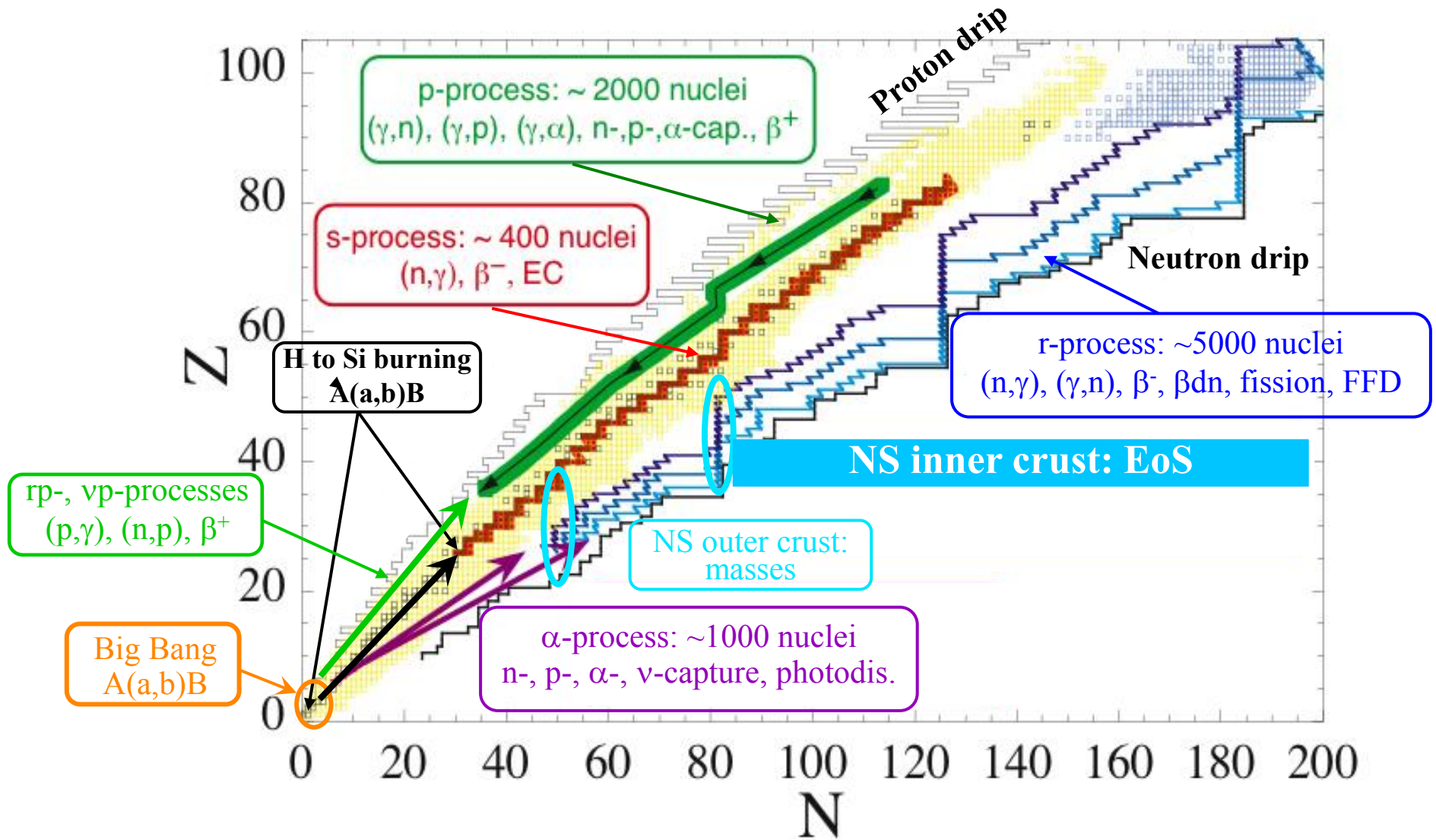


**Towards more accurate and reliable
predictions
for nuclear (astrophysics) applications**

S. Goriely

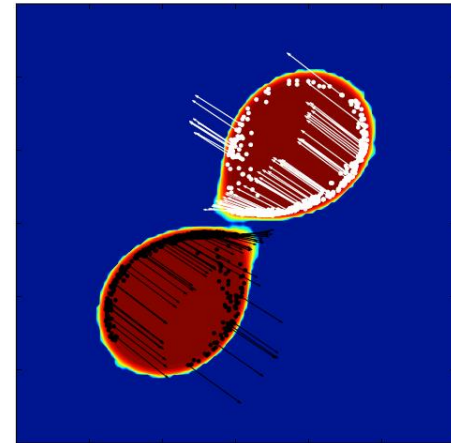
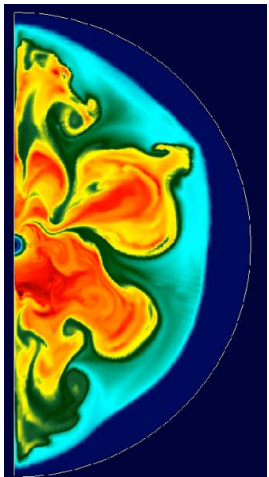
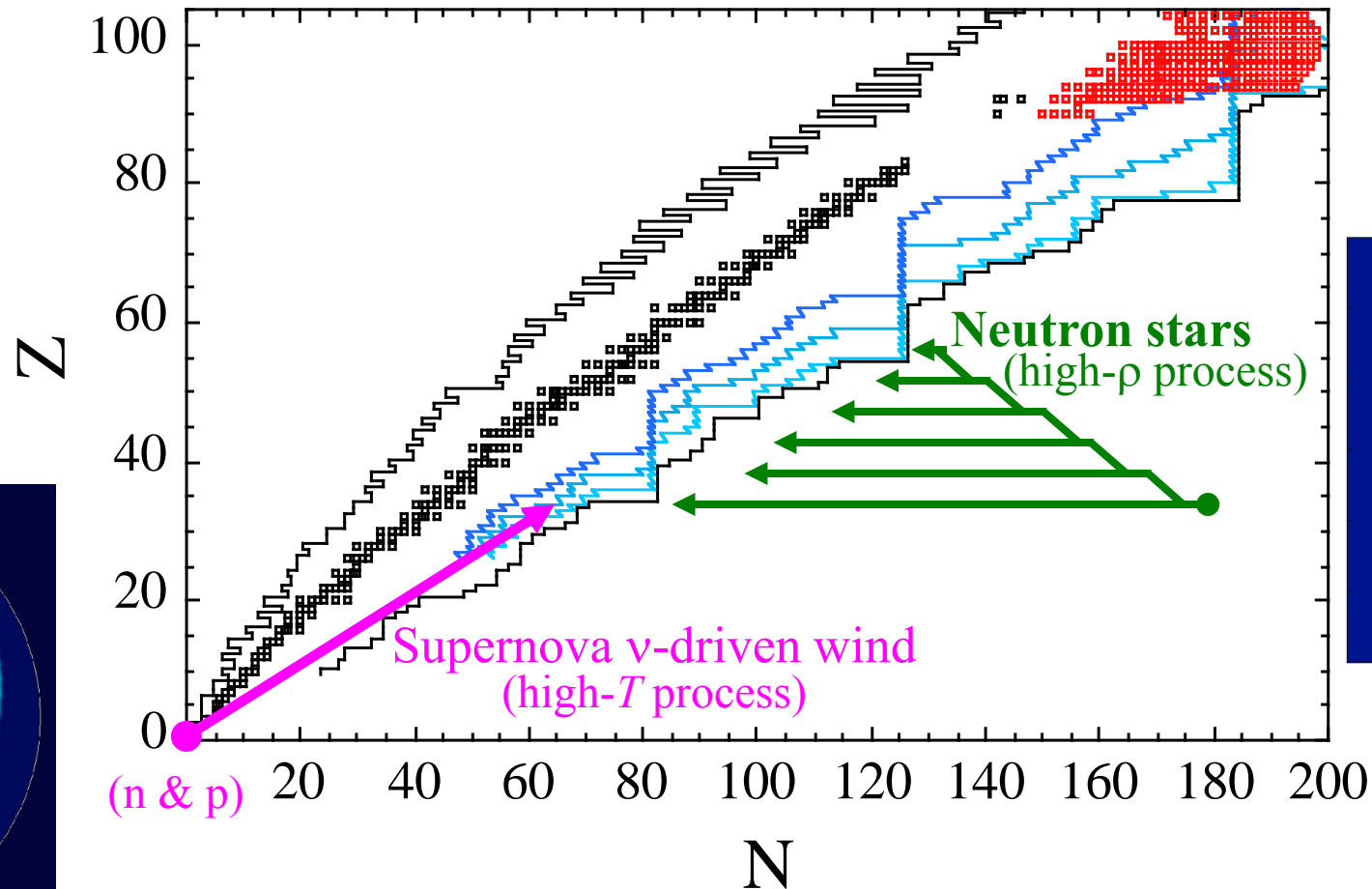
Institut d'Astronomie et d'Astrophysique - Brussels University

Many different nuclear needs for many different nuclear astrophysics applications



The r-process nucleosynthesis responsible for half the elements heavier than iron in the Universe

one of the still unsolved puzzles in nuclear astrophysics
... the r-process site remains unknown ...

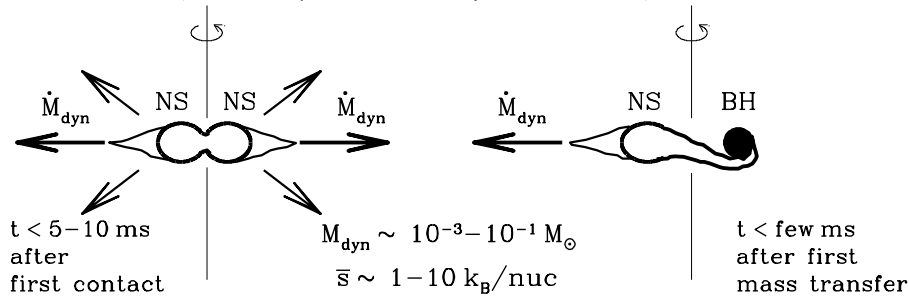


Neutron Star Mergers: a (very) promising r-process site

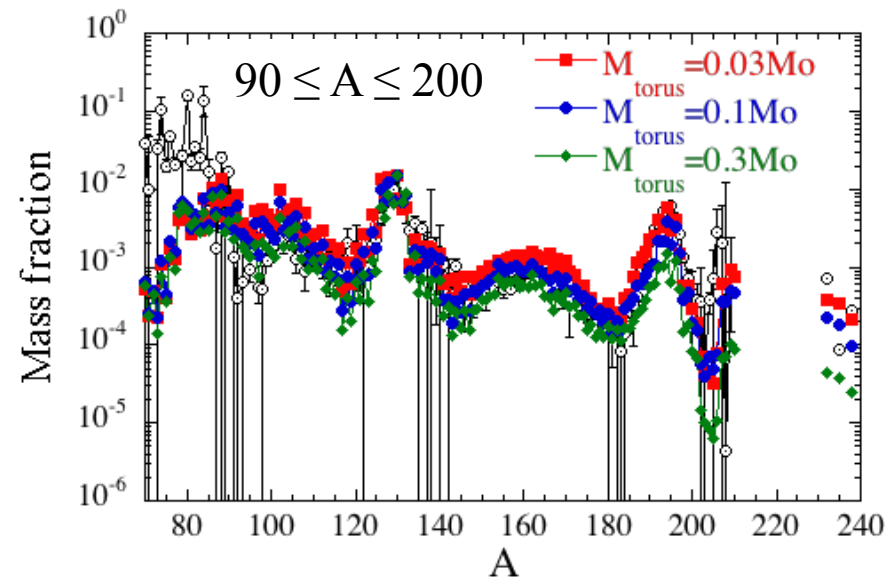
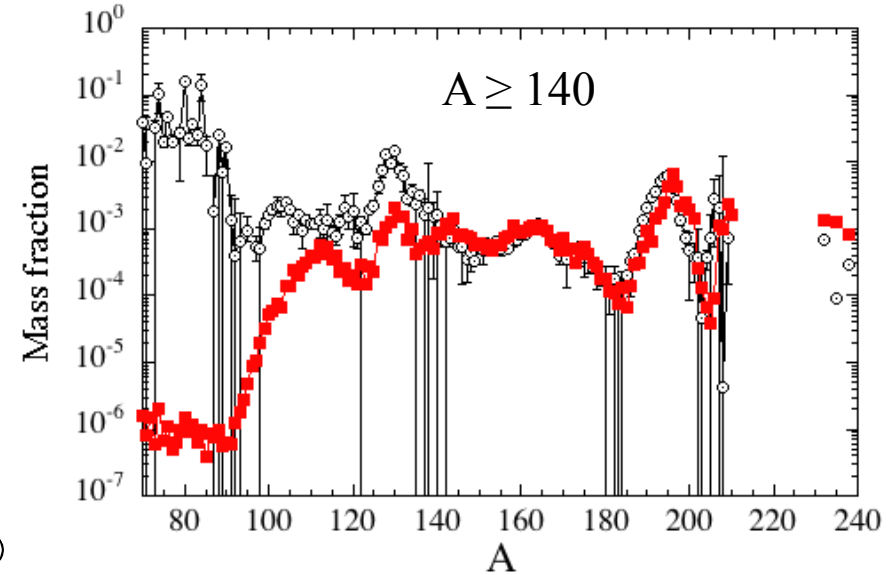
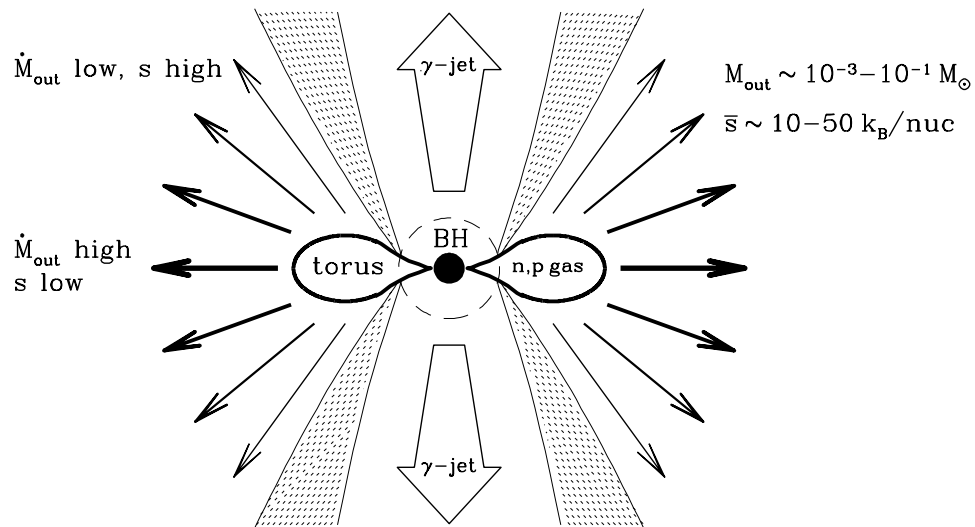
3D hydrodynamical simulations : Just, Bauswein, Janka et al. MNRAS (2014)

Mass loss phases during NS-NS and NS-BH merging

- 1. Merger Phase** Prompt/dynamical ejecta
(due to dynamic binary interaction)

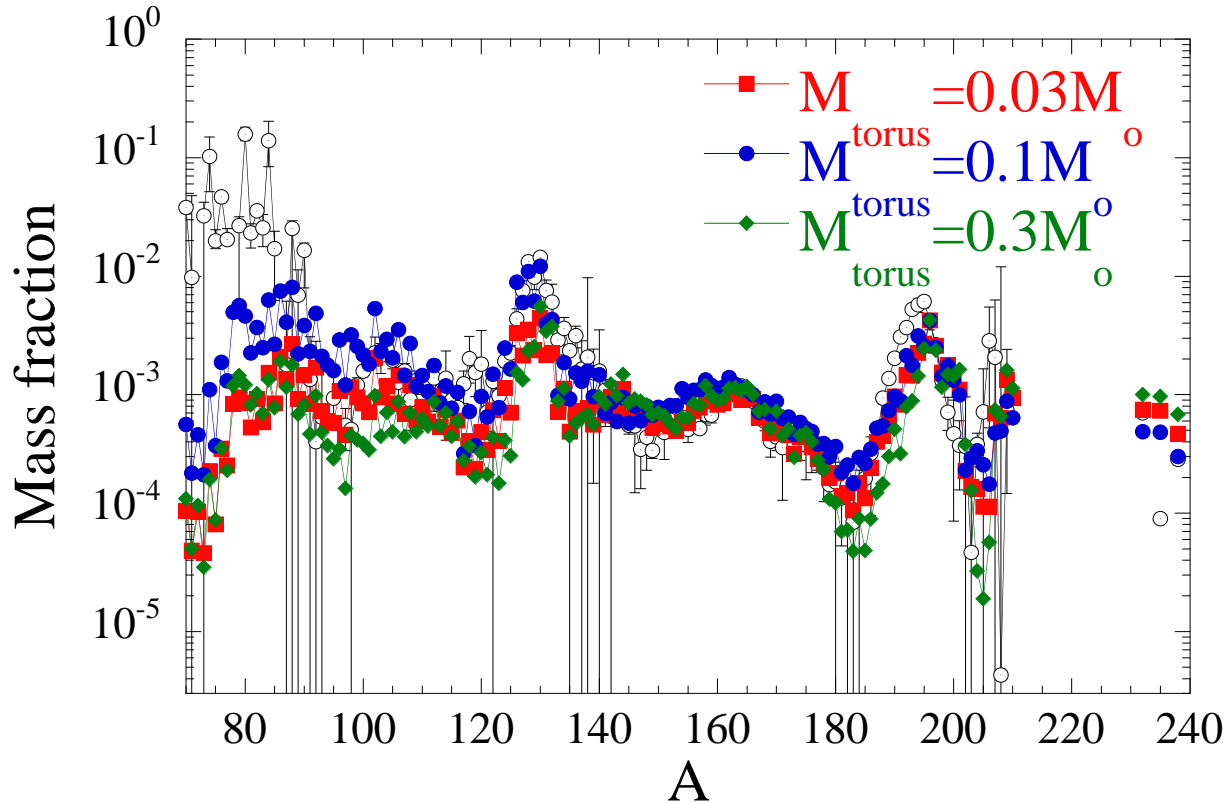


- 2. BH-Torus Phase** Disk ejecta
(due to ν heating, viscosity/magn. fields, recombination)



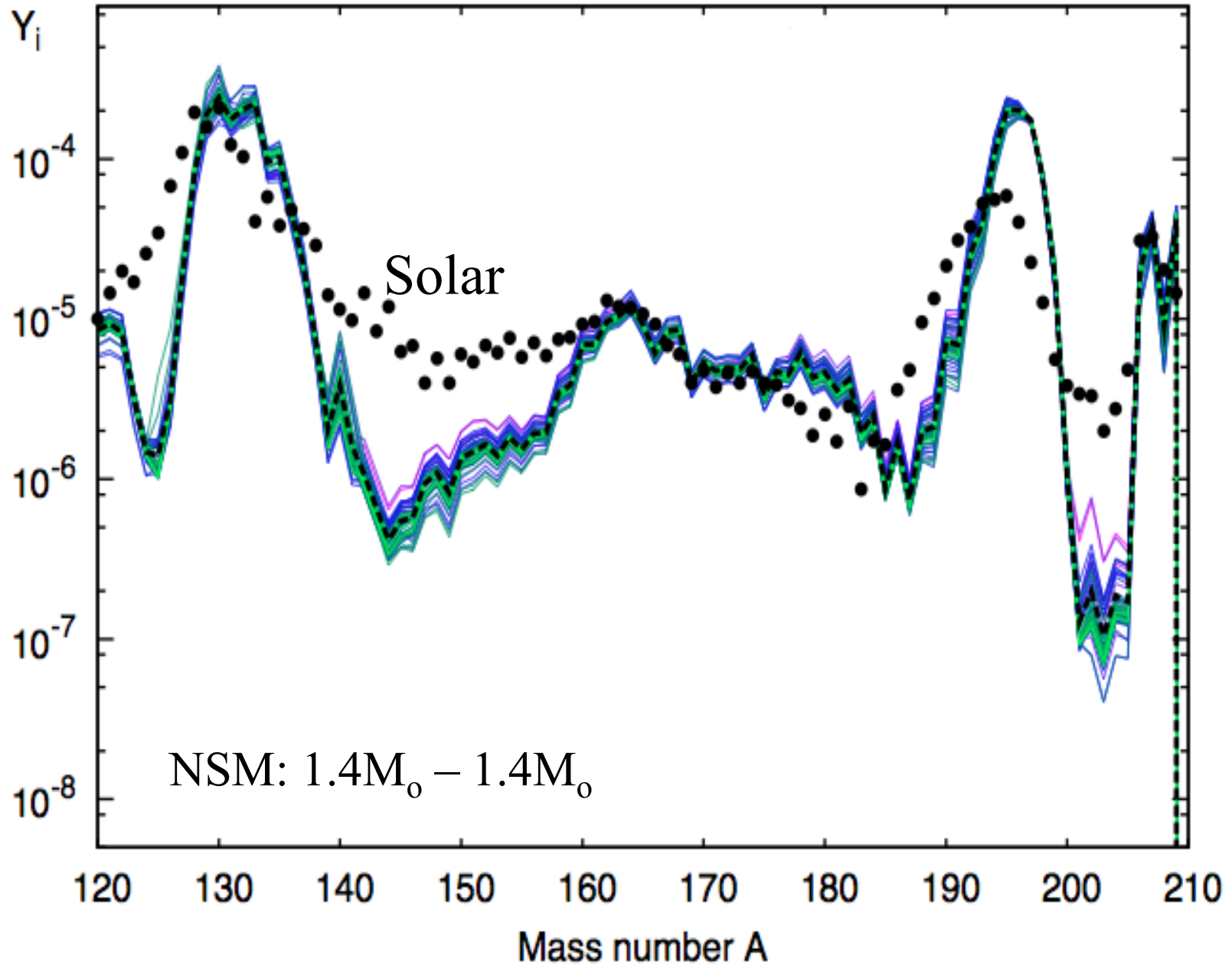
Composition of the consistently combined Dynamical + Disk ejecta

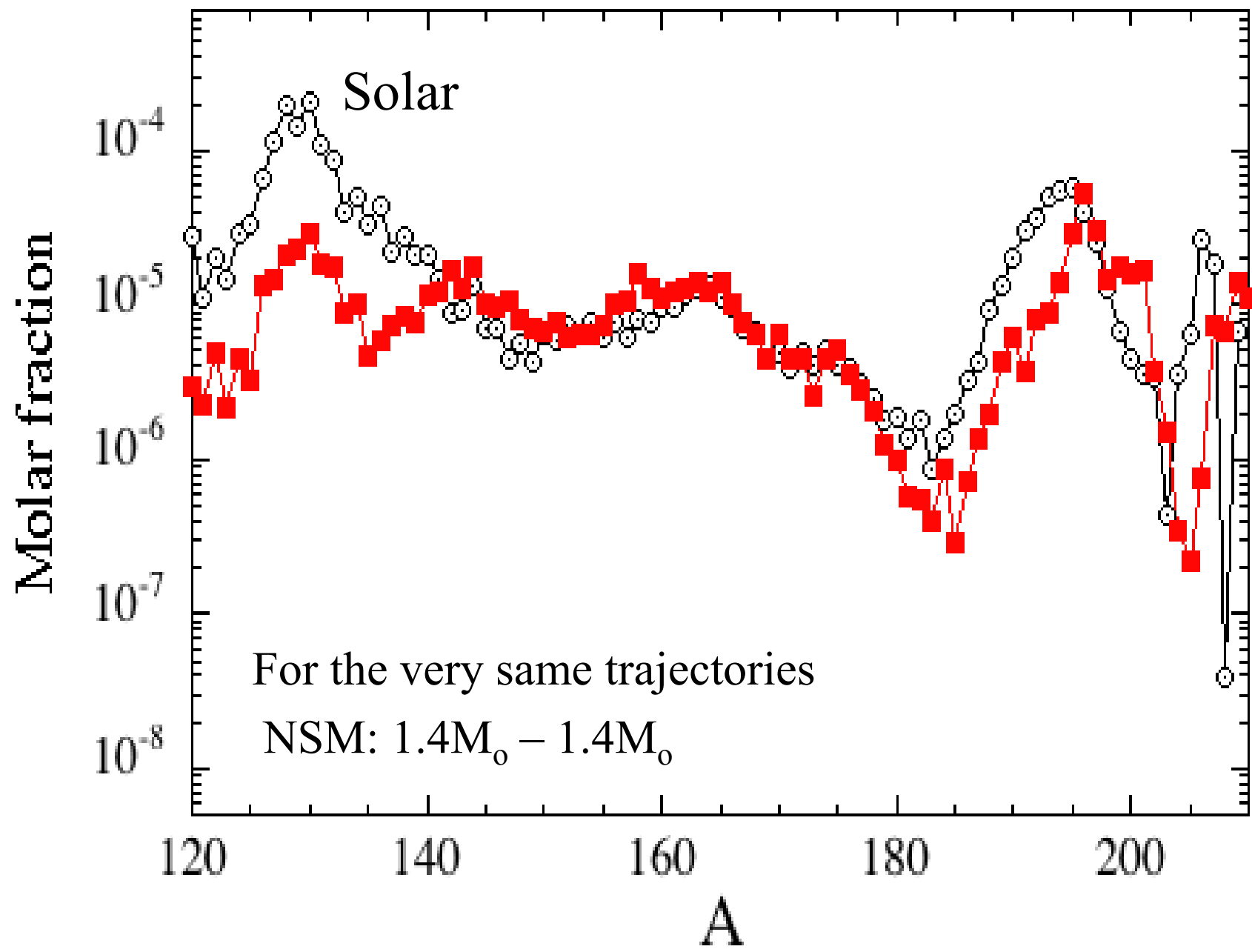
3D hydrodynamical simulations : Just, Bauswein, Janka et al. MNRAS (2014)

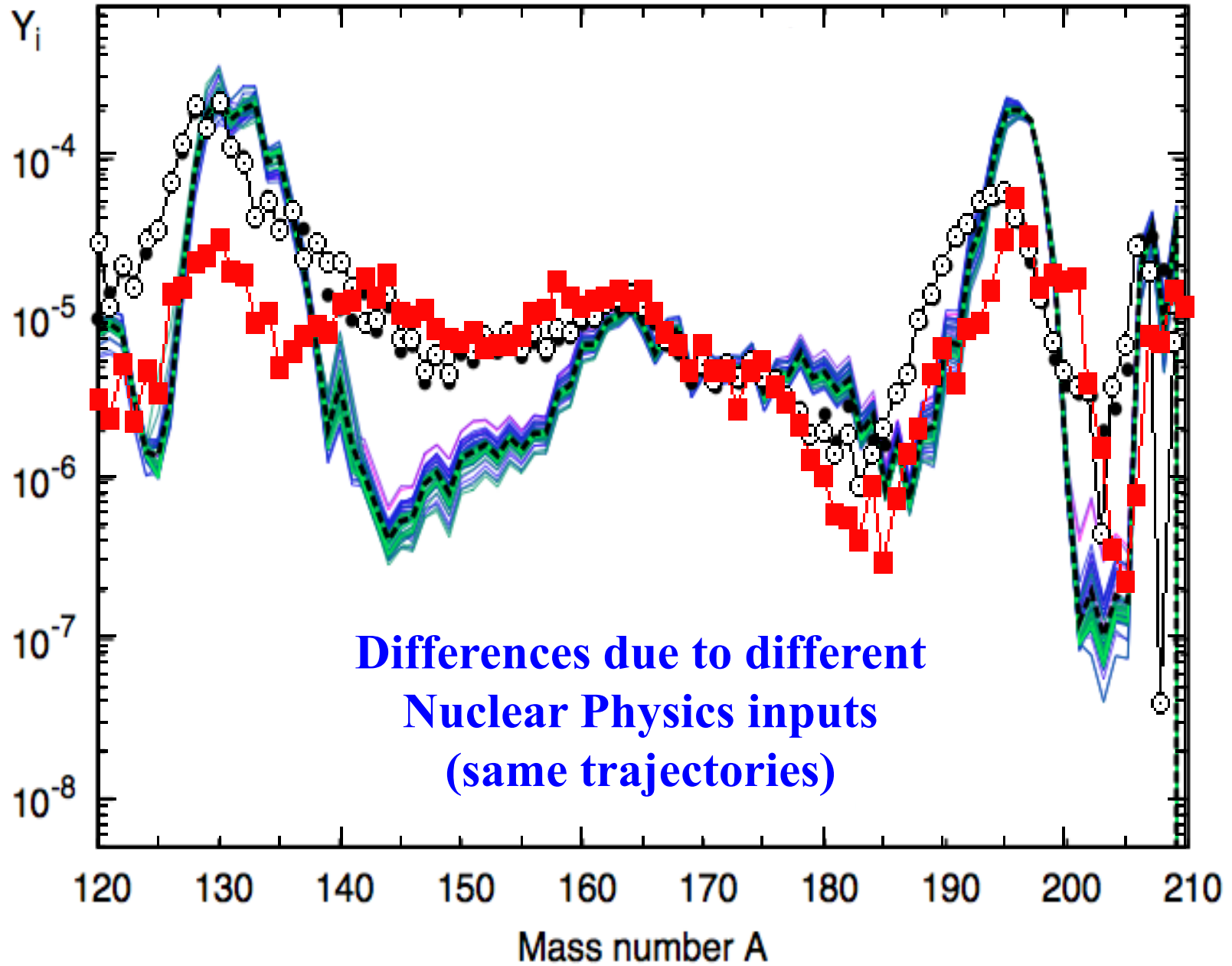


Robust production of all $A \geq 90$ r-nuclei with a rather solar distribution
but very much dependent on the adopted nuclear physics !

Newtonian SPH calculations (Korobkin et al. 2012; Rosswog et al. 2013)





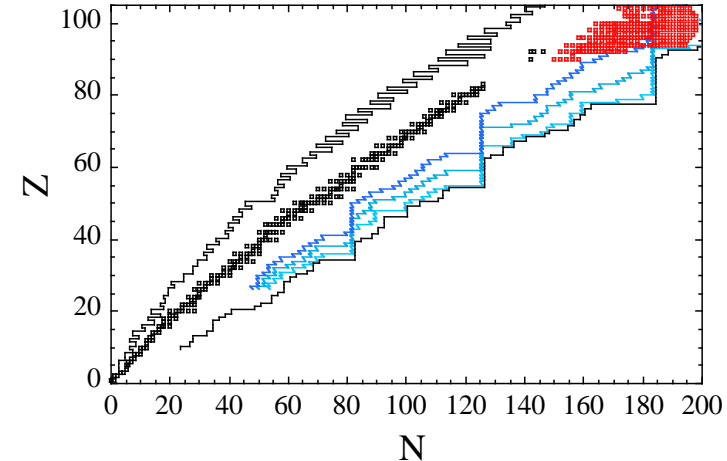
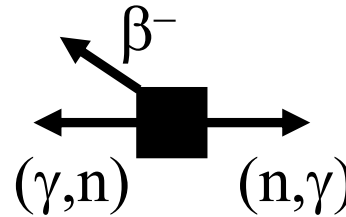


Nuclear needs for r-process nucleosynthesis

$(n,\gamma) - (\gamma,n) - \beta$ competition & Fission recycling

Main needs

- β -decay
- (n,γ) and (γ,n) rates
- Fission (nif , sf , βdf) rates
- Fission Fragments Distributions



Nucleosynthesis requires RATES for some 5000 nuclei !

(and not only masses or β -decay along the oversimplified so-called “r-process path”)

➡ simulations rely almost entirely on theoretical predictions

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

PHENOMENOLOGICAL DESCRIPTION



UNIVERSAL GLOBAL « MICROSCOPIC » DESCRIPTION

UNIVERSAL: capable of predicting *all properties* of relevance

GLOBAL: capable of predicting the properties of *all nuclei*

« MICROSCOPIC »: for more « controlled » *extrapolations* from valley of stability to drip lines

...An approach that can also provide new insight for other applications...

(Global « microscopic » models can nowadays compete with phenomenological models)

A challenge that will require a continued effort for more than the next decade

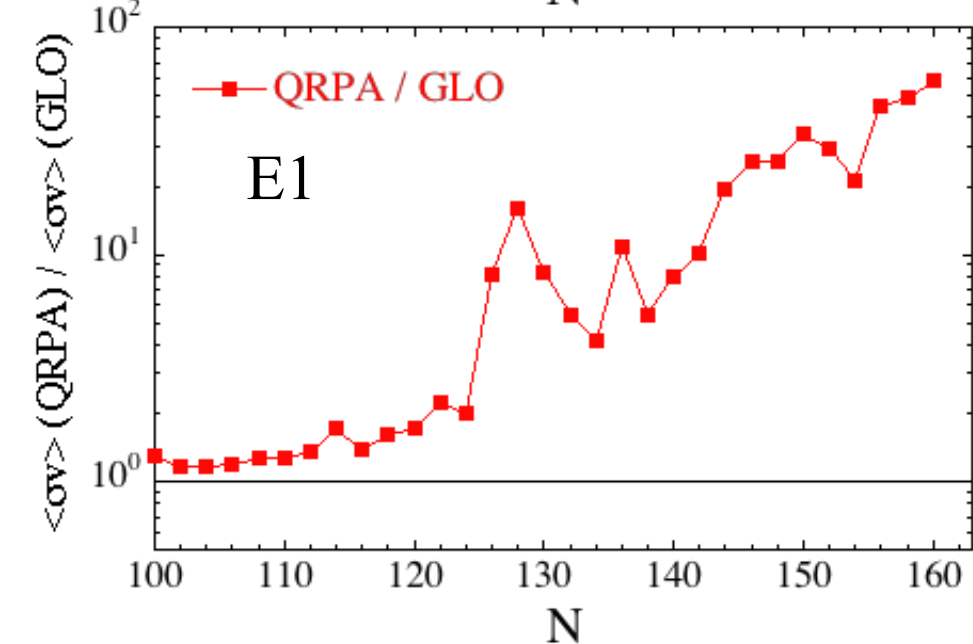
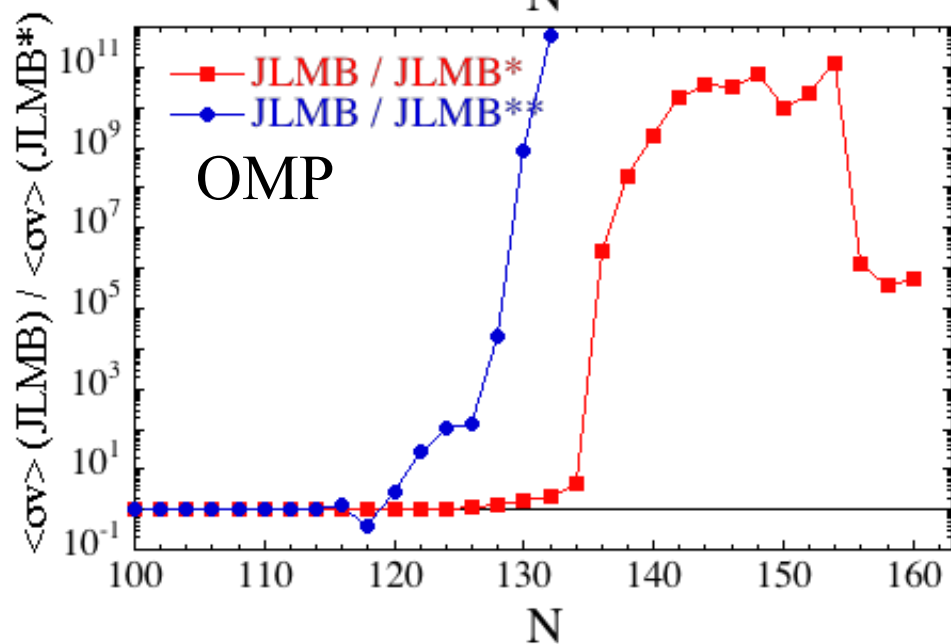
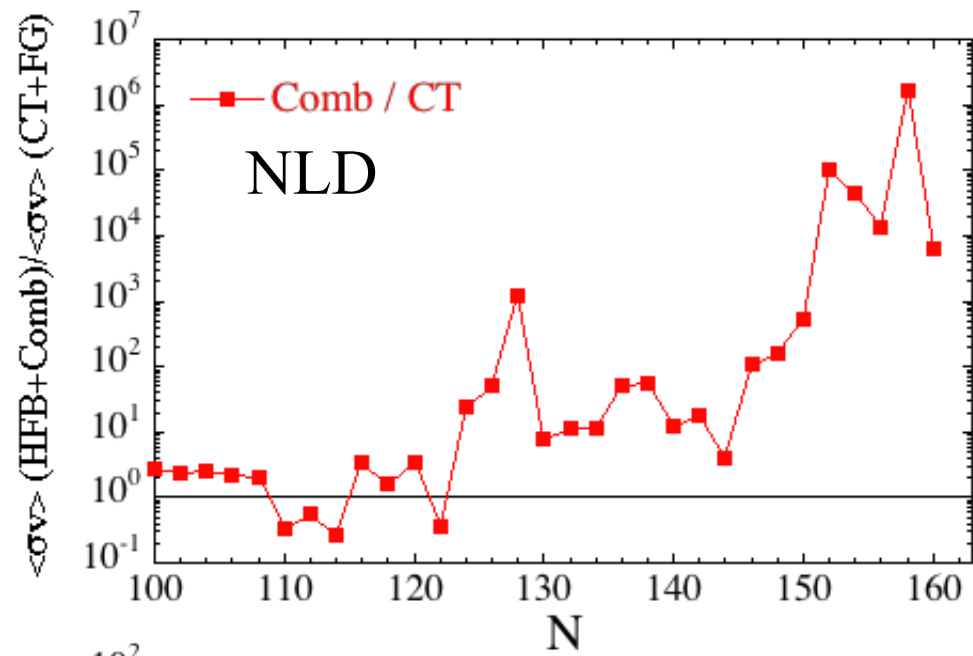
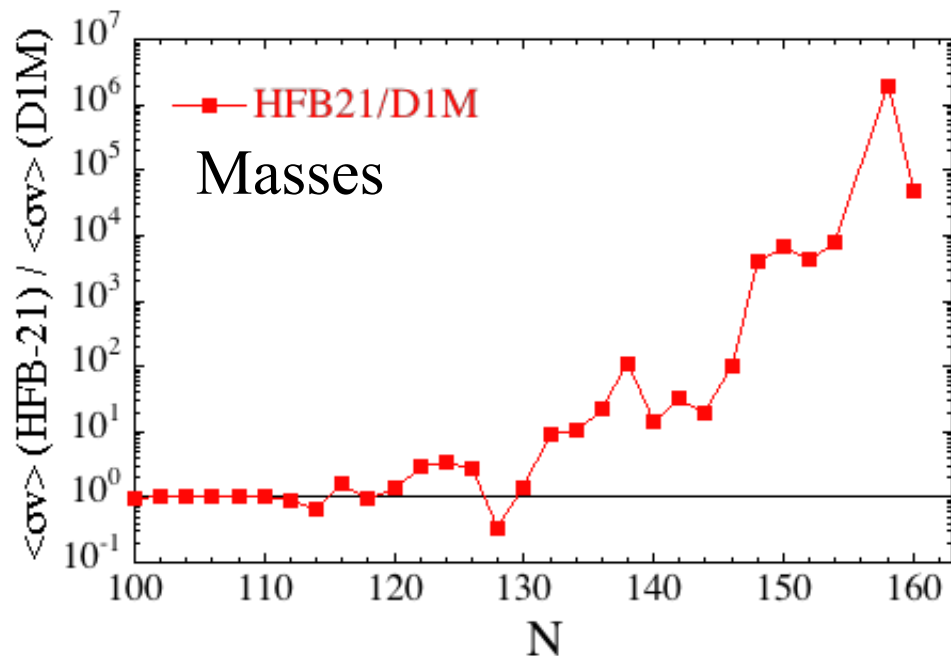
STILL MANY OPEN QUESTIONS FOR THE NEXT DECADE

- **The reaction model**
 - **CN vs Direct capture for low- S_n reactions**
- **Nuclear inputs to the reaction model** (almost no exp. data !)
 - **GS properties:** masses (correlations - GCM, odd-nuclei)
 - **E1-strength function:** GDR tail, PR, $\varepsilon_\gamma=0$ limit, T-dep, PC
 - **Nuclear level Densities (at low E):** J- and π -description, pairing, shell and collective effects & damping
 - **Optical potential:** the low-E isovector imaginary component
 - **Fission:** fission paths, NLD at the saddle points, FFD
- **The β -decay rates**
 - **Forbidden transitions, deformation effects, odd-nuclei, PC**

We are still far from being capable of estimating *reliably* the radiative neutron capture and β -decay of exotic n-rich nuclei
(and fission properties even for known nuclei)

Models exist, but corresponding uncertainties are usually not estimated

Illustration of the impact on the $_{70}\text{Yb}(n,\gamma)$ rates at $T=10^9\text{K}$



Nuclear mass models

Nuclear mass models provide all basic nuclear ingredients:

Mass excess (Q-values), deformation, GS spin and parity

but also the major nuclear structure properties

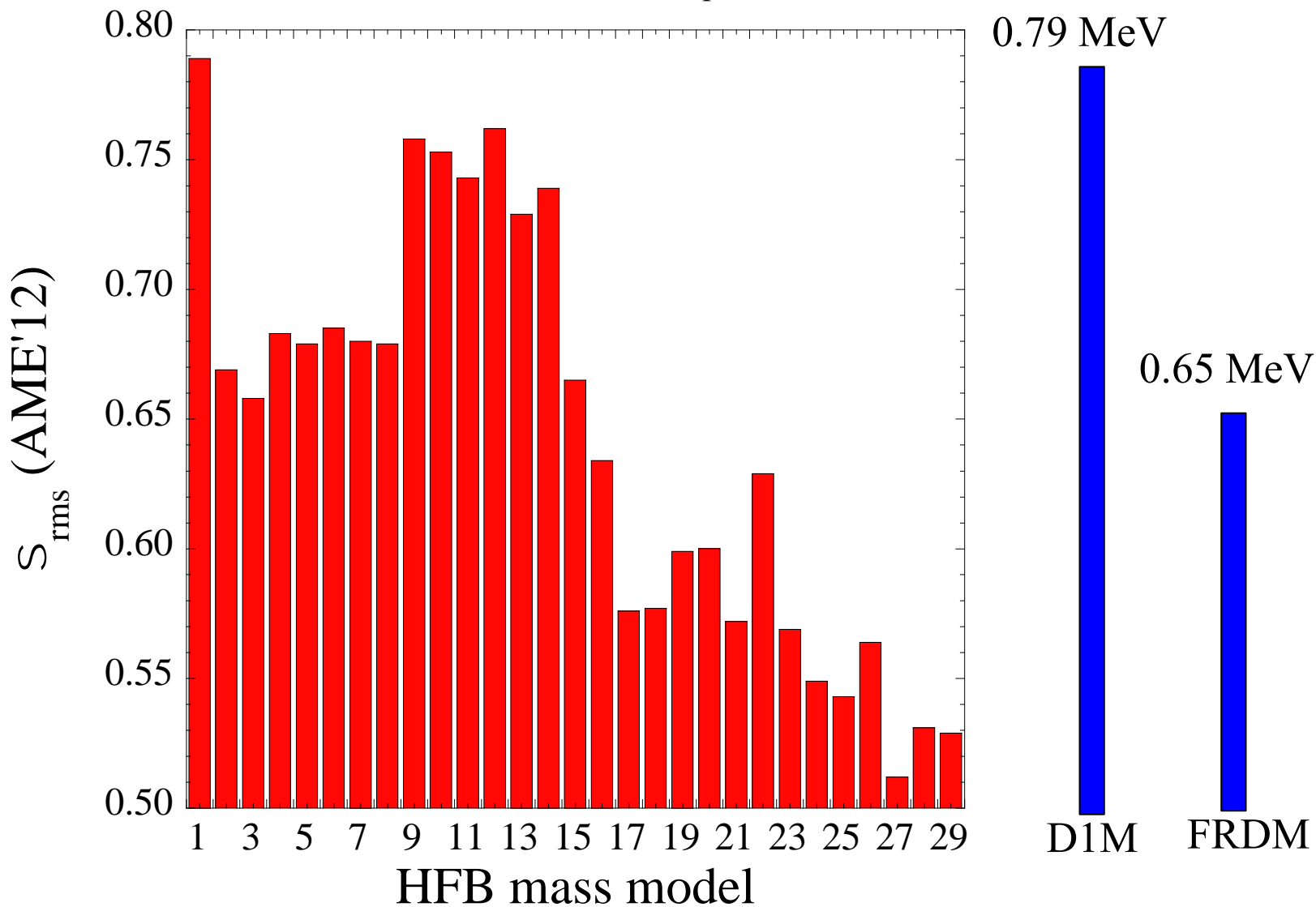
**single-particle levels, pairing strength, density distributions, ...
in the GS as well as non-equilibrium (e.g fission path) conf.**

Building blocks for the prediction of ingredients of relevance in the determination of nuclear reaction cross sections and β -decay rates, such as

- nuclear level densities
- γ -ray strengths
- optical potentials
- fission probabilities
- etc ...

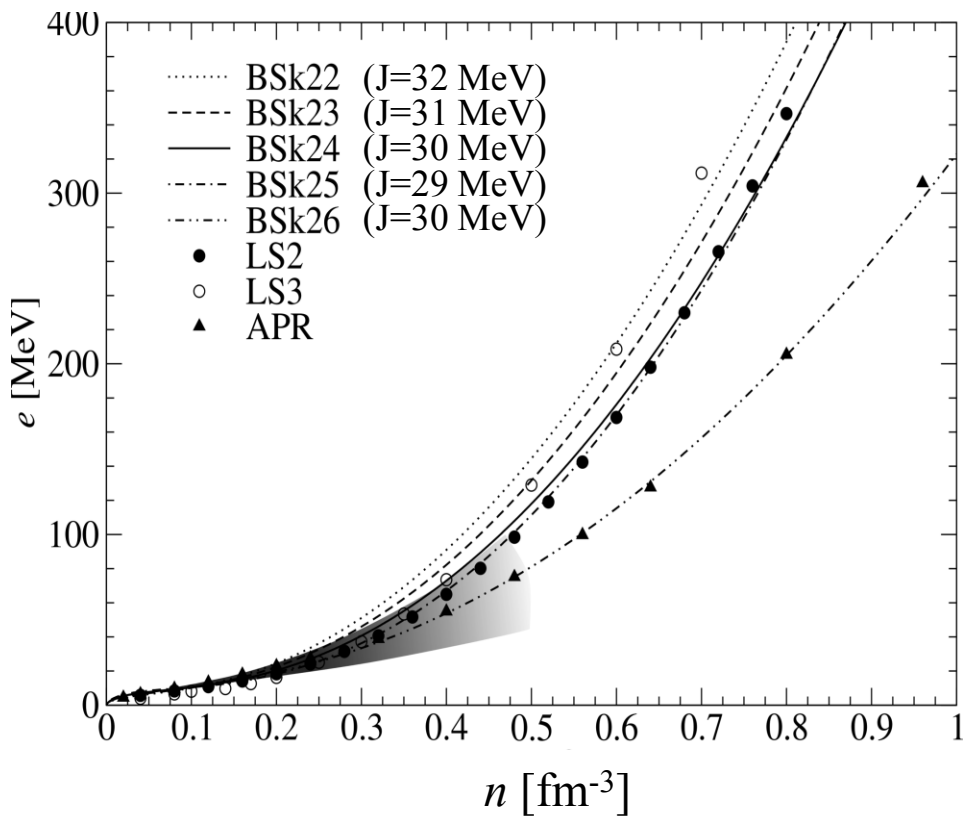
Adjustement of mean-field interactions to all (2353) experimental masses within the Hartree-Fock-Bogolyubov framework

29 Skyrme HFB mass models with $0.5 < \sigma_{\text{exp}} < 0.8$ MeV (2353 masses, AME'12)

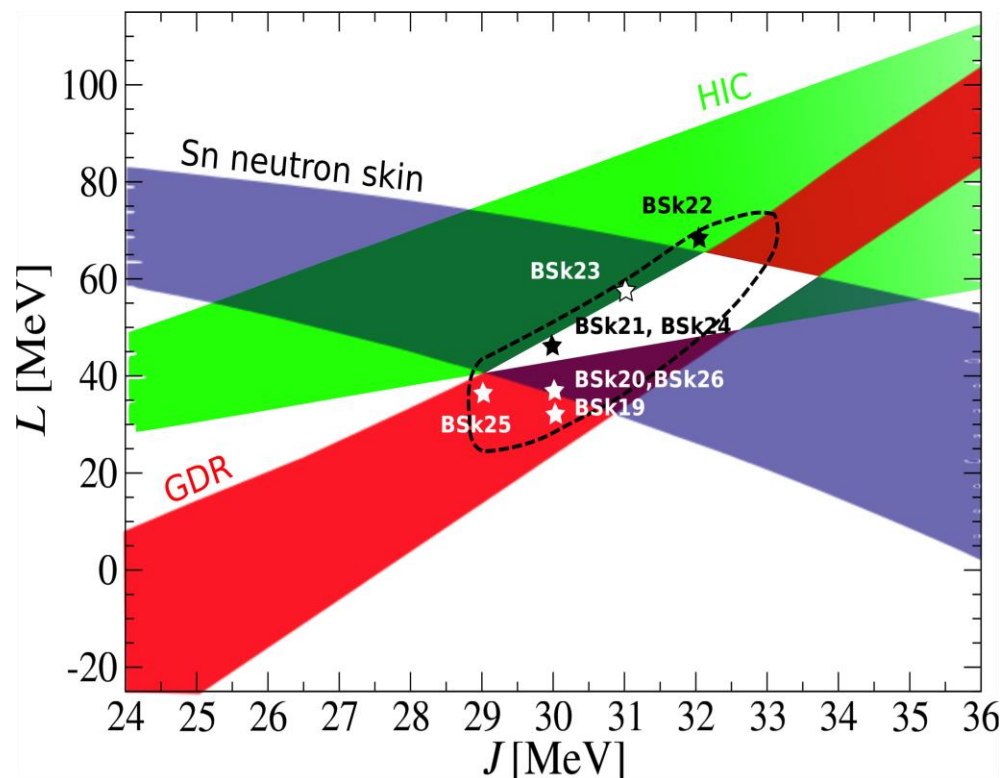


Nuclear matter properties & constraints from “realistic calculations”

Energy per nucleon in neutron matter



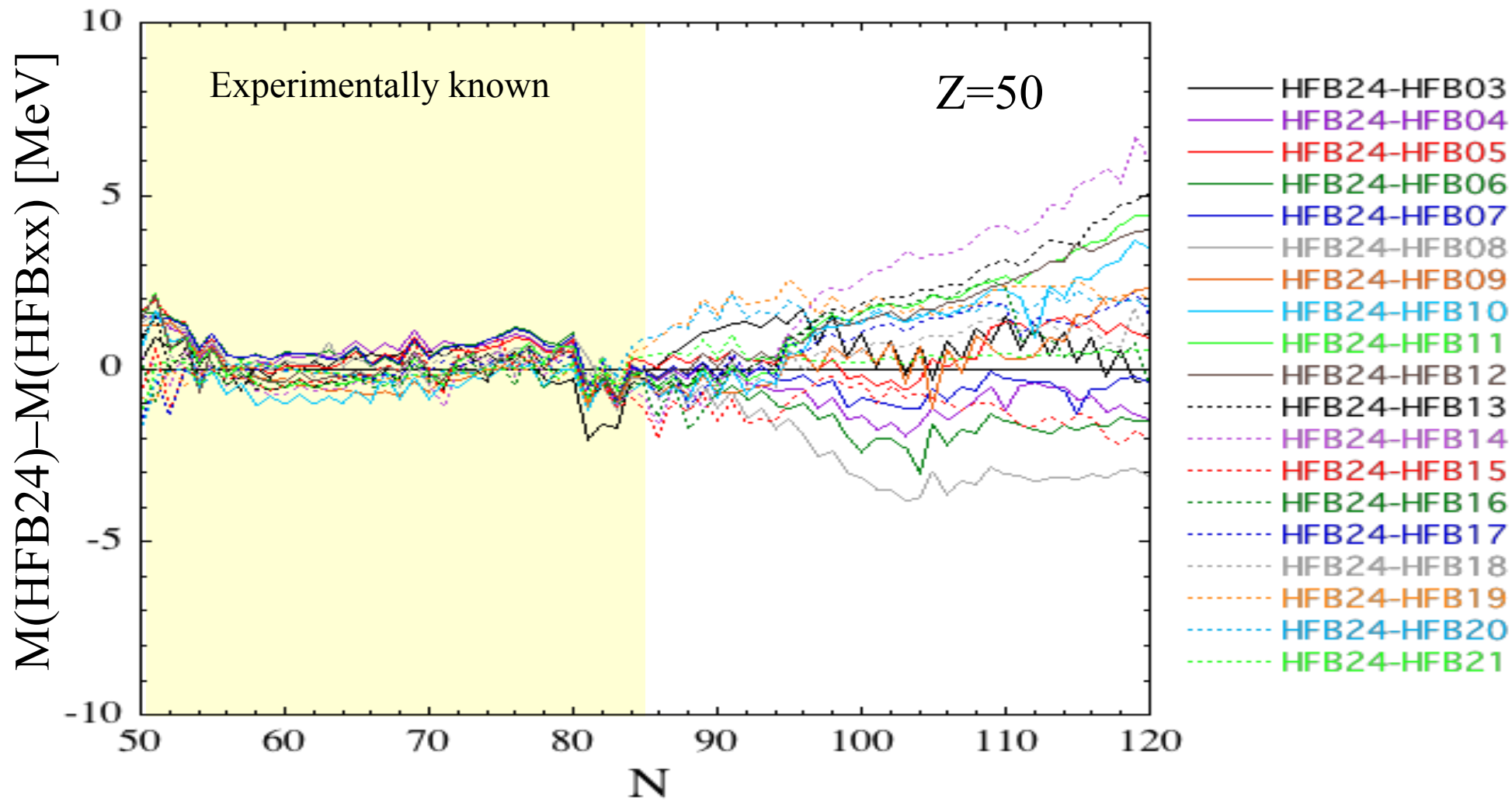
J - L symmetry energy parameters



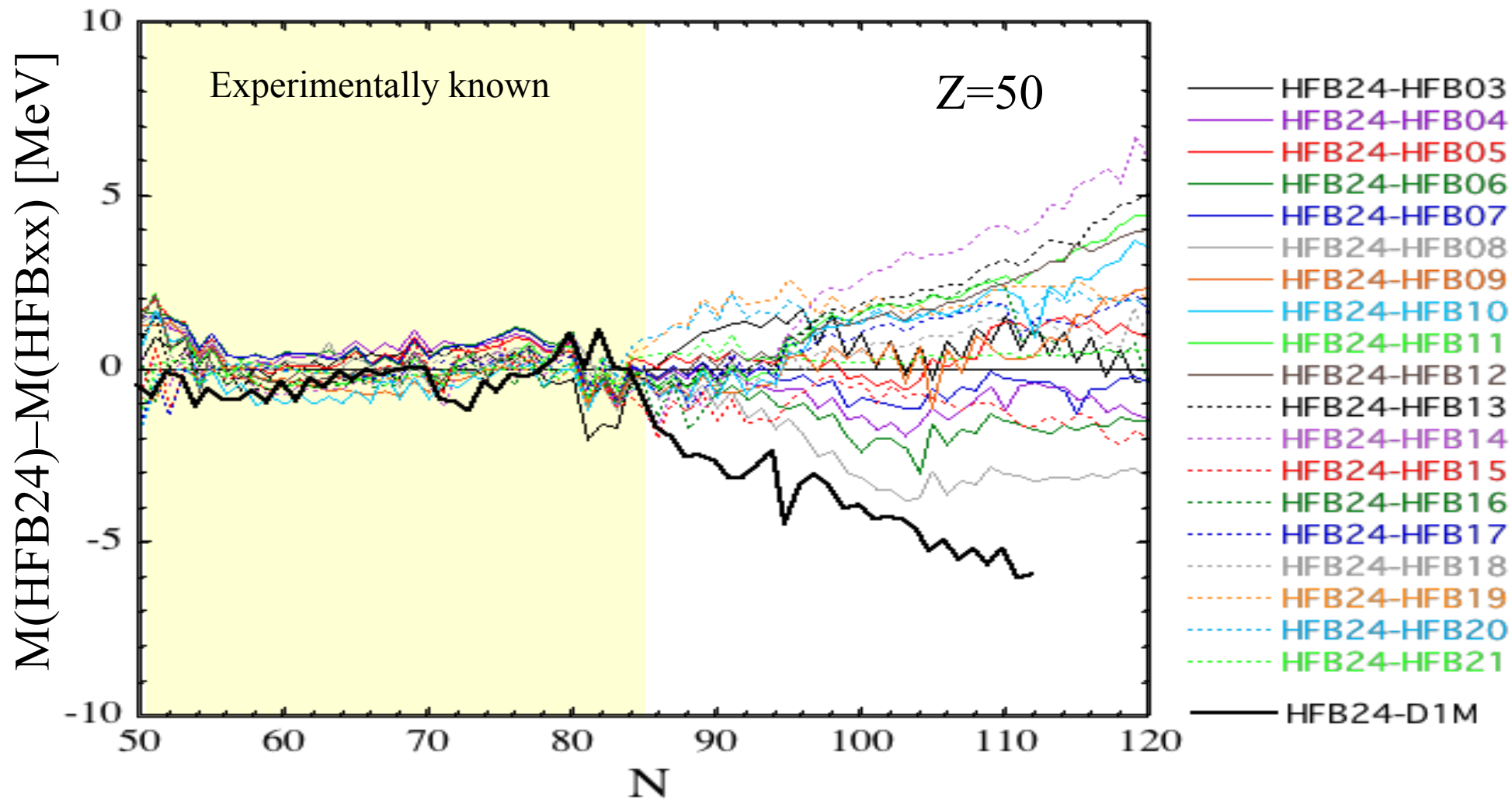
- Stable neutron matter at all polarisations (no ferromagnetic instability)
- Effective masses in agreement with realistic predictions $M_s^* > M_v^*$
- Maximum NS mass : $M_{\text{max}} > 2.0 M_\odot$ for HFB-20–26 as constrained by observation

$$M_s^* / M = 0.80 \quad \& \quad M_v^* / M \sim 0.70$$

Uncertainties of mass extrapolation in HFB mass models

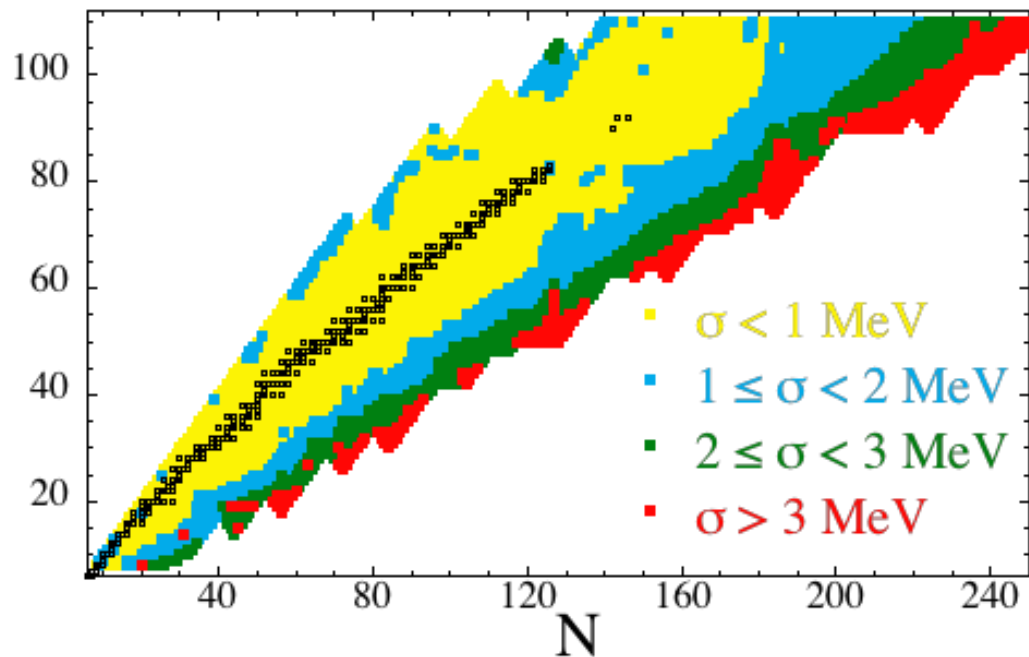


Uncertainties of mass extrapolation in HFB mass models



Uncertainties of mass extrapolation in HFB mass models

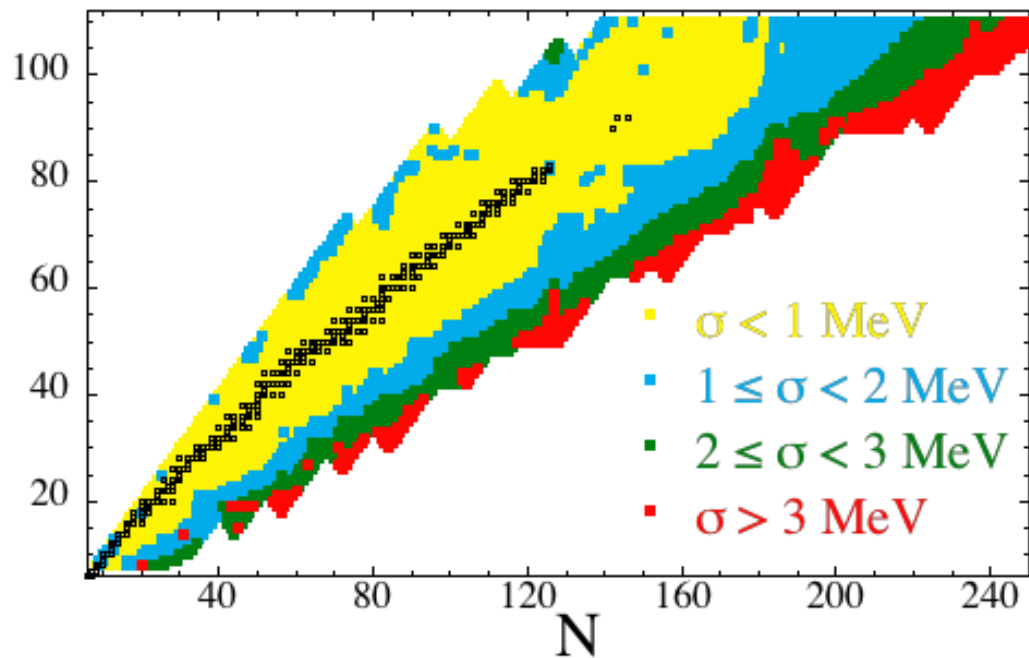
1σ uncertainties between the
29 HFB mass models
($0.51 < \sigma_{\text{exp}} < 0.79$ MeV)



But what about statistical
uncertainties
corresponding to variation
of HFB parameters in the
vicinity of a given
minimum ??

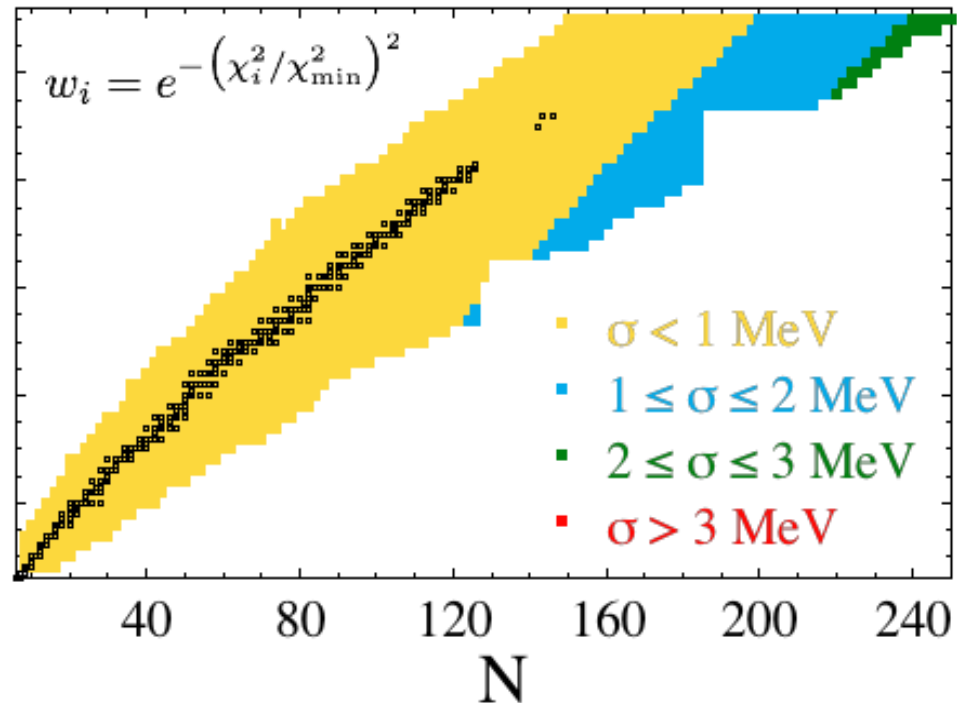
Uncertainties of mass extrapolation in HFB mass models

1σ uncertainties between the
29 HFB mass models



Need to keep on scanning the large
parameter space and model uncertainties,
also responsible for local variations due to
shell/pairing/correlation effects

1σ statistical uncertainties
around HFB-24 mass models



Backward-Forward MC method:
29300 HFB runs for different sets of the
model parameters following a Gaussian
distribution centered on BSk24 constrained
by experimental masses

Future challenges for modern mass models

- 1. To include the state-of-the-art theoretical framework**
 - To include explicitly correlations (quadrupole, octupole, ...) → GCM
 - To include relevant degrees of freedom for deformation (triaxility, l-r symmetry, ...)
 - To include proper description for odd nuclei
 - To include “extended” interactions (tensor, D2-type, ...)

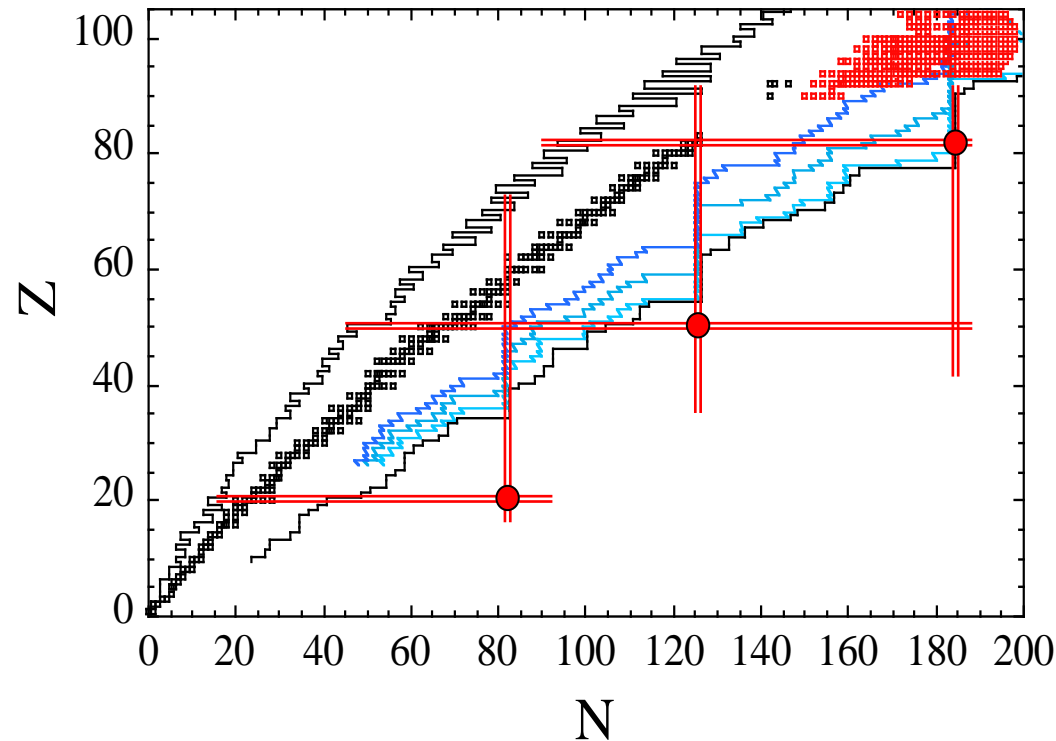
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- 2. To reproduce as many “observables” as possible (“exp.” & “realistic”)**
 - Experimental masses (rms < 0.8 MeV)
 - Radii and neutron skins
 - Fission and isomers
 - Infinite nuclear matter properties (Symmetric, Neutron matter)
 - Giant resonances
 - Spectroscopy
 - Neutron Star maximum mass
 - Etc...

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 - Etc...
- 3. To consider different frameworks**
 - Relativistic, non-relativistic
 - Skyrme-type, Gogny-type (D1 & D2 interactions), DDME, PC, ...
 - Non-empirical, Shell Model, etc...

...but significant improvement for the next decade may lie in (absolute or differential) constraints from *ab-initio* calculations (CC, SCGF, IMSRG, ...) based on 2- and 3-nucleon forces for specific nuclei, eg. doubly magic but also semi-magic chains (cf talk of T. Duguet)



P.S. including constraints on the n-Nucleus optical potential, in particular its isospin dependence

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 ($A \sim 110-160$) by fission recycling
- heating of the matter (affecting the light curve)
- production of radiocosmochronometers (U, Th)

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

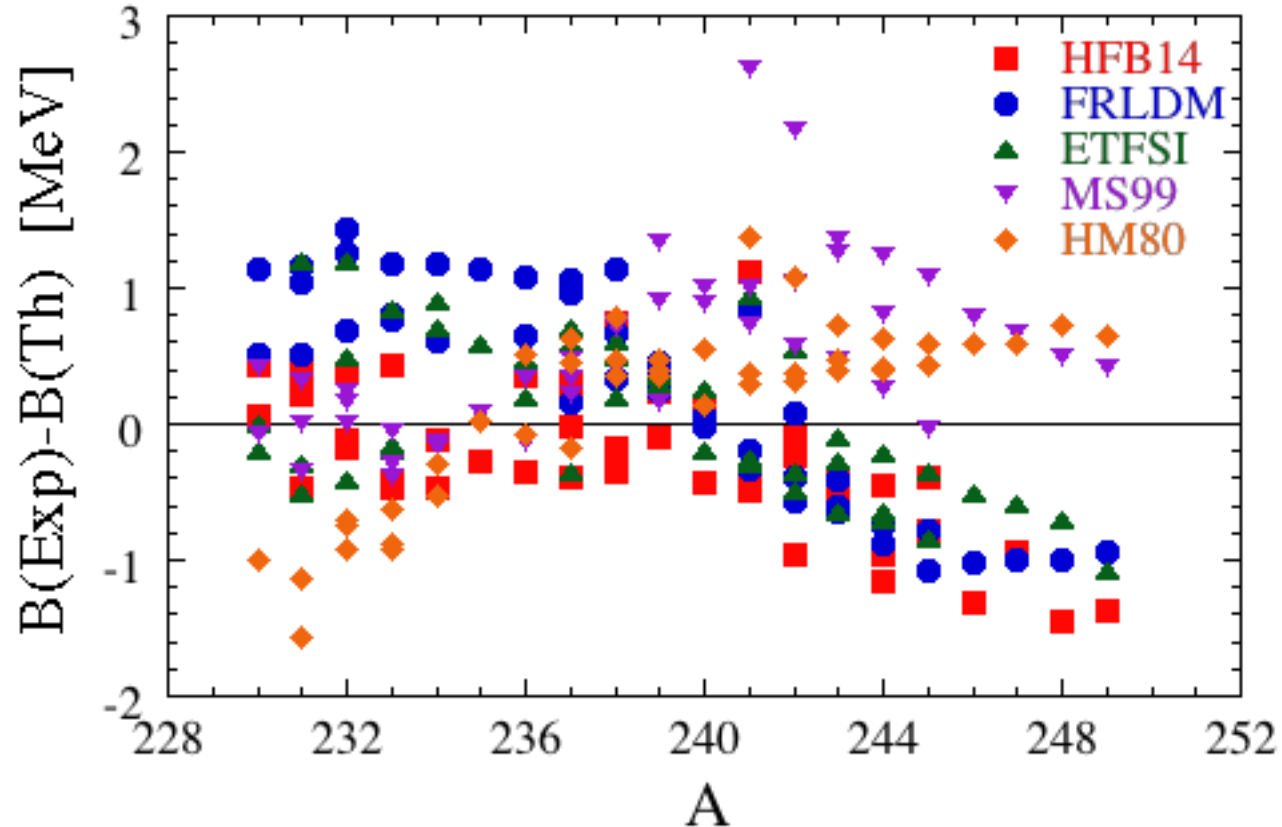
+ coupling with competitive n-, γ -, β -channels

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 !)

Description of the primary fission barriers by global models

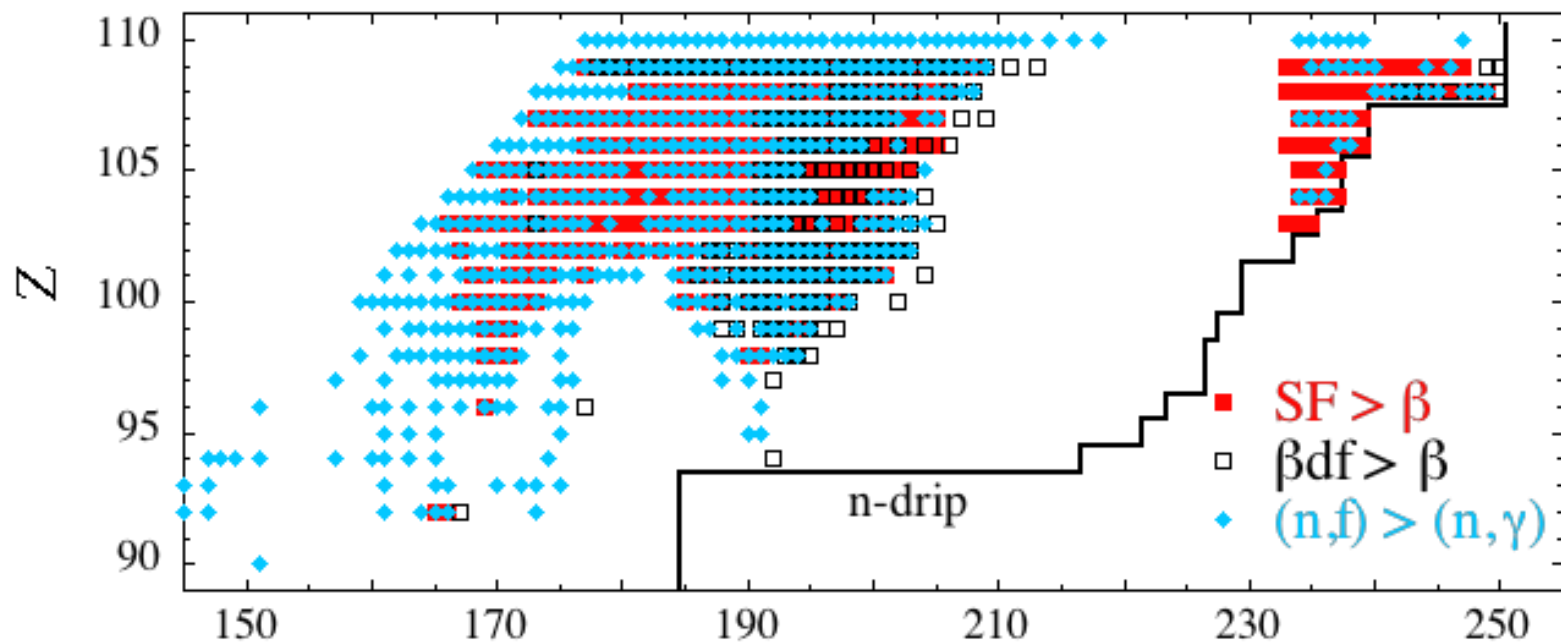
45 « empirical » primary barriers $88 \leq Z \leq 96$ (RIPL-3)



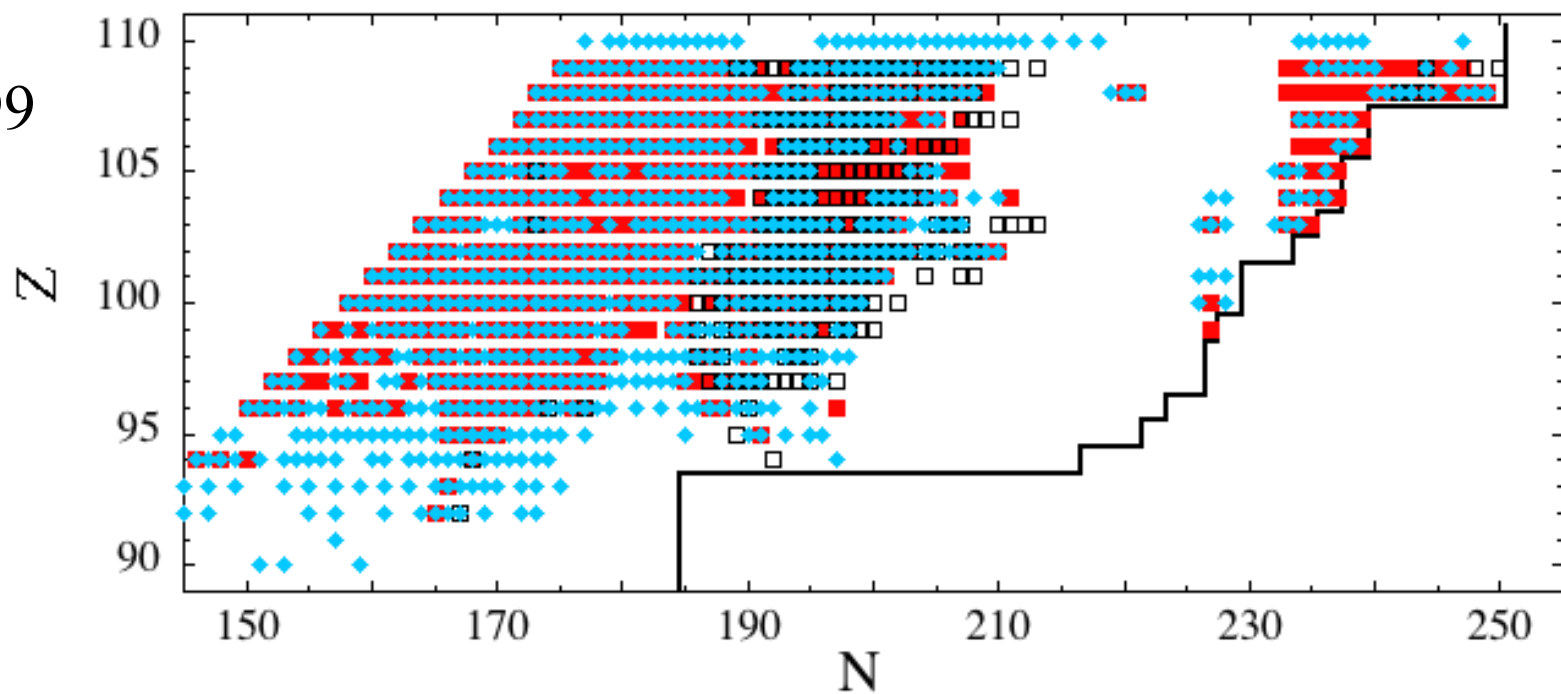
Model	σ [MeV]
HFB-14	0.60
FRLDM	0.81
ETFSI	0.57
MS99	0.82
HM80	0.66

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
 (cf talk of N. Dubray)

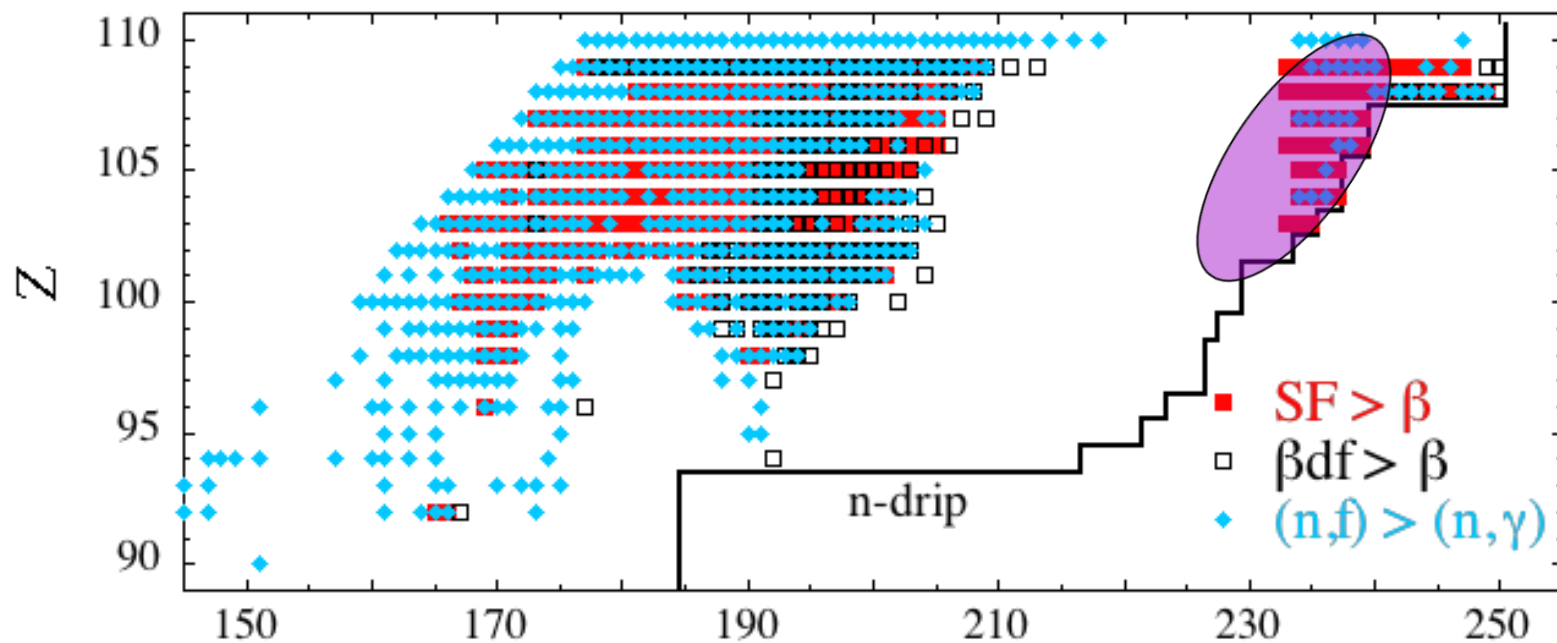
HFB-14



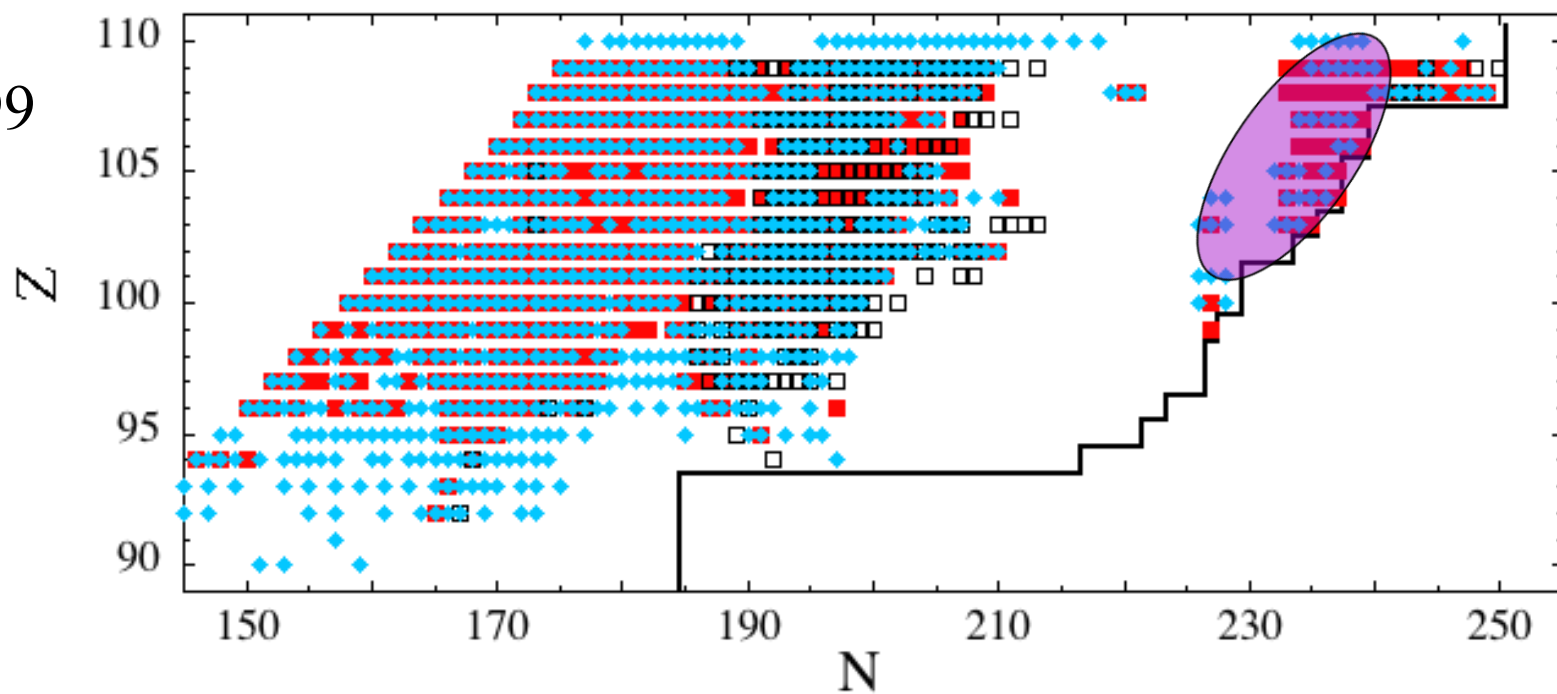
TF: MS99



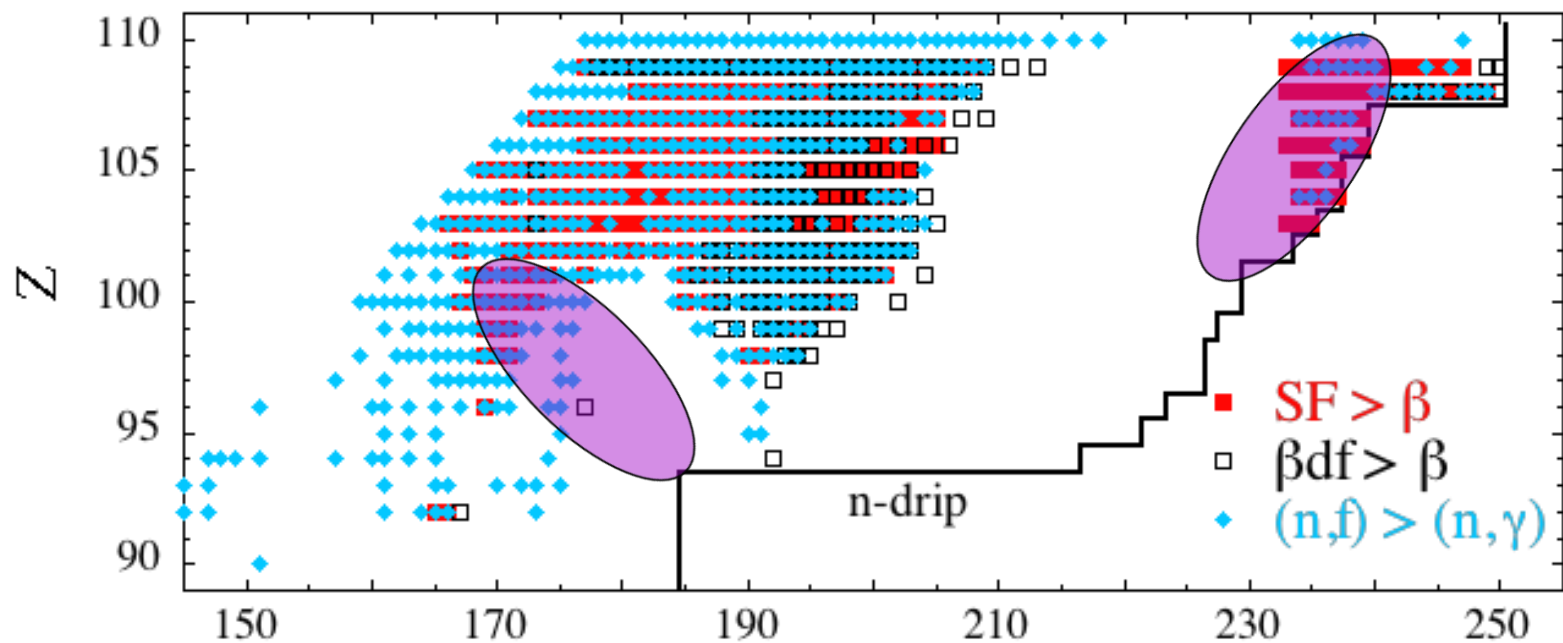
HFB-14



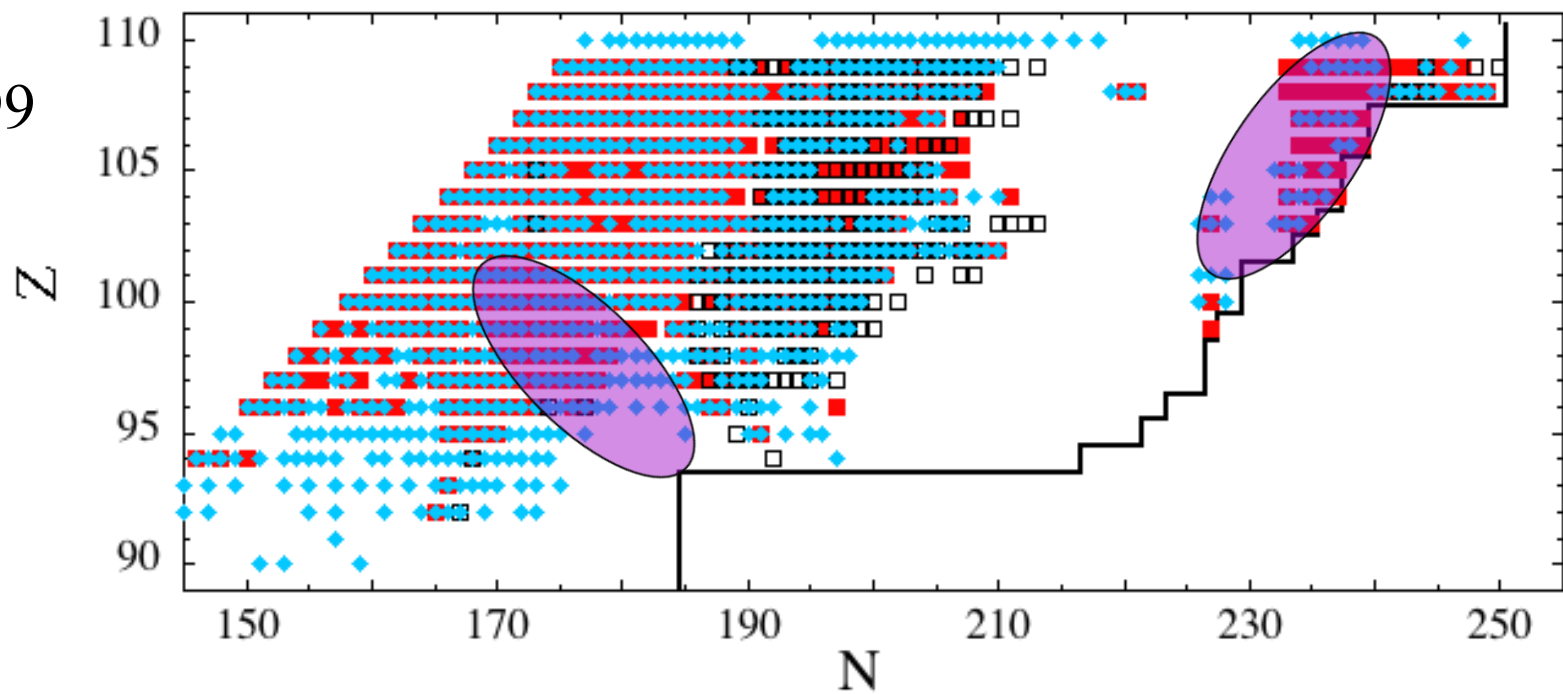
TF: MS99



HFB-14



TF: MS99



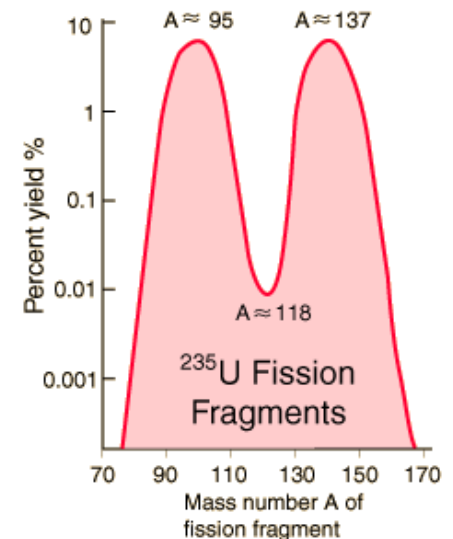
Fission Fragment Distribution

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

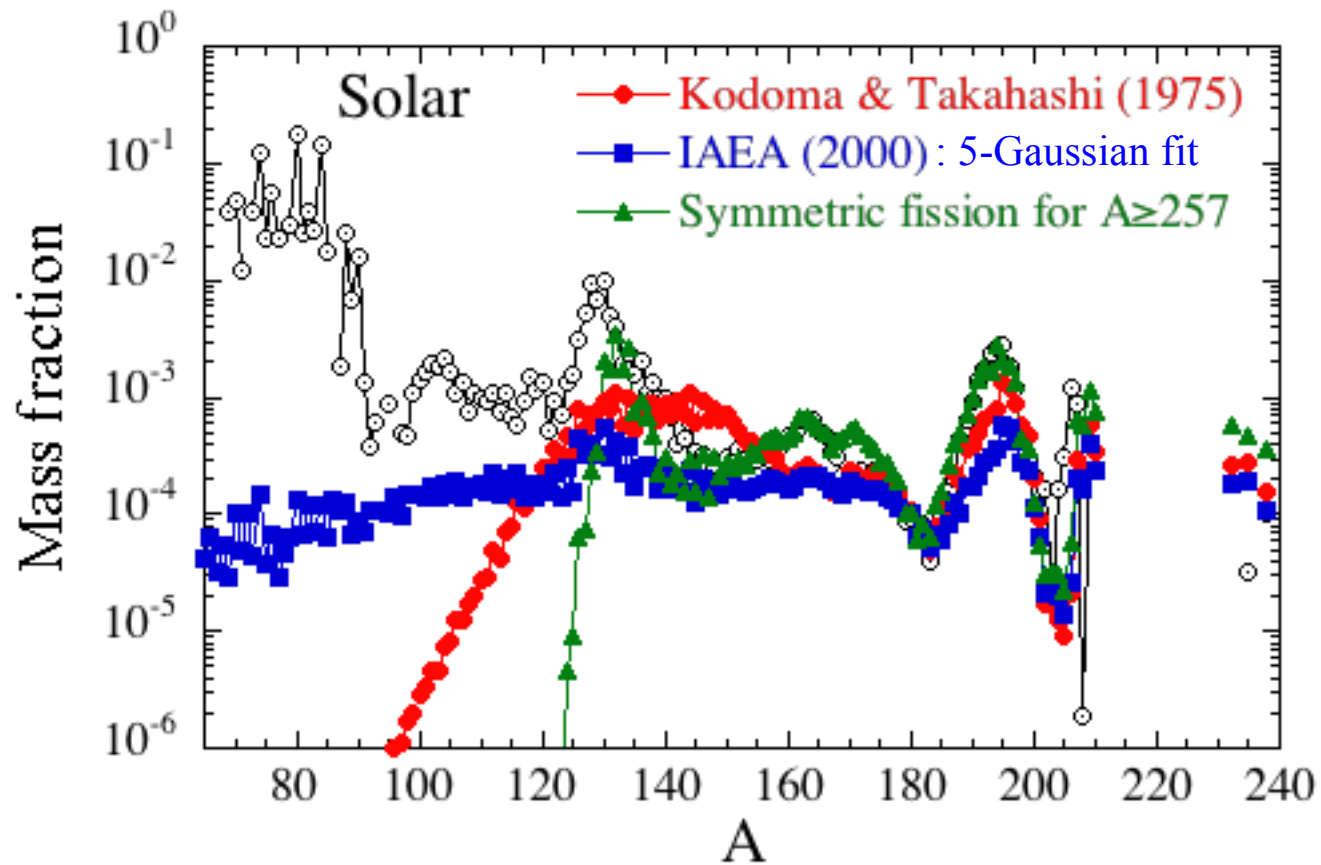
- Final r-abundance distribution ($110 \leq A \leq 170$) shaped by the FFD
- Emission of prompt neutrons that will be at late times

Many different phenomenological approaches exist, based on systematics, i.e highly-parametrized multi-Gaussian-type fits, with adjustment 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.)



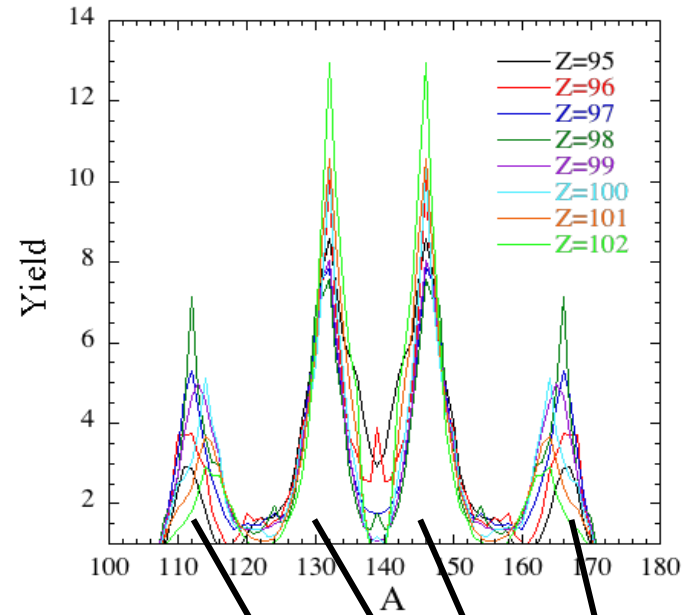
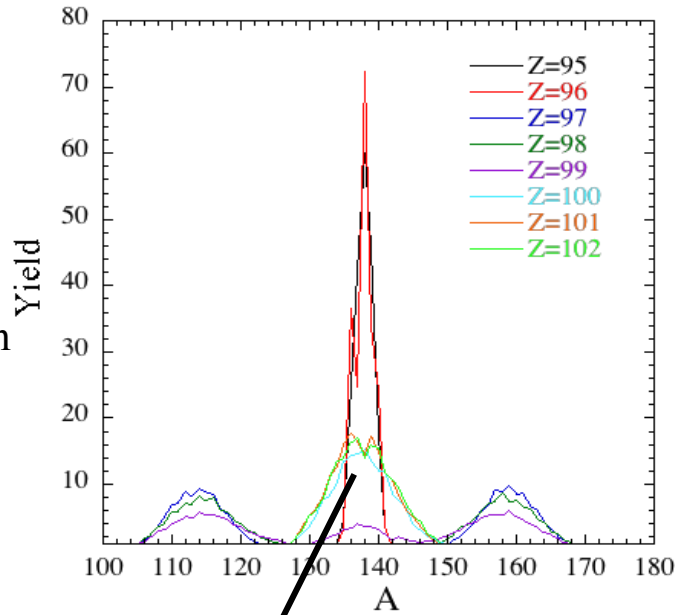
The FFD lottery



Sensitivity to the fission fragment distribution along the $A=278$ isobar (from the $N=184$ closed shell)

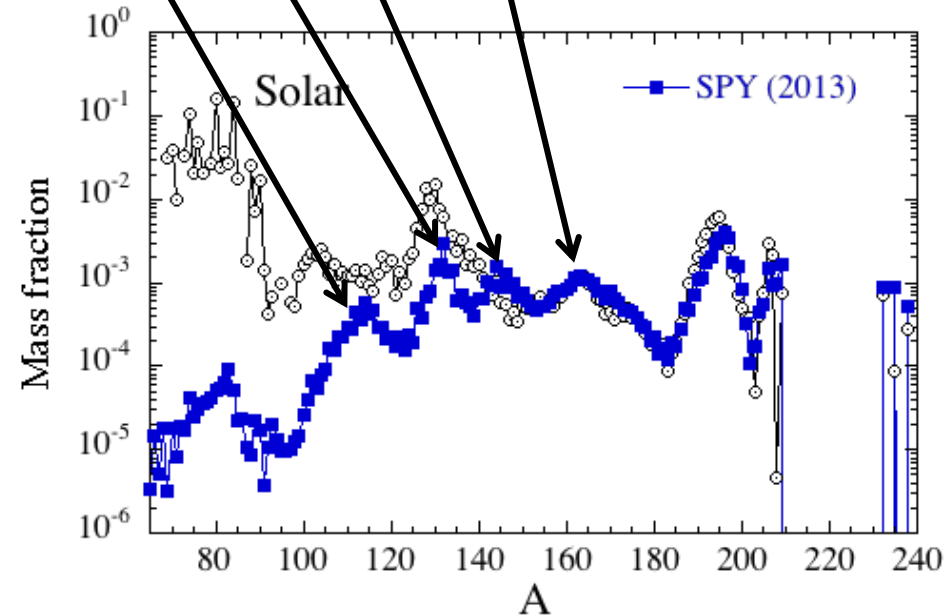
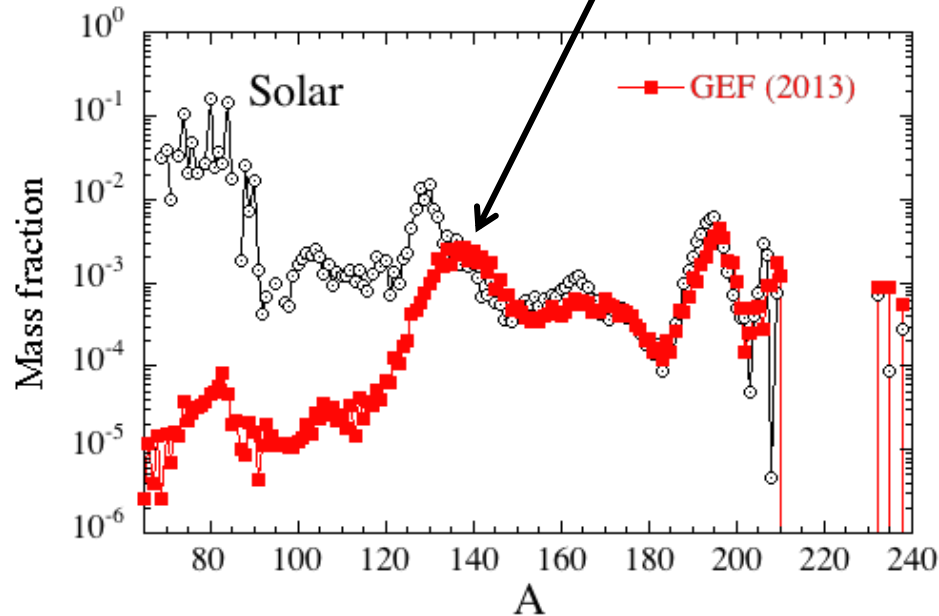
GEF v1.4
K. Schmidt et al. (2013)

Semi-empirical mic-mac Scission Point model

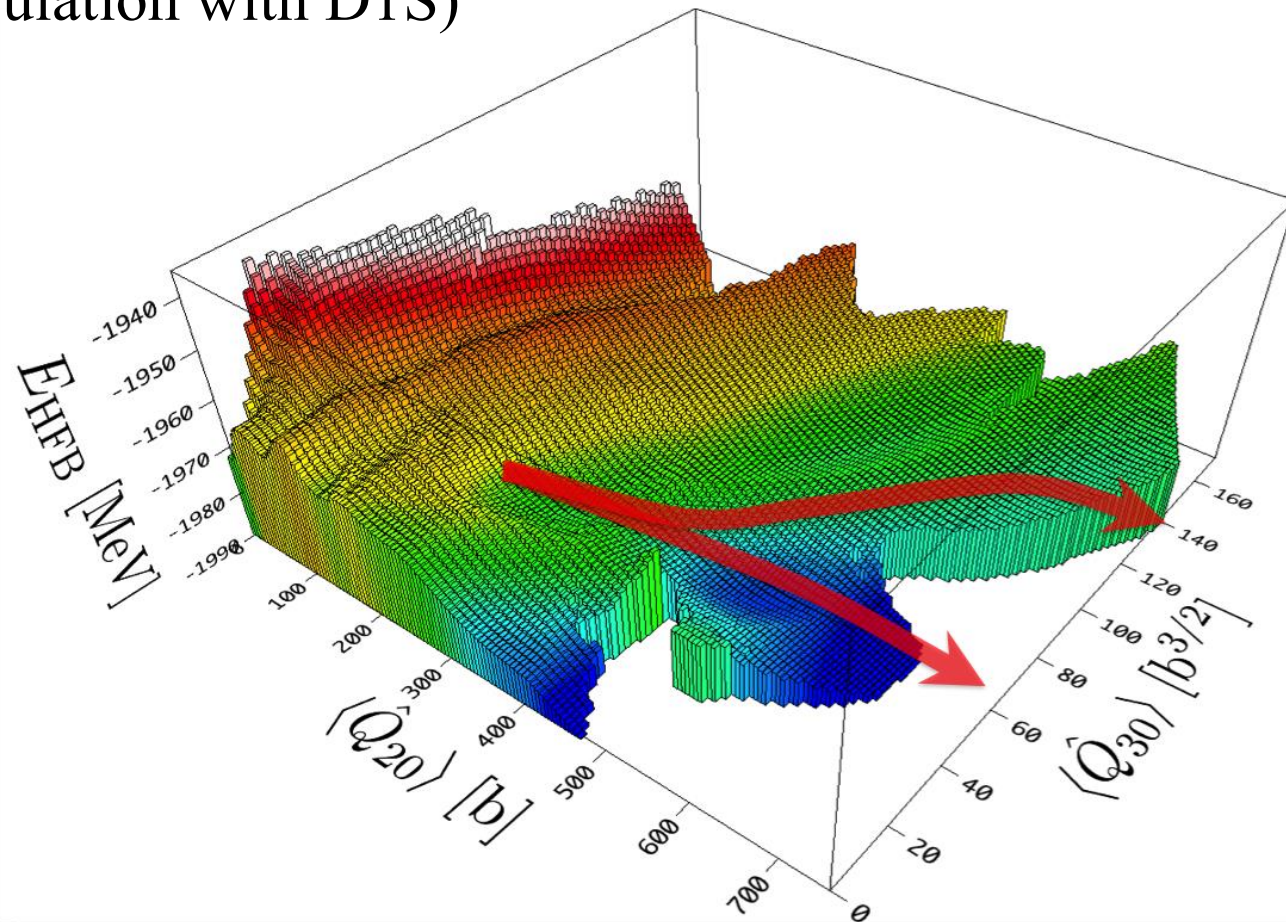


SPY:
S. Panebianco et al. (2013)

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



Qualitative confirmation through the ^{278}Cf potential energy surface (HFB calculation with D1S)



N. Dubray

Need qualitative and quantitative calculations, e.g from a time-dependent formalism based on the GOA of the time-dependent GCM

(Goutte et al. 2005, Bernard et al. 2011)

The fundamental role of β -decay rates

(including β_{dn} & β_{df})

Gross Theory :

the β -strength function is estimated by folding one-particle strength function via a simple pairing scheme taking into account the corresponding sum rules and even-odd effects.

QRPA approach (Skyrme, Gogny, RMF) with some level of approximations:

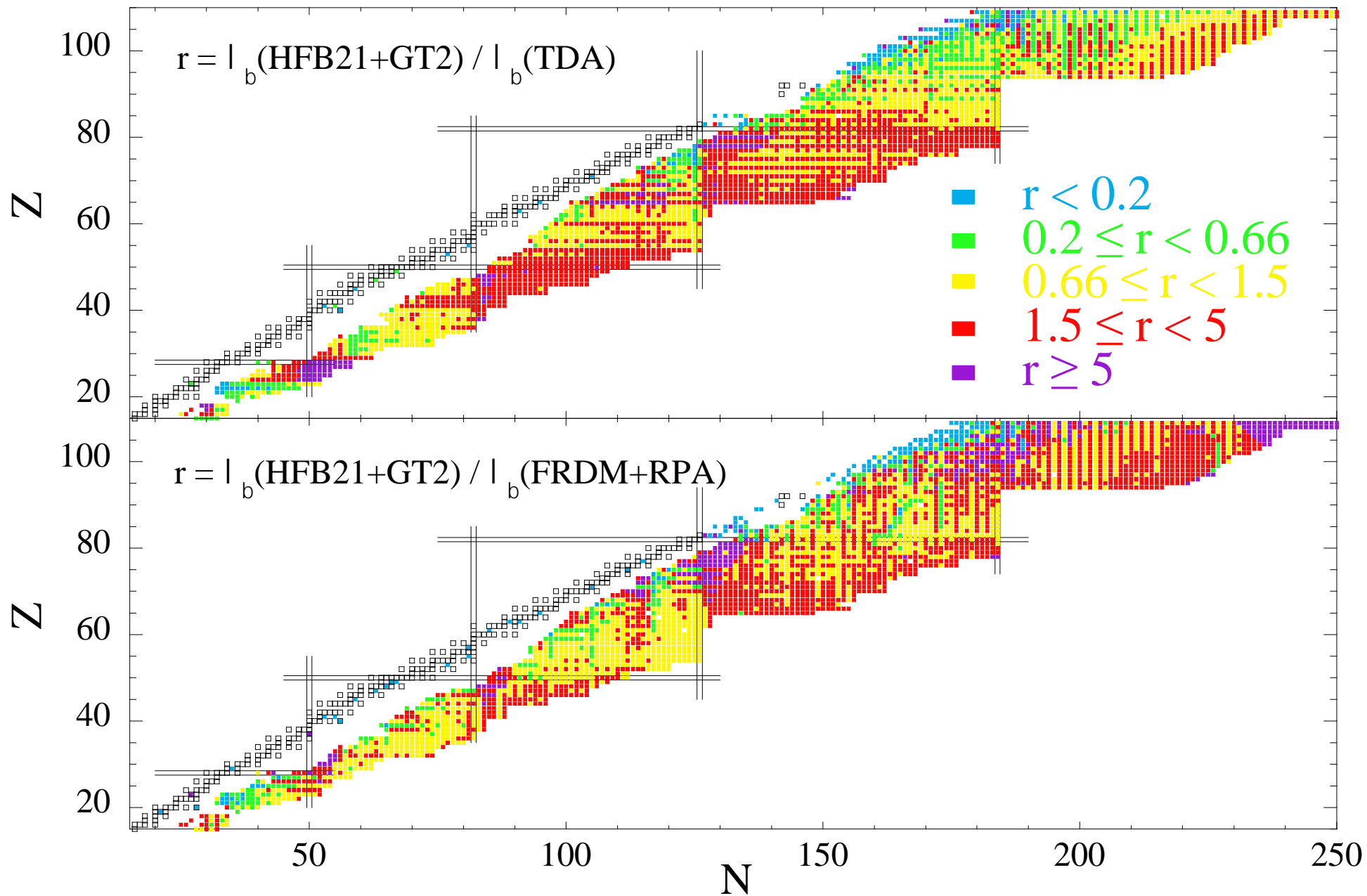
TDA, separable interactions, inconsistency between Ground & Excited states, spherical approximation, GT only, ...

Recent work within

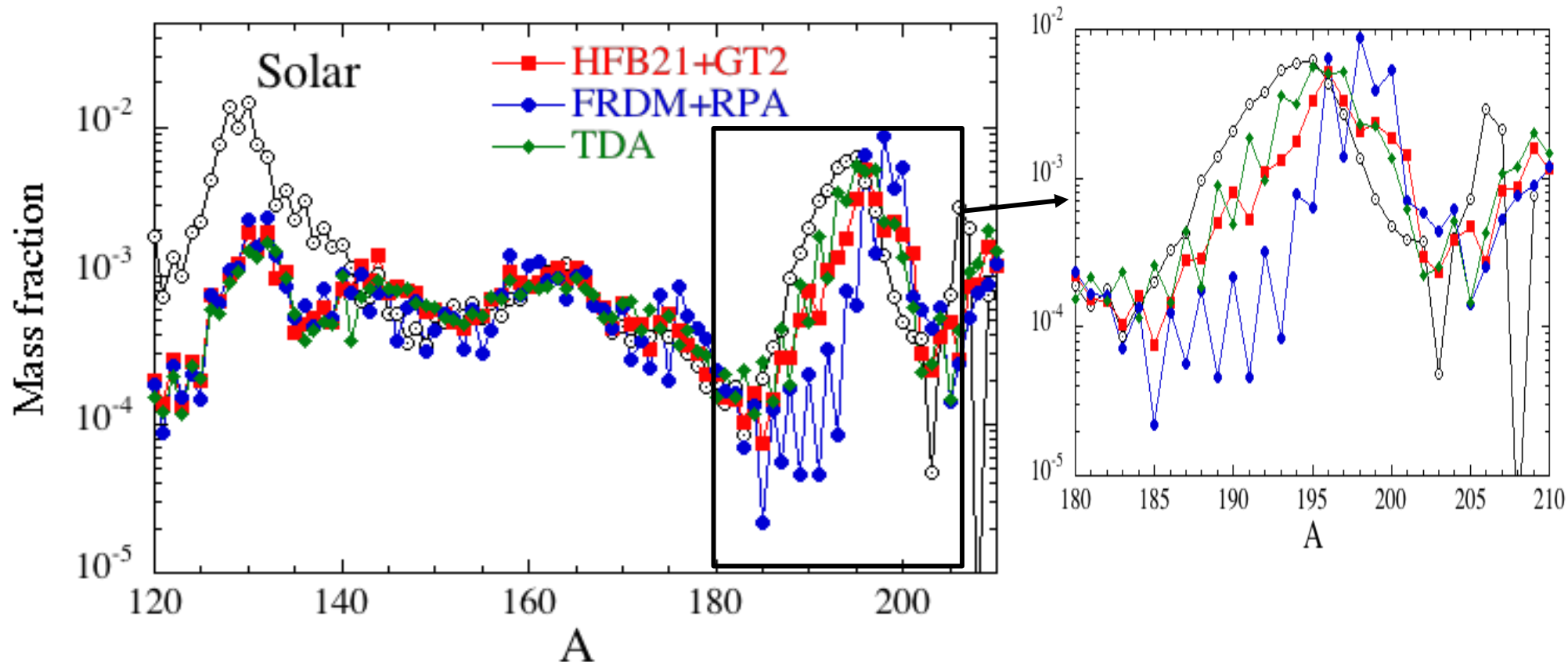
- EDF+Fermi Liquid Theory (Borzov 2010): spherical, FF incl.
- RHB+QRPA (Marketin et al. 2014): spherical, FF incl.
- Gogny HFB+QRPA (Martini & Péru 2014): def, GT, no FF (yet)

In practice, only a few complete tables (publicly) available

- Tachibana et al. (1990): HFB + Gross Theory 2 (GT + FF)
- Klapdor et al. (1984): Tamm-Dancoff approximation
- Möller et al. (2003): FRDM + QRPA & gross theory for FF



Impact of β -decay rates on the r-process nucleosynthesis in NS mergers



Large impact of the β -decay rate – set the synthesis timescales
(β dn also influences the location of the peak with the late capture of neutrons released)

→ Need at least deformed “microscopic” calculation (HFB+QRPA)
including GT+FF transitions, odd nuclei, PC,

Conclusions

Astrophysics simulations are now able to provide consistent robust nucleosynthesis models for the r-process

(3D relativistic hydro simulations of the NS Mergers and BH-torus phases)

Calculated r-abundance distributions remain essentially affected by

- **β -decay: better than factor 1.5**
- **neutron capture (nuclear input models as well as reaction models: CN, DC): better than factor 2 around $S_n \sim 2-3\text{MeV}$, 10 at drip lines ?**
- **Fission probabilities (barriers within \sim few 100keVs) and fission fragment distributions**

The best Nuclear Physics input should be provided

- **More theoretical work based on “MICROSCOPIC” approaches**
- **Consistent estimate of the model & parameter uncertainties**

That should keep us busy for the next decade... for sure...