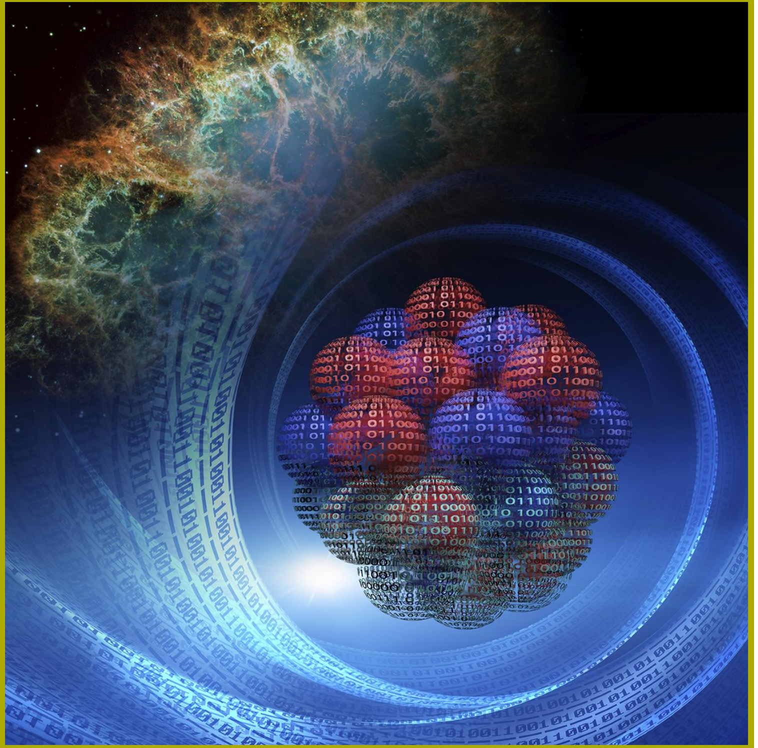
WOUTER RYSSENS



Andy Sproles, ORNL

Towards..

A global view of nuclear structure

W. Ryssens

19th of March 2025

wryssens.com

wryssens@ulb.be

BLU-ULB BRUSSELS LABORATORY OF THE UNIVERSE

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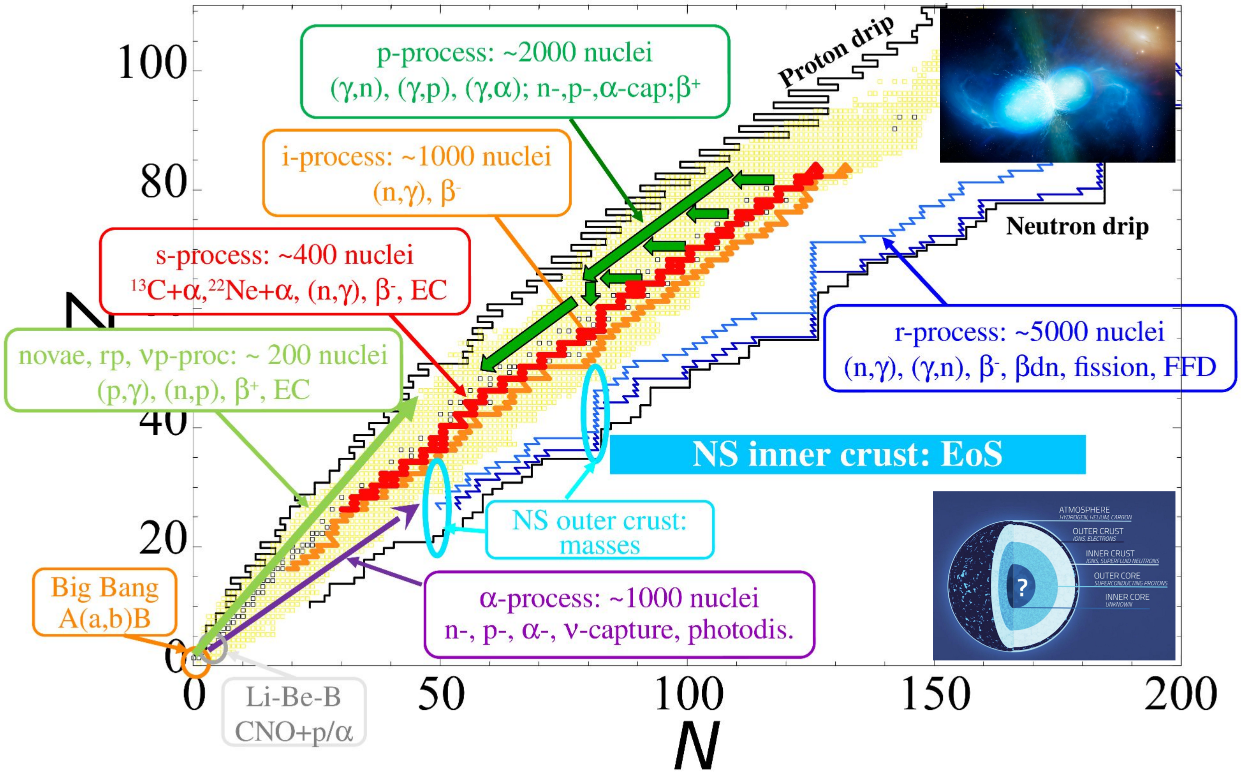
A small clarification...

A small clarification...

Introduction



Skyrme **E**nergy **D**ensity **F**unctionals (**EDF**s)

$$E \sim \int d^3r \left[C^\rho \rho(\mathbf{r})\rho(\mathbf{r}) + C^\tau \tau(\mathbf{r})\rho(\mathbf{r}) + \dots \right]$$

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Local densities and currents of a wavefunction

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Coupling constants (~ **25** parameters) fitted to data

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2. more (pseudo-) observables simultaneously
   “more” = both **<u>scale</u>** and **<u>diversity</u>**!

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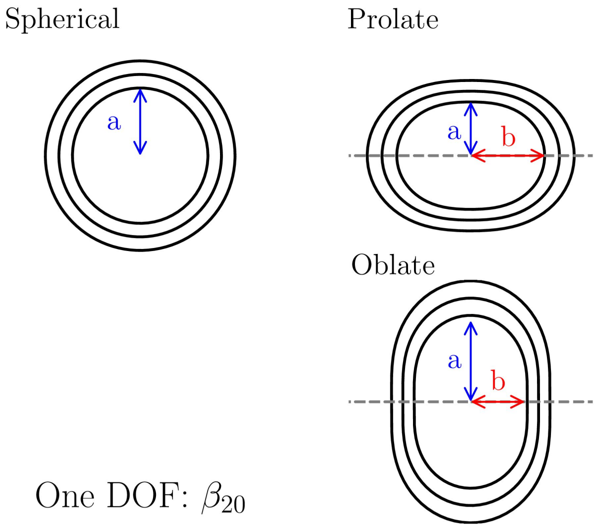
Local densities and currents of a wavefunction

Progress?

1. more physics in the wavefunction
2. more (pseudo-) observables simultaneously
   "more" = both **scale** and **diversity**!
3. search for a "better" EDF form

Large-scale models in 1-2 dimensions

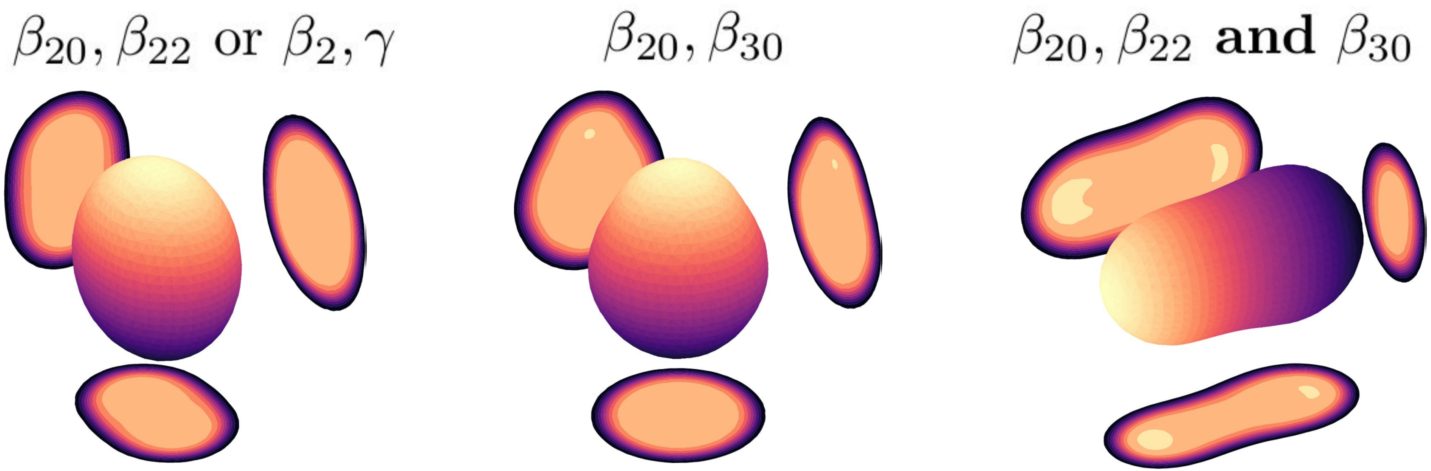


One DOF: β_{20}

Nuclear deformation

- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
- intuitive interpretation

Large-scale models in 1-2-3 dimensions



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More general configurations

- triaxial shapes
- reflection asymmetry
- elongated shapes

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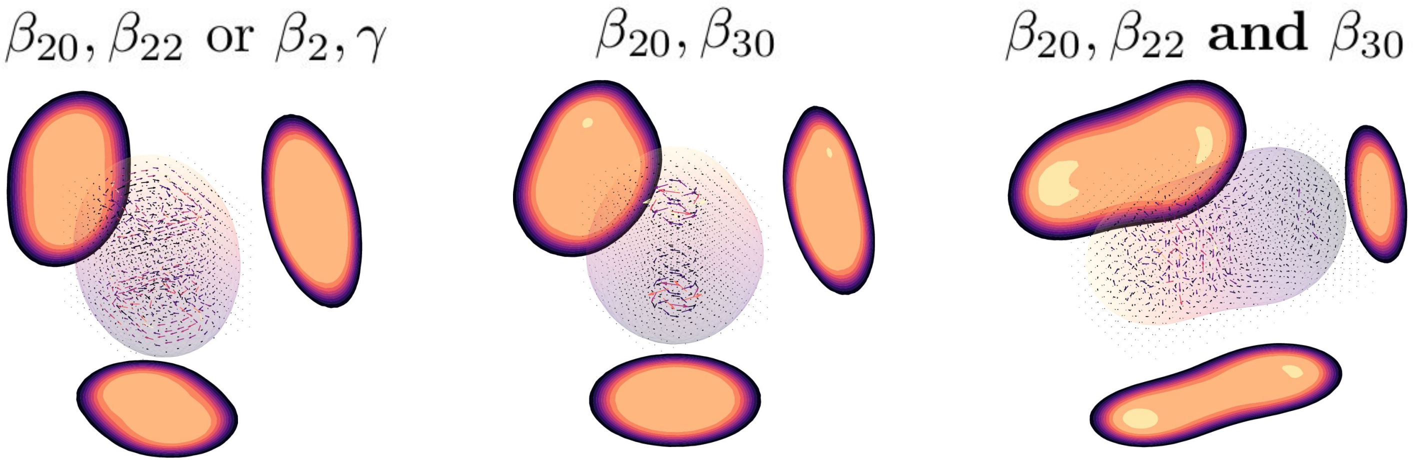

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More general configurations

- triaxial shapes
- reflection asymmetry
- elongated shapes
- spin densities and currents

Brussels-**Sk**yrme-on-a-**G**rid: BSkG

BSkG1: G. Scamps et al., EPJA **57**, 333 (2021).
BSkG2: W. Ryssens et al., EPJA **58**, 246 (2022).
W. Ryssens et al., EPJA **59**, 96 (2023).
BSkG3: G. Grams et al., EPJA **59**, 270 (2023).
BSkG4: G. Grams et al., arXiv:2411.08007 (2024).

BSkG1

- fitted to 2457 masses
- fitted to 884 charge radii
- includes triaxial deformation

Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741			
S_n [MeV]	0.466			
Radii [fm]	0.024			
Prim. barriers [MeV]				
Sec. barriers [MeV]				
Fission isomers [MeV]				
Max. NS mass [$M_\odot$]				

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Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741	0.678		
S_n [MeV]	0.466	0.500		
Radii [fm]	0.024	0.027		
Prim. barriers [MeV]	0.88	0.44		
Sec. barriers [MeV]	0.87	0.47		
Fission isomers [MeV]	1.0	0.49		
Max. NS mass [$M_\odot$]				

BSkG2

- <u>complete</u> time-reversal breaking
- fit to 45 reference fission barriers
  + 28 fission isomers

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Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741	0.678	0.631	
S_n [MeV]	0.466	0.500	0.442	
Radii [fm]	0.024	0.027	0.024	
Prim. barriers [MeV]	0.88	0.44	0.33	
Sec. barriers [MeV]	0.87	0.47	0.51	
Fission isomers [MeV]	1.0	0.49	0.34	
Max. NS mass [$M_\odot$]	1.8	1.8	2.3	

BSkG2

- <u>**complete**</u> time-reversal breaking
- fit to 45 reference fission barriers
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BSkG3

- extended Skyrme EDF form
- supports massive neutron stars

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BSkG3: G. Grams et al., EPJA **59**, 270 (2023).
BSkG4: G. Grams et al., EPJA **61,** 35 (2024).

BSkG1

- fitted to 2457 masses
- fitted to 884 charge radii
- includes triaxial deformation

BSkG4

- pairing reproduces advanced INM calculations
- ideal for TD simulations in NS crust

Rms σ	BSkG1	BSkG2	BSkG3	BSkG4
Masses [MeV]	0.741	0.678	0.631	0.633
S_n [MeV]	0.466	0.500	0.442	0.402
Radii [fm]	0.024	0.027	0.024	0.025
Prim. barriers [MeV]	0.88	0.44	0.33	0.36
Sec. barriers [MeV]	0.87	0.47	0.51	0.53
Fission isomers [MeV]	1.0	0.49	0.34	0.33
Max. NS mass [$M_\odot$]	1.8	1.8	2.3	2.3

BSkG2

- <u>**complete**</u> time-reversal breaking
- fit to 45 reference fission barriers + 28 fission isomers

BSkG3

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G. Scamps et al., EPJA **57**, 333 (2021).
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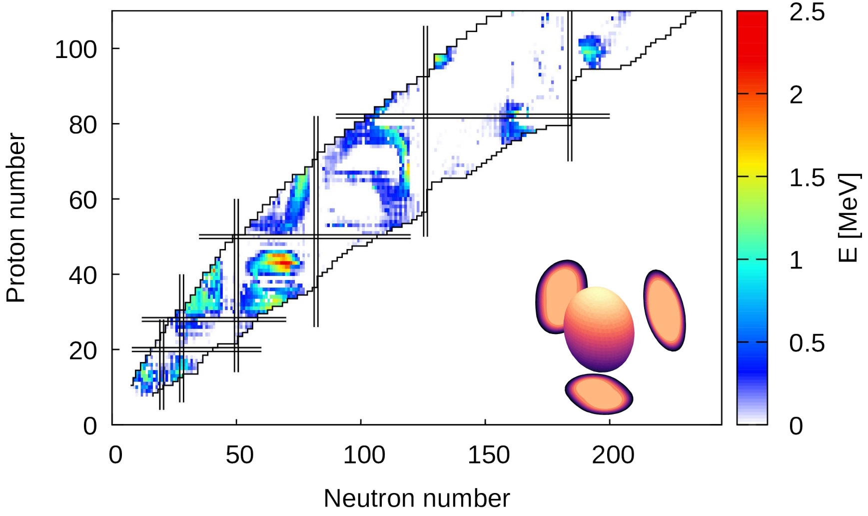

Triaxial deformation

- many nuclei are affected
- effects up to 2.5 MeV near Z~44

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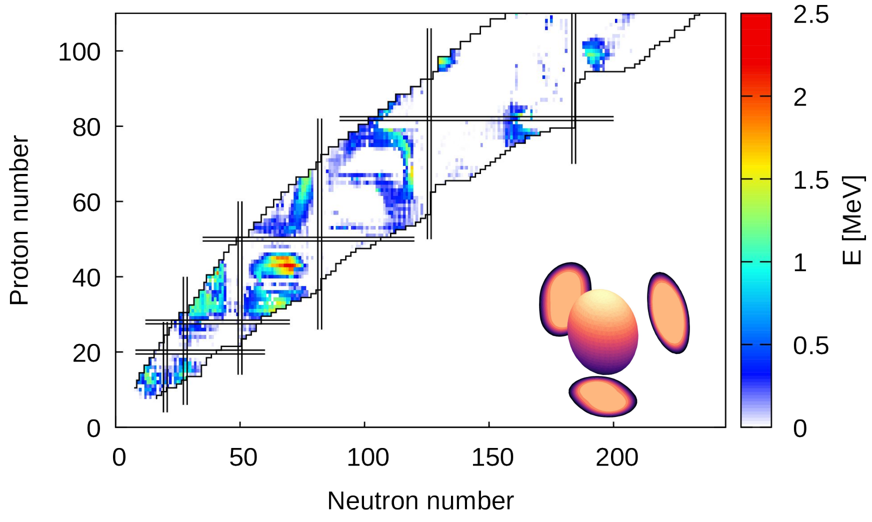
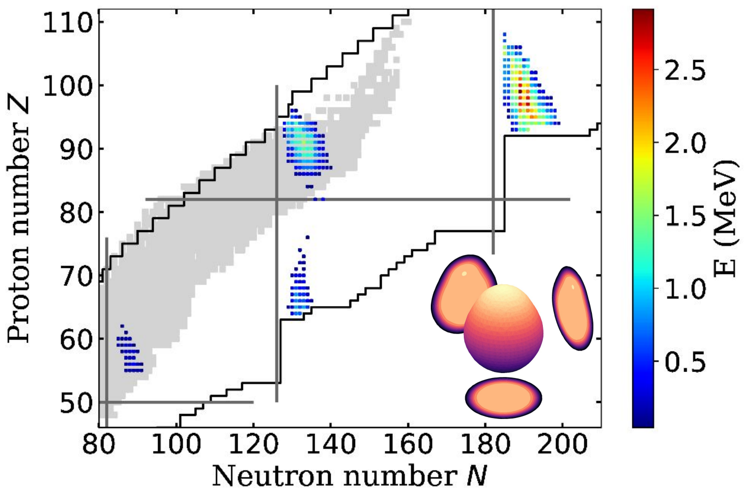




Triaxial deformation

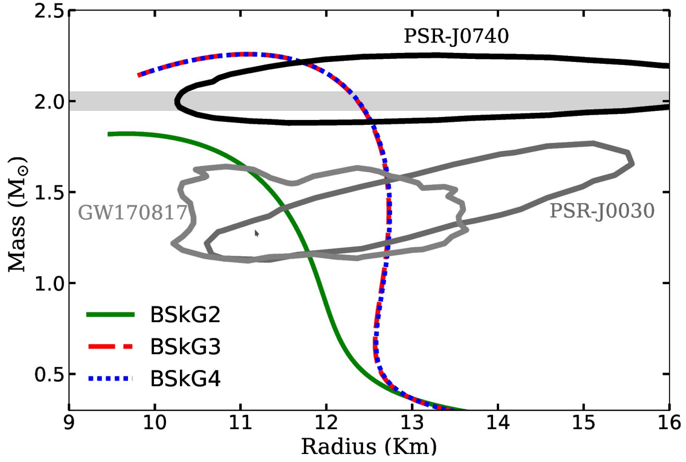
- many nuclei are affected
- effects up to 2.5 MeV near Z~44

Reflection asymmetry

- small number of known nuclei affected
- Near N=184:
  - large effect up to 2.5 MeV
  - dripline modified
  - fission properties modified

Neutron stars

G. Grams et al., EPJA **59**, 270 (2023).



Stiffer EoS

- results in higher maximum mass
- usually incompatible with masses

Neutron stars

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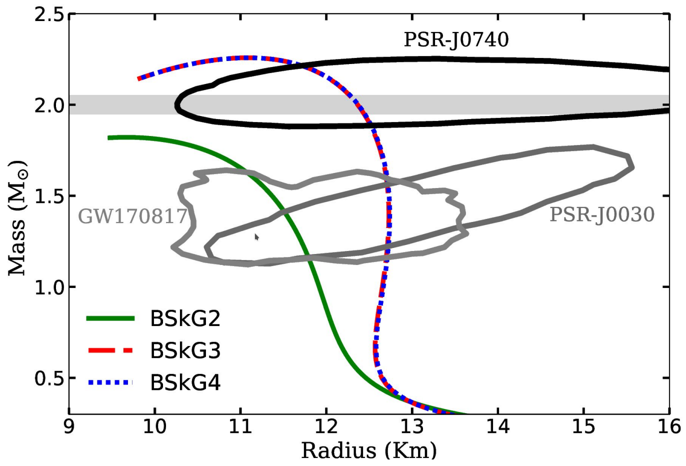


$$
\begin{aligned}
\mathcal{E}_{t,\mathrm{e}}(\mathbf{r}) = {} & C_t^{\rho\rho}(\rho_0)\,\rho_t^2(\mathbf{r}) + \boxed{C_t^{\rho\tau}(\rho_0)}\,\rho_t(\mathbf{r})\,\tau_t(\mathbf{r}) \\
& + C_t^{\rho\nabla J}\,\rho_t(\mathbf{r})\,\nabla\cdot\mathbf{J}_t(\mathbf{r}) \\
& + C_t^{\rho\Delta\rho}\,\rho_t(\mathbf{r})\,\Delta\rho_t(\mathbf{r}) \\
& + \boxed{C_t^{\nabla\rho\nabla\rho}(\rho_0)}\,\nabla\rho_t(\mathbf{r})\cdot\nabla\rho_t(\mathbf{r}) \\
& + \boxed{C_t^{\rho\nabla\rho\nabla\rho}(\rho_0)\,\rho_t(\mathbf{r})\nabla\rho_0(\mathbf{r})\cdot\nabla\rho_t(\mathbf{r})}
\end{aligned}
$$

Stiffer EoS

- results in higher maximum mass
- usually incompatible with masses

Extended density dependencies

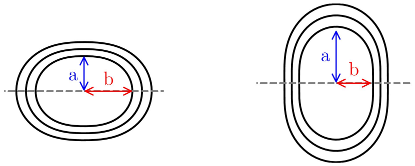
- originally to cure instabilities
- 6 additional parameters

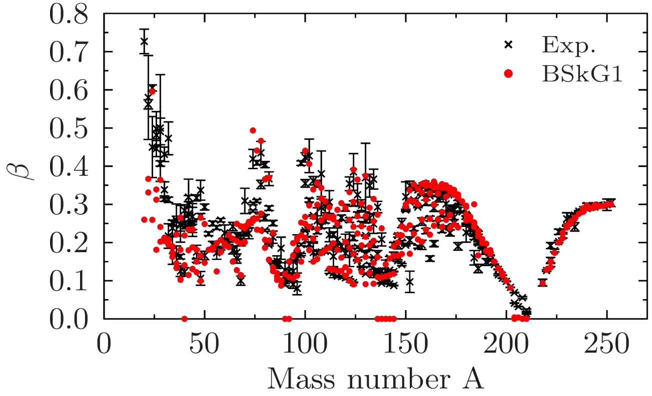
... two are fractional powers!

Deformations

G. Scamps et al., EPJA **57**, 333 (2021).
G. Grams et al., arXiv:2411.08007 (2024).
W.R. et al., Phys. Rev. Lett. **130**, 212302 (2024).

“Ordinary” quadrupole deformation





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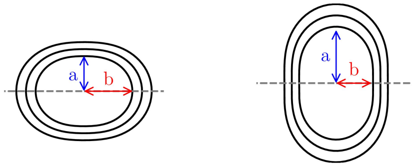
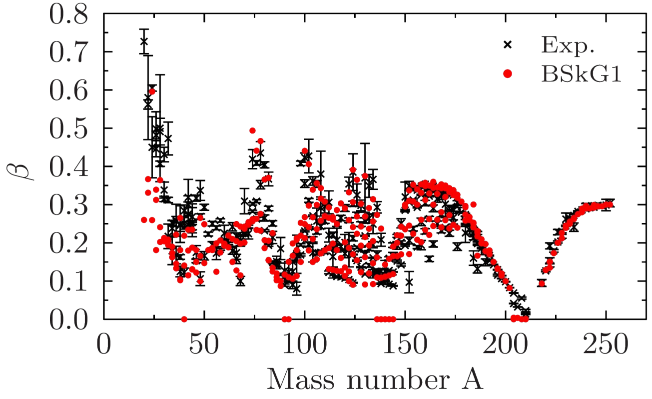
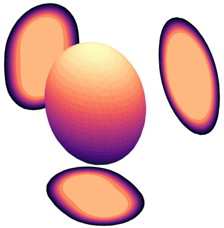
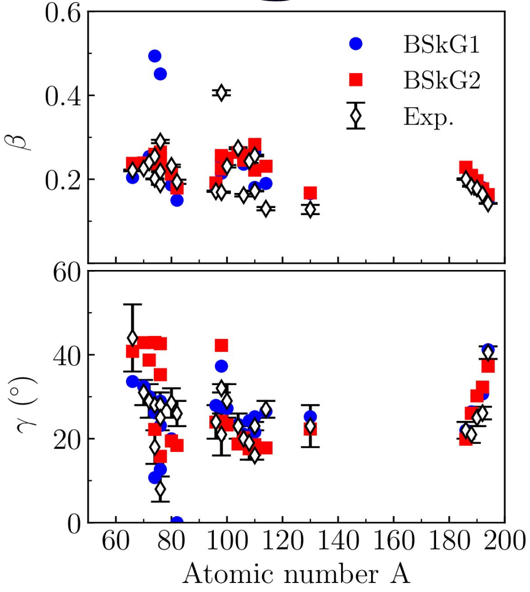




… and triaxial deformation …





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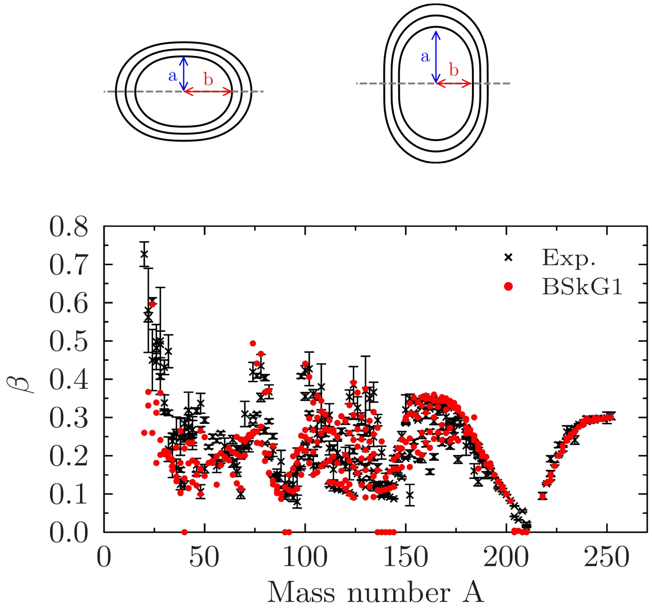

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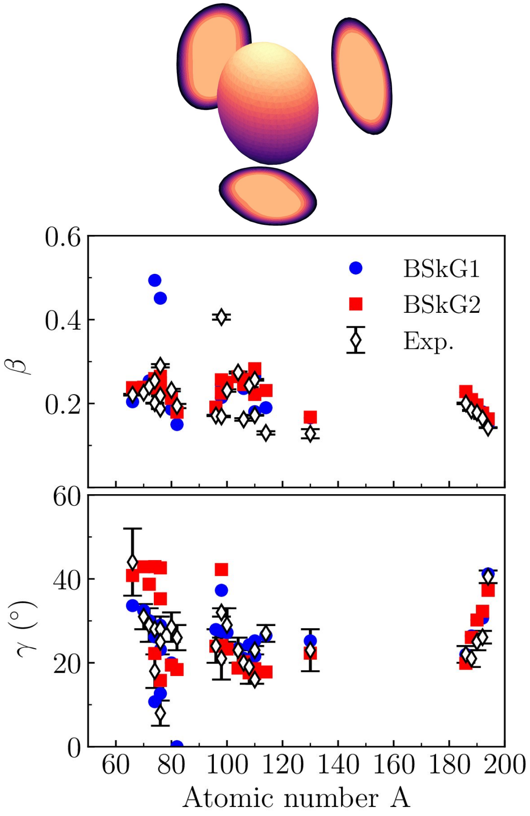
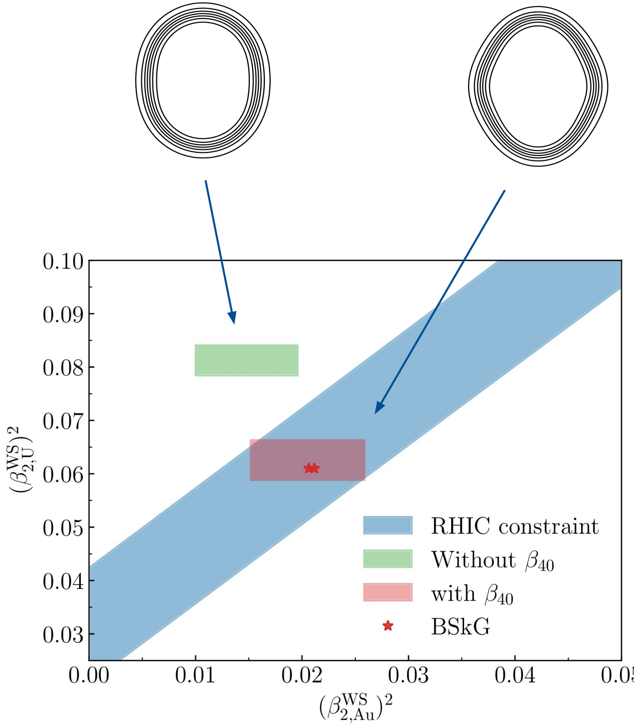


… and even hexadecapole!



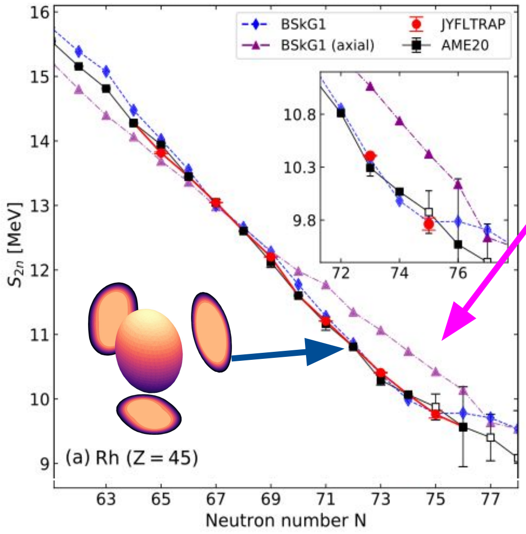
Z ~ 44

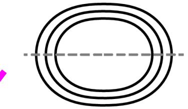
Known spectra indicate triaxial deformation

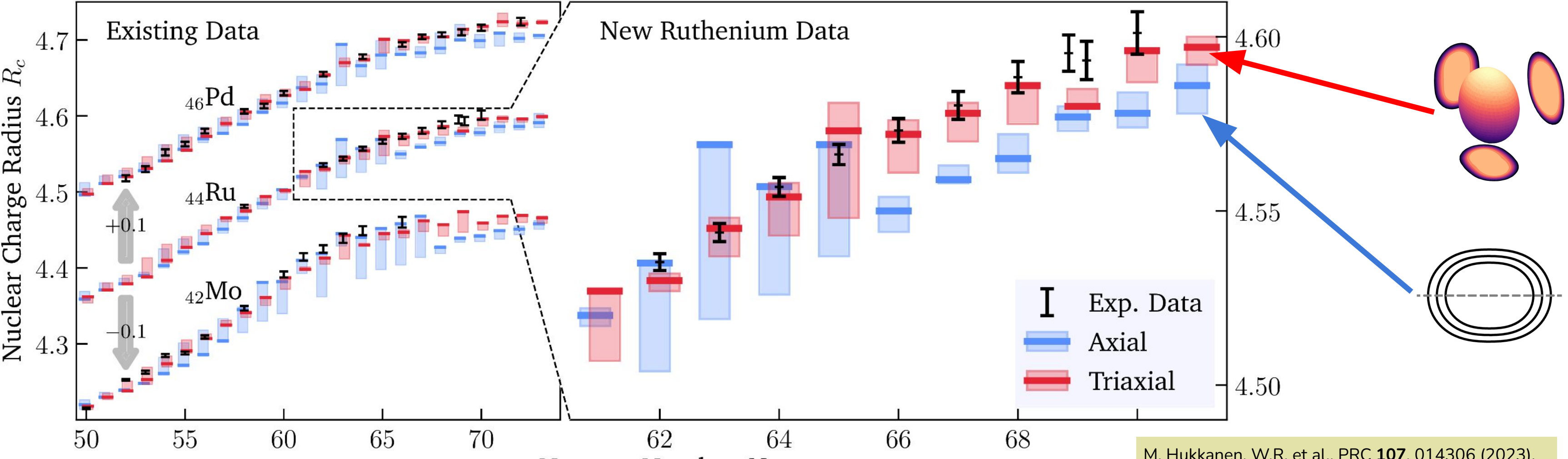
Triaxiality:

- impacts masses
- explains existence of isomers

M. Hukkanen, W.R. et al., PRC **107**, 014306 (2023).







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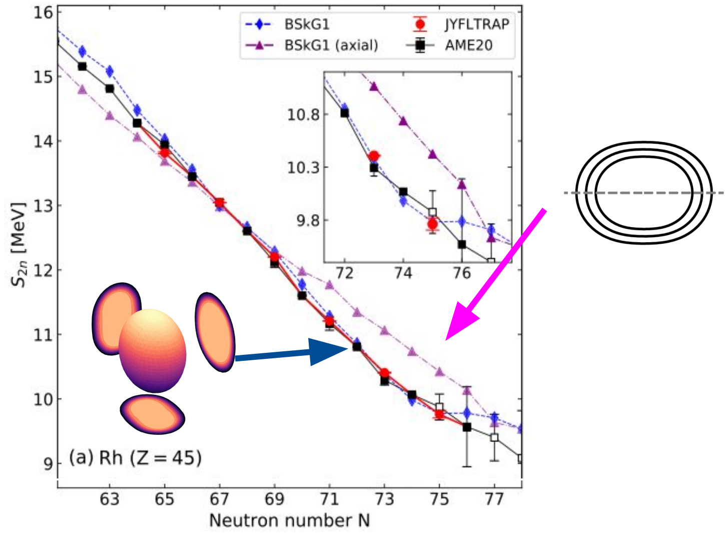

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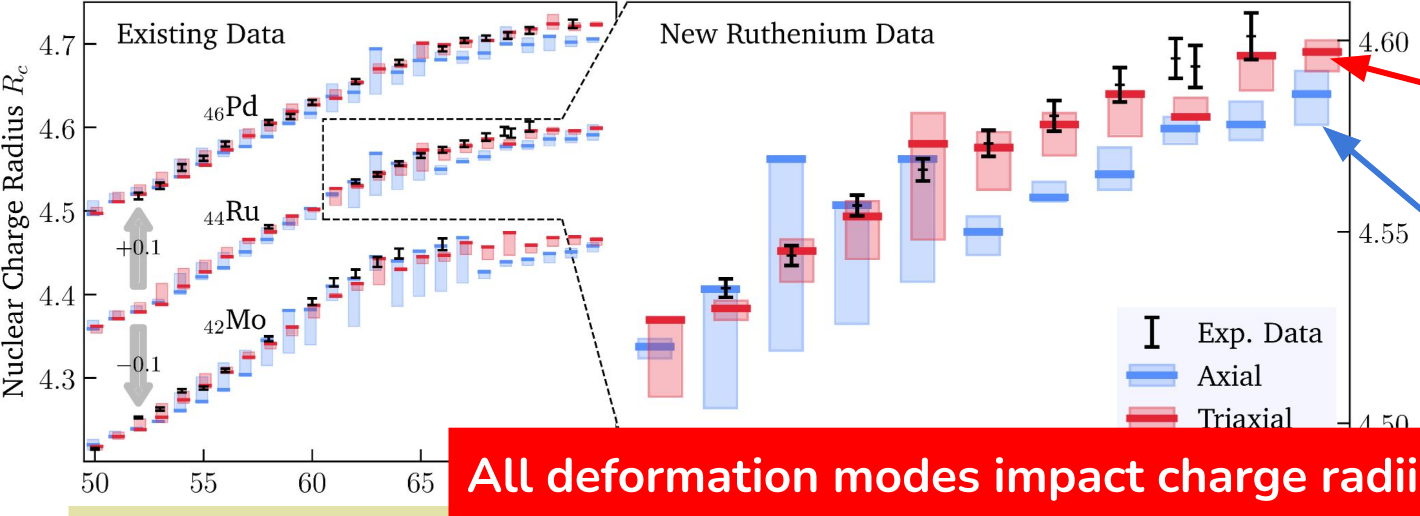
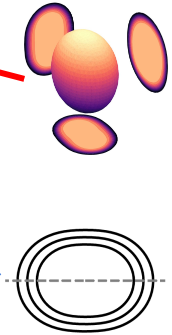
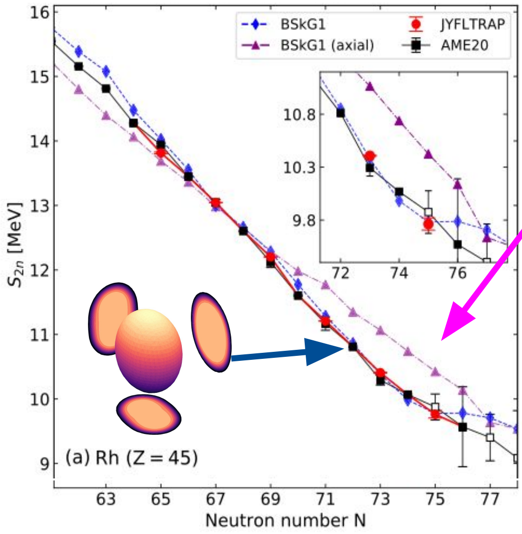


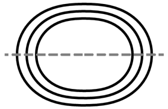
All deformation modes impact charge radii!

B. Maa□, W.R. et al., arXiv:2503.07841 (2025)

RC **107**, 014306 (2023).







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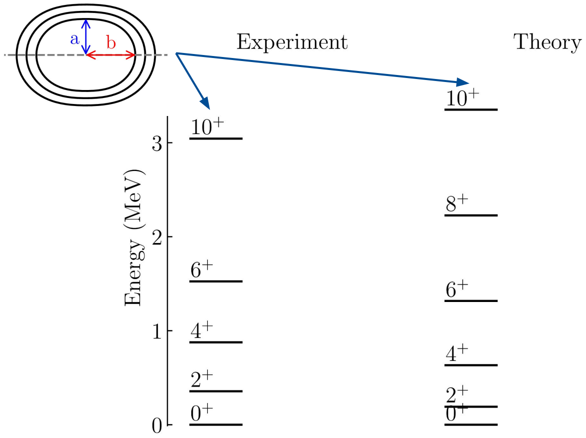
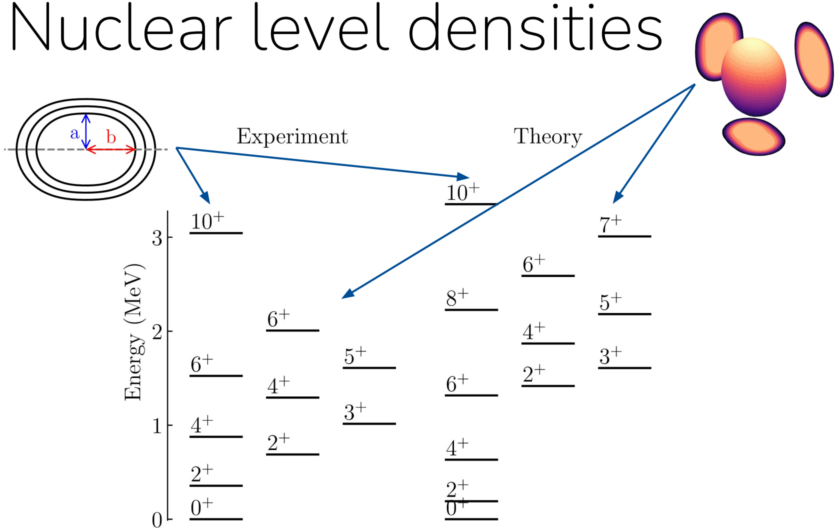
Nuclear level densities



Symmetries dictate NLDs

- larger collective enhancement

Nuclear level densities



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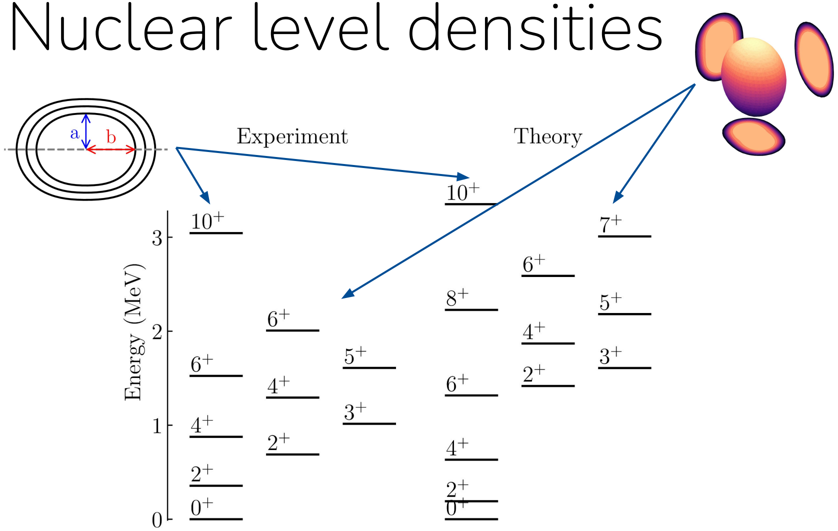
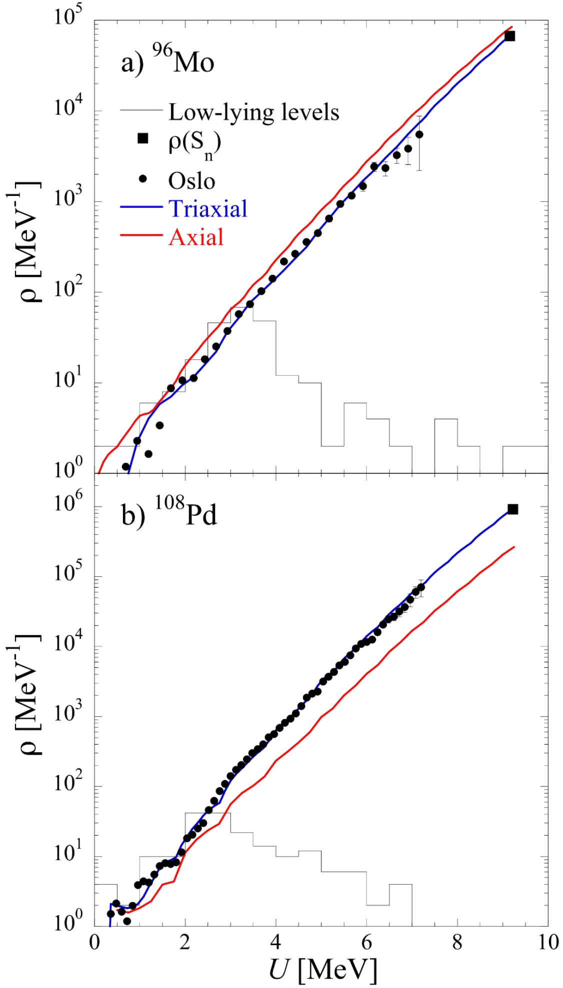


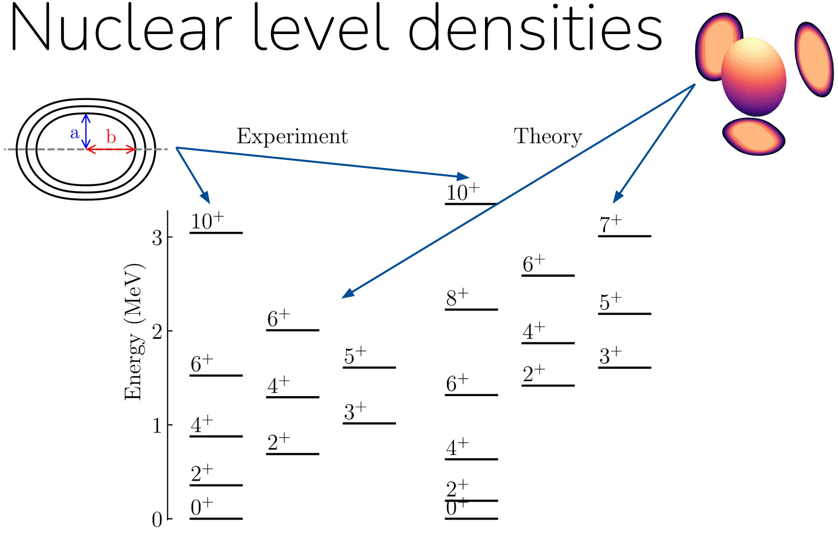


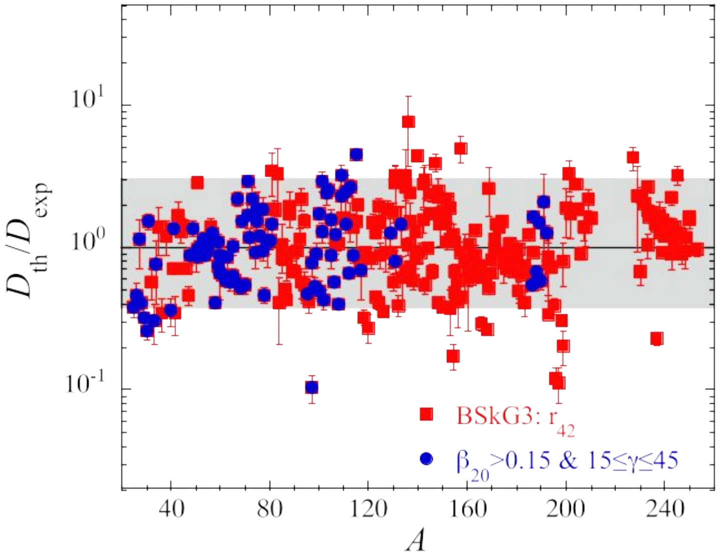
Symmetries dictate NLDs

- larger collective enhancement
- combinatorial calculation of NLDs
- … but the story is not so simple!

Nuclear level densities

S. Goriely et al., in preparation.





Symmetries dictate NLDs

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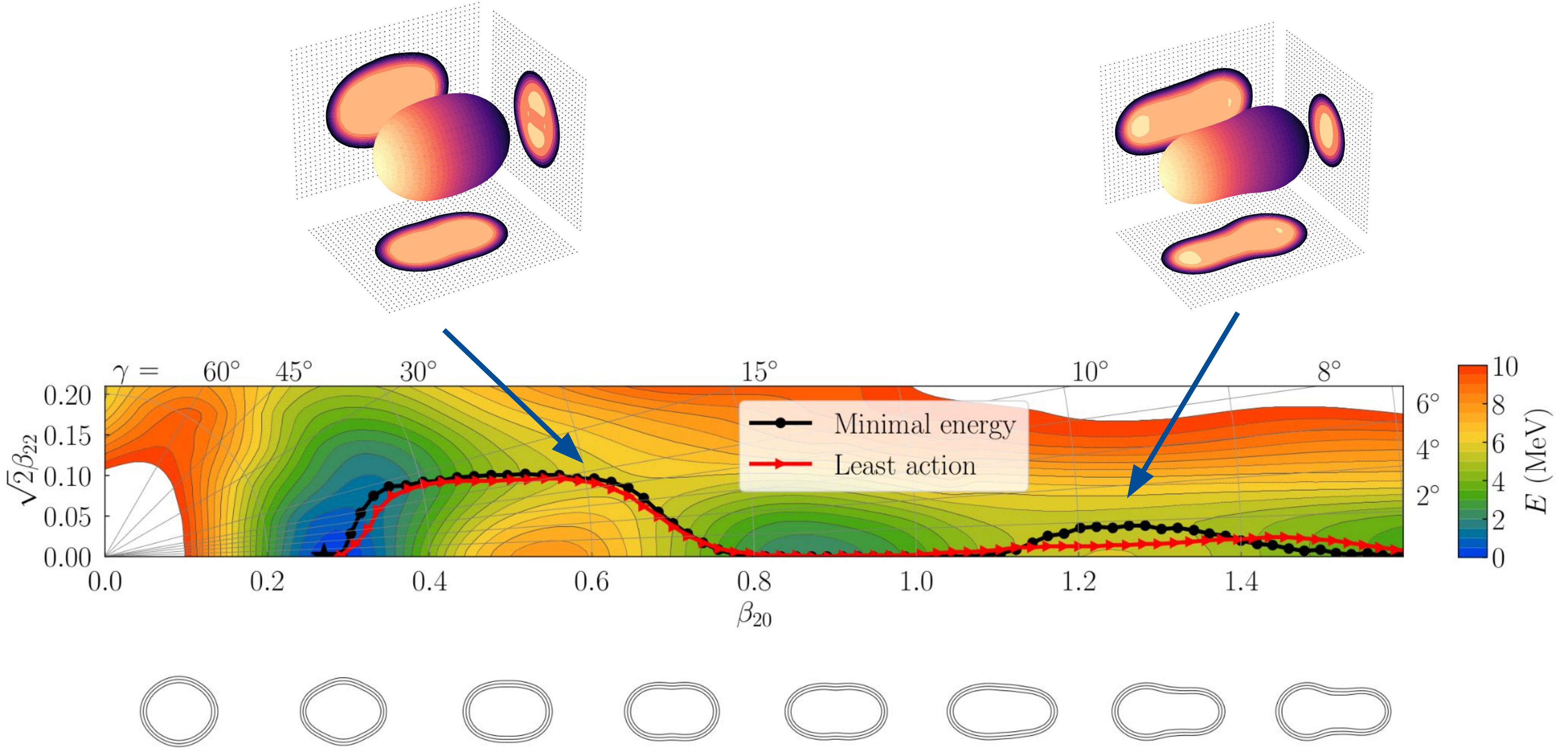
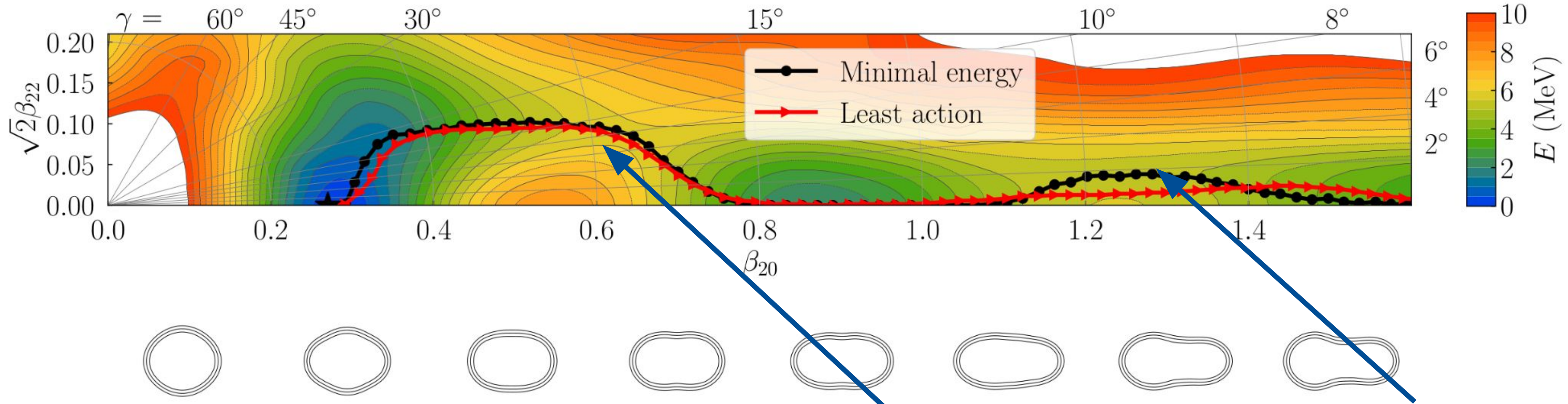
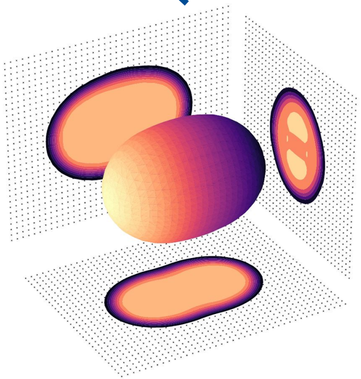
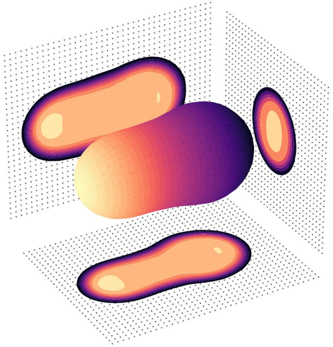
$$f_{\mathrm{rms}} = \exp\left[\frac{1}{N_e}\sum_i^{N_e}(\ln r_i)^2\right]^{1/2} = 1.96\,.$$



$\gamma =$ 60° 45° 30° 15° 10° 8°
$\sqrt{2}\beta_{22}$
0.20 0.15 0.10 0.05 0.00
6° 4° 2°
Minimal energy
Least action
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4
β_{20}
10 8 6 4 2 0
E (MeV)



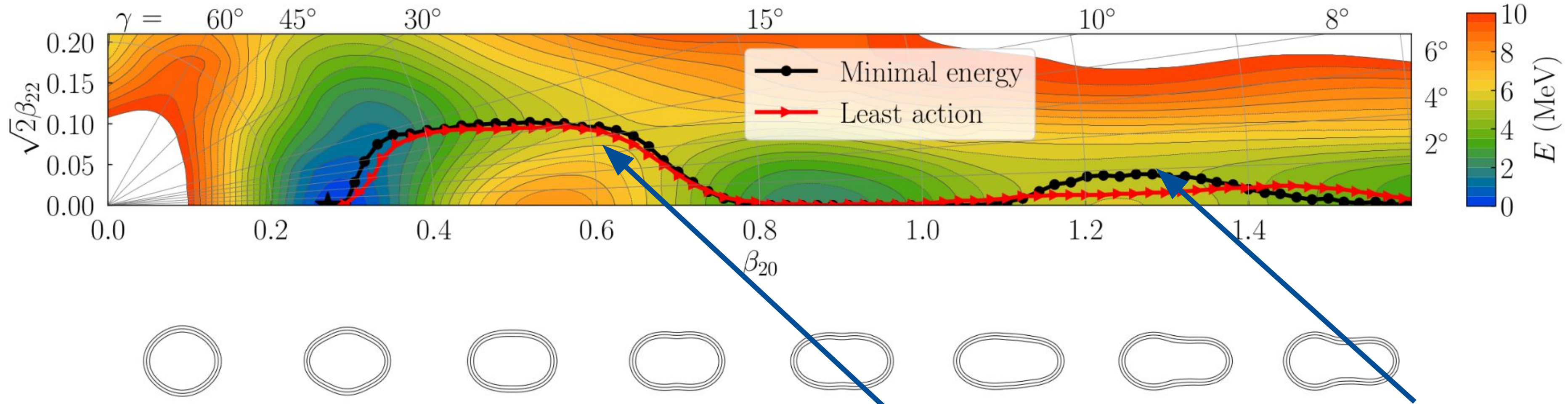


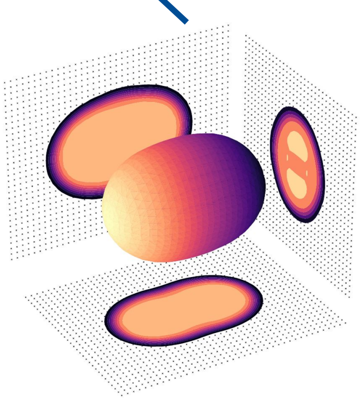


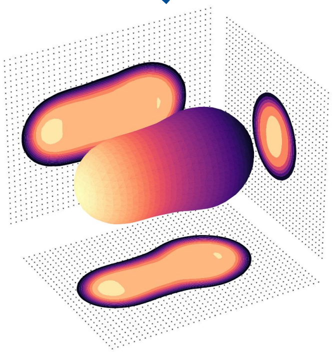
Fission barriers

- empirical barriers reproduced < 500 keV
- microscopic calculation of inertia

W. R. et al., EPJA **59**, 96 (2023).
S. Bara et al. & A. Sánchez-Fernández et al., in preparation.



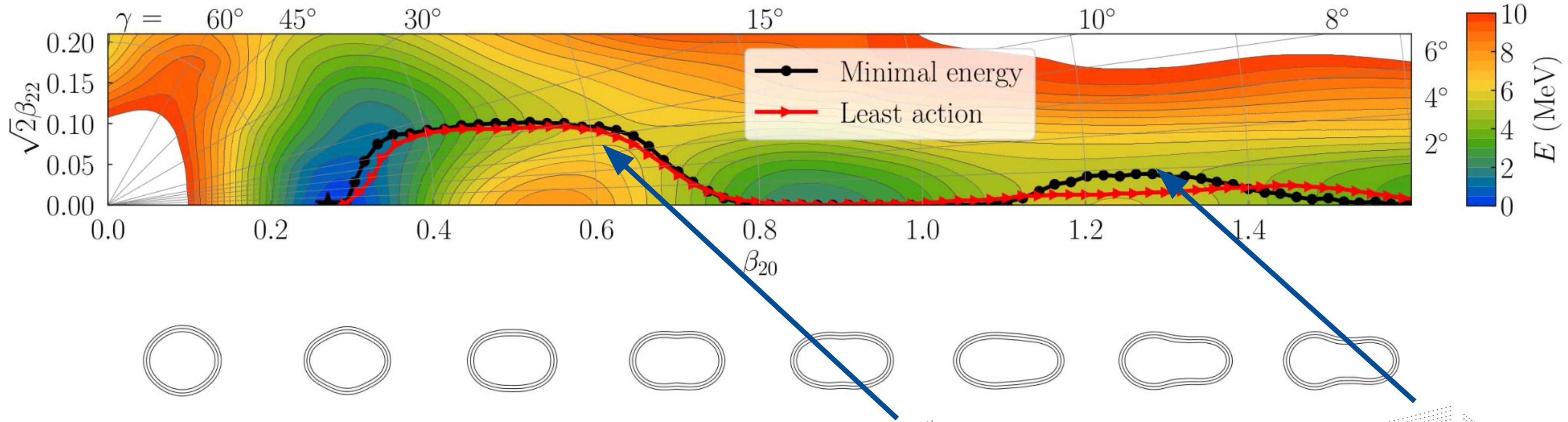


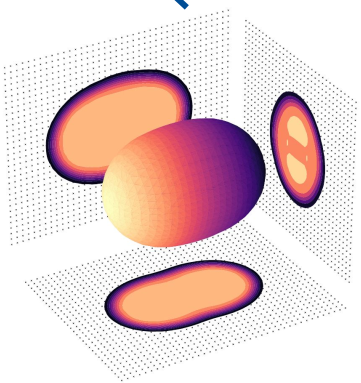


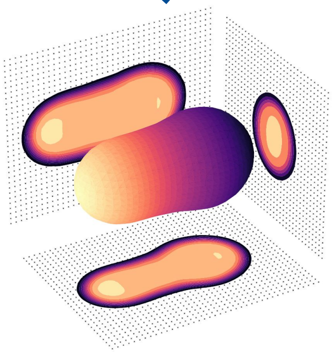
Fission barriers

- empirical barriers reproduced < 500 keV
- microscopic calculation of inertia
- β-delayed fission study underway

W. R. et al., EPJA **59**, 96 (2023).
S. Bara et al. & A. Sánchez-Fernández et al., in preparation.







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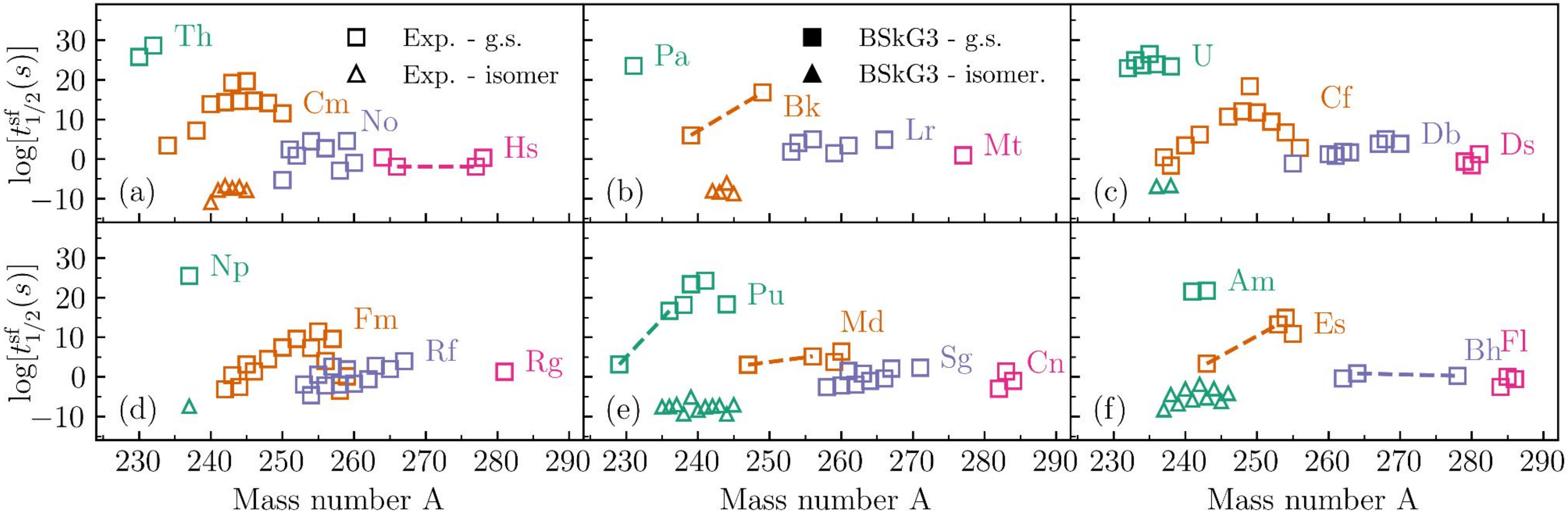
✅ 2700/3000 fission rates calculated

W. R. et al., EPJA **59**, 96 (2023).
S. Bara et al. & A. Sánchez-Fernández et al., in preparation.

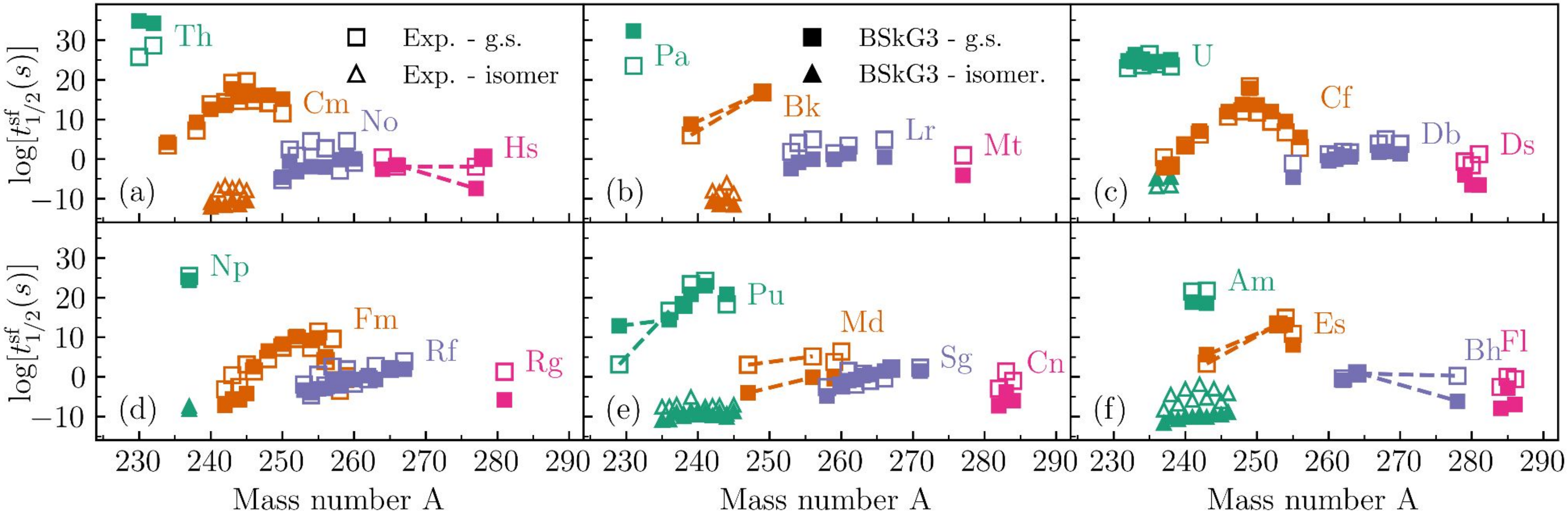


Spontaneous fission half-lives

Experimental data:

- 124 ground state half-lives
- 34 half-lives of isomeric states

… that span **> 40** orders of magnitude!



A. Sánchez-Fernández et al., submitted to PRL

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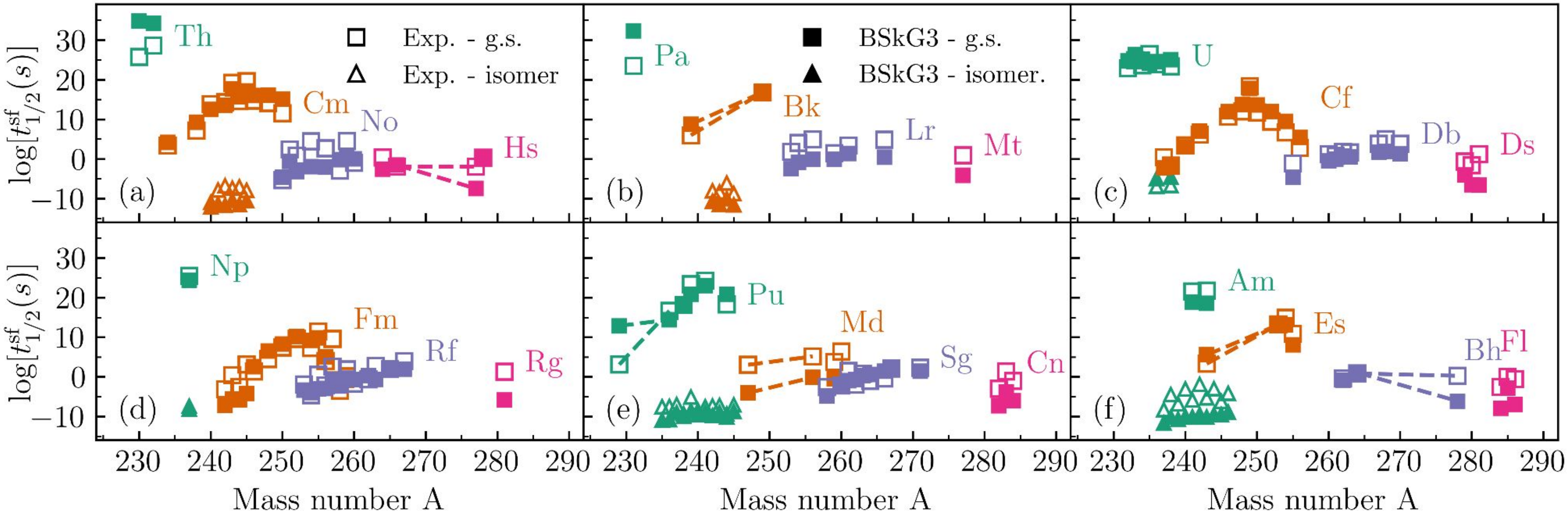
... at scale from microscopic models!

- comparable best mic-mac models
- ... without adjustable parameters!



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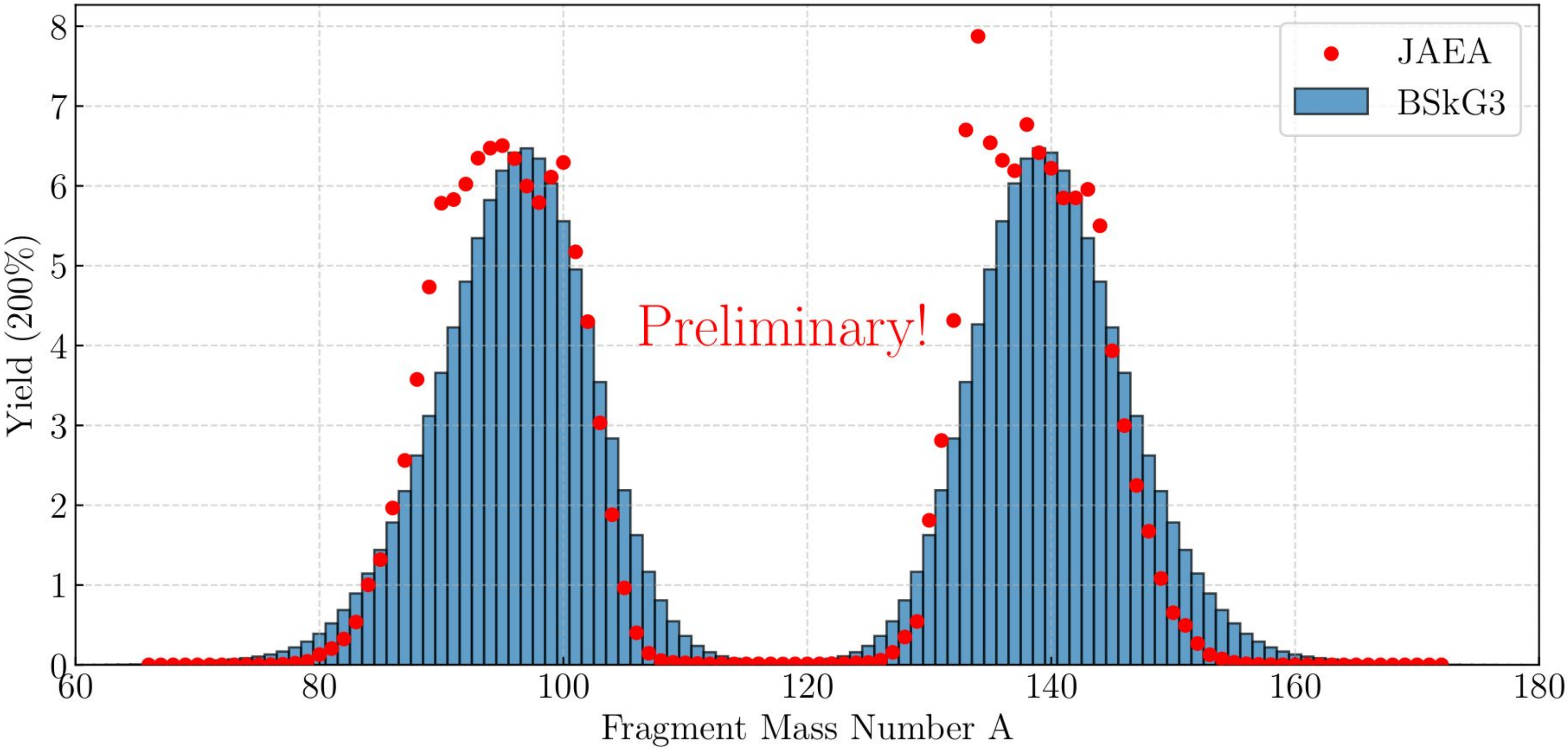
… that span > **40** orders of magnitude!

… at scale from microscopic models!

- comparable best mic-mac models
- … without adjustable parameters!
- also for BSkG2/4/5
- half-lives in the model adjustment

Fission fragments coming up!

A. Sánchez-Fernández et al., in preparation.



Investment in computing

MOCCa

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Density functional theory with MOCCa

- algorithms for speed and robustness
- algorithms for EDF implementation
- open-source in 2026

Investment in computing

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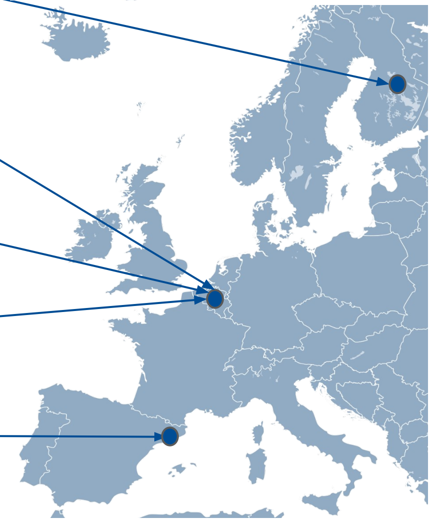
      '.___.'
```

EuroHPC Joint Undertaking

VLAAMS SUPERCOMPUTER CENTRUM — Vlaanderen is supercomputing

CÉCI

Cenaero



Density functional theory with MOCCa

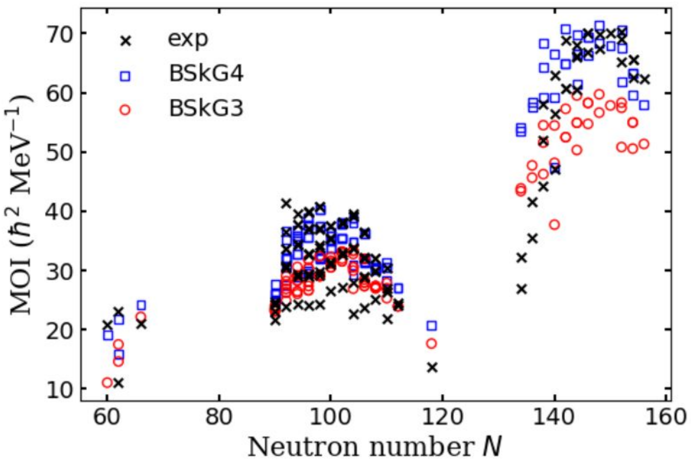
- algorithms for speed and robustness
- algorithms for EDF implementation
- open-source in 2026
- MOCCa school v0 done!

Raw computing power

- CÉCI & VSC: academic support in Belgium
- TIER-1 resources by Cenaero
    - Lucia - ranked 388th - our development workhorse
- TIER-0 resources by EuroHPC
    - MN 5 - ranked 11th - large scale fission
    - LUMI - ranked 8th - nuclear pasta

The future

Future stops: rotational properties

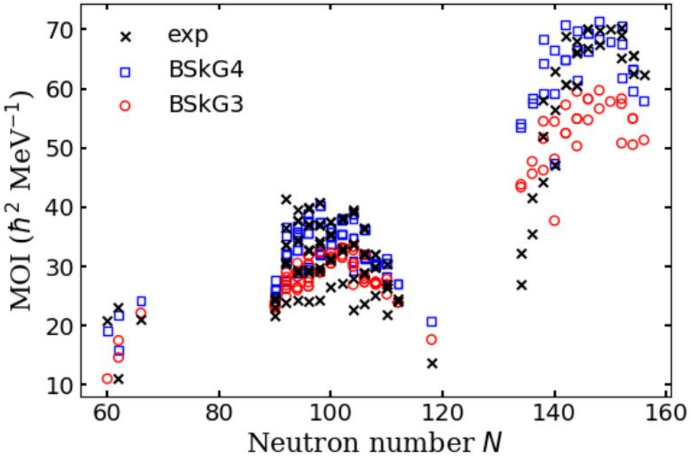


Moments of inertia

- calculated through explicit cranking (rotational bands also accessible!)

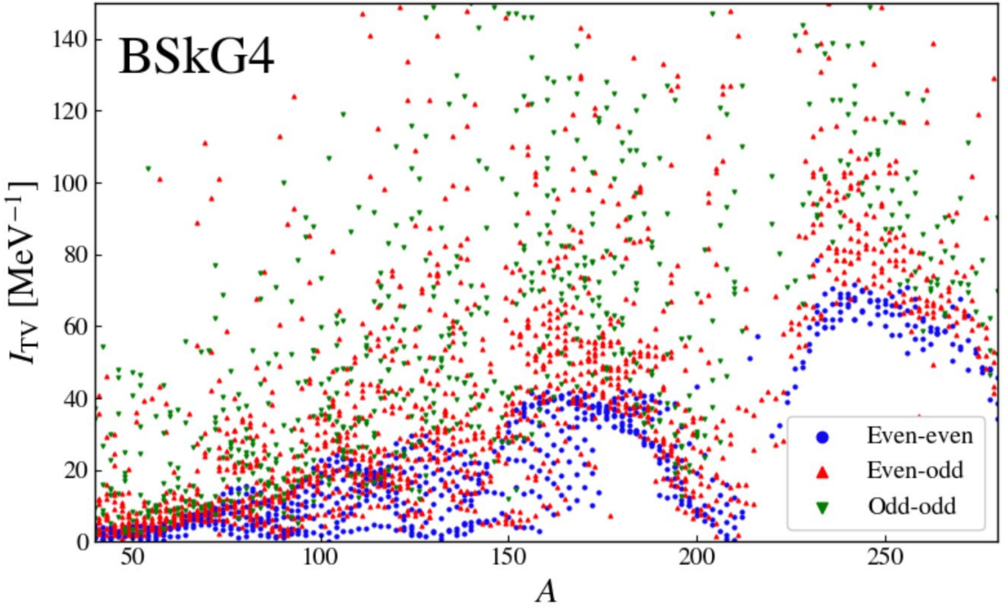
Future stops: rotational properties

L. Gonzales-Miret et al., in preparation



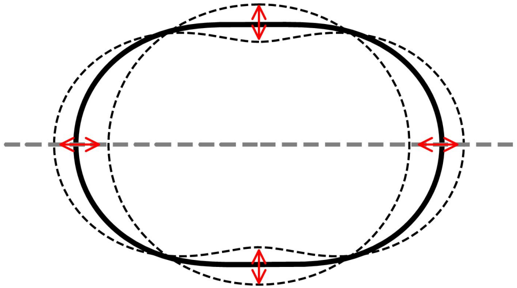
Moments of inertia

- calculated through explicit cranking (rotational bands also accessible!)
- .... also of odd-mass and odd-odd nuclei!
- sensitive to time-odd terms and pairing
- characterizes spurious collective motion
- ... and will impact masses!



Future stops: FAM-QRPA

P. Demol et al., in preparation



Linear response

- FAM algorithm for scaling
- symmetry-breaking
- extended EDFs

Future stops: FAM-QRPA

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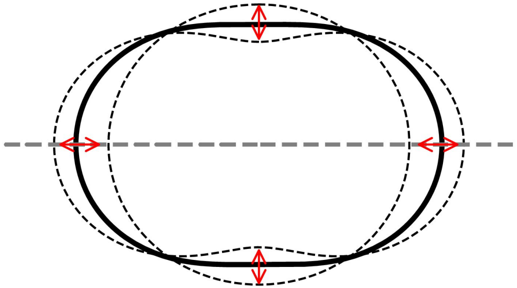

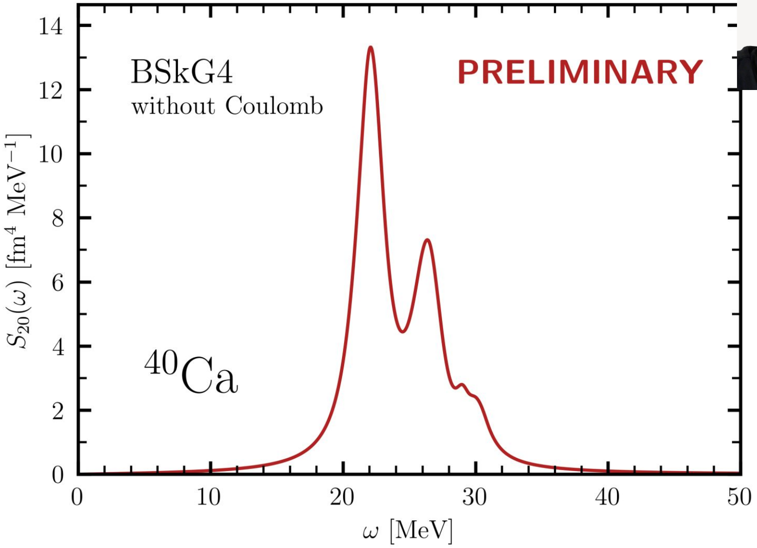

Linear response

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Electroweak strength functions

- photon capture/dissociation rates
- radiative neutron capture rates
- β-decay rates

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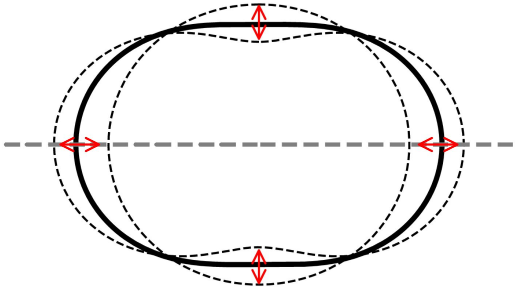

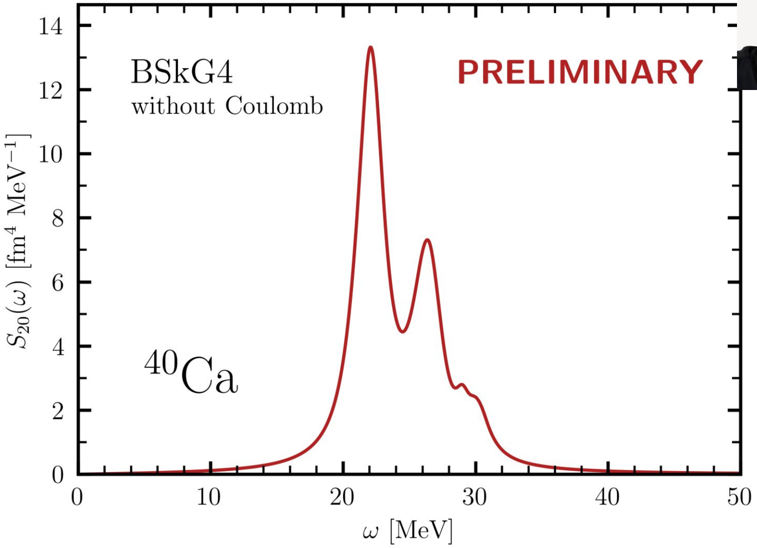

Linear response

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- photon capture/dissociation rates
- radiative neutron capture rates
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- ❗ feedback into model adjustment

BSkG5

G. Grams et al., in preparation.

$$
\begin{aligned}
\mathcal{E}^{(0)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1} \left[A^{(0,1)}_{\mathrm{t,e}} \left(D^{1,1}_t\right)^2 + A^{(0,2)}_{\mathrm{t,e}} \left(D^{1,1}_0\right)^\alpha \left(D^{1,1}_t\right)^2 \right], \\
\mathcal{E}^{(2)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1} \left[A^{(2,1)}_{\mathrm{t,e}} D^{1,1}_t \left(\Delta D^{1,1}_t\right) + A^{(2,2)}_{\mathrm{t,e}} D^{1,1}_t D^{(\nabla,\nabla)}_t + A^{(2,3)}_{\mathrm{t,e}} \sum_{\mu\nu} C^{1,\nabla\sigma}_{t,\mu\nu} C^{1,\nabla\sigma}_{t,\mu\nu} + A^{(2,4)}_{\mathrm{t,e}} D^{1,1}_t \left(\nabla \cdot C^{1,\nabla\times\sigma}_t\right) \right], \\
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N2LO EDF

- **systematic** expansion in gradients
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BSkG5

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\end{aligned}
$$

Rms σ	BSkG4	BSkG5
Masses [MeV]	0.633	0.637
S_n [MeV]	0.402	0.407
Radii [fm]	0.025	0.028
Prim. barriers [MeV]	0.36	0.36
Sec. barriers [MeV]	0.53	0.53
Fission isomers [MeV]	0.33	0.42

N2LO EDF

- **systematic** expansion in gradients
- next-to-next-to-leading order
- original motivation: spectroscopy
- massively complicates things

… what if we improve INM first?

- same global quality as BSkG4
- density dependence as standard Skyrme
- k-dependent effective mass, cf. **Gogny**

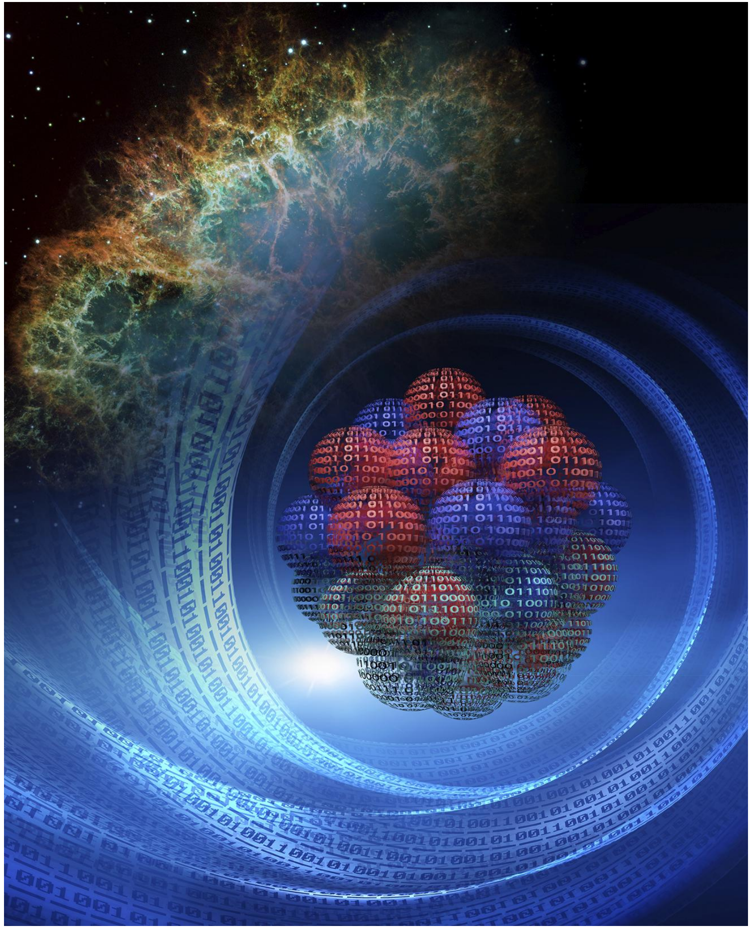
… all with **LESS** parameters!

Conclusion

We build **large-scale**, **microscopic** models for (astro) applications.

Large-scale = **thousands** of nuclei and **many observables.**
Microscopic = simple wave functions yet complex **symmetry breaking.**

-



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The BSkG models

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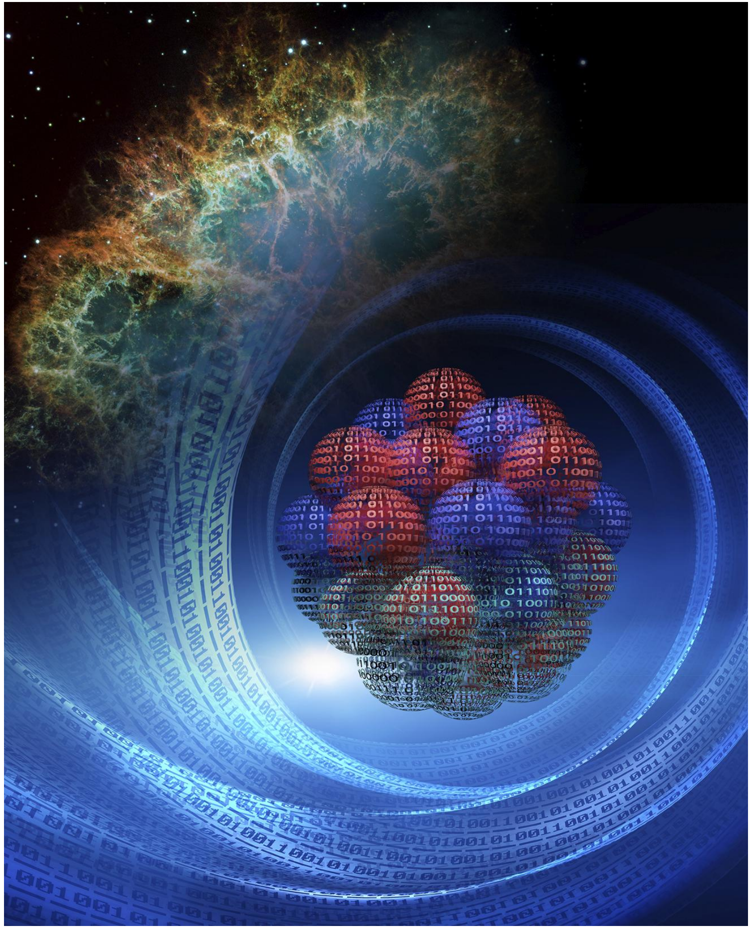
- competitive for masses and charge radii
- unmatched for fission properties
- consistent with NS constraints
- constantly benchmarked on experiment



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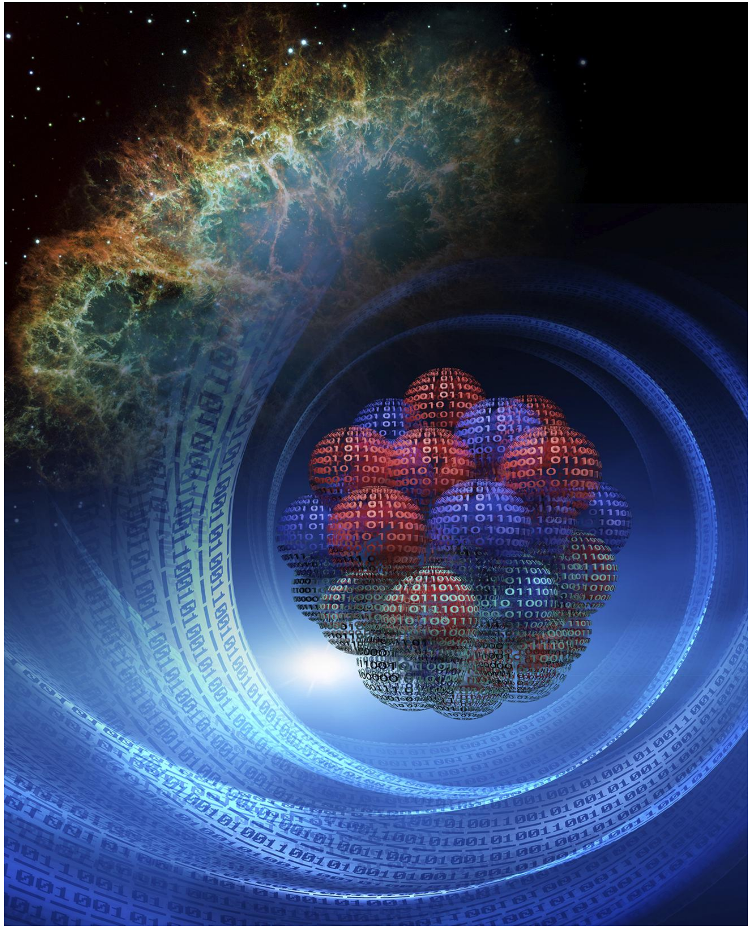
3. more with less: BSkG5



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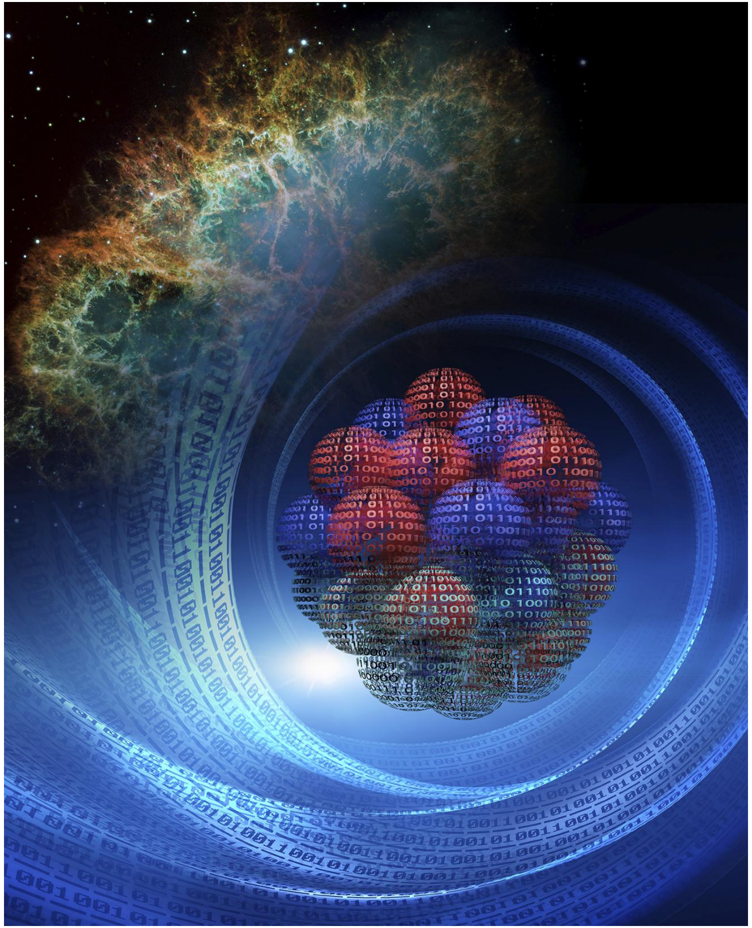
Soon-ish:

1. We will deliver the **first complete set of nuclear structure data** for r-process simulations based on a single model.
2. .... and we will be able to repeat that feat!



Thank you for...

...... all the wonderful work!

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N. Shchechilin

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M. Bender

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+ several experimental teams!

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