Progress in the modelling of nuclear inputs for r-process simulations

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In collaboration with

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- S. Hilaire, S. Péru (CEA, France)
- O. Just, A. Bauswein (GSI)
- H-.T. Janka, R. Glas (MPA)






Content

1. Progress in the modelling of some nuclear ingredients
   - Nuclear masses
   - Fission probabilities and fragment distributions
   - neutron-Nucleus optical model potentials
2. Radiative transfer calculation of Kilonovae
   - Revised calculation of HFR atomic opacities
   - Impact of mass and β-decay models
   - Impact of optical model potential

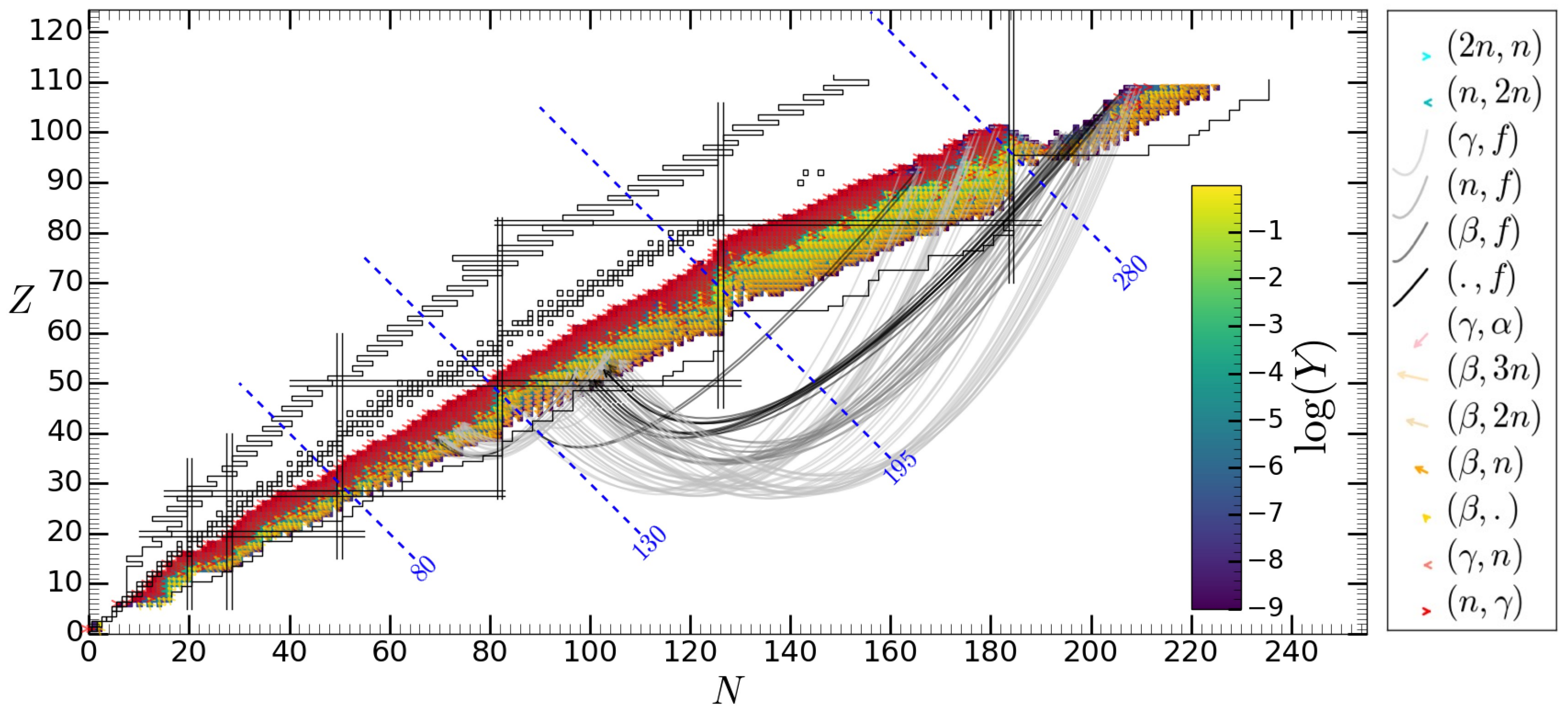
One major uncertainty in r-process: nuclear physics input

(n,γ) – (γ,n) – β competition & Fission

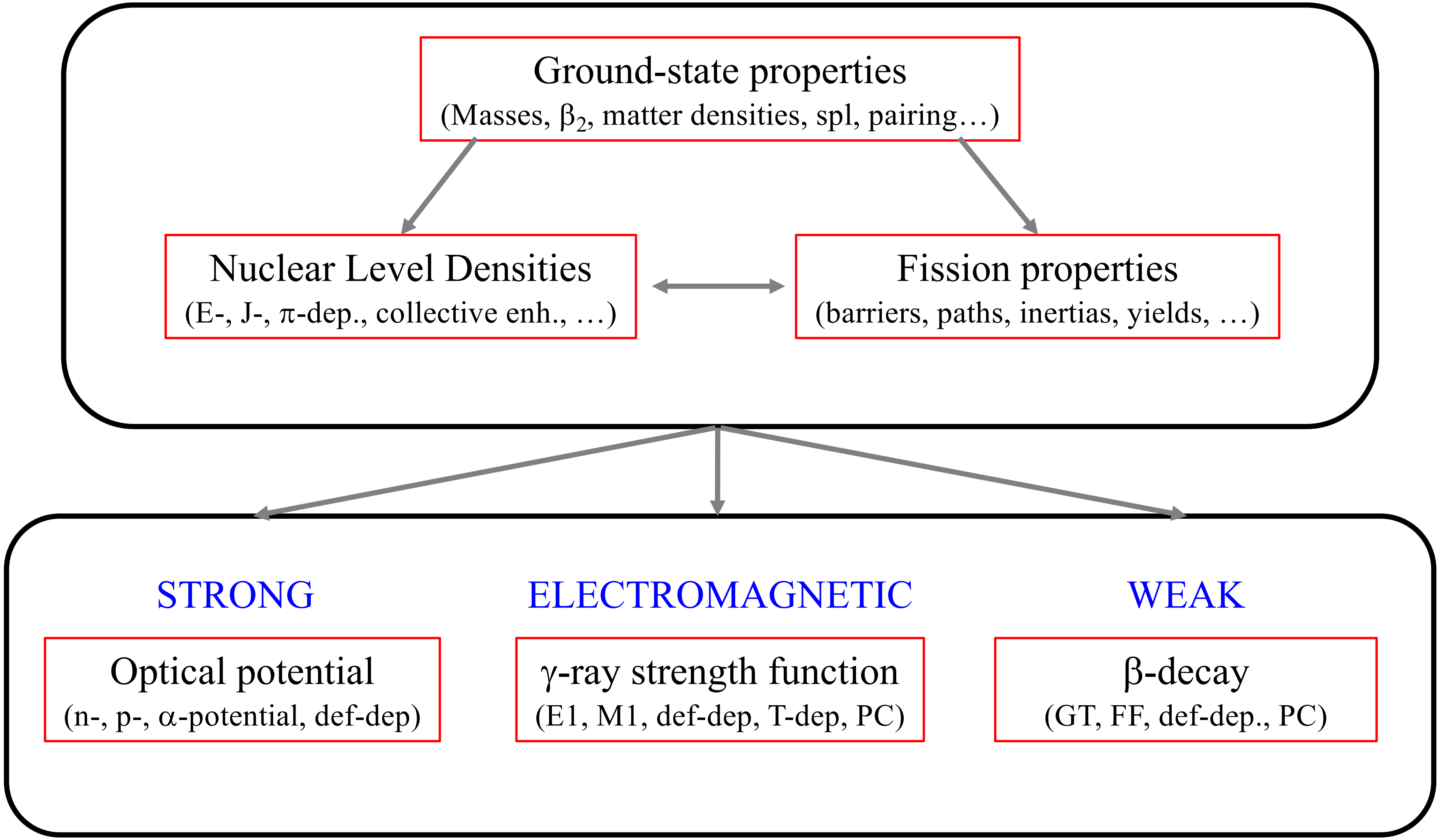
- β-decay rates
- (n,γ) and (γ,n) rates – Masses (S_n)
- Fission (*nif, sf, βdf*) rates
- Fission Fragments Distributions

Still many open questions

some 5000 nuclei with $Z \leq 110$ involved on the n-rich side; essentially no data

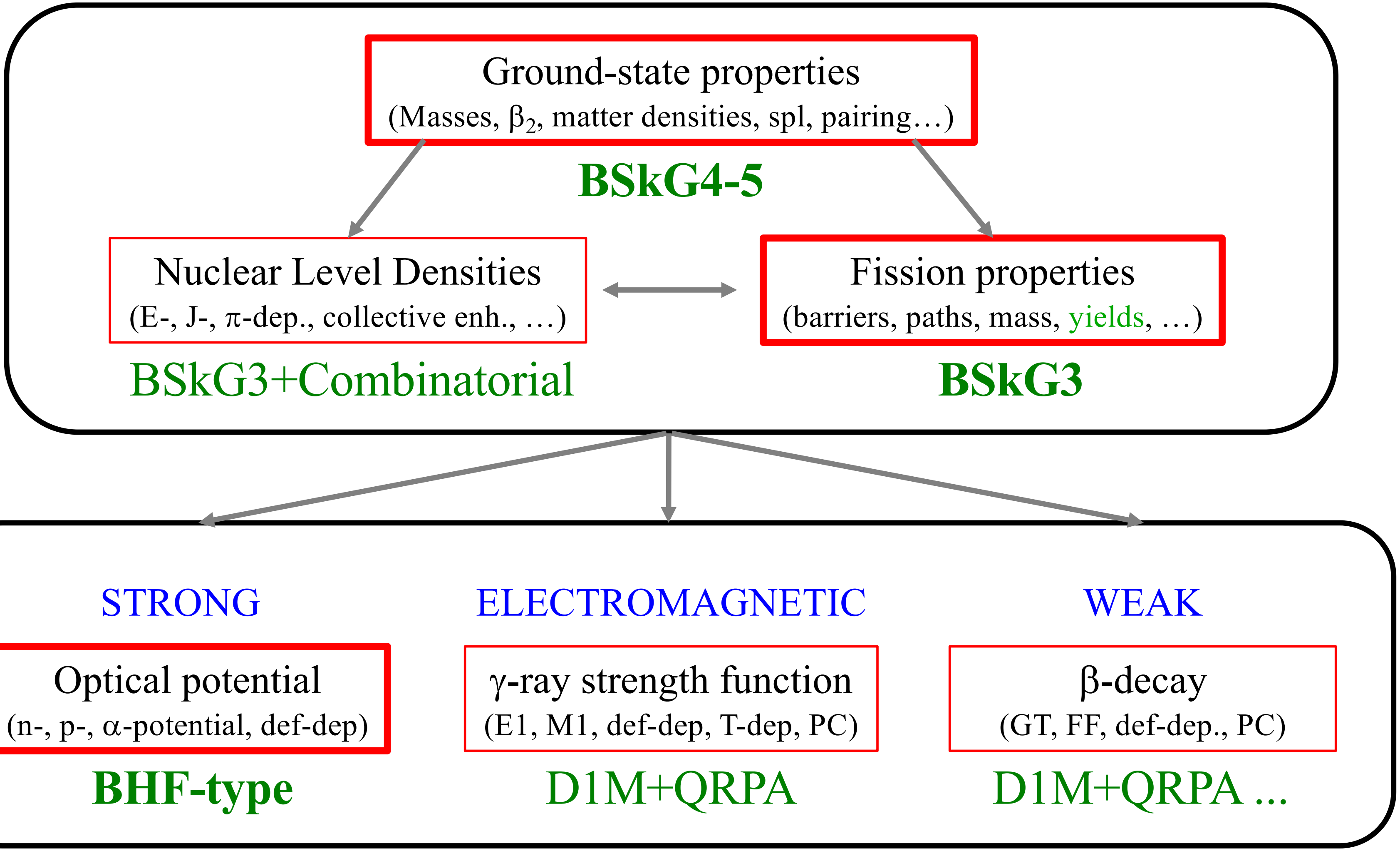


Nuclear inputs to nuclear reaction & decay calculations



Some new efforts to improve the nuclear predictions for r-process applications

Nuclear inputs to nuclear reaction & decay calculations



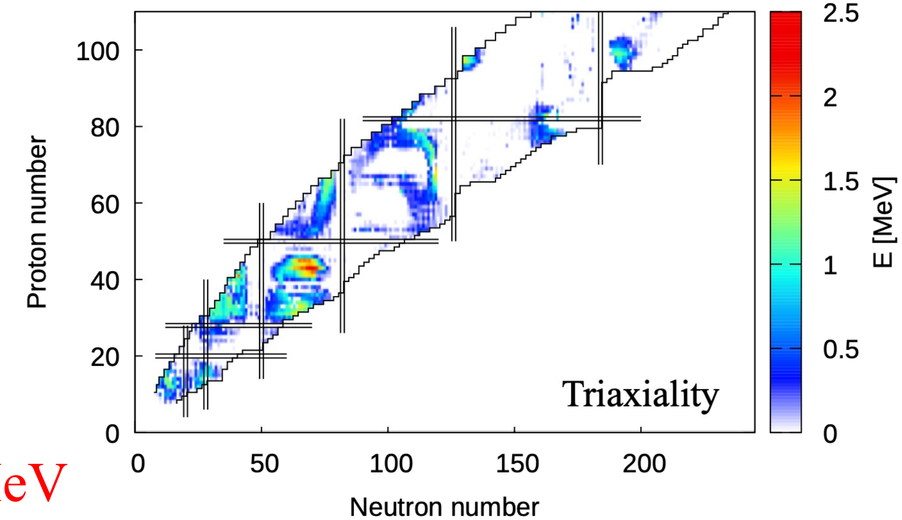
"Microscopic" approach is a necessary but not a sufficient condition !
"(Semi-)Microscopic" models must be competitive in reproducing exp. data !

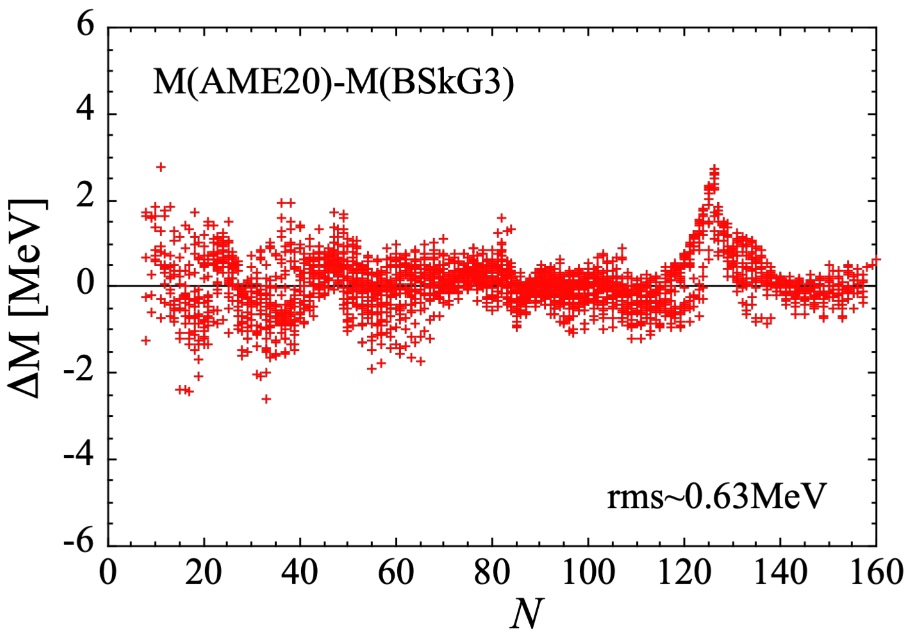
BSkG3 HFB nuclear mass models

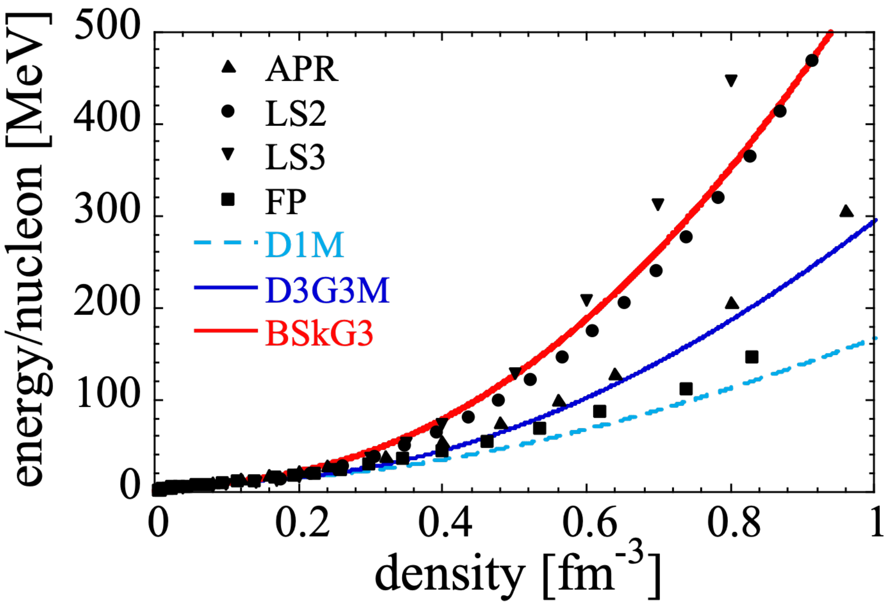
Grams, Ryssens et al. (EPJA 59, 270, 2023)

Skyrme-HFB mass model: BSkG3

- Triaxiality, time-reversal symmetry breaking & octupole GS deformation
- Microscopic pairing from "realistic" calculations
- Stiff EoS (NS max mass M=2.2M$_o$)
- Accurate masses: σ(2457M)=0.63MeV
- Accurate fission barriers σ(45B_f)=0.33MeV



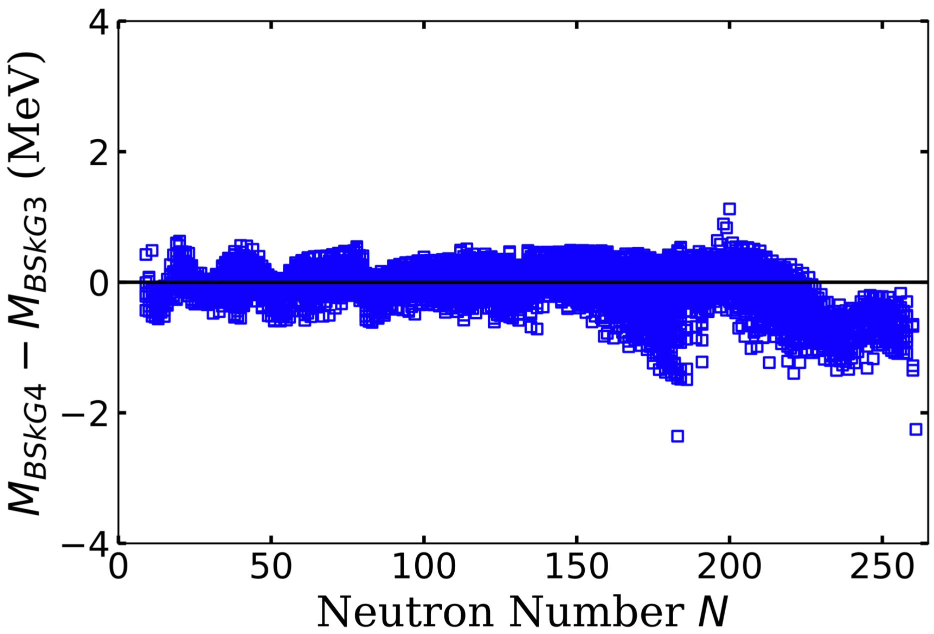




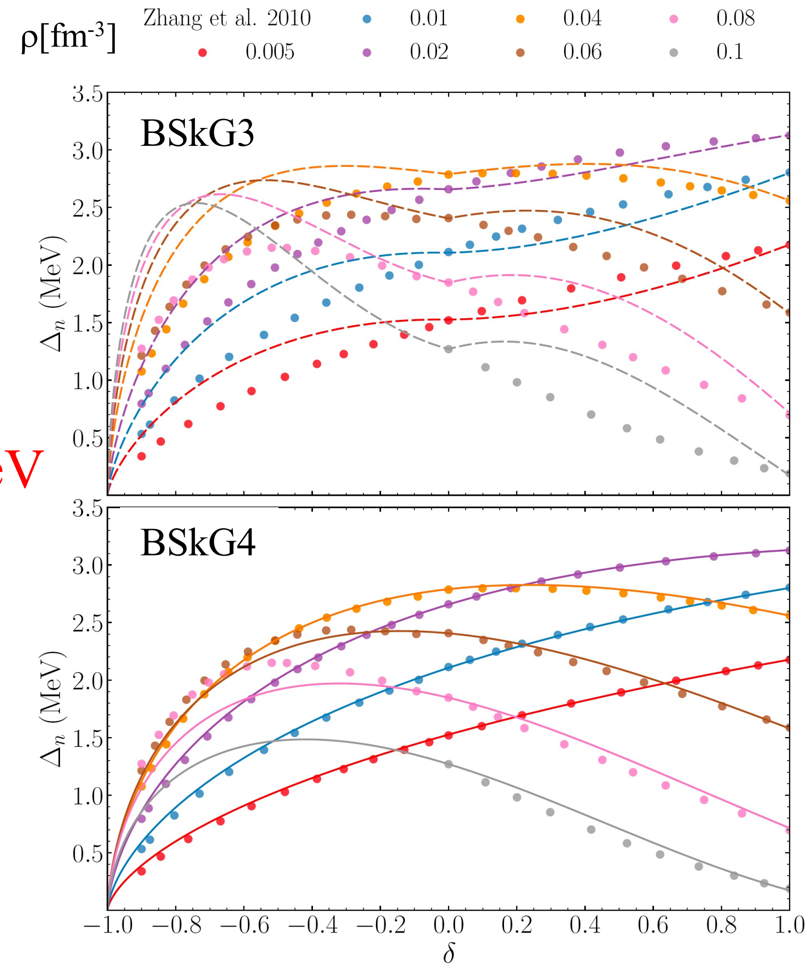
New BSkG4 HFB nuclear mass models

New Syrme-HFB mass model: BSkG4

- Triaxiality, time-reversal symmetry breaking & octupole GS deformation
- **Refined treatment of the isospin dependence of the pairing gaps in asymmetric nuclear matter**
- Stiff EoS (NS max mass M=2.2M$_o$)
- Accurate masses: σ(2457M)=0.63MeV
- Accurate fission barriers σ(45B_f)=0.36MeV



neutron pairing gaps in asymmetric INM



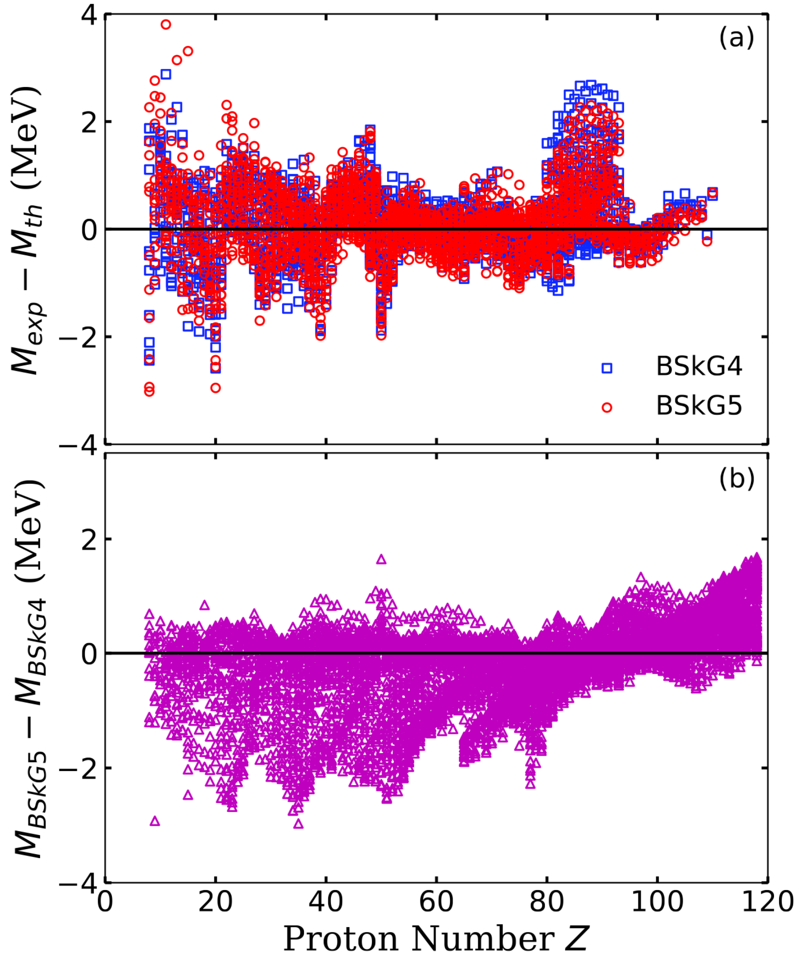
Grams, Ryssens et al. (EPJA 61, 35, 2025)

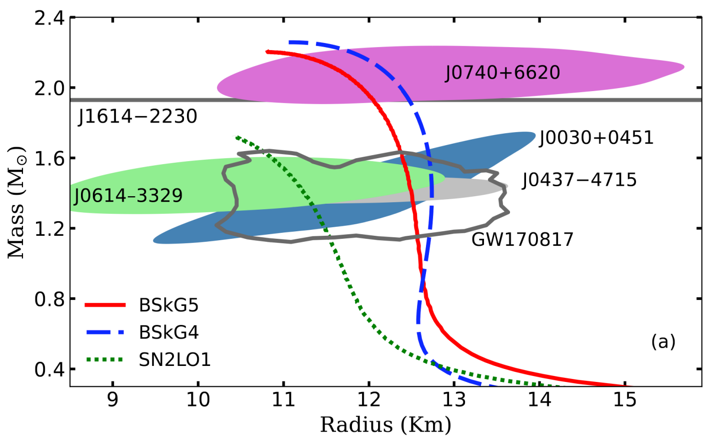
New BSkG5 HFB nuclear mass models

Grams, Ryssens et al. (PLB879, 140590, 2026)

Recent Skyrme-HFB mass model: BSkG5

- **First N2LO mass model**: central terms with 4 additional gradients
- Triaxiality, time-reversal symmetry breaking & octupole GS deformation
- Improved description of the isospin dependence of the pairing as in BSkG4
- Stiff EoS (NS max mass M=2.2M$_o$)
- Accurate masses: σ(2457M)=0.65MeV
- Accurate fission barriers σ(45B_f)=0.43MeV

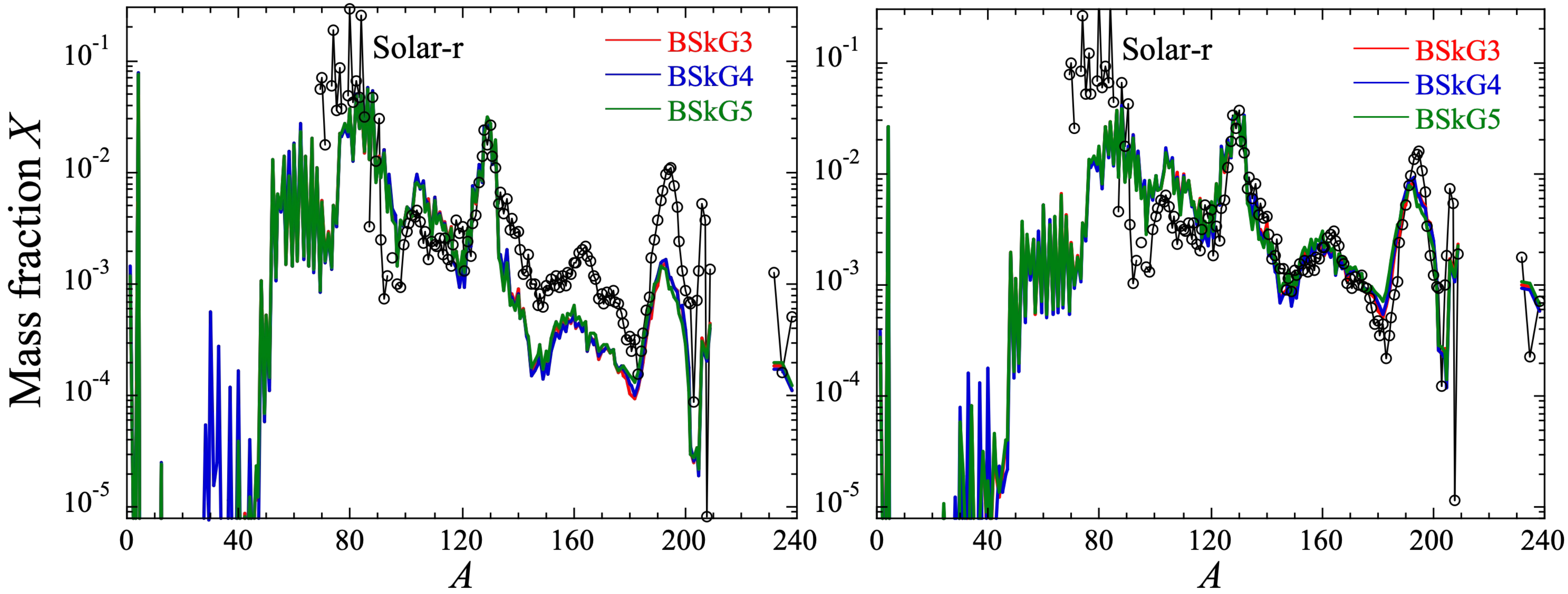




Impact of new BSkG5 HFB nuclear mass models

Long-lived collapse: 1.375 – 1.375 M_o Short-lived collapse: 1.20 – 1.60 M_o

Just et al. (2023)



Only impact of masses on the (n,γ) and (γ,n) reactions rates...

→ Impact of masses on β-decay rates or fission probabilities not yet studied

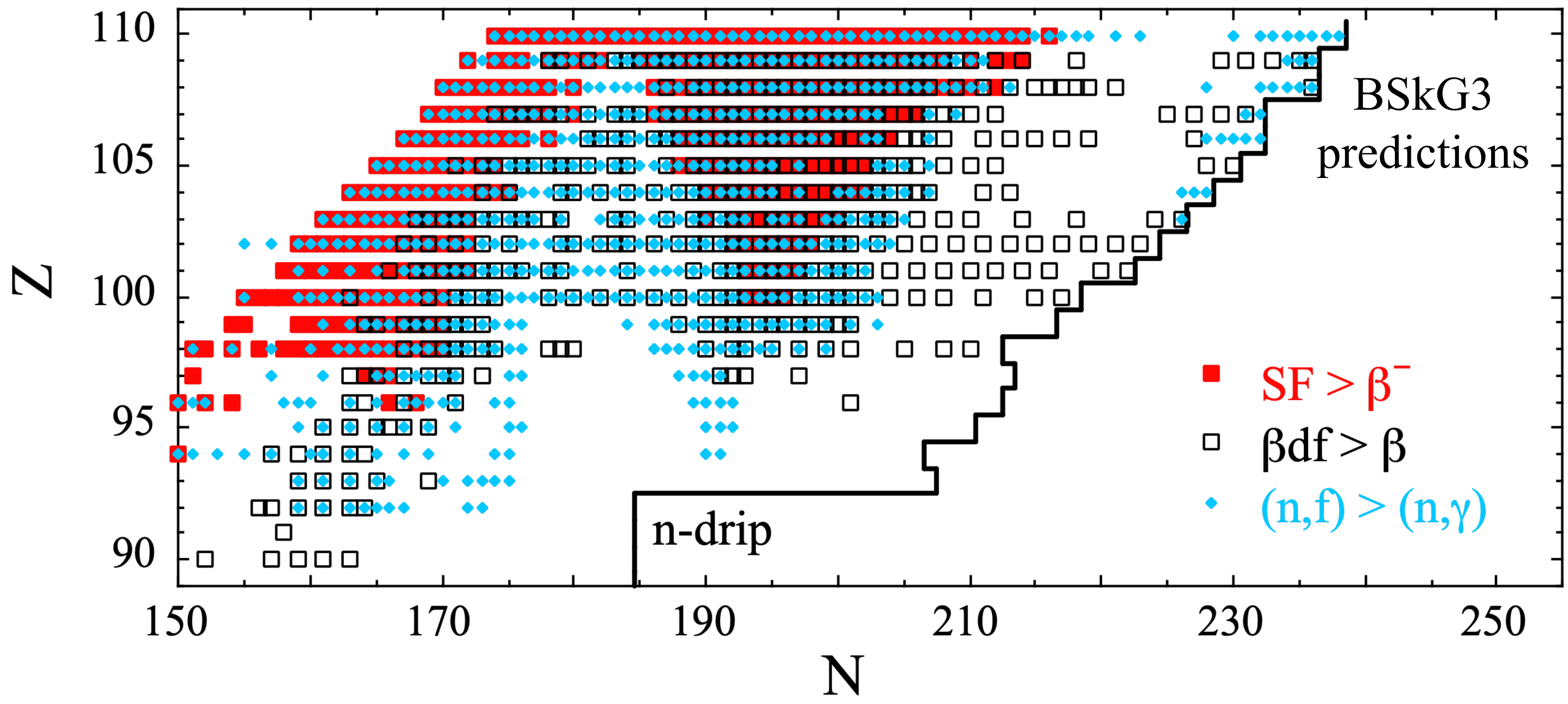
BSkG6 (N2LO with improved quadrupole corrections) to follow ...

Impact of fission on the r-process in NSM

Fission processes and fission fragments distributions of relevance in low-Y_e trajectories for estimating the

- termination point of the r-process (recycling, heating, prod of SH)
- production of Pb-peak elements
- production of cosmochronometers (U, Th) and other tracers (^{254}Cf)
- production of light species (A~110-160) by fission recycling

Detailed calculation of fission probabilities (*sf, nif, βdf*) for about 2000 nuclei

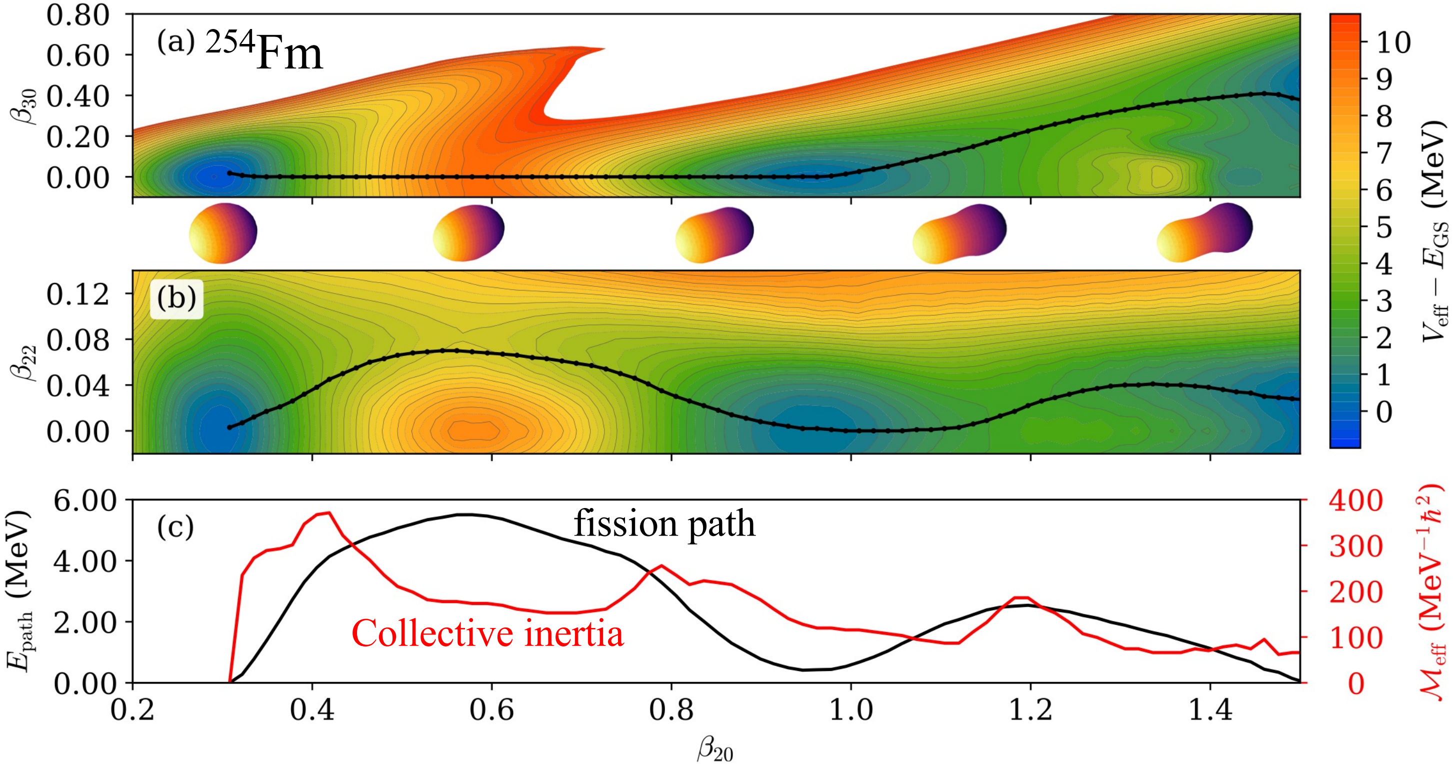


Fission (*sf, nif, βdf*) is the most complex nuclear physics process to model

1. Calculation of the multi-dimensional PES to determine fission paths and collective inertias

(β_{20},β_{30})

(β_{20},β_{22})

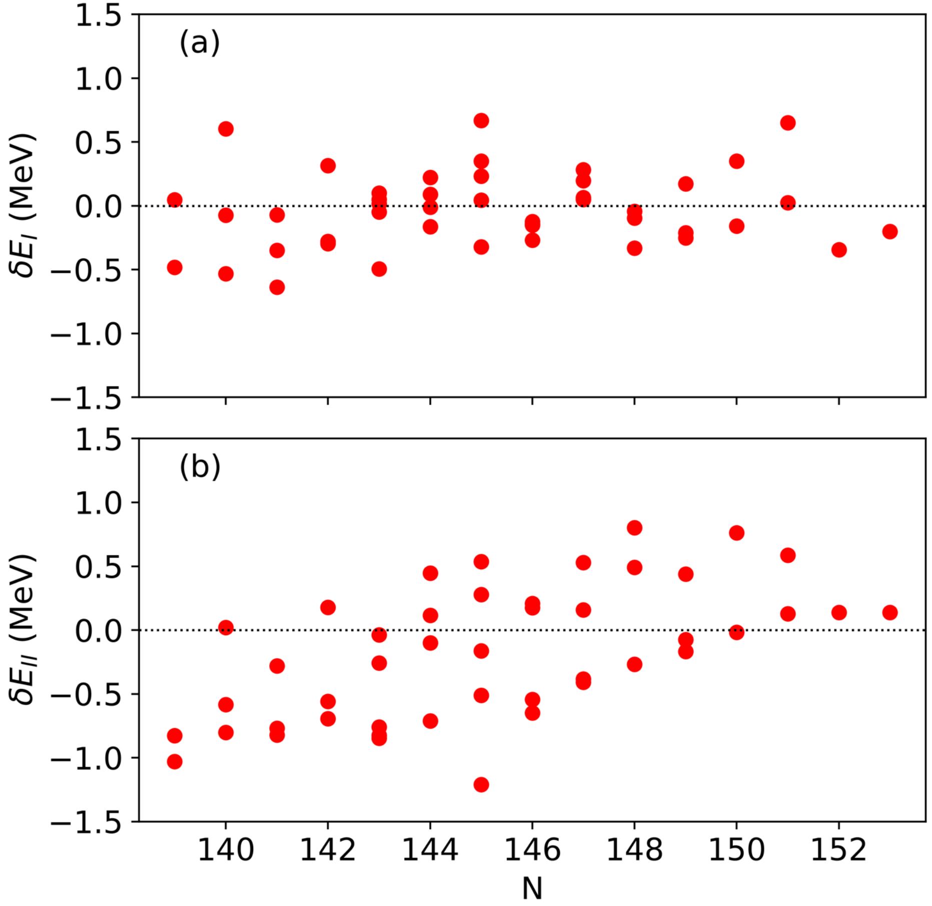


→ Fission barriers, fission paths, collective inertias....

The primary (i.e. highest) barrier plays the most crucial role

BSkG3: Remarkable description of primary fission barriers (**σ=0.33MeV**)

Triaxial- **and** octupole-deformed barriers



(Δ=0.5 MeV → ~3-6 orders of magnitude on SF $T_{1/2}$)

rms deviations on 45 $Z > 90$ nuclei wrt known (RIPL3) fission barriers/wells

	BSkG3
σ(M) [MeV]	0.63
σ(E_I) [MeV]	**0.33**
σ(E_{II}) [MeV]	0.57
σ(E_{iso}) [MeV]	0.39

	HFB-14	FRLDM	BCPM
σ(M) [MeV]	0.76	0.81	1.58
σ(E_I) [MeV]	0.60	0.81	1.48
σ(E_{II}) [MeV]	0.69	1.41	0.75
σ(E_{iso}) [MeV]	1.07	1.00	0.78

Extended to ~3500 nuclei ($70 \leq Z \leq 118$) for r-process simulations ...

(~ 1 year of calculations)

2. Calculation of the *sf, nif*, and *βdf* rates starting from the BSkG3 PES

- SF half-life calculated by least action integral

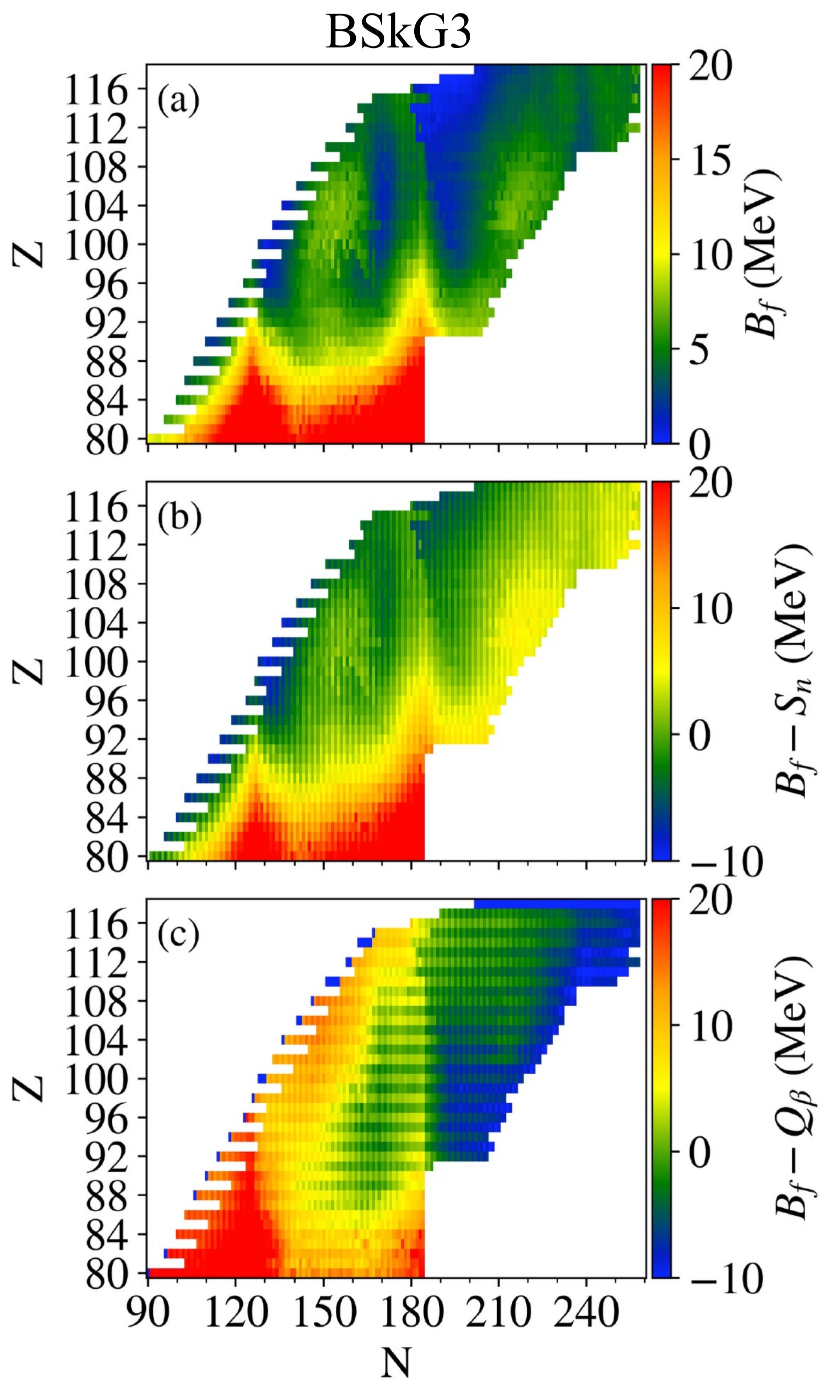
  Significant if $B_f \lesssim 4$ MeV

- (*n,f*) calculated with TALYS
  (including NLD at saddle points)

  Significant if $B_f < S_n$

- βdf calculated using a β-feeding distribution from D1M+QRPA and TALYS de-excitation scheme

  Significant if $B_f < Q_\beta$



Comparison of BSkG3 SF with semi-empirical formula (Khuyagbaatar 2020)

Formula often used in r-process simulations (e.g. WinNet)

$$T_{\rm sf} = \frac{\ln 2}{nT} \quad \text{where} \quad T = \frac{1}{1 + \exp[2\pi B_f / \hbar\omega]}$$

n = frequency of barrier assaults $\quad n = \omega / 2\pi$

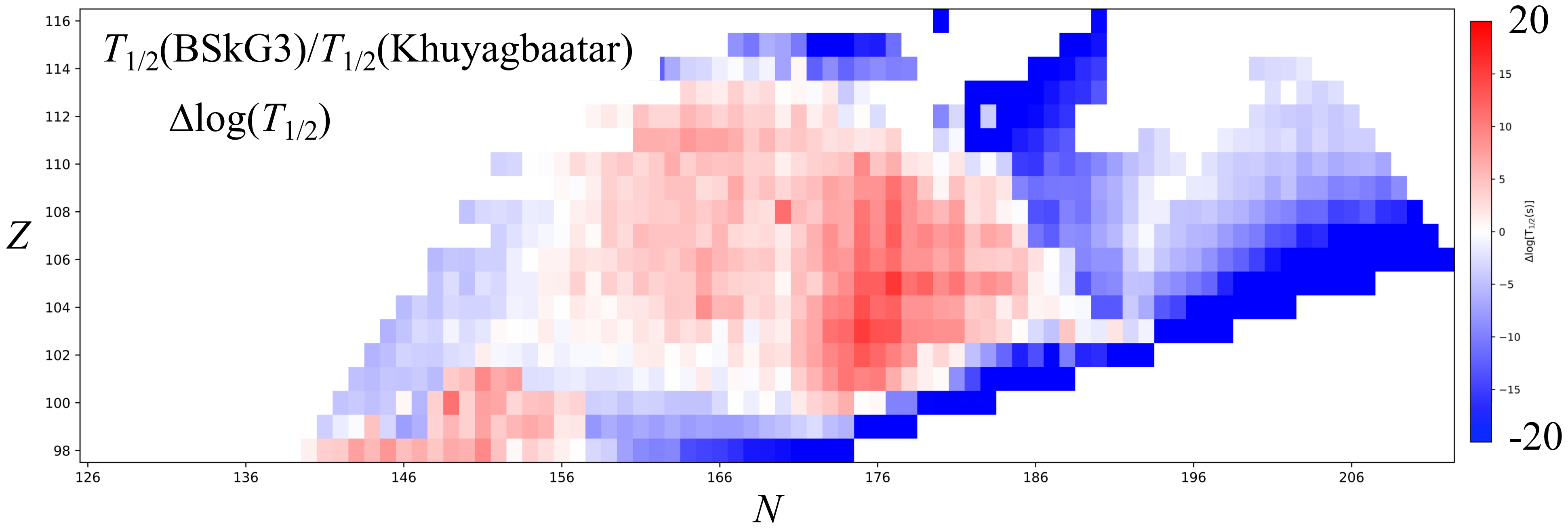
using ETFSI primary barriers → barrier width fitted to SF data

$$\hbar\omega = -0.02534 \cdot (Z^2/A)^2 + 2.10736 \cdot Z^2/A - 42.7659$$

For GS: 107 exp $T_{1/2}$

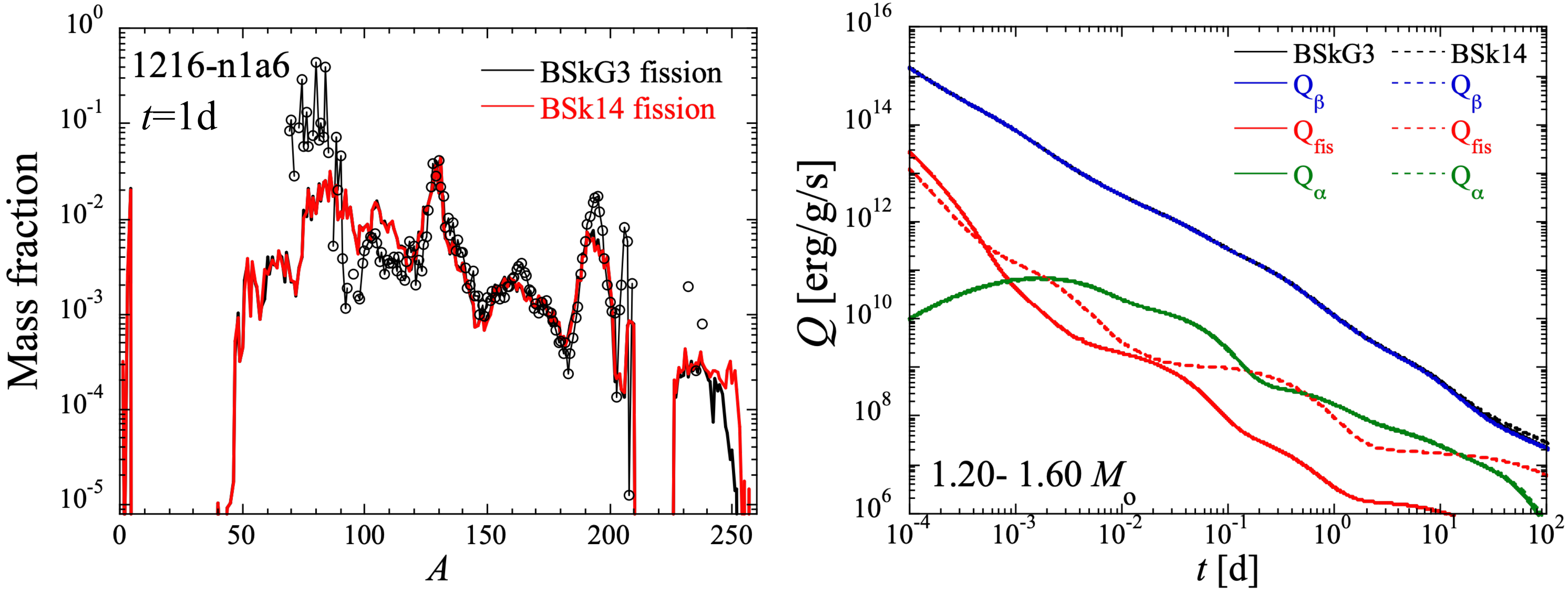
BSkG3: $f_{\rm rms}$=1.5 10^3

Khuyagbaatar: $f_{\rm rms}$=3.1 10^6

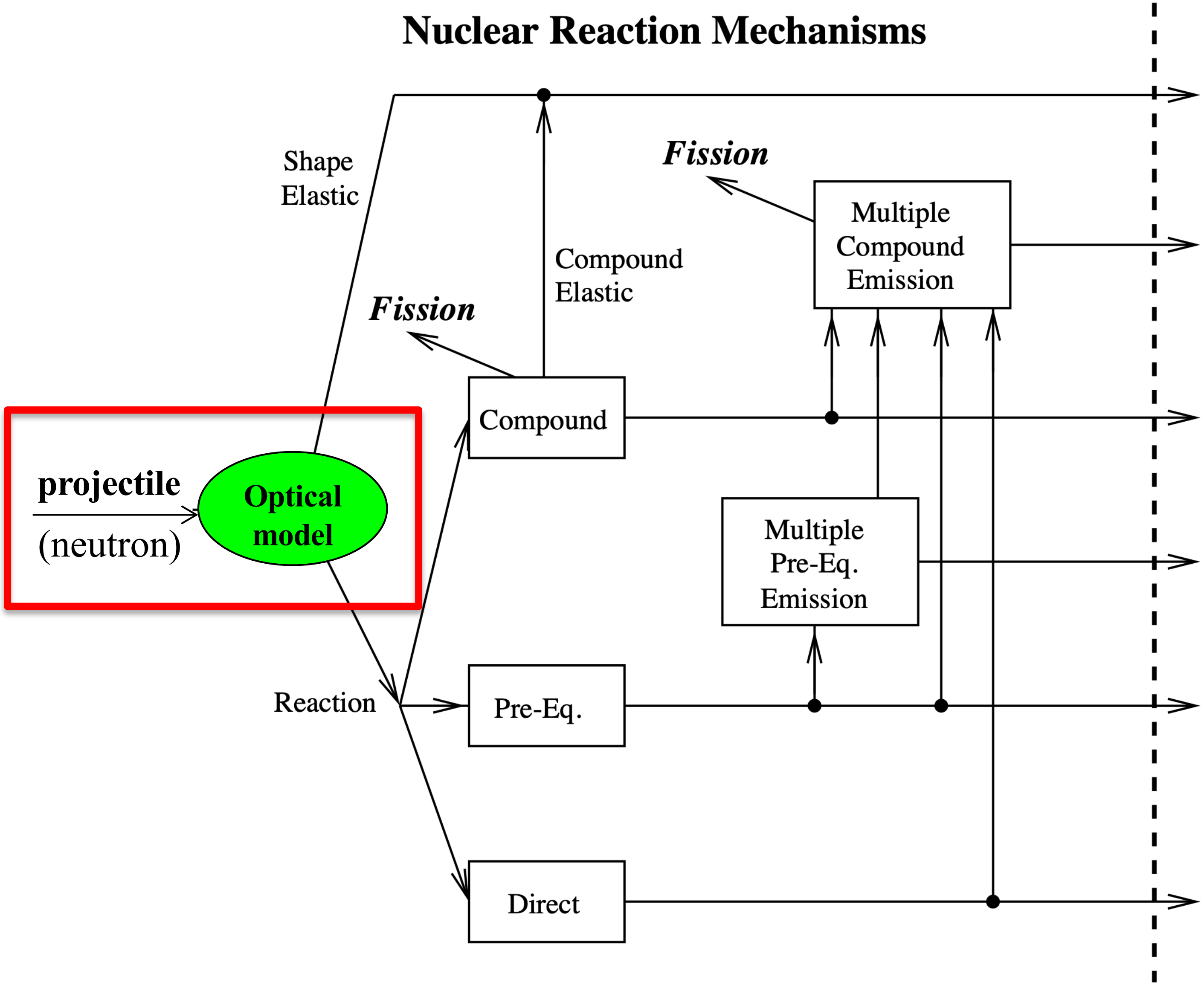


Impact of the fission probabilities

Short-lived collapse: 1.20 – 1.60 M_o

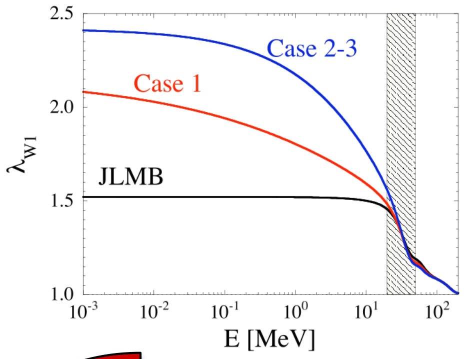


Impact of the neutron optical potential on the r-process in NSM

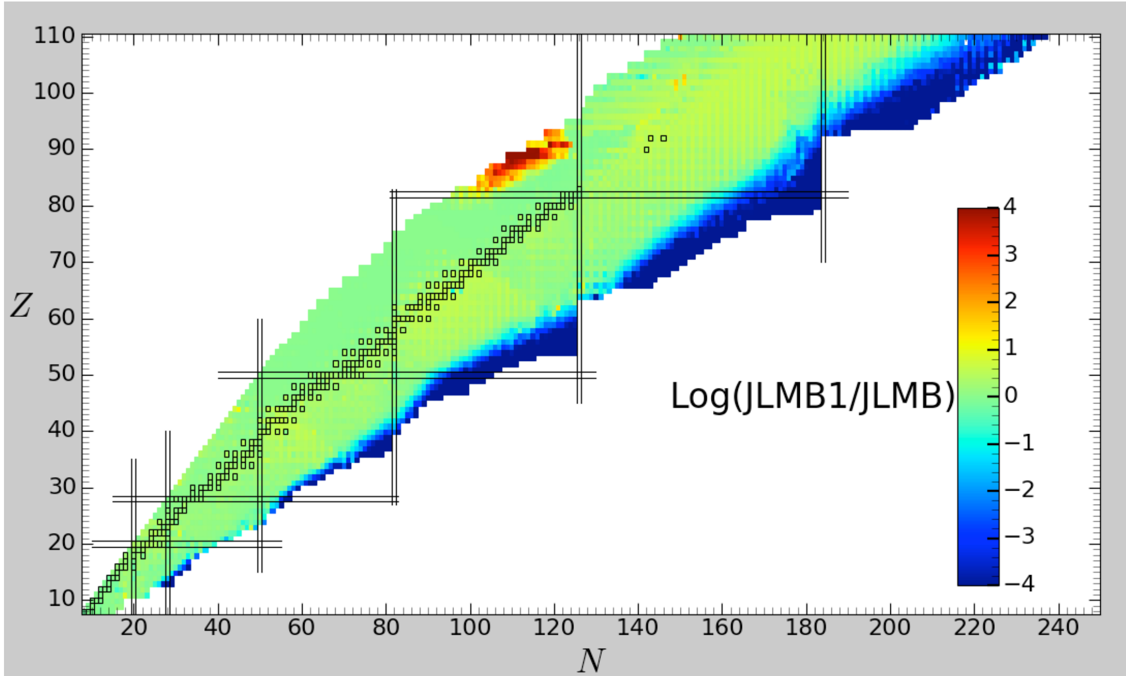


Impact of the OMP on (n,γ) is small unless the n-absorption becomes negligible for n-rich nuclei

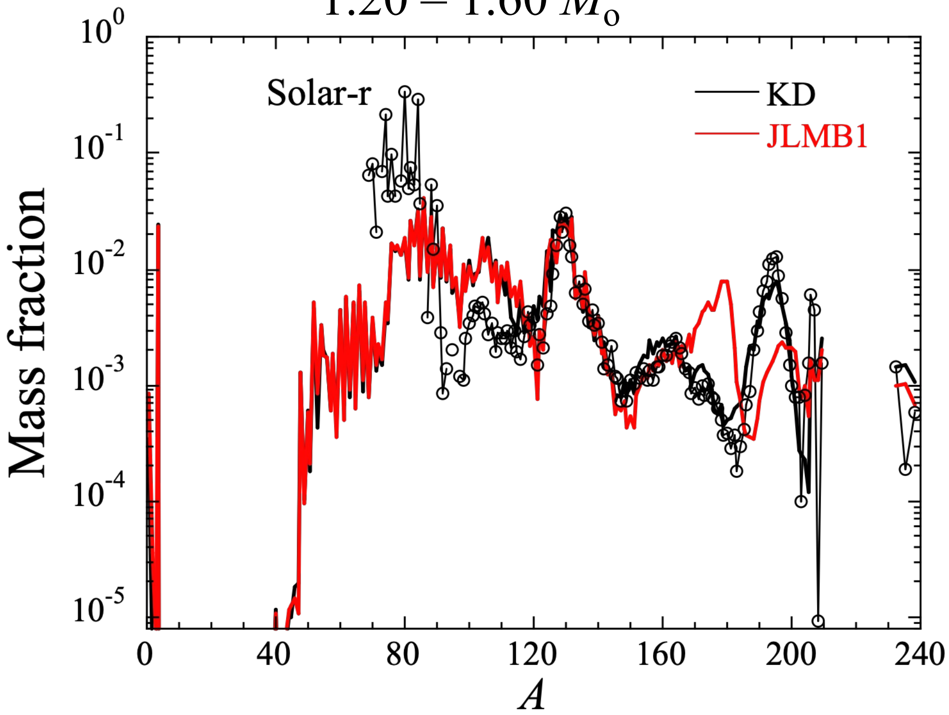
JLMB* (Case 1): HF+DC

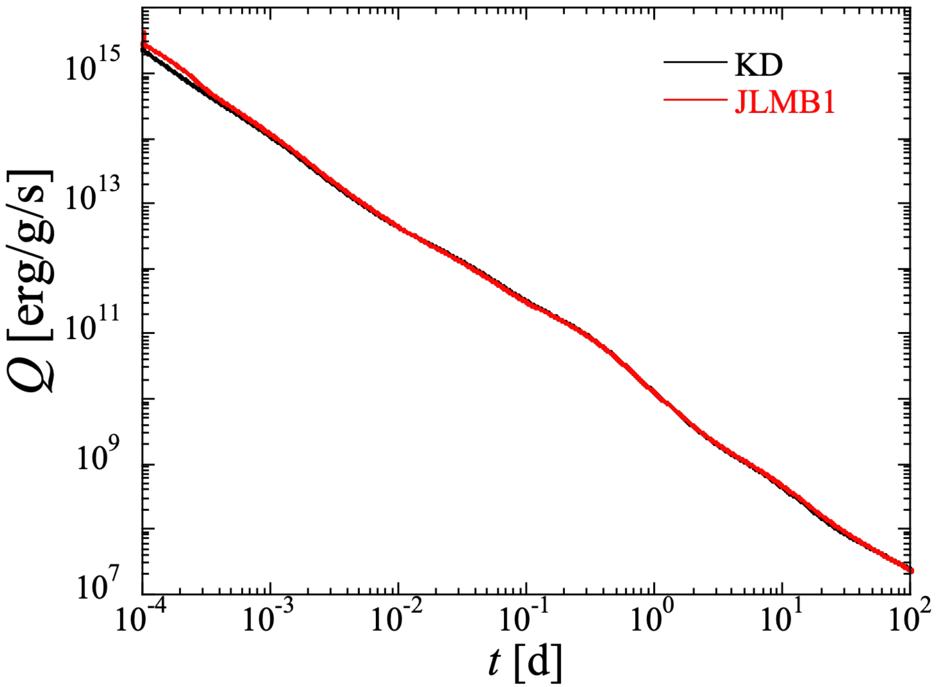


SG & Delaroche (PLB 2007)

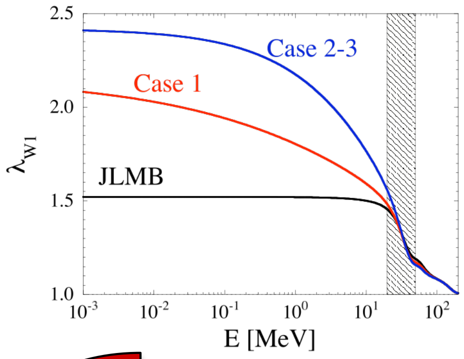


Short-lived collapse:
1.20 – 1.60 M_o

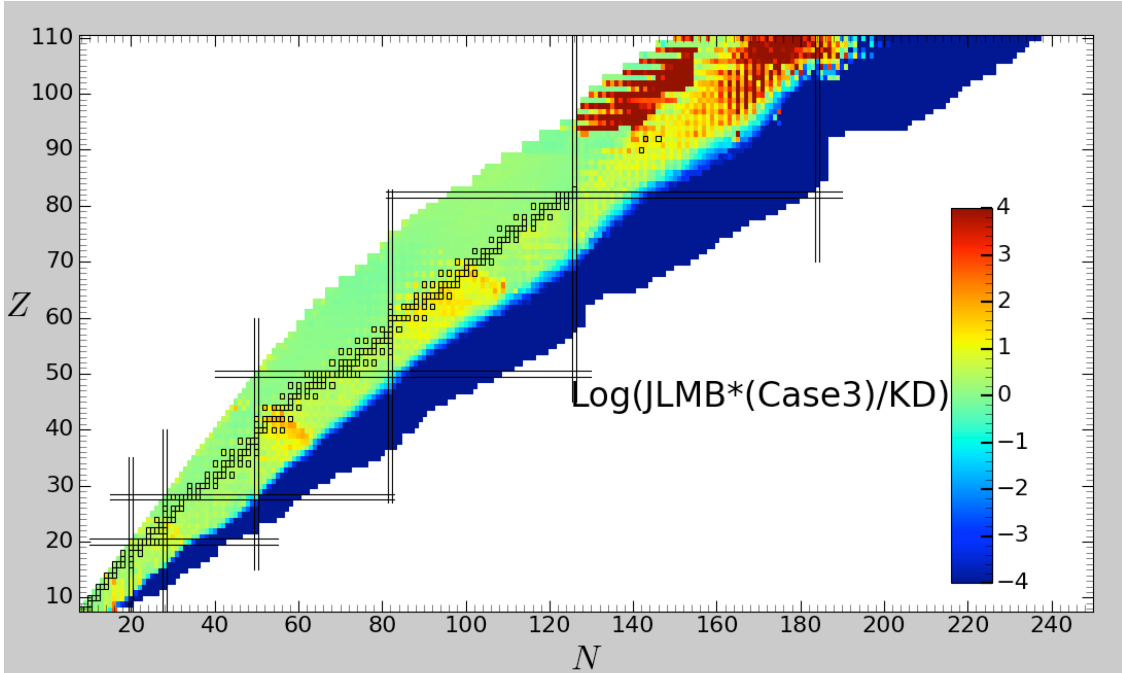




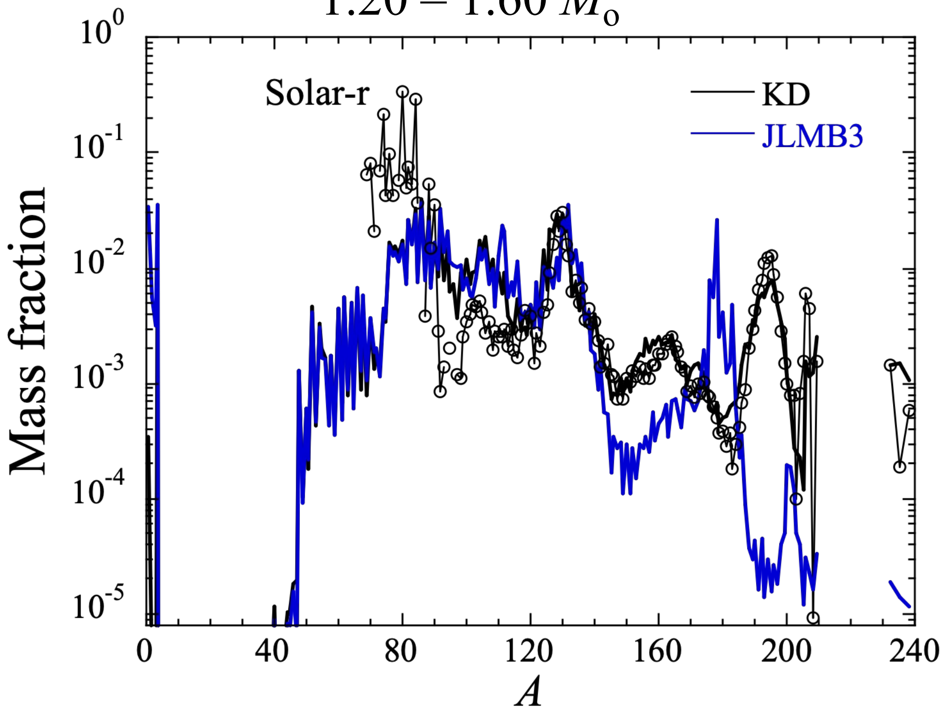
JLMB* (Case 3): HF+DC

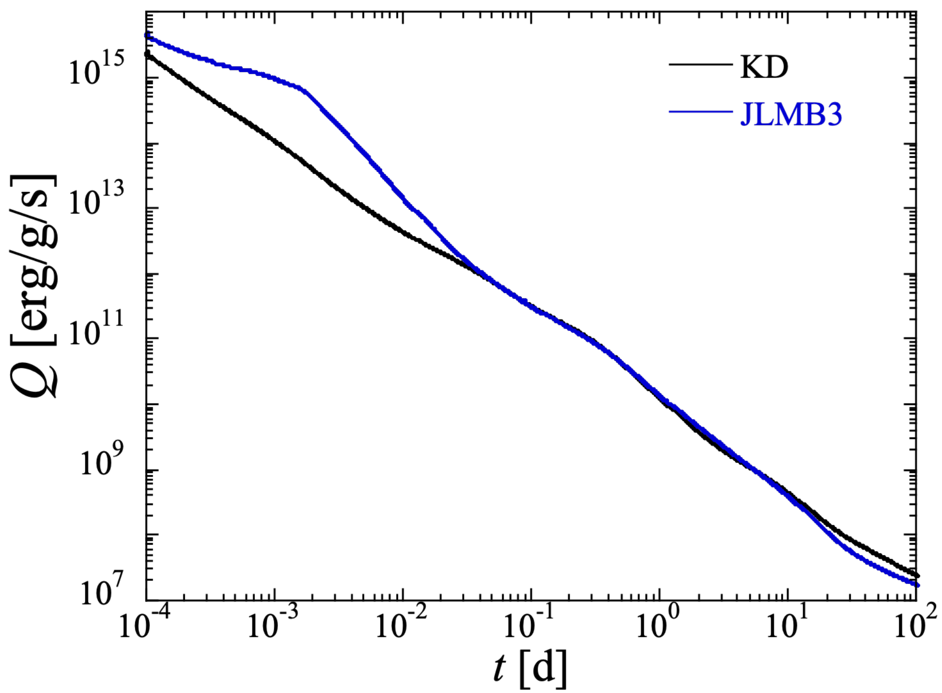


SG & Delaroche (PLB 2007)



Short-lived collapse:
1.20 – 1.60 M_o

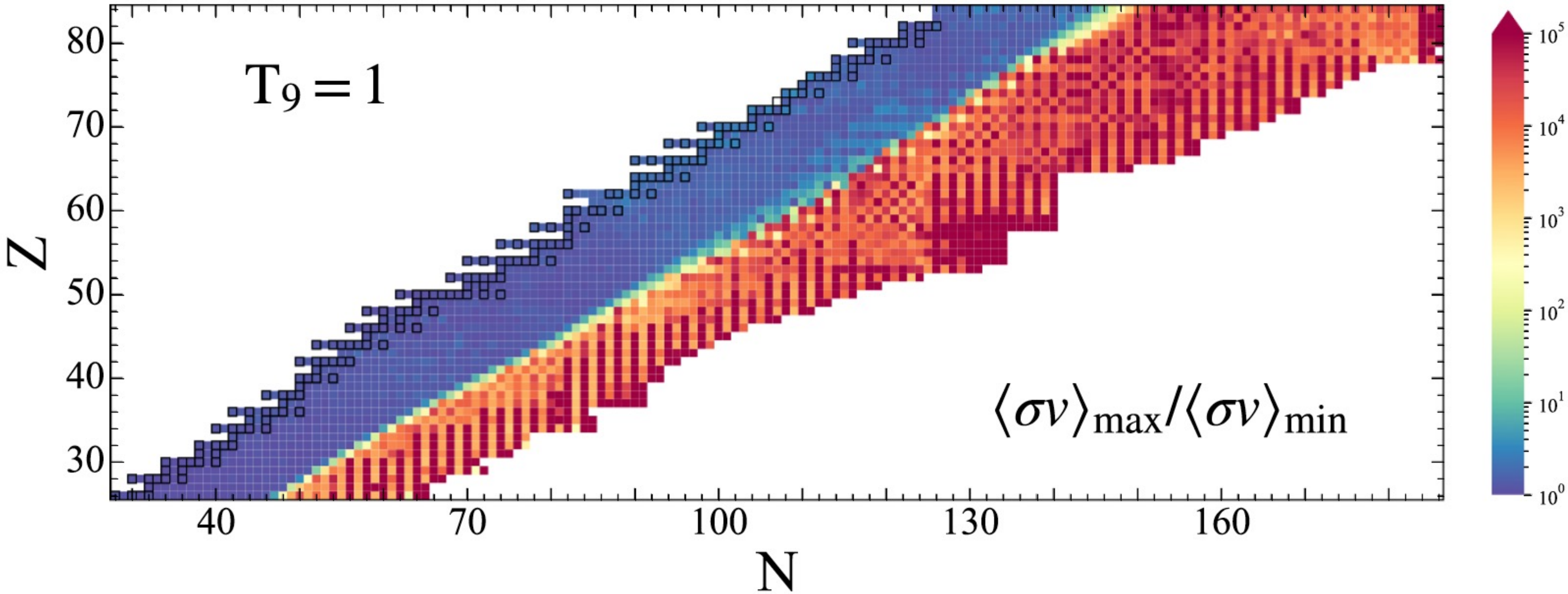




Recent new global OMP calculation: Whitehead et al. (2021; PRL 127 182502)

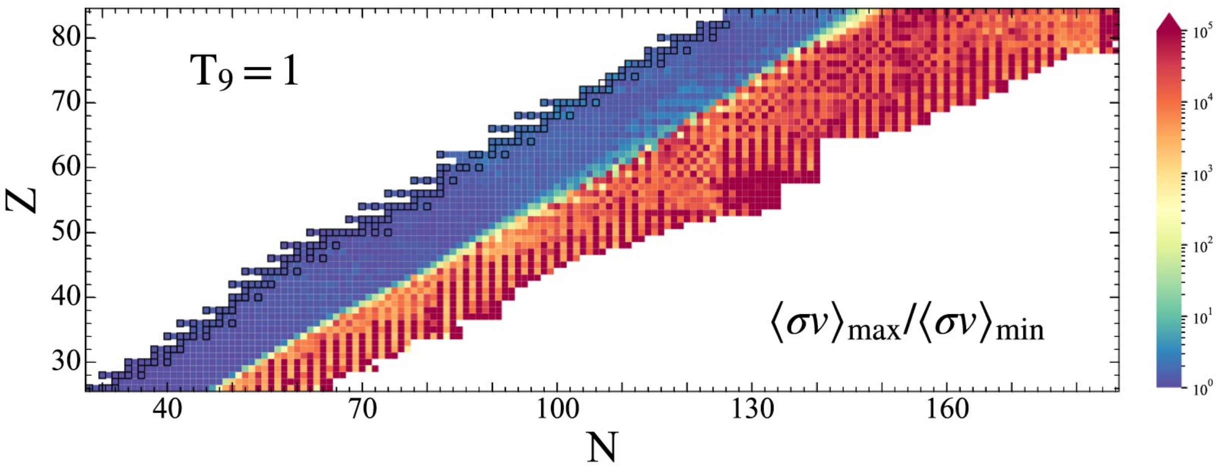
Fully microscopic global nucleon-nucleus optical potential obtained within the framework of many-body perturbation theory using realistic nuclear interactions from chiral effective field theory, including **uncertainty quantification associated with the chiral interaction**

Uncorrelated *parameter* uncertainties

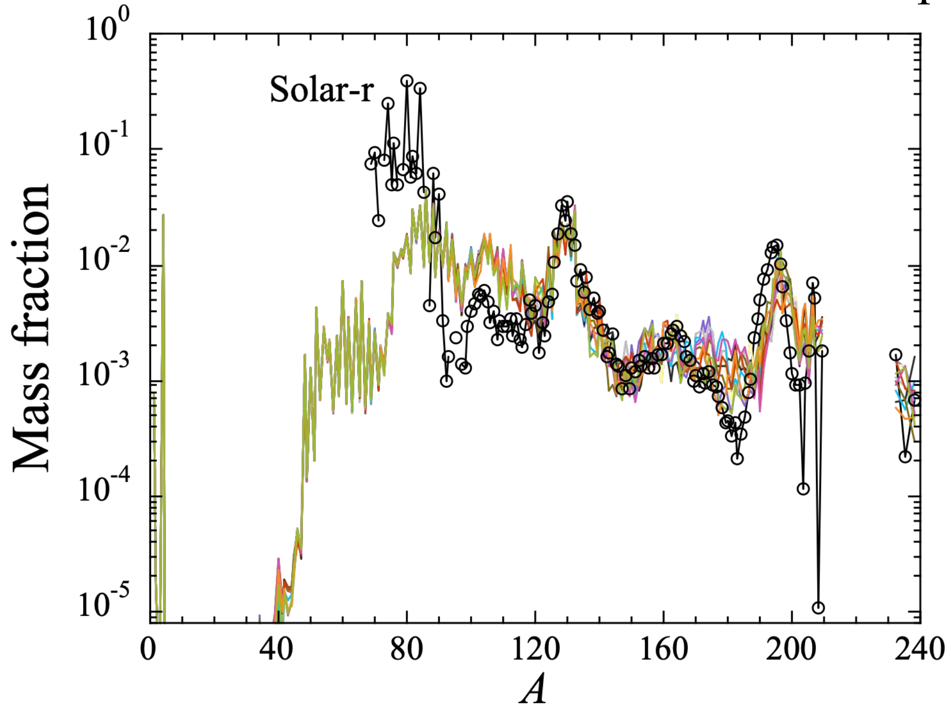


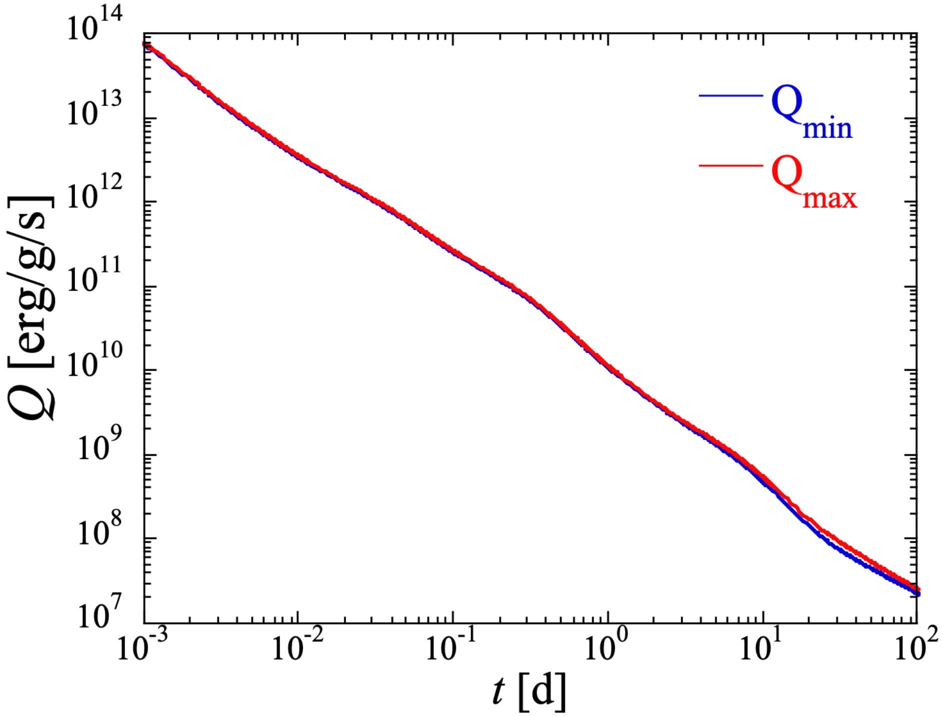
Wang et al. (2026, PLB 872, 140056)

Recent new global OMP calculation: Whithead et al. (2021; PRL 127 182502)

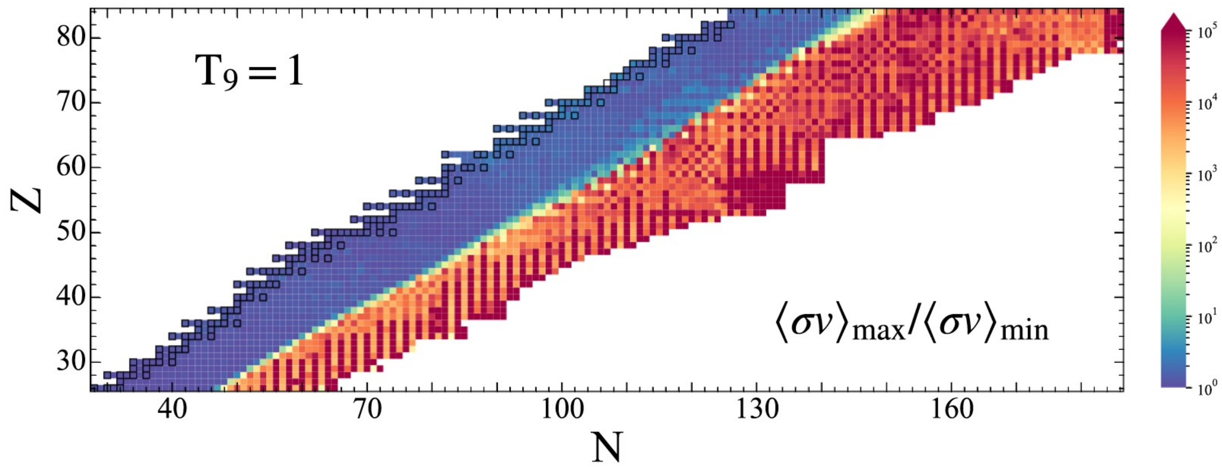


Short-lived collapse: 1.20 – 1.60 M_o

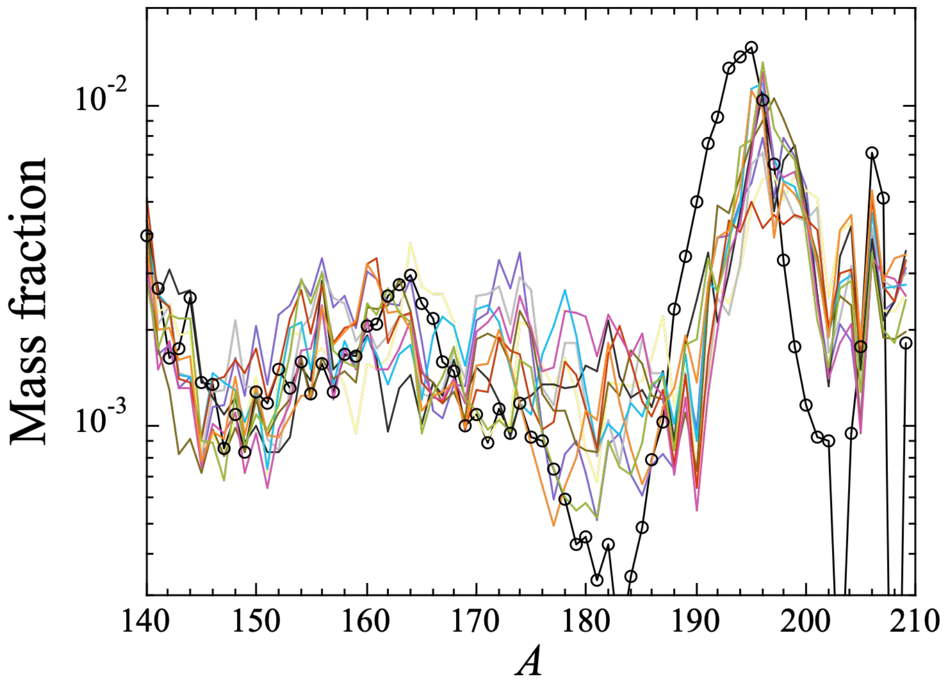


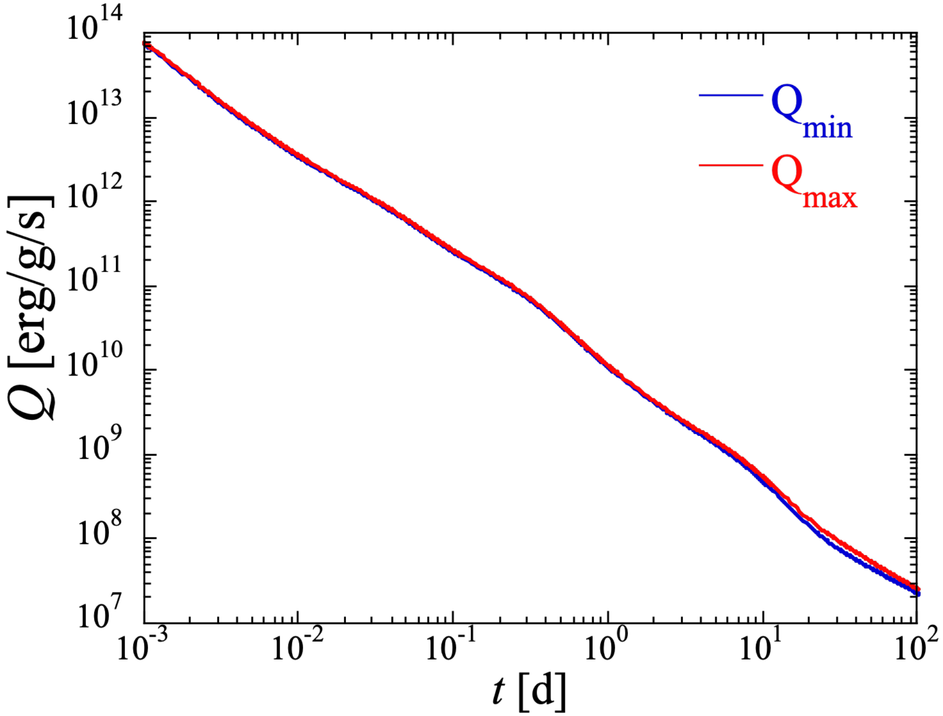


Recent new global OMP calculation: Whithead et al. (2021; PRL 127 182502)



Short-lived collapse: 1.20 – 1.60 M_o

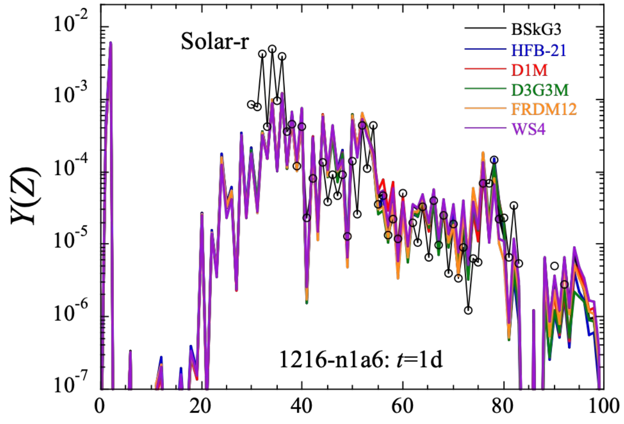




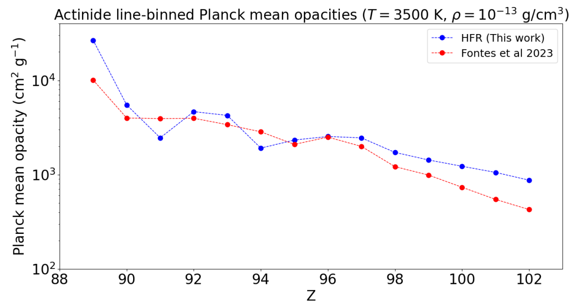
r-process nucleosynthesis and Kilonova radiation transfer

Determination of the KN lightcurve and spectra based on

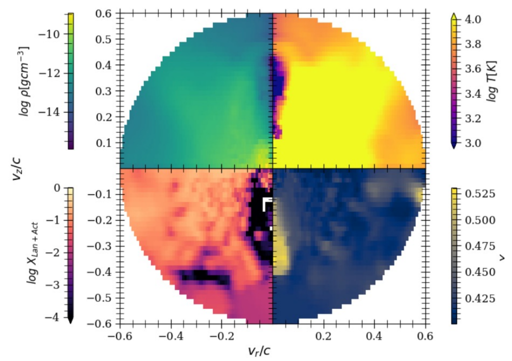
- Nucleosynthesis yields and decay heat calculated at ULB along each trajectory of NSM hydrodynamic simulations (O. Just et al. – GSI)



- Line-binned opacities calculated using the HFR method for elements, including lanthanides and actinides, Z = 20–103 (J. Deprince - U. Mons)



- KN light curves and spectra calculated using Implicit Monte Carlo Radiation Transport code **SuperNu** (Wollaeger et al. 2021; G. Wagle – ULB)

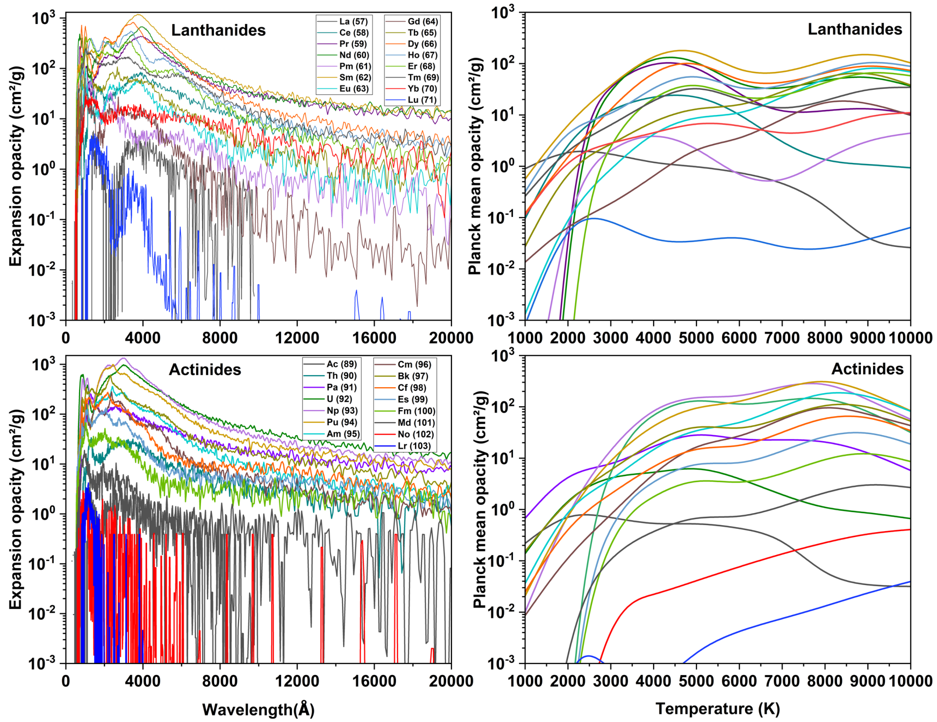


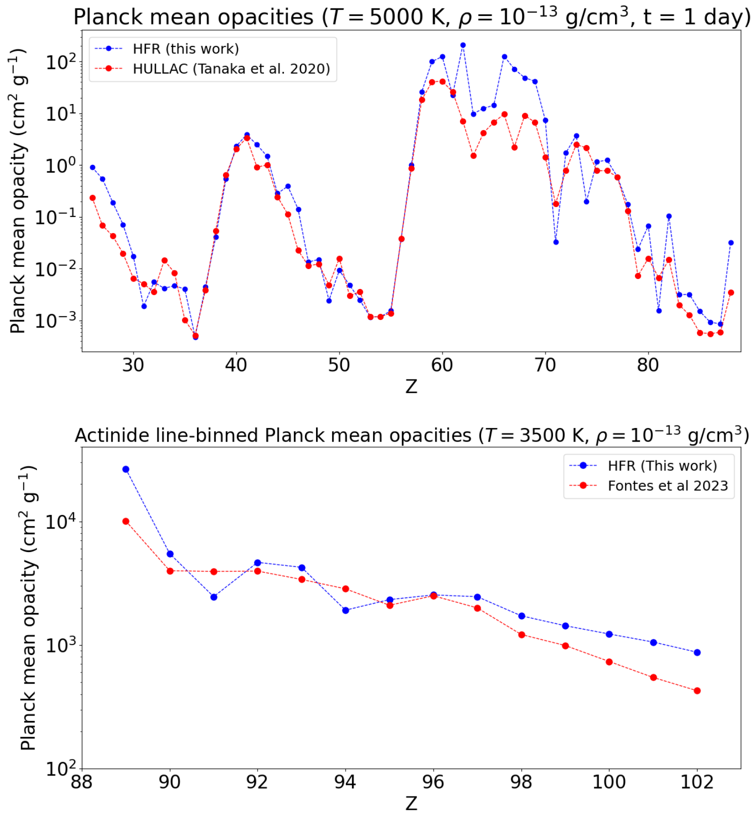
A&A, 696, A32 (2025)
https://doi.org/10.1051/0004-6361/202452967

Astronomy & Astrophysics

Kilonova ejecta opacity inferred from new large-scale HFR atomic calculations in all elements between Ca ($Z = 20$) and Lr ($Z = 103$)

J. Deprince[1,2,⋆], G. Wagle[2], S. Ben Nasr[1], H. Carvajal Gallego[1], M. Godefroid[3], S. Goriely[2], O. Just[4,5], P. Palmeri[1], P. Quinet[1,6], and S. Van Eck[2]





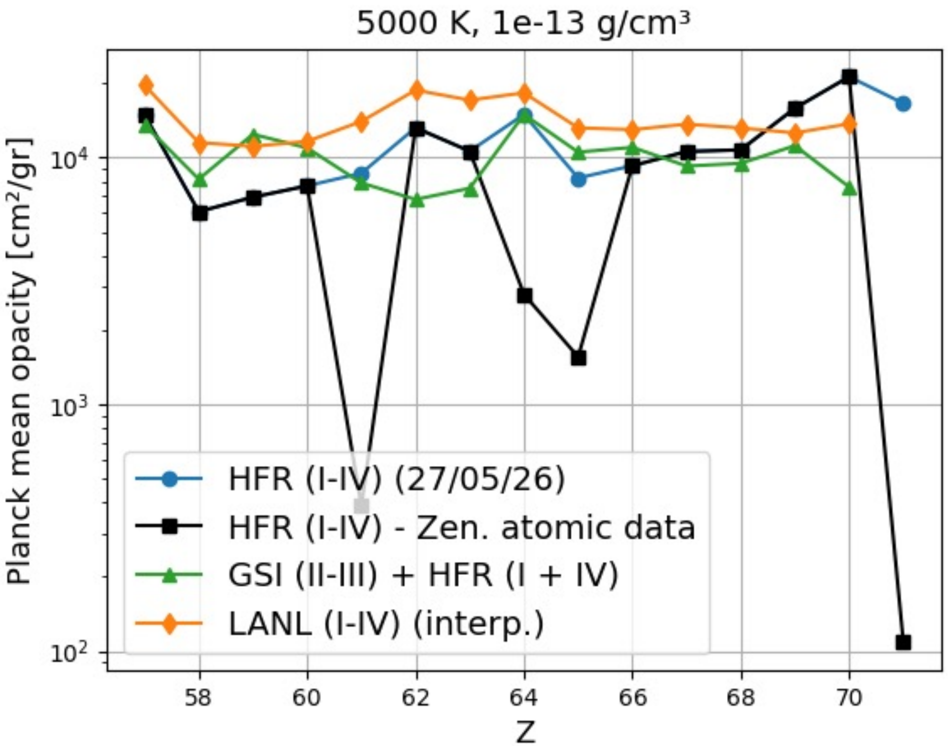
Data available on Zenodo: https://zenodo.org/records/14017952 (DOI:10.5281/zenodo.14017952)

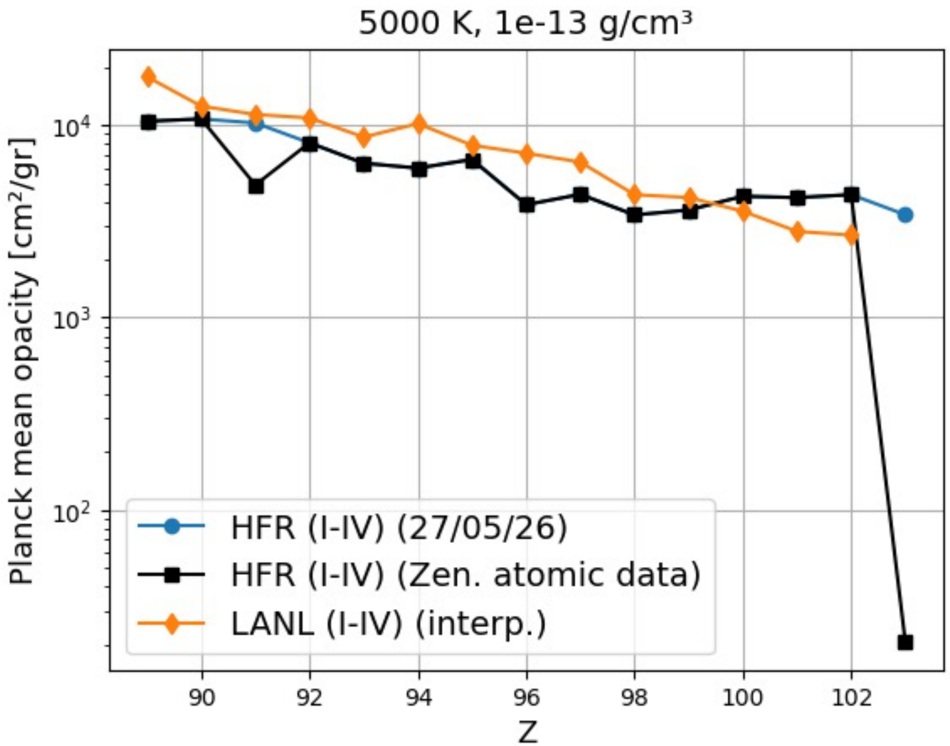
Natalia Thomas

All HFR atomic data and opacities for Lanthanides and Actinides have been reviewed

Jerome Deprince

Line-binned opacities at *T*=5000K and $\rho=10^{-13}$ g/cm^3





HFR (U. Mons - ULB) - Ionization stages (I-IV) for Z = 1, 2, and 20 - 103, not calibrated

FAC (GSI) - Ionization stages (II-III) for Z = 57 - 71, calibrated (Flörs et al. 2026)

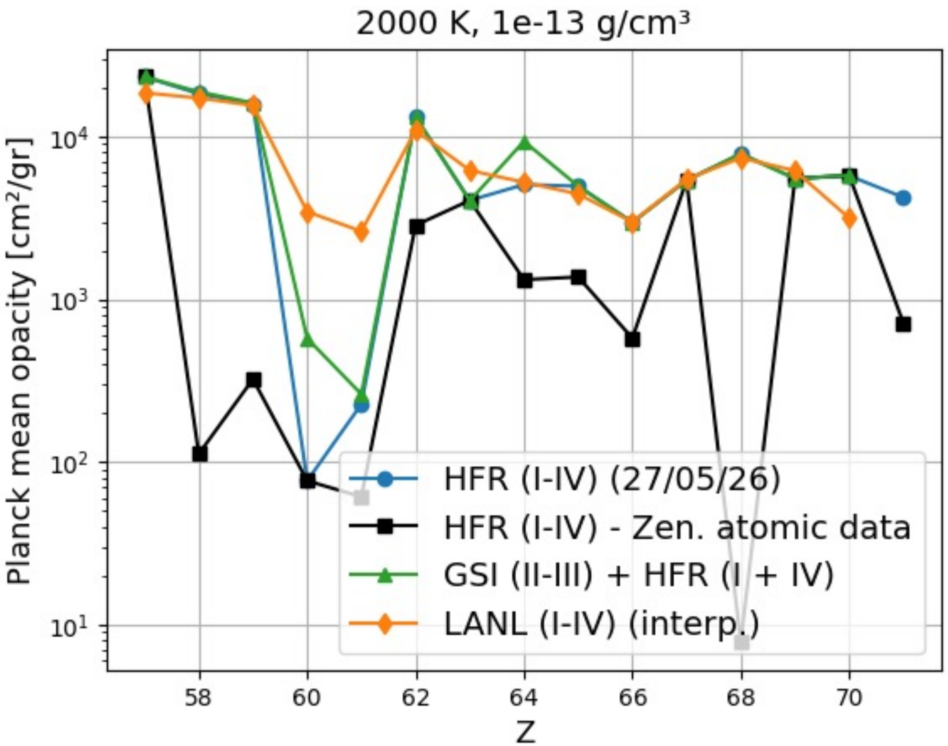
HFR (LANL) - Opacity tables from NIST/LANL, Z = 57 - 71, 89 - 102 (Fontes et al. 2020, 23)

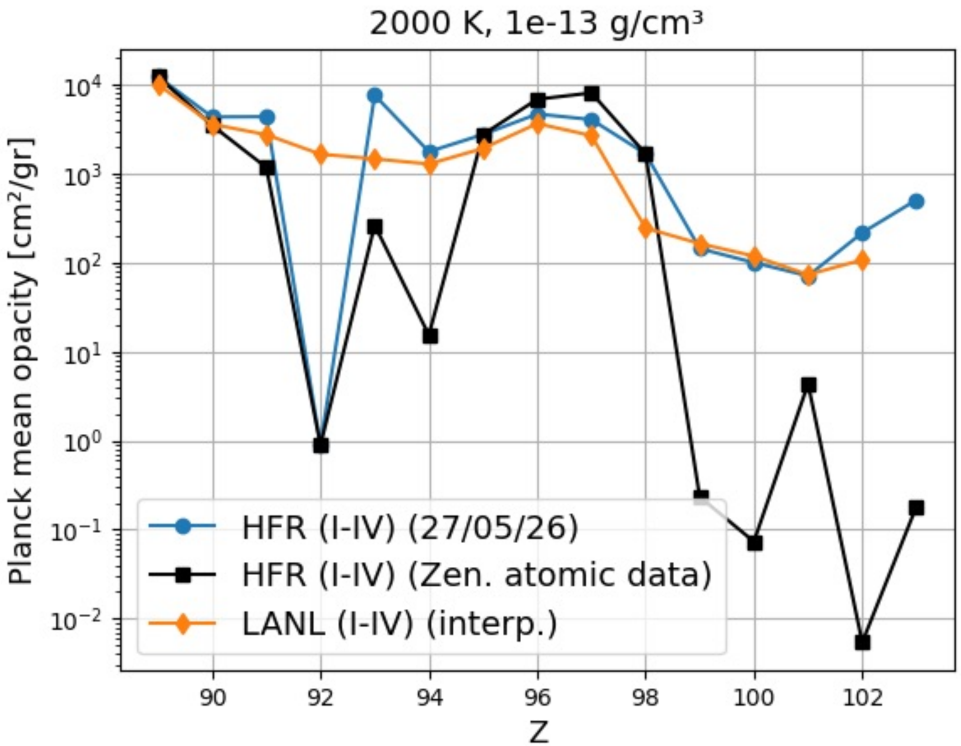
Natalia Thomas

All HFR atomic data and opacities for Lanthanides and Actinides have been reviewed

Jerome Deprince

Line-binned opacities at T=2000K and $\rho=10^{-13}$ g/cm^3



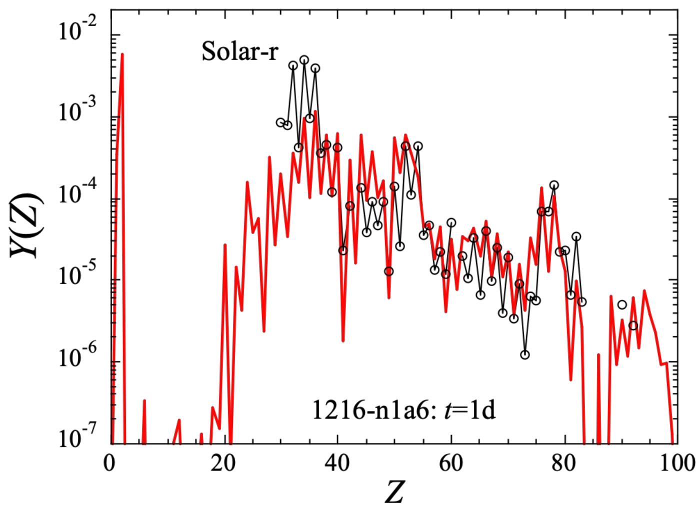


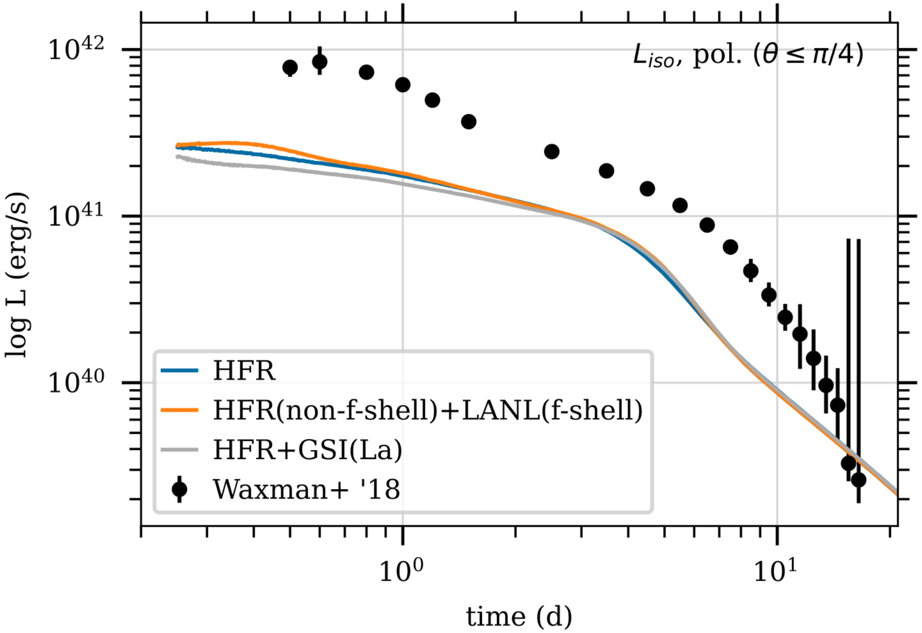
Data on Zenodo to be updated ... soon... Nd I and U I may still be underestimated

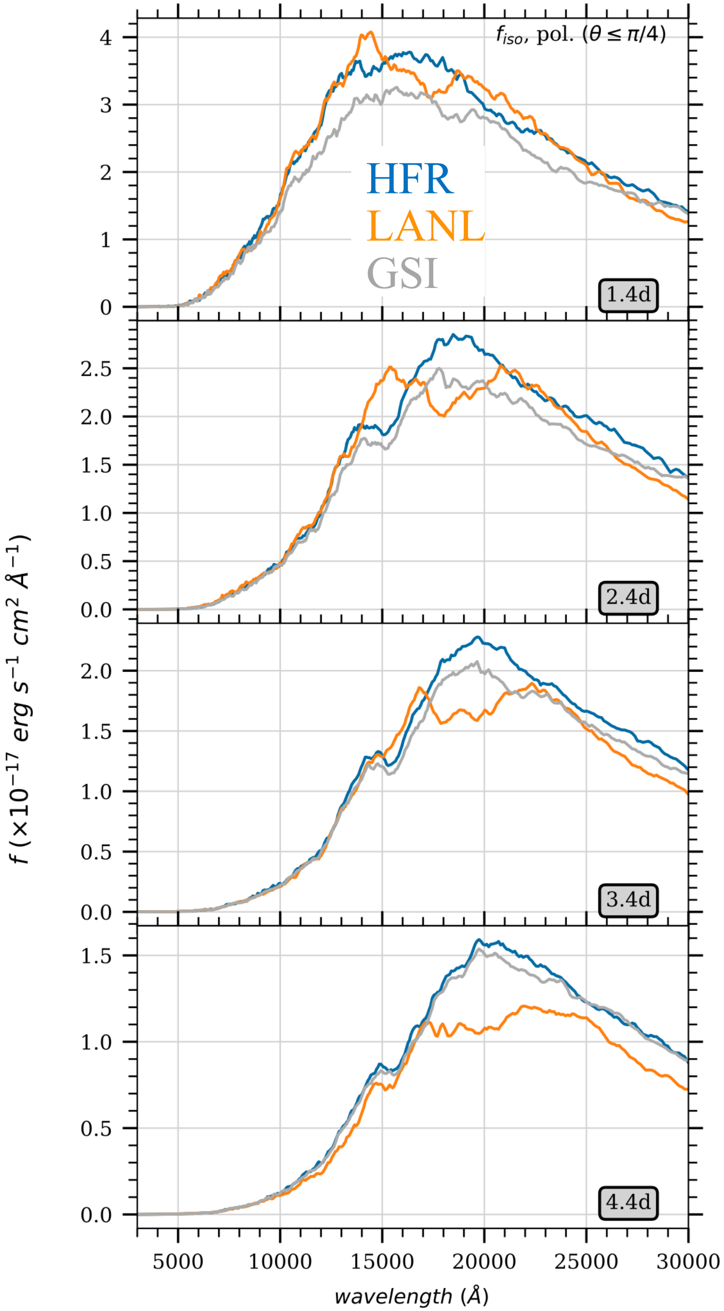
Gururaj Wagle

Sensitivity of the light curve and spectra w.r.t. opacity tables

Short-lived collapse: 1.20 – 1.60 M_{o}





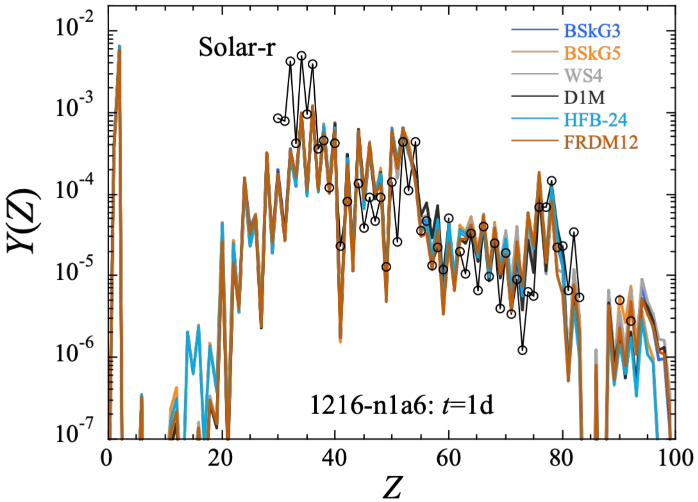


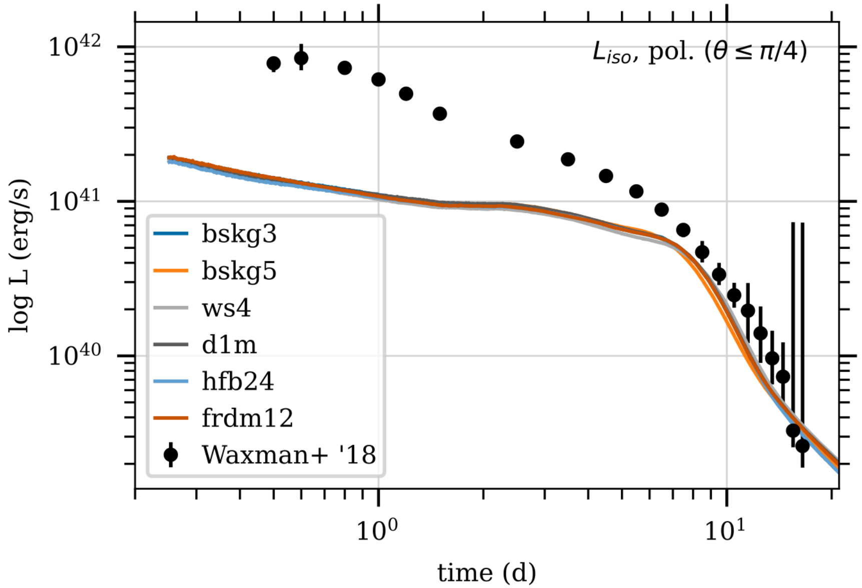
Relatively similar light curves but rather different spectral distributions

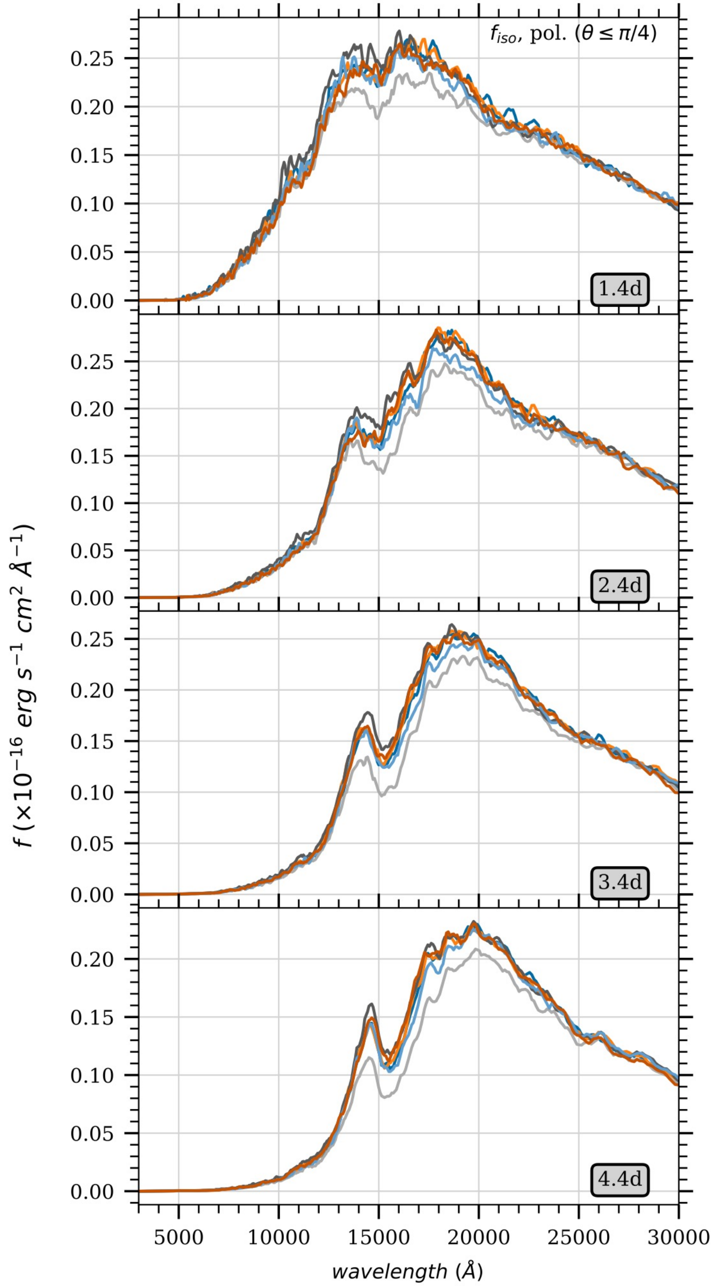
Gururaj Wagle

Propagation of mass model uncertainties to the light curve and spectra

Short-lived collapse: 1.20 – 1.60 M_o







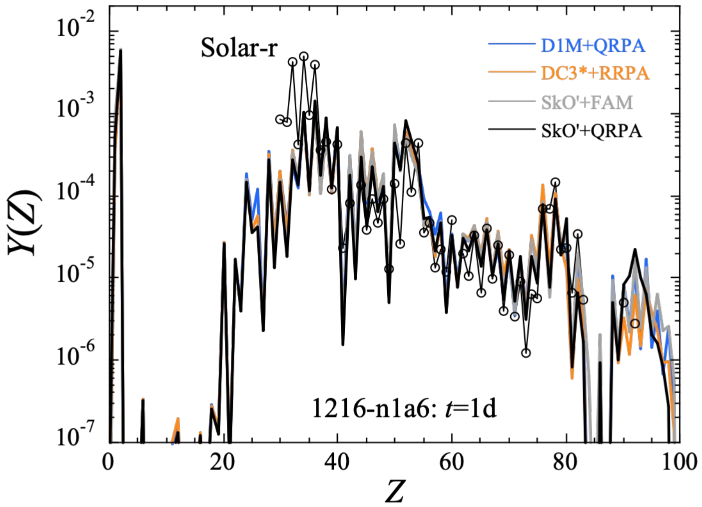
Relatively similar light curves and spectral distributions

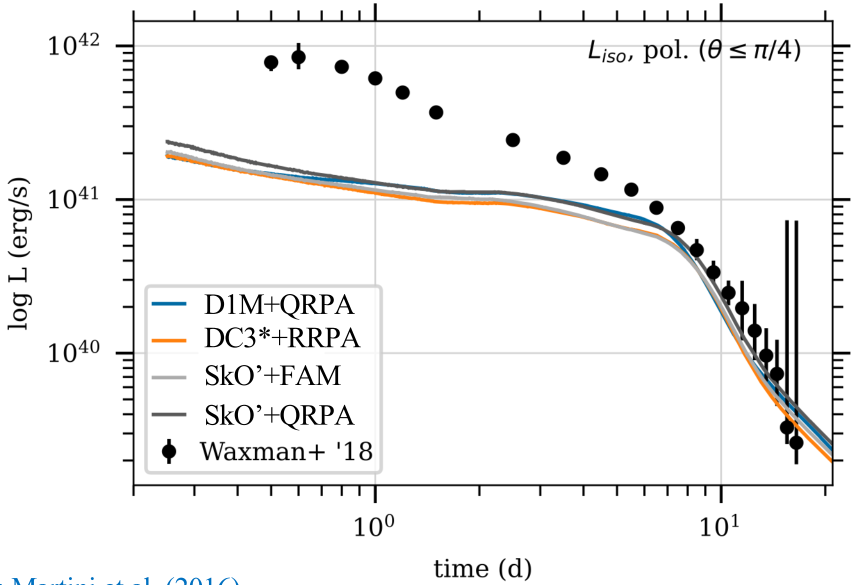
(except for WS4 mass model)

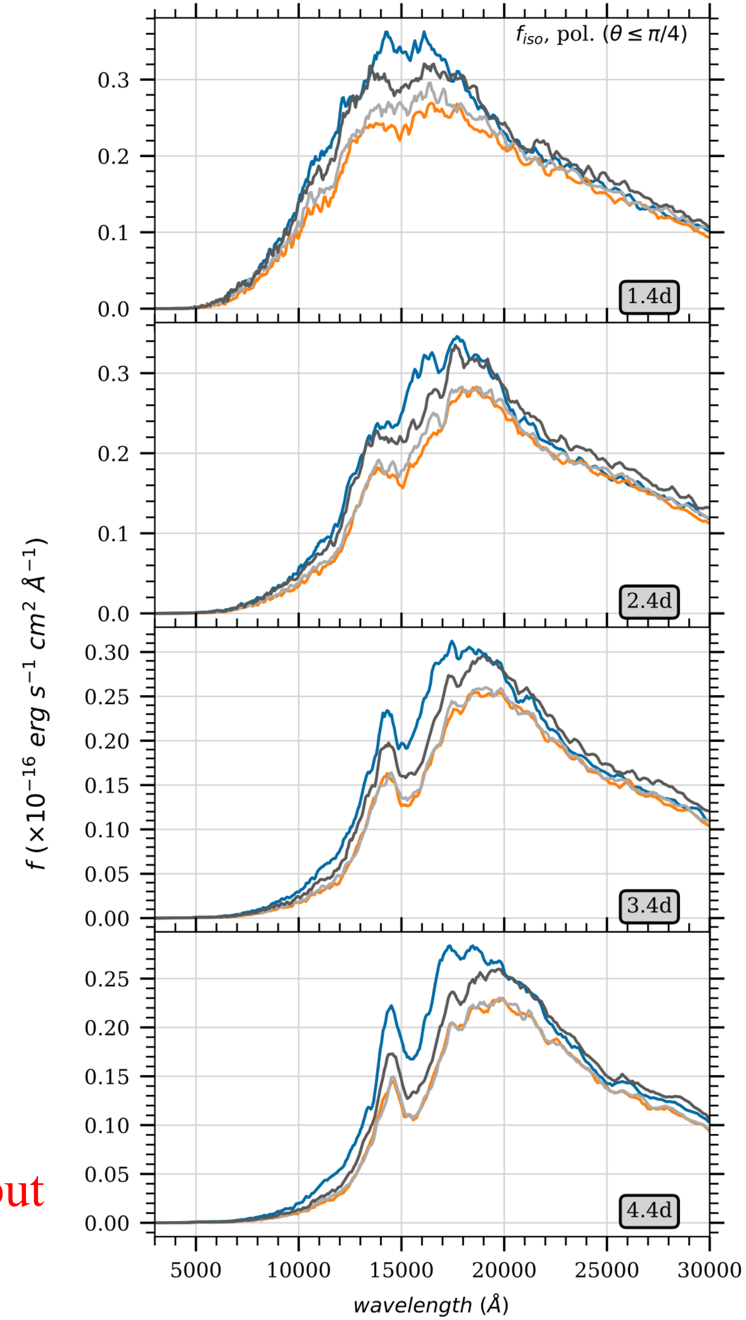
Gururaj Wagle

Propagation of β-decay model uncertainties to the light curve and spectra

Short-lived collapse: 1.20 – 1.60 $M_{\odot}$







D1M+QRPA : Martini et al. (2016)

DC3*+RRPA: Marketin et al. (2016)

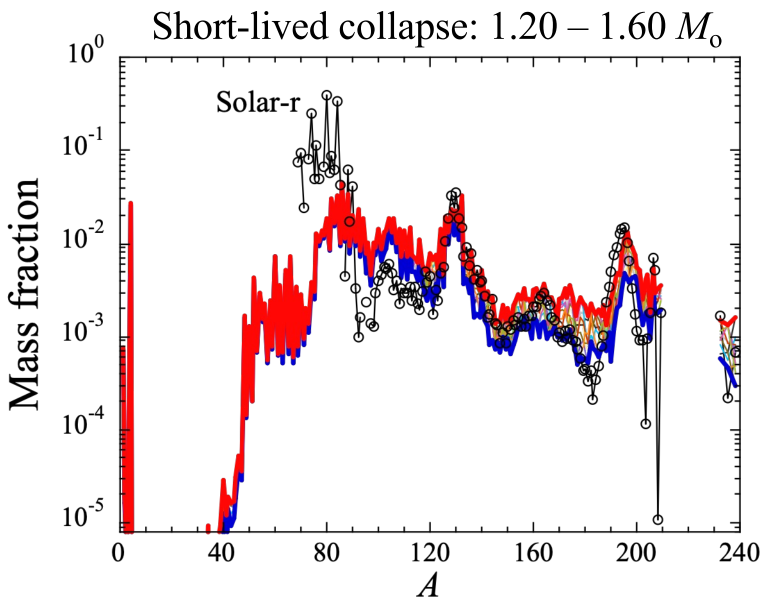
SkO'+FAM: Ney et al. (2020)

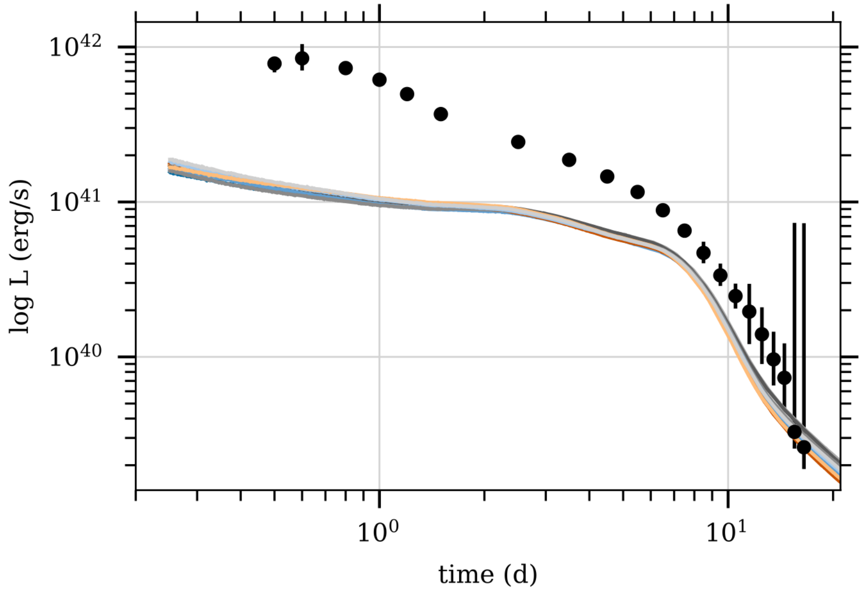
SkO'+QRPA: Minato et al. (2022)

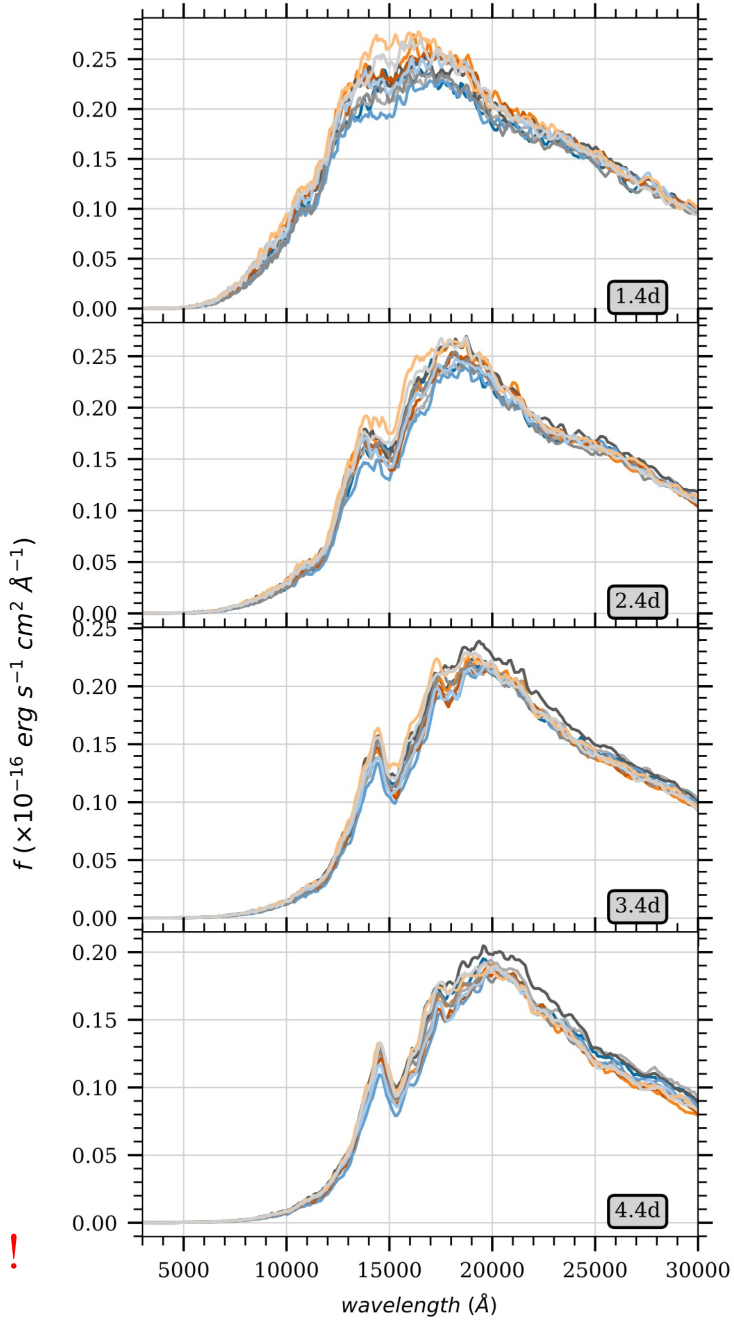
Relatively similar light curves but
≠ spectral distributions

Gururaj Wagle

Propagation of OMP uncertainties to the light curve and spectra







Relatively similar light curves but ≠ spectral distributions !

THANK YOU
FOR
YOUR ATTENTION