic" models must be competitive in reproducing exp. data !

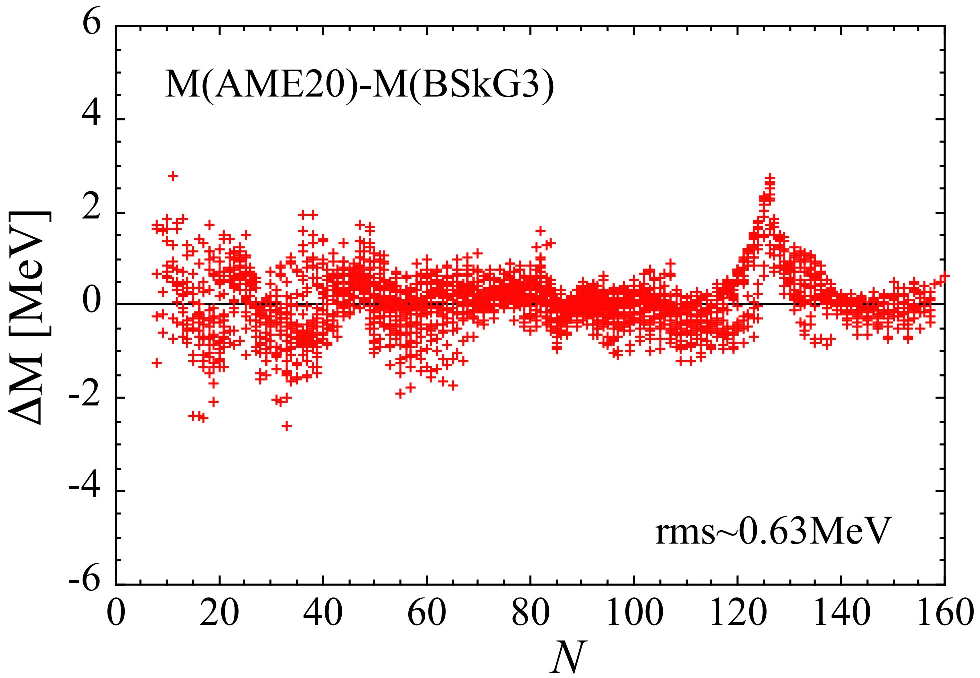
BSkG3 HFB nuclear mass models

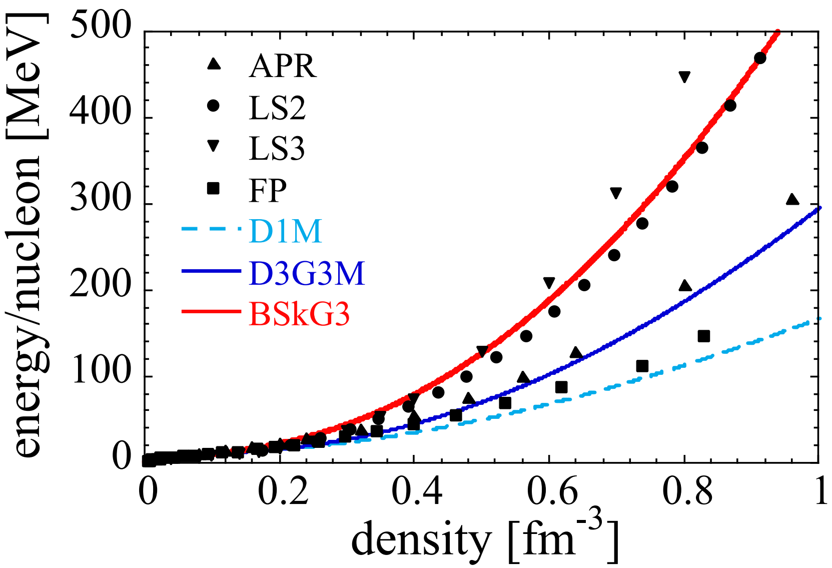
Grams, Ryssens et al. (EPJA 59, 270, 2023)

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



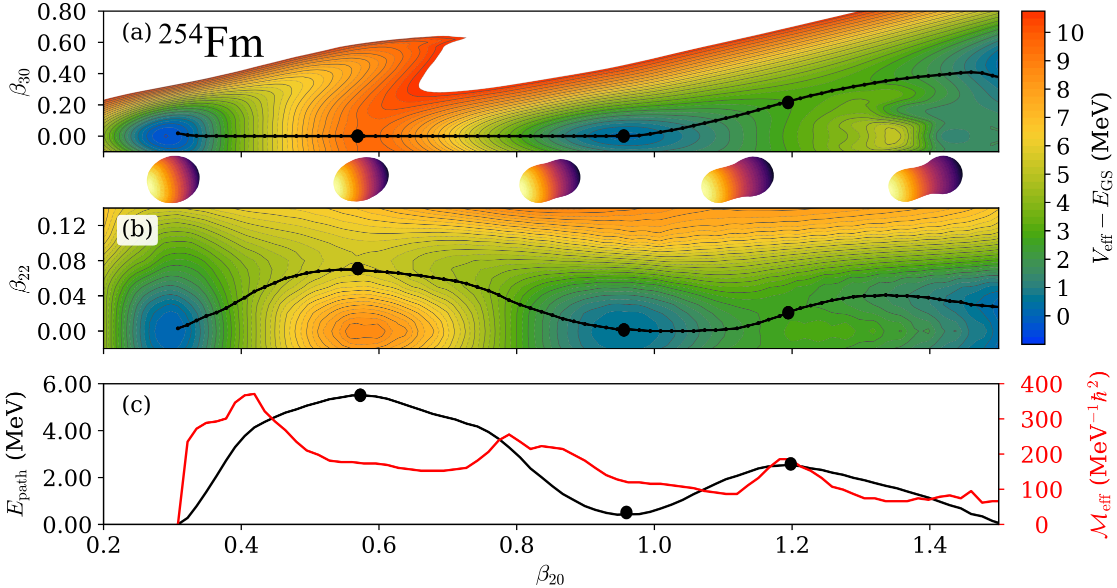




BSkG3: Remarkable description of fission properties

cf Sánchez Fernández et al. (2025)

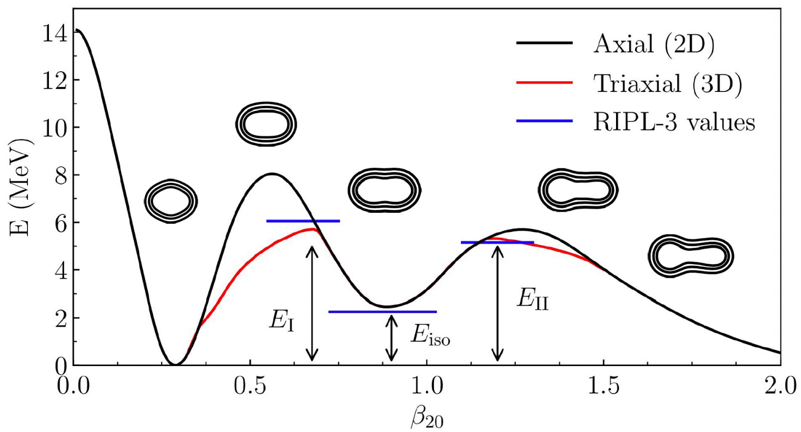
- Fission barriers



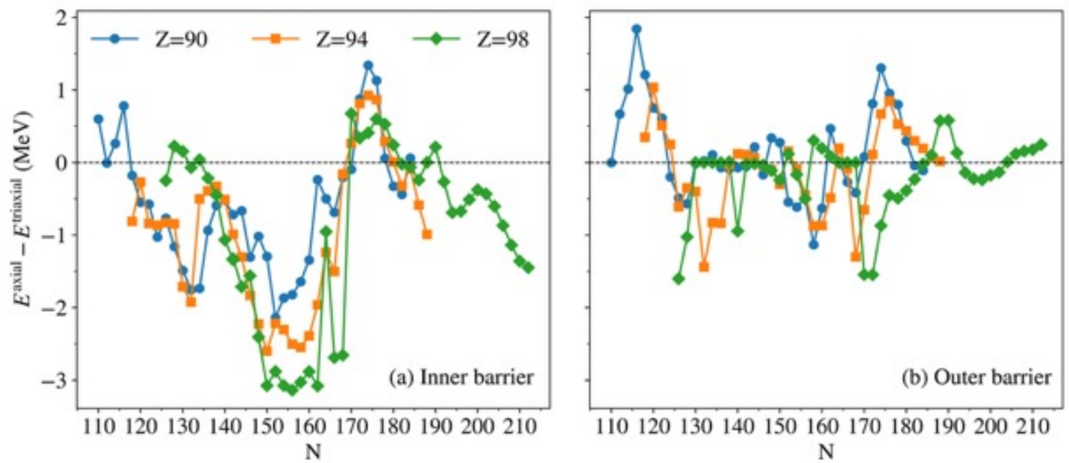
Deviations of the primary barrier wrt to RIPL-3 ones

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



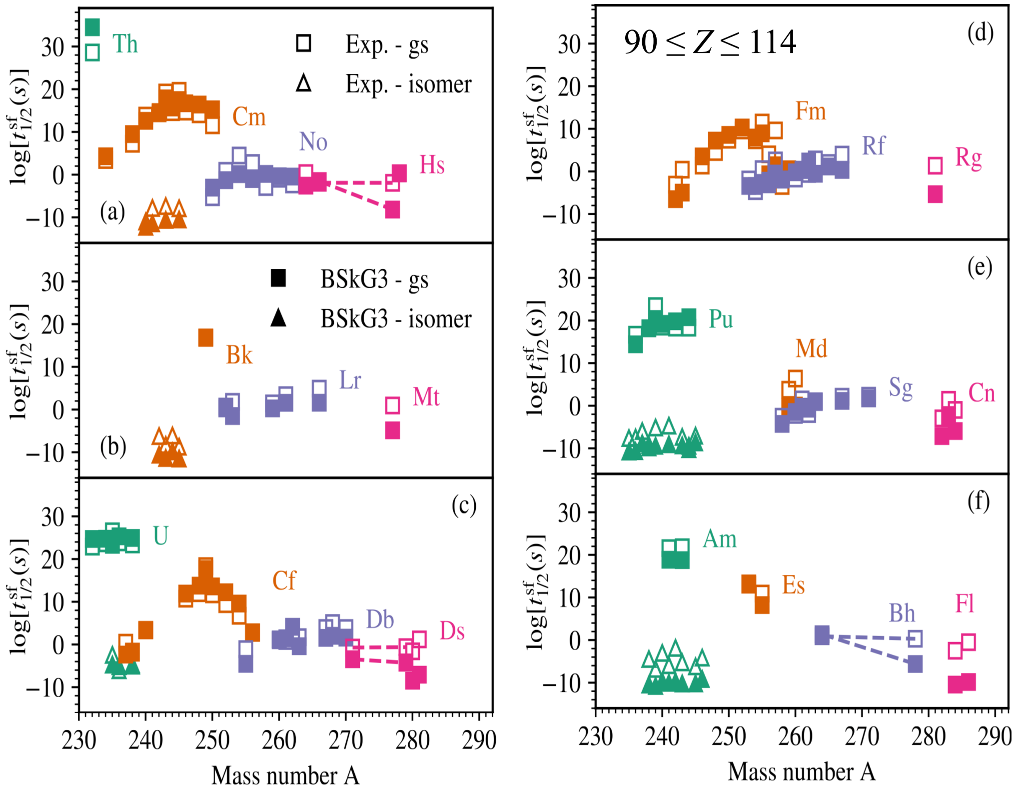
Impact of triaxiality on the barrier height



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

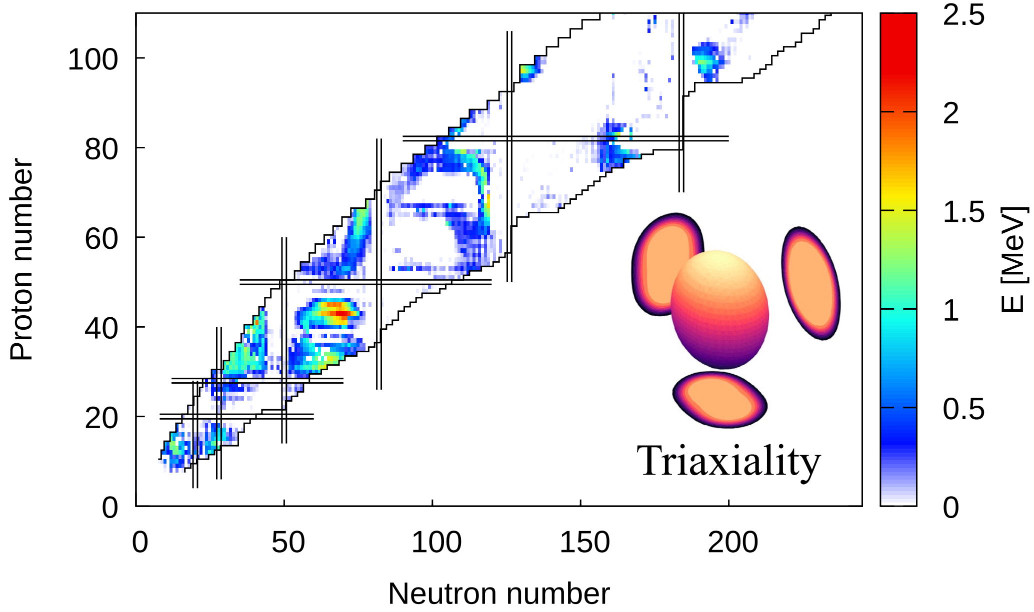
$$f_{\rm rms} = \exp\left[\frac{1}{N}\sum_i^N (\ln r_i)^2\right]^{1/2}$$

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

Nuclear Level densities

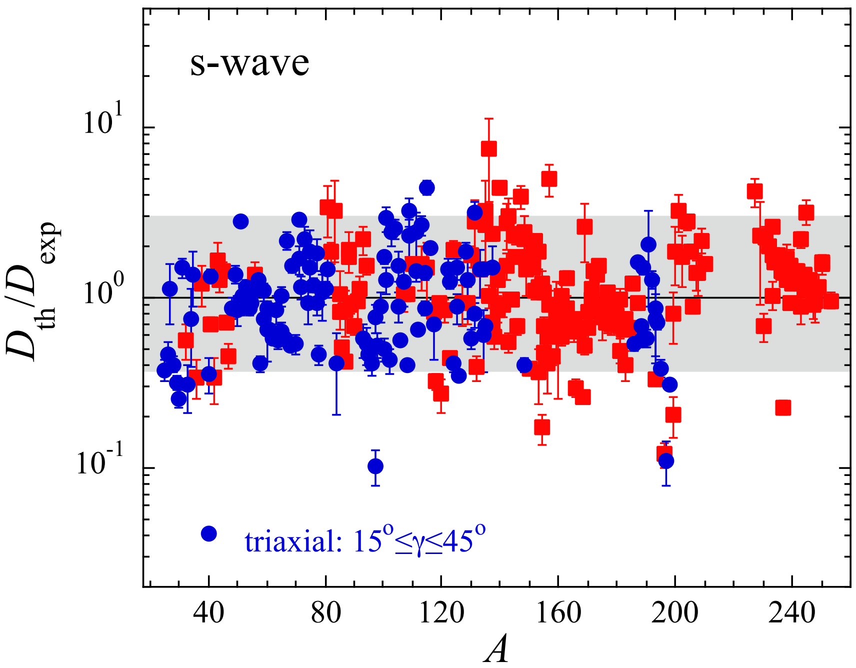
New *combinatorial* predictions based on the BSkG3 nuclear structure properties

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



Comparison with experimental data

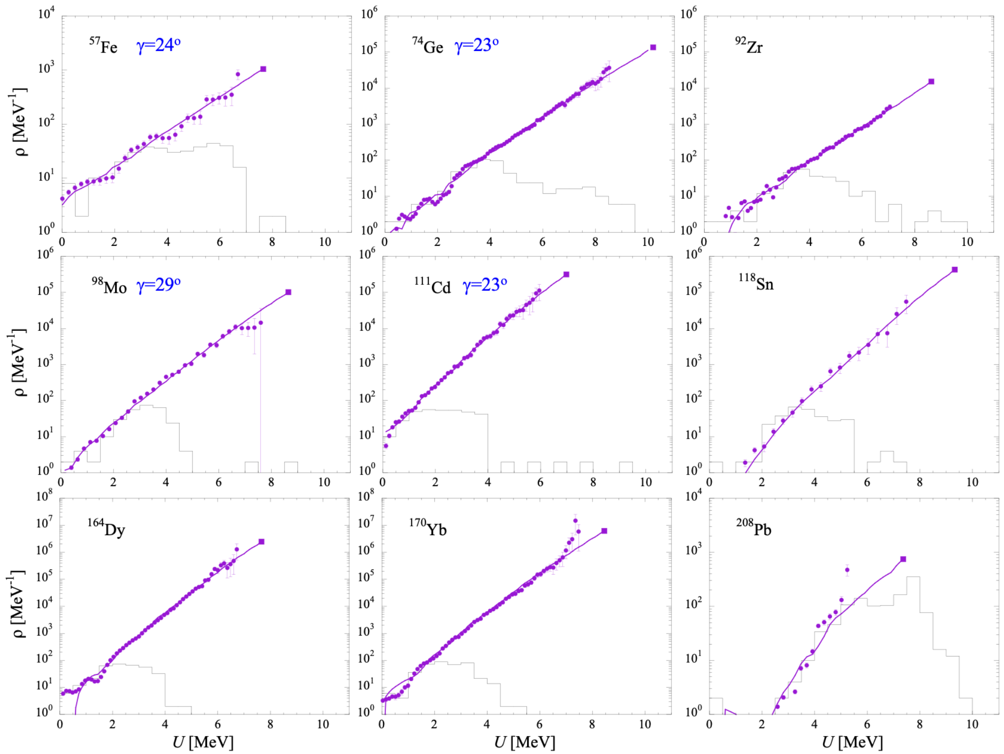
s-wave neutron resonance spacings at S_n



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

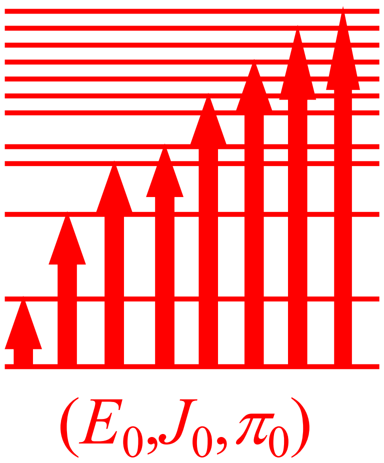


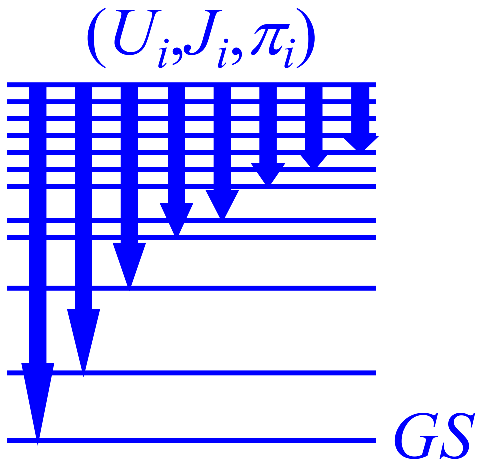
(after renormalisation on D_0)

Photon Strength Function

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

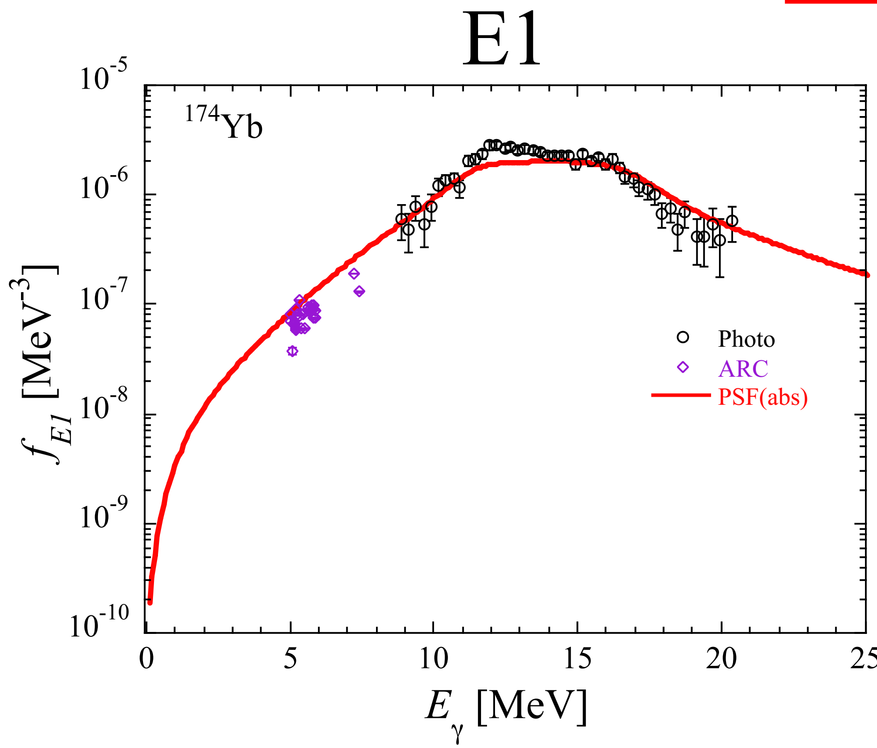
In particular: (γ,n), (γ,p), (γ,α) (n,γ), (p,γ), (α,γ)

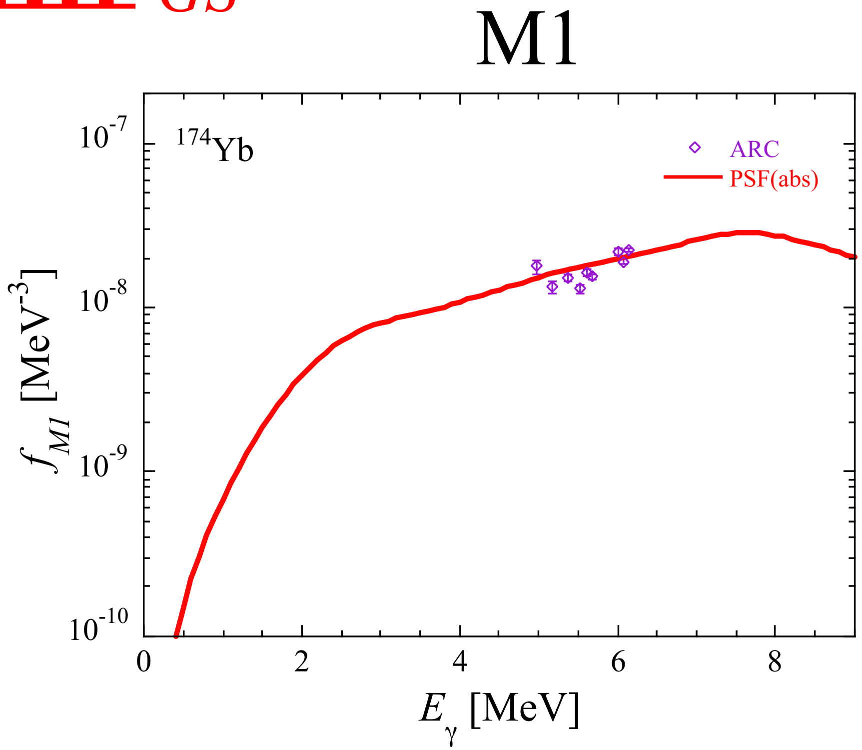




QRPA photoabsorption PSF from the GS

Gogny-HFB+QRPA

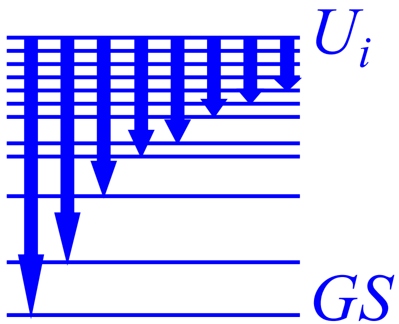




Successful in describing photo, ARC, NRF, ... data

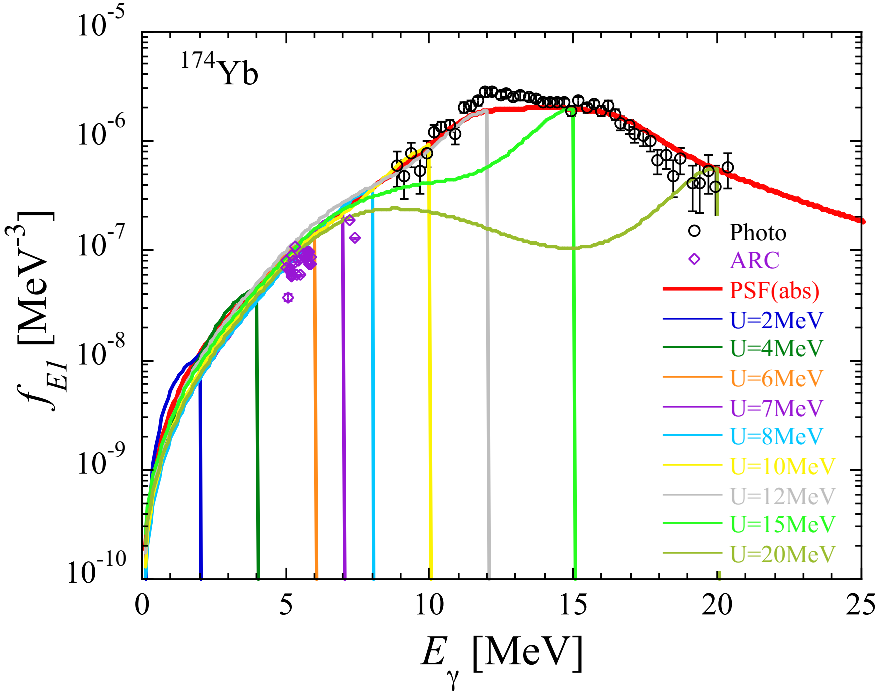
QRPA de-excitation PSF at an initial energy U_i

deformed ^{174}Yb



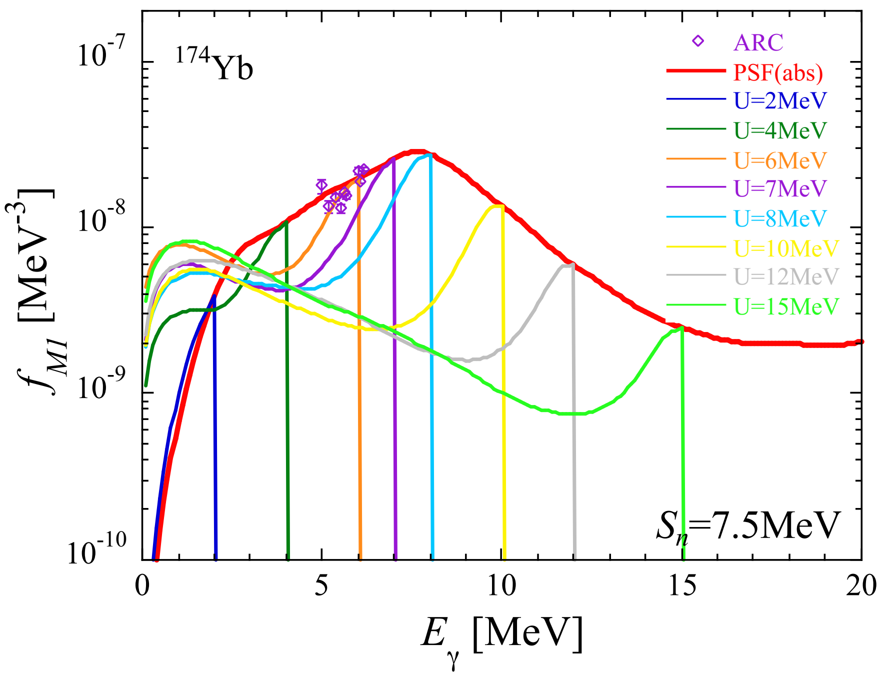
Gogny-HFB+QRPA

E1



Negligible low-energy E1 enhancement

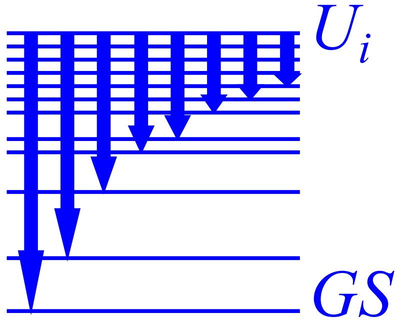
M1



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

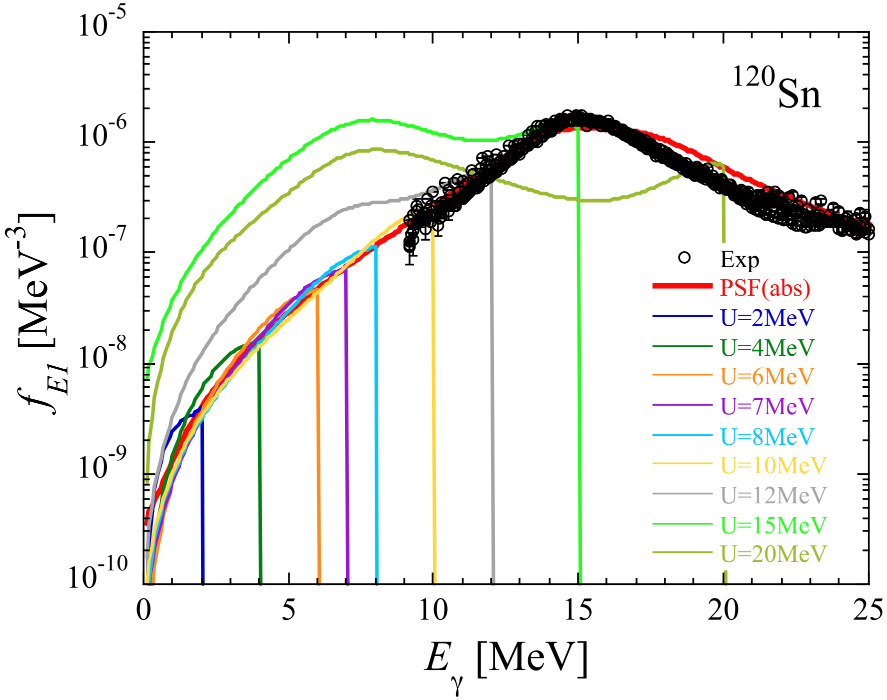
QRPA de-excitation PSF at an initial energy U_i

spherical ^{120}Sn

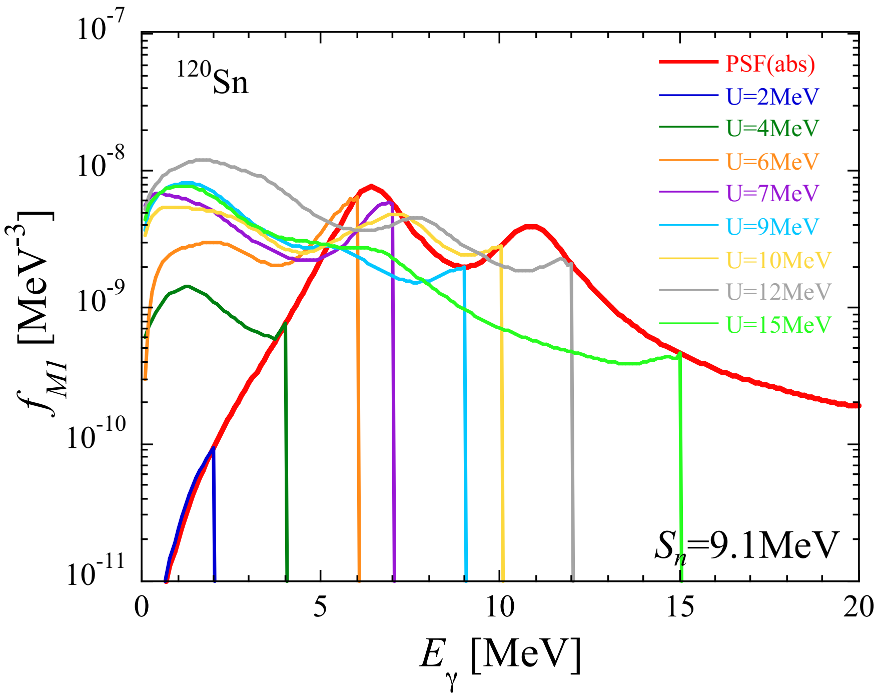


Gogny-HFB+QRPA

E1



M1

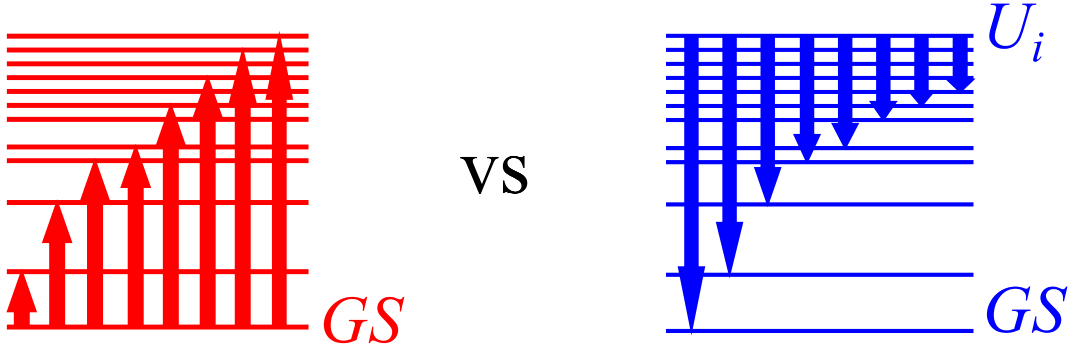


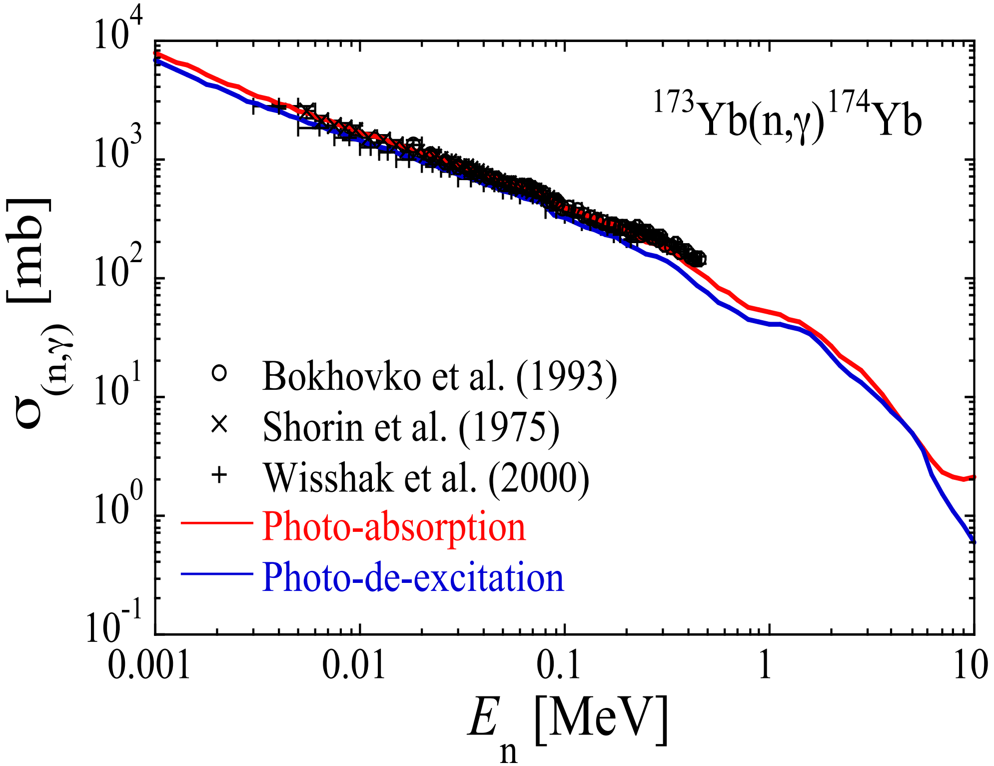
Non-negligible low-energy E1 enhancement at E_γ>10MeV

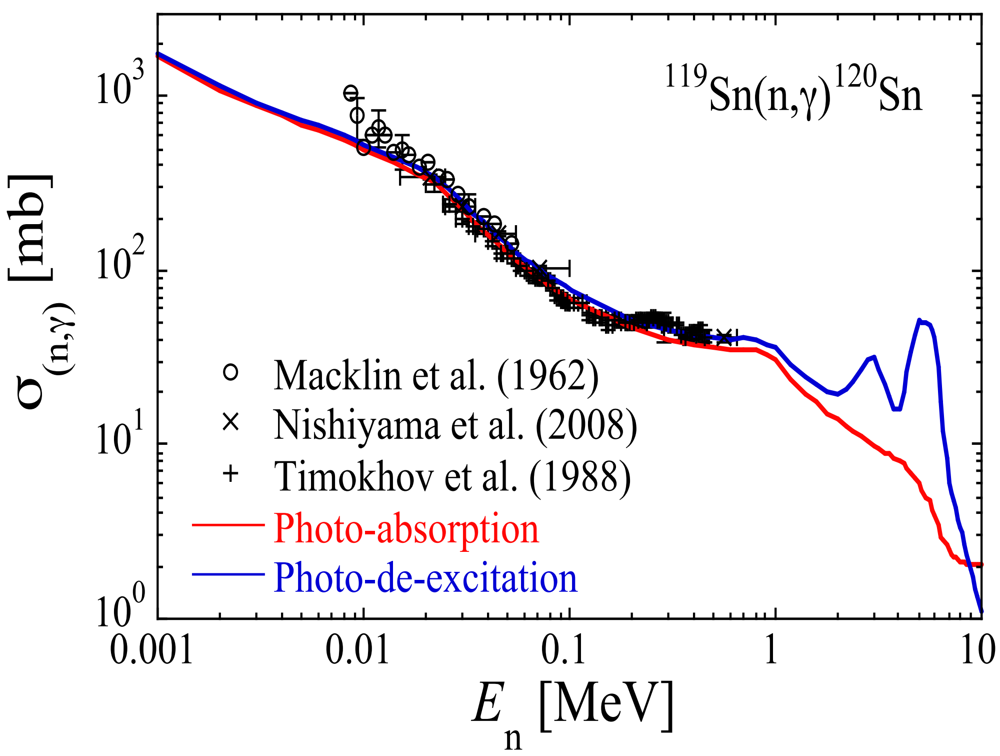
Significant low-energy M1 enhancement ("upbend") but also reduction at higher E_γ

Note: - 2 billions CPU hours for about 160 e-e Z<80 nuclei
- Coherent use of the QRPA phonon energies to estimate NLD by a combinatorial approach

QRPA de-excitation PSF at an initial energy U_i





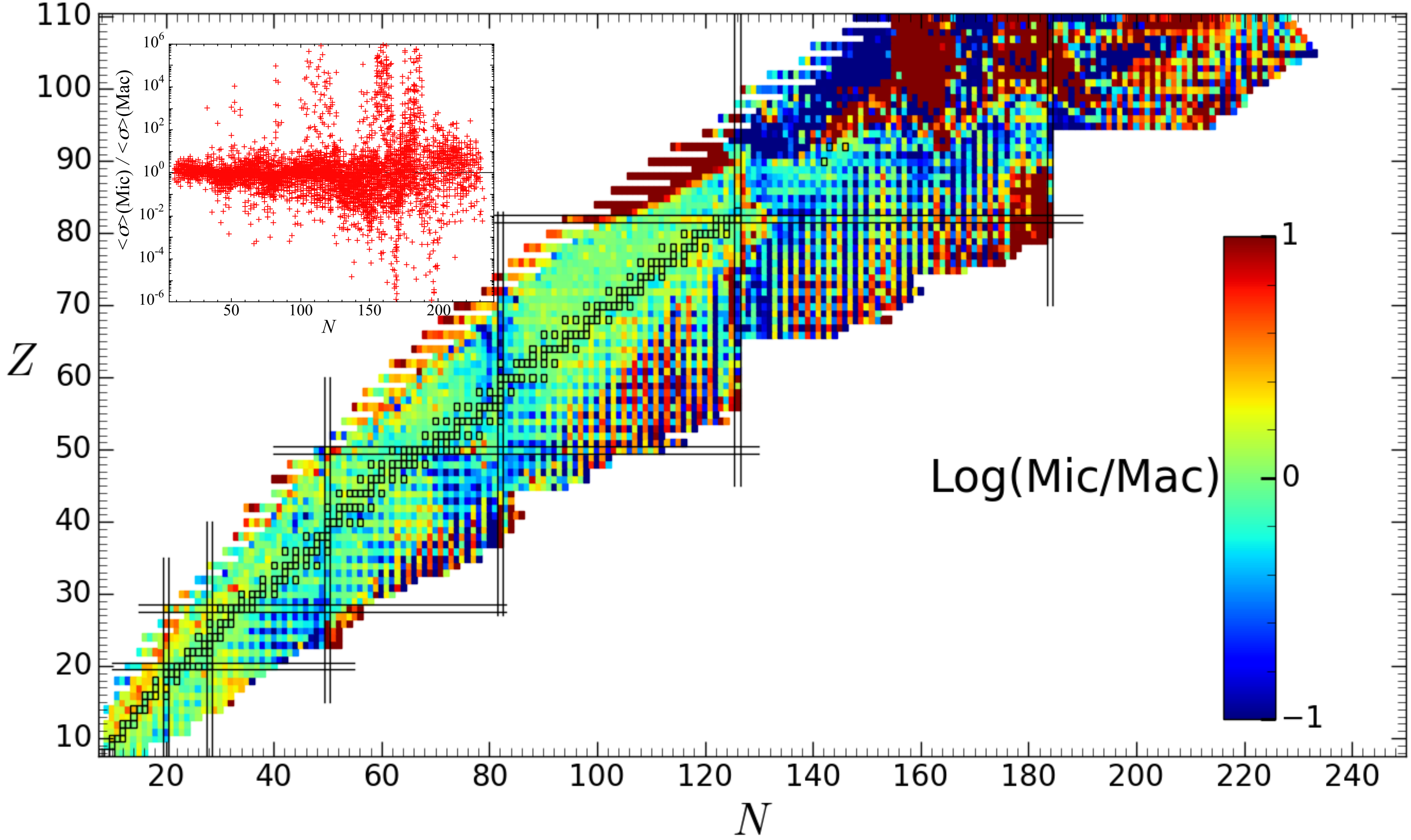


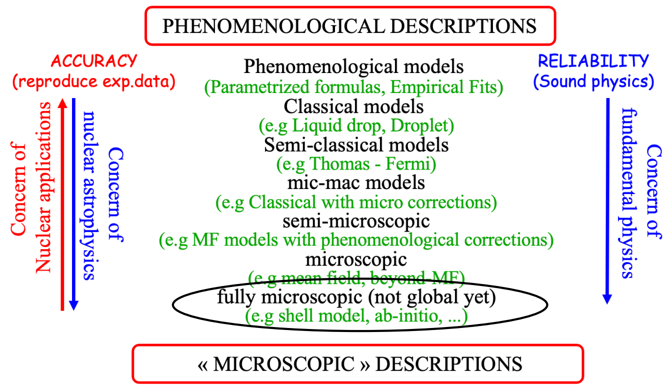
Application to cross section calculations and implication for nucleosynthesis still ongoing

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

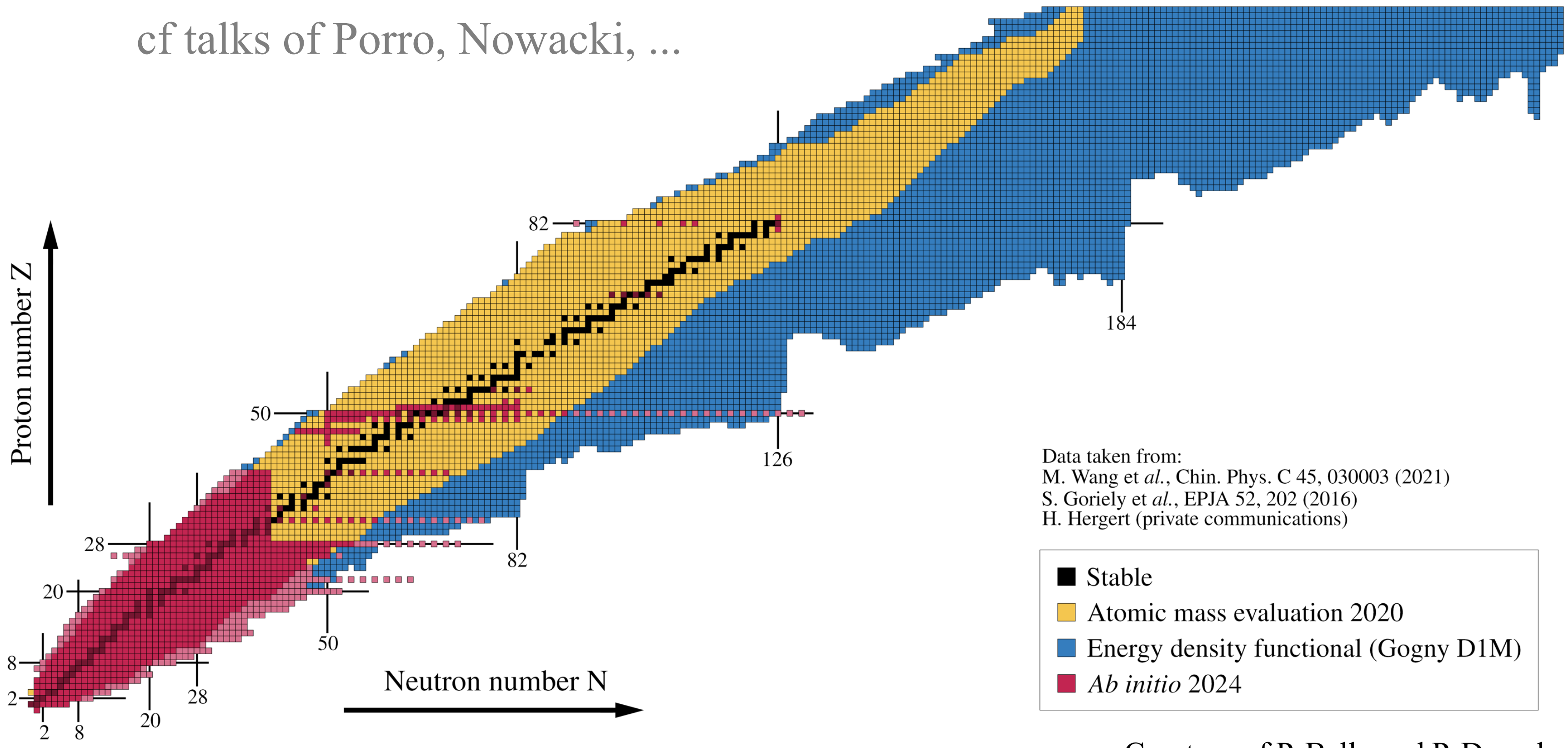




Impressive progress in *Shell* & *Ab-initio* models

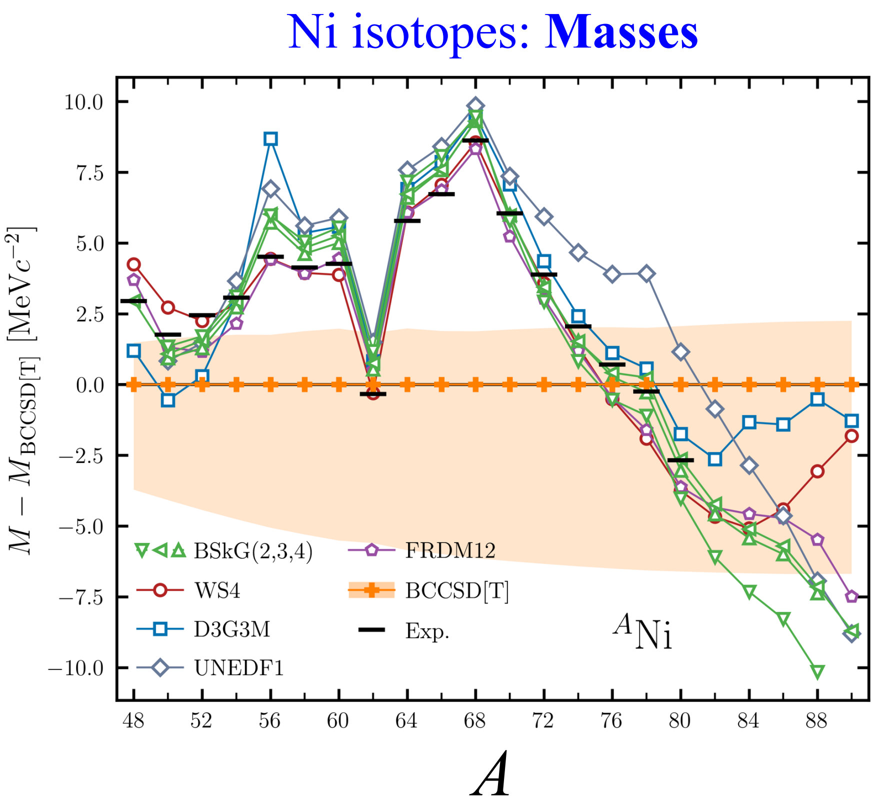
- Self-consistent Green's function (e.g. Soma, 2002; Barbieri et al. 2022)
- In-medium similarity renormalization group (e.g. Hergert et al. 2016)
- Coupled cluster (e.g. Hagen et al. 2014, Demol 2024)
- Many-body perturbation theory (e.g. Tichai et al. 2020)

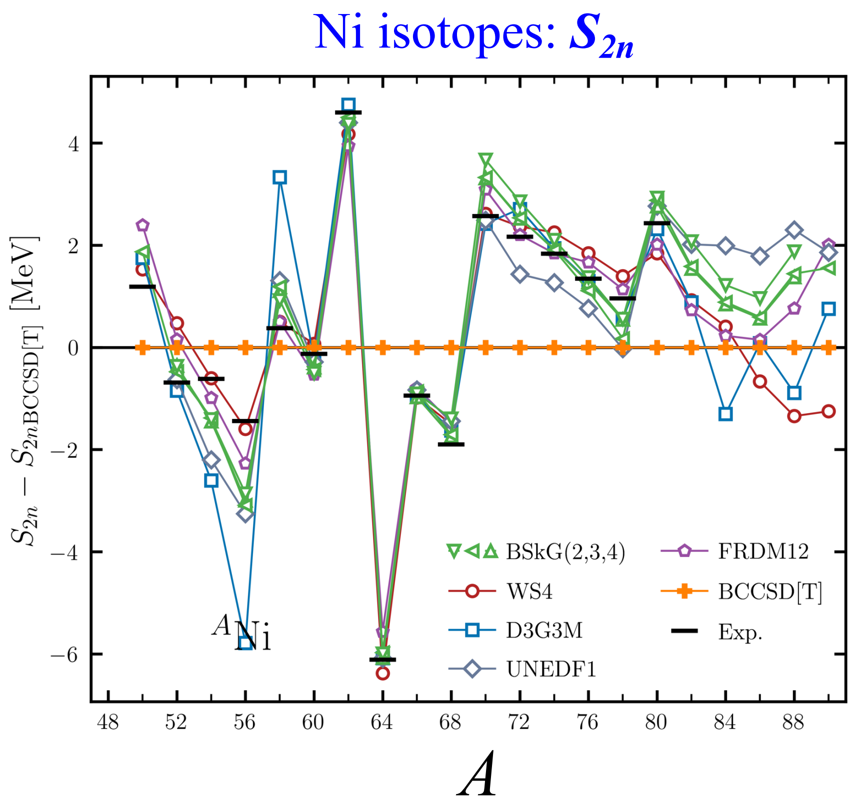
cf talks of Porro, Nowacki, ...



Courtesy of P. Bally and P. Demol

Comparison between BCCSD[T] *ab-initio* predictions with mass models





Courtesy of P. Demol

Future developments may allow us to use *ab-initio* models as reference calculation far away from experimentally known regions

Conclusions

- **Major progress achieved and efforts ongoing**
  - Reaction model (e.g. TALYS)
  - 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/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

THANK YOU
FOR
YOUR ATTENTION