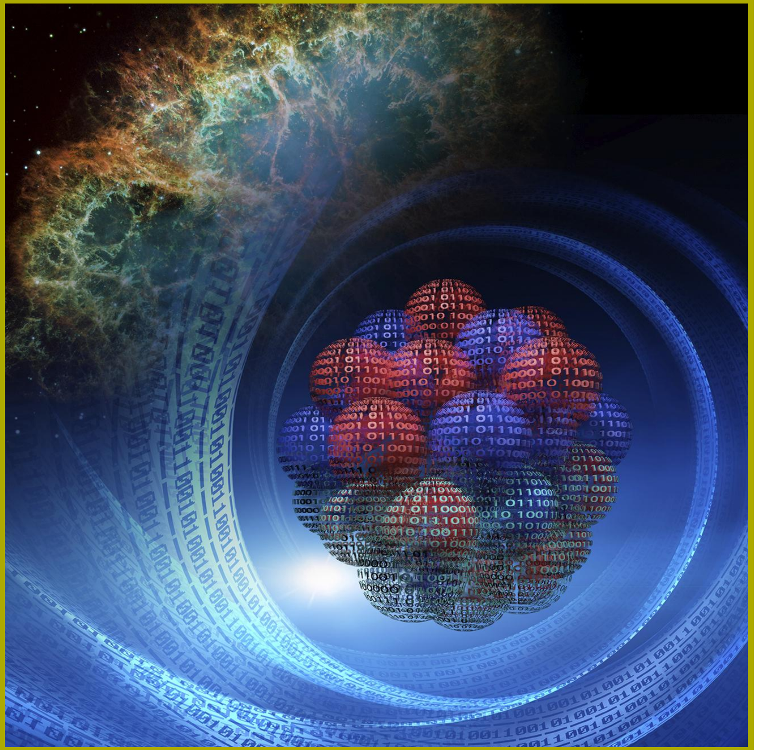
WOUTER RYSSENS



Andy Sproles, ORNL

Microscopic models of nuclear structure at scale

W. Ryssens
S. Bara, G. Grams, A Sanchez-Fernandez, N. Shchechilin, M. Bender, N. Chamel, S. Hilaire and S. Goriely

12th of December 2025

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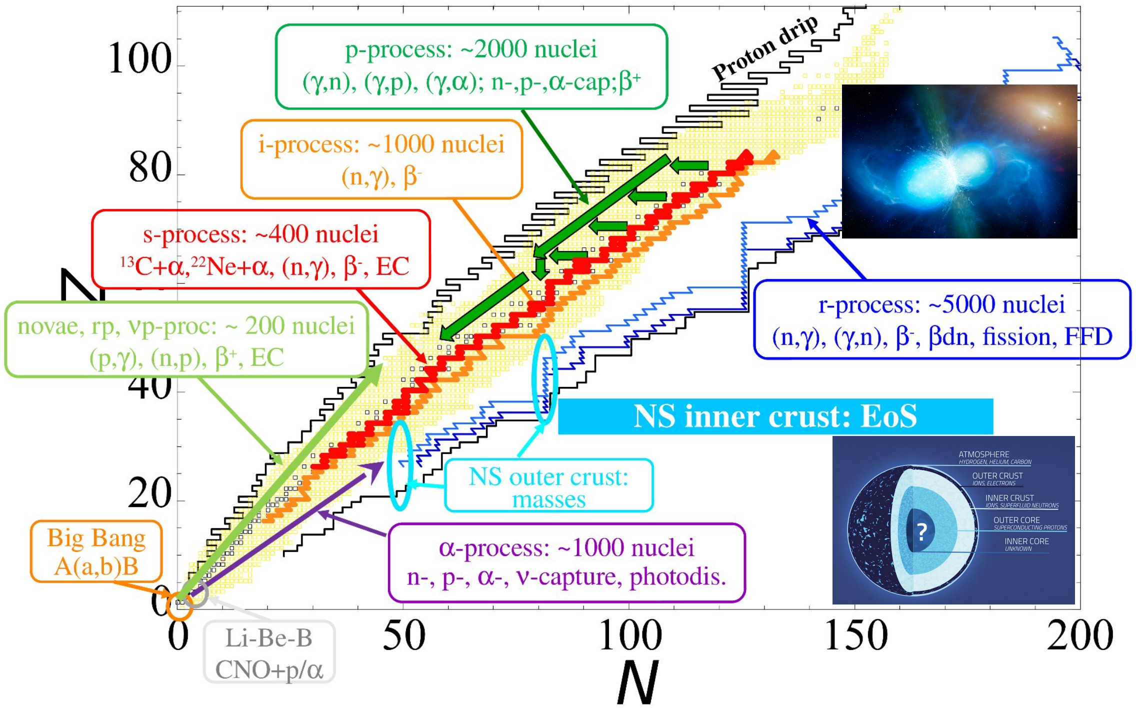
BRUSSELS LABORATORY OF THE UNIVERSE

LA LIBERTÉ DE CHERCHER

The nuclear chart and the processes traversing it

Extrapolations in

- nucleon number
- energy
- temperature
- density
- ……



The nuclear chart and the processes traversing it

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- nucleon number
- energy
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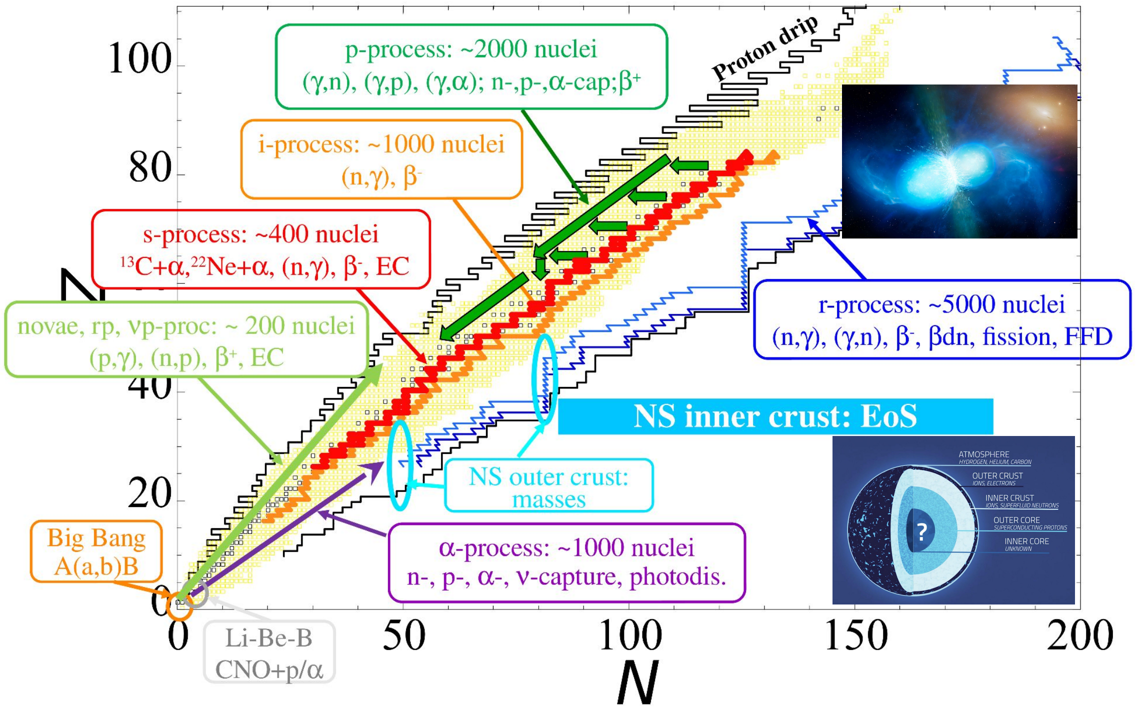
- density
- ……

and all of that for
- **~7000** nuclei
- **many** reactions



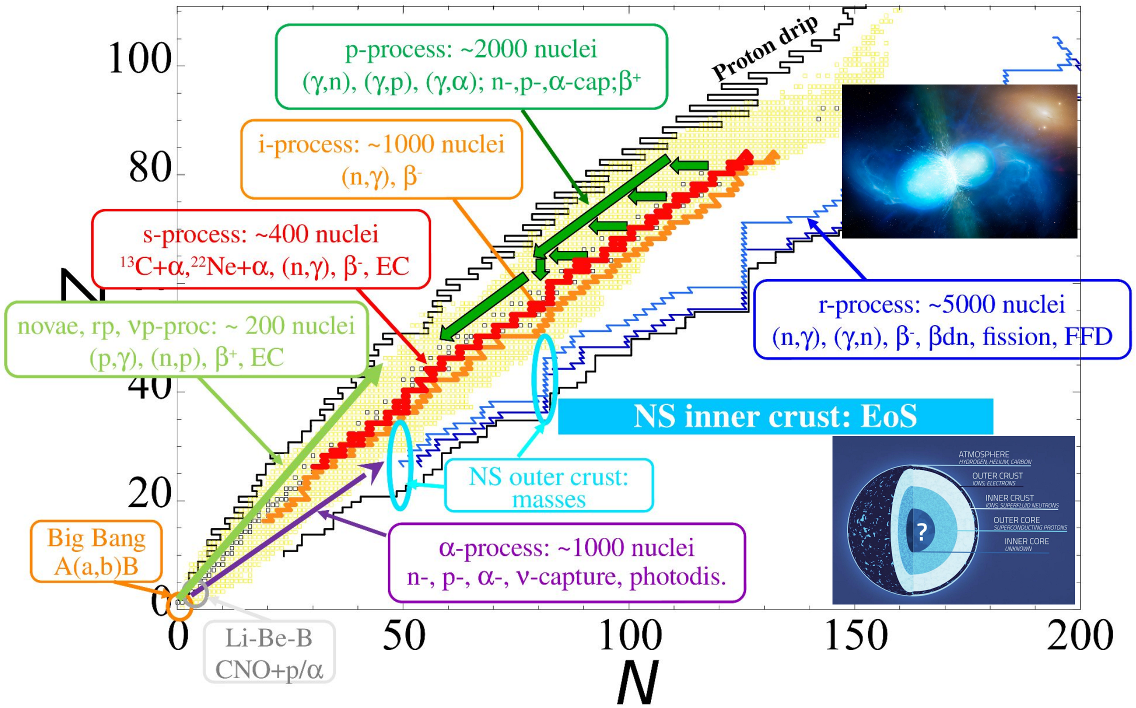
The nuclear chart and the processes traversing it

Extrapolations in
- nucleon number
- energy
- temperature
- density
- ……

and all of that for
- **~7000** nuclei
- **many** reactions

We need structure models that are

1. **predictive**….
2. but **complete!**



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

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

Energy

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

Local densities and currents of a wavefunction

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Local densities and currents of a wavefunction

Progress?

1. more physics in the wavefunction

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1. more physics in the wavefunction
2. more (pseudo-) observables simultaneously
   “more” = both **scale** and **diversity**!

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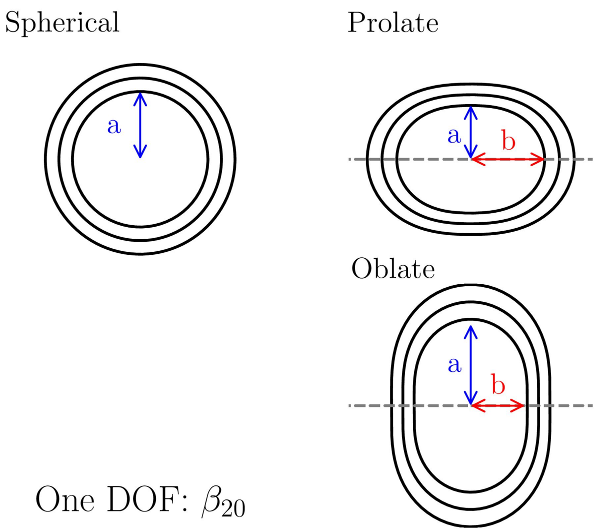
Local densities and currents of a wavefunction

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

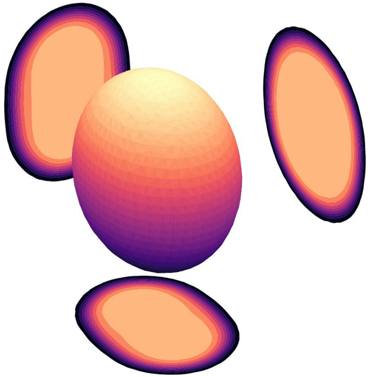


Nuclear deformation

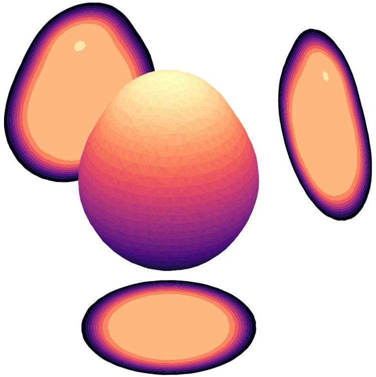
- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
- intuitive interpretation

Large-scale models in 1-2-3 dimensions

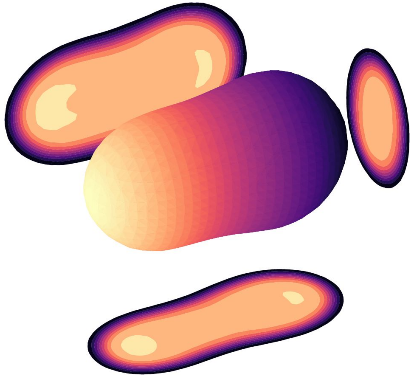
β_{20}, β_{22} or β_2, γ



β_{20}, β_{30}



β_{20}, β_{22} **and** β_{30}



Nuclear deformation

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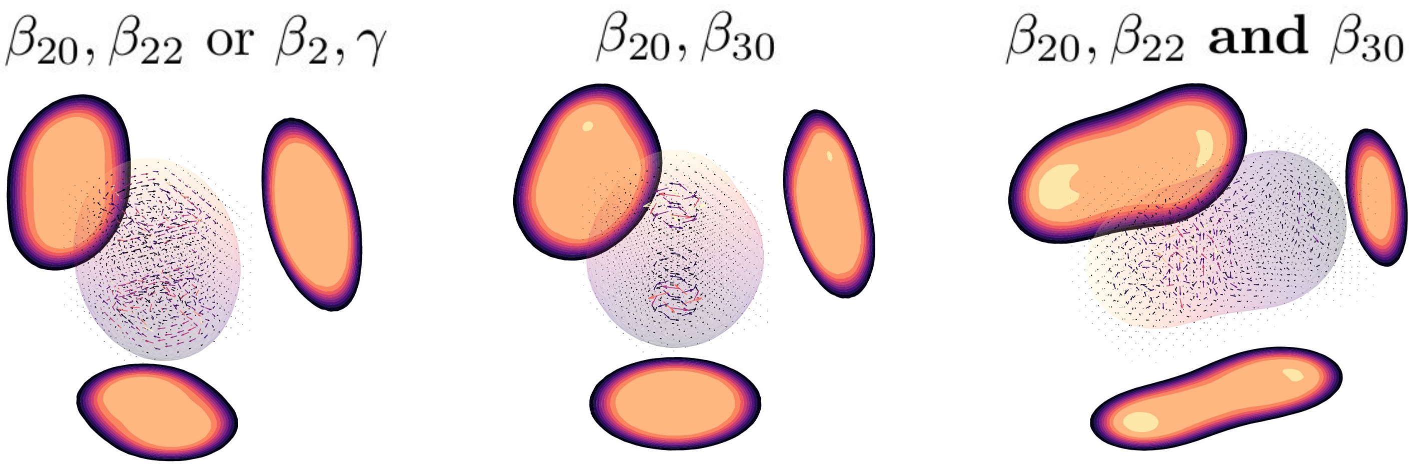
More general configurations

- triaxial shapes
- reflection asymmetry
- elongated shapes

Large-scale models in 1-2-**3** dimensions



Nuclear deformation

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

More general configurations

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

Brussels-Skyrme-on-a-Grid: 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 [$M_\odot$]				

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

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- fitted to 2457 masses
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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

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

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BSkG1

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

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

- **complete** time-reversal breaking
- fit to 45 reference fission barriers
  + 28 fission isomers

BSkG3

- extended Skyrme EDF form
- supports massive neutron stars

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

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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

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

- extended Skyrme EDF form
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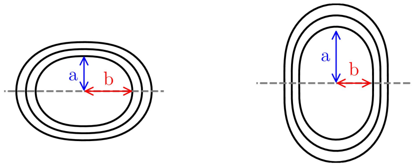
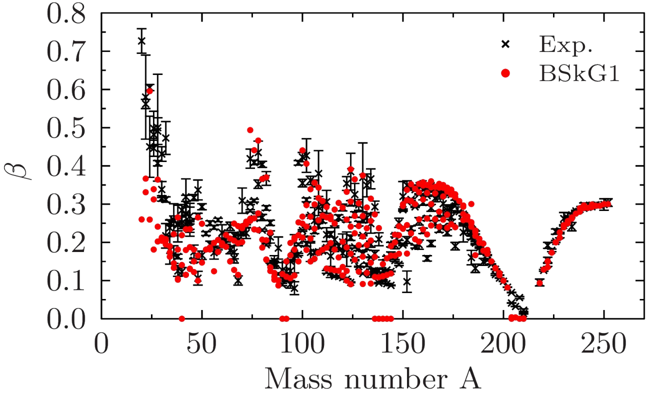
Deformations

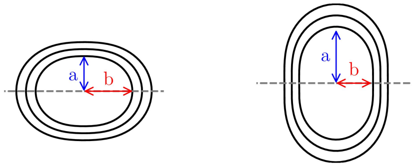
“Ordinary” quadrupole deformation

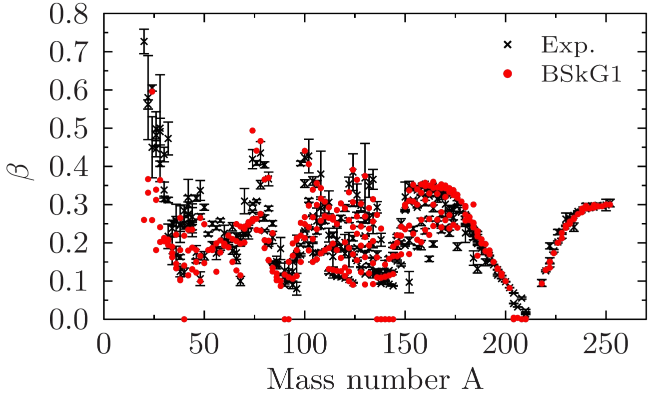


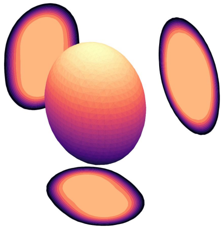


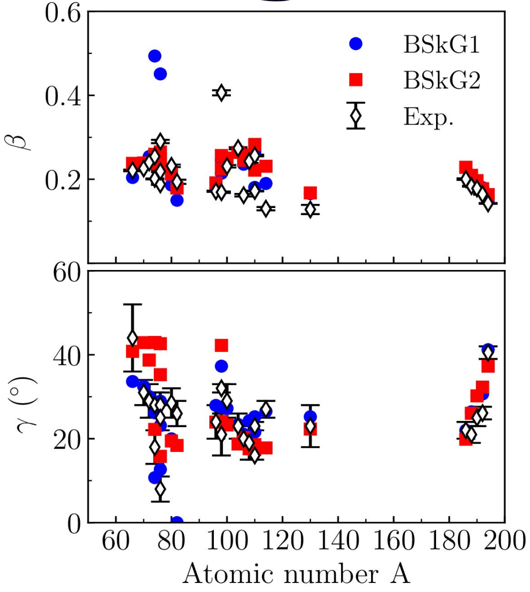
Deformations

“Ordinary” quadrupole deformation ... and triaxial deformation ...





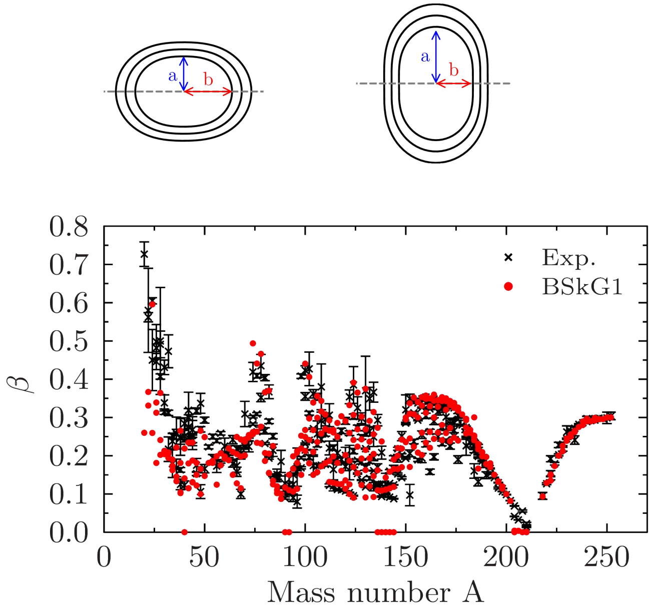




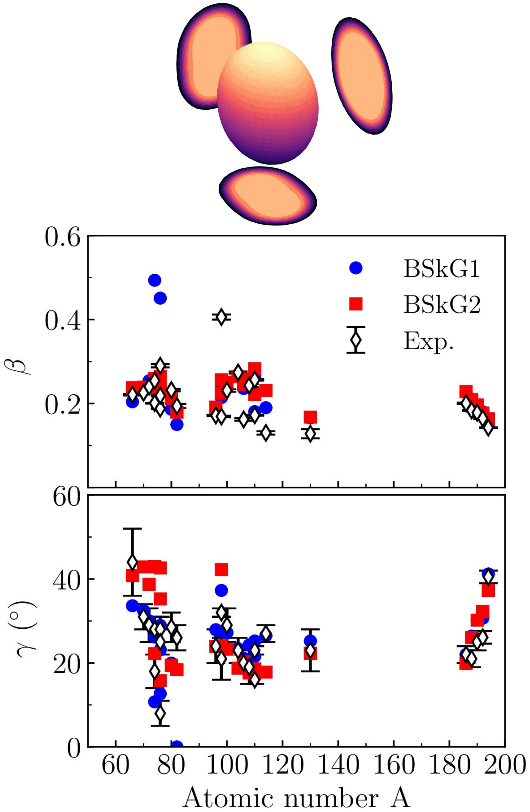
Deformations

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).

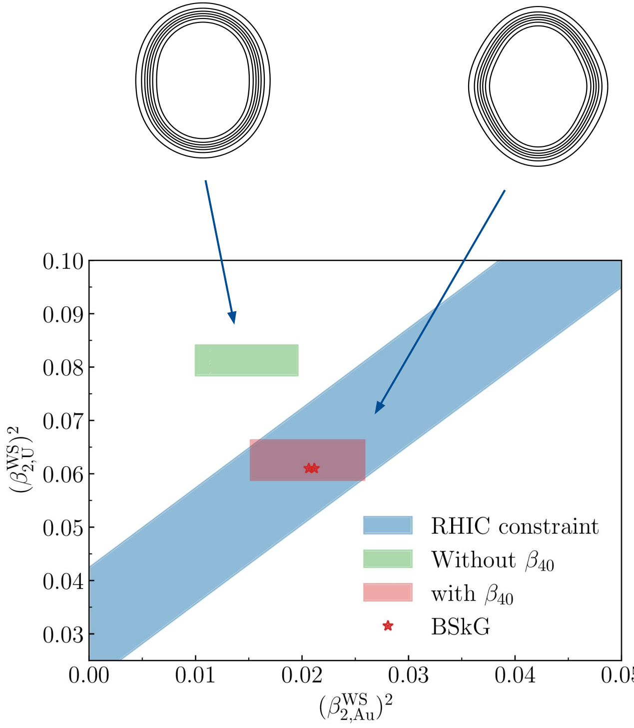
“Ordinary” quadrupole deformation



… and triaxial deformation …



… and even hexadecapole!



Masses

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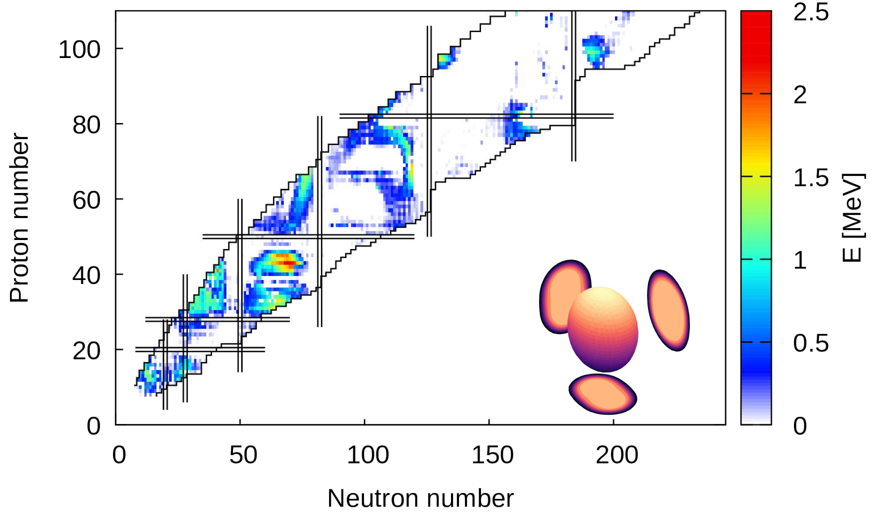

Triaxial deformation

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

Masses

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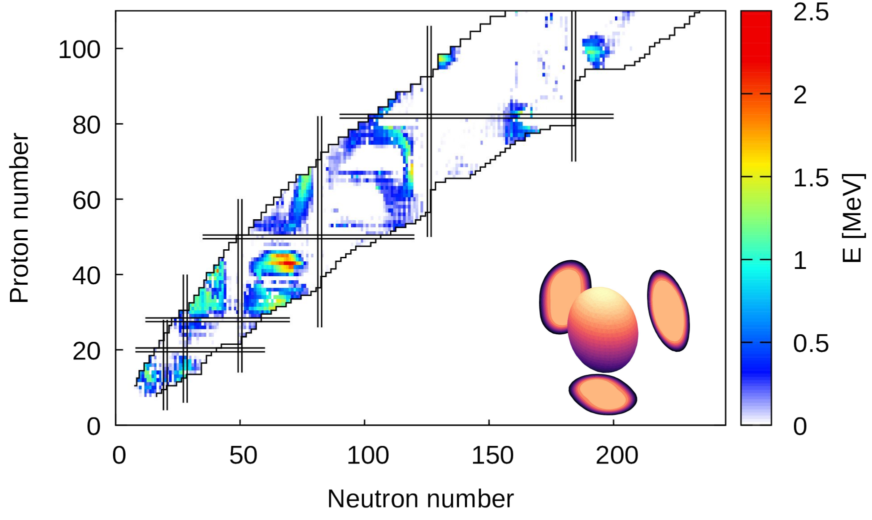
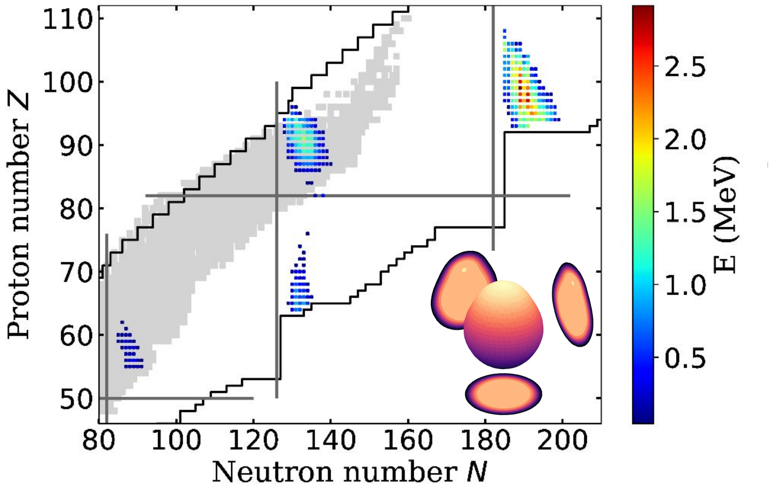




Triaxial deformation

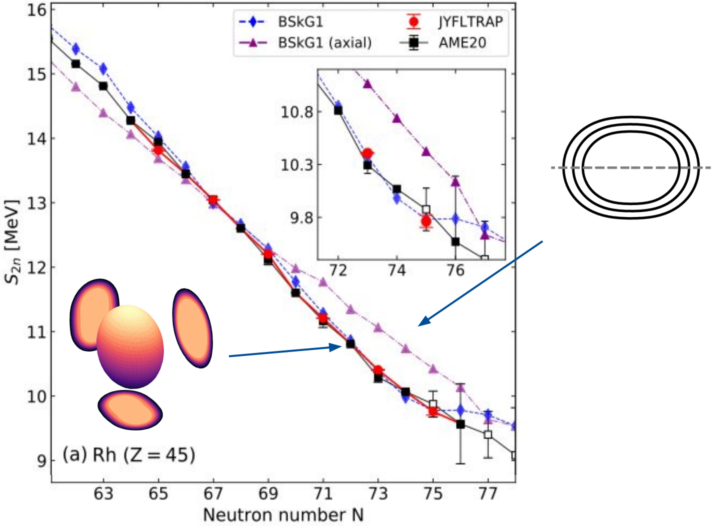
- many nuclei are affected
- effects up to 2.5 MeV near Z~44

Reflection asymmetry

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

Structure near Z ~ 44

M. Hukkanen, W.R. et al., PRC **107**, 014306 (2023).
M. Hukkanen, W.R. et al., PRC **108**, 064315 (2023).
M. Hukkanen, W.R. et al., PLB **856**, 138916 (2024).
M. Stryjczyk, W. R. et al., arXiv:2409.15016 (2024).



+ explanation of isomerism in odd-odds

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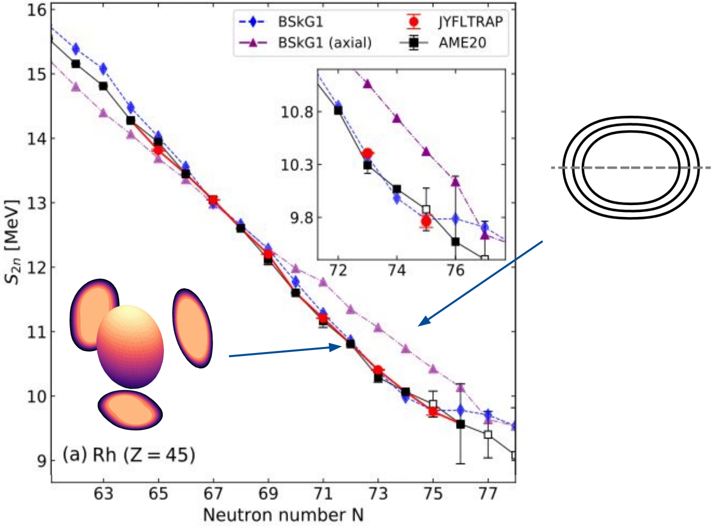
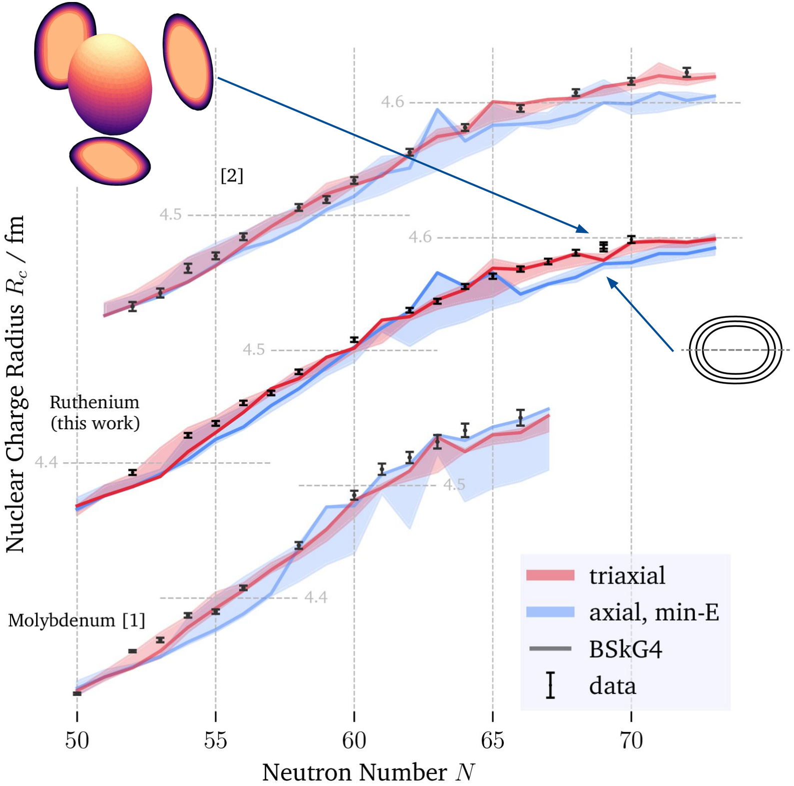
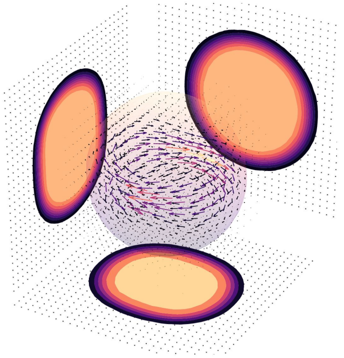
M. Hukkanen, W.R. et al., PLB **856**, 138916 (2024).
M. Stryjczyk, W. R. et al., arXiv:2409.15016 (2024).
B. Maass et al., in preparation.

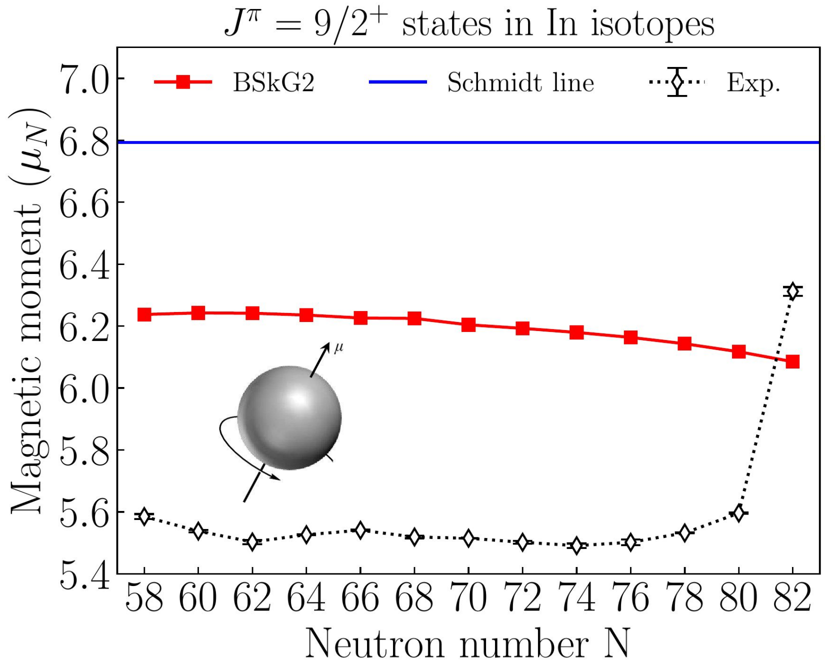


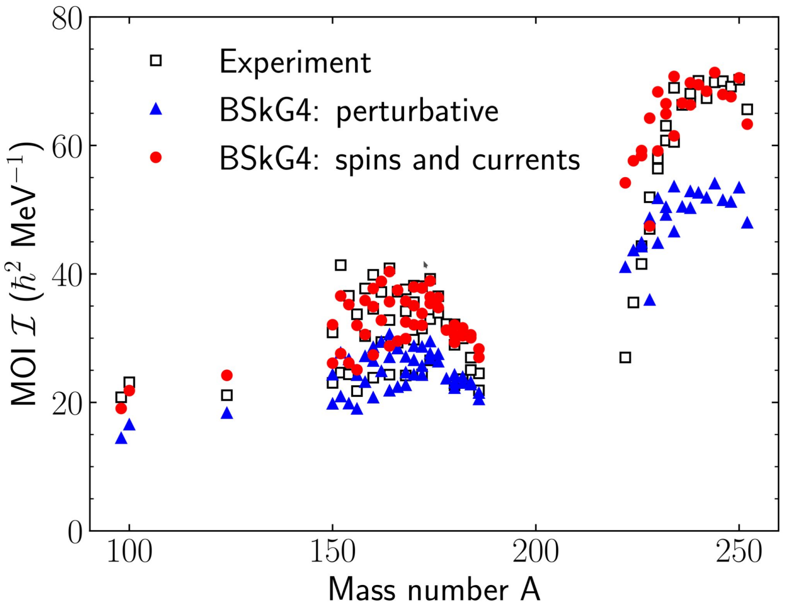


+ explanation of isomerism in odd-odds

Time-odd channel

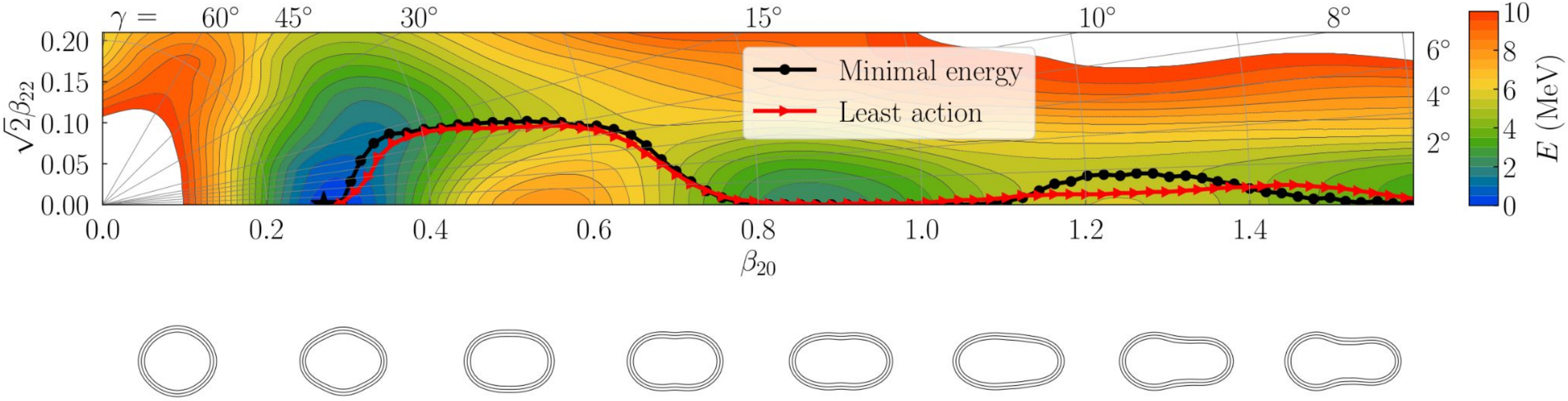






Fission barriers

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



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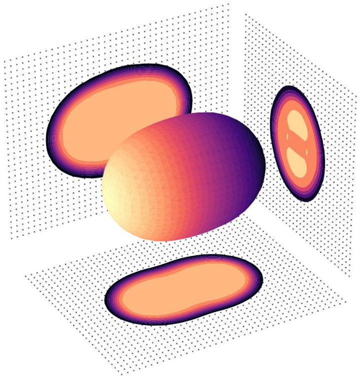

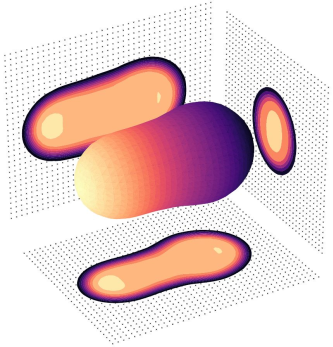

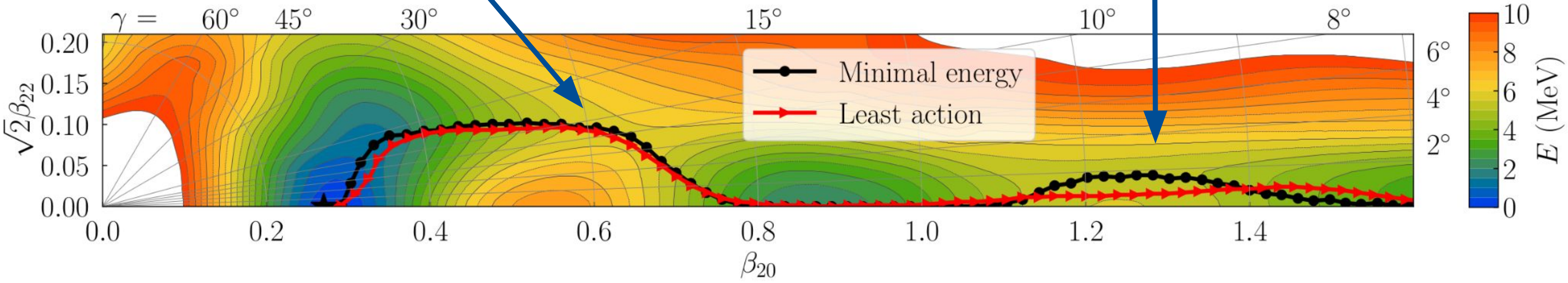

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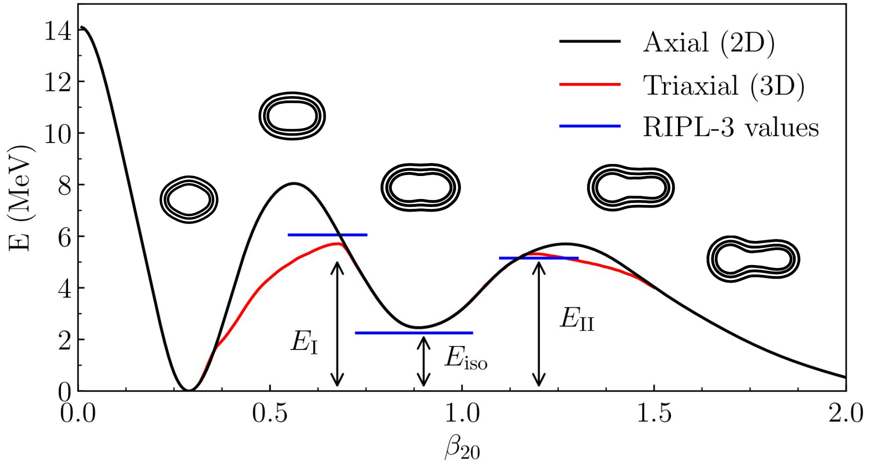

Fission properties of 45 actinide nuclei

- includes odd-A and odd-odds
- **<u>all</u>** inner barriers: triaxial
- **<u>all</u>** outer barriers: octupole + triaxial

... even with consistent inertia's!

Fission

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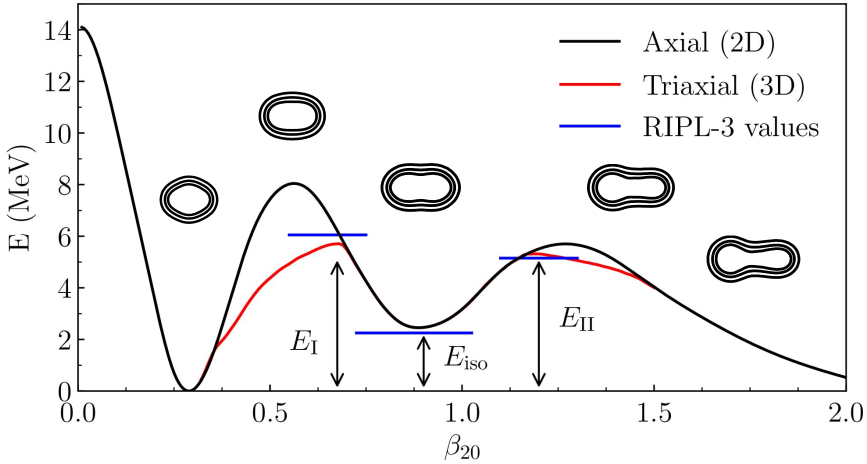

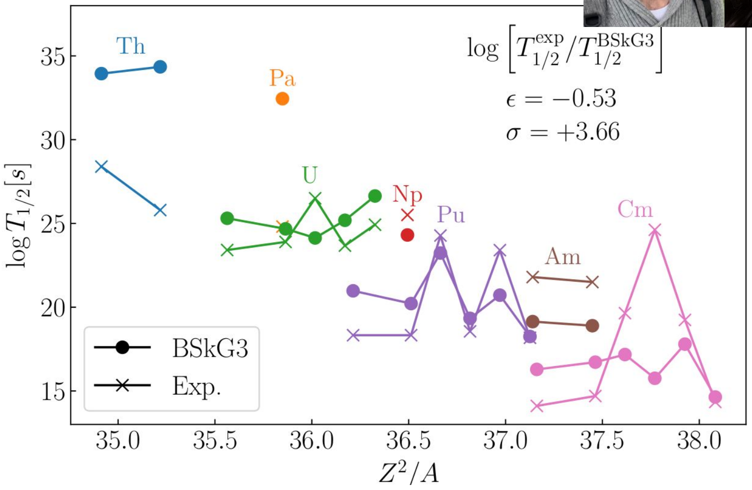

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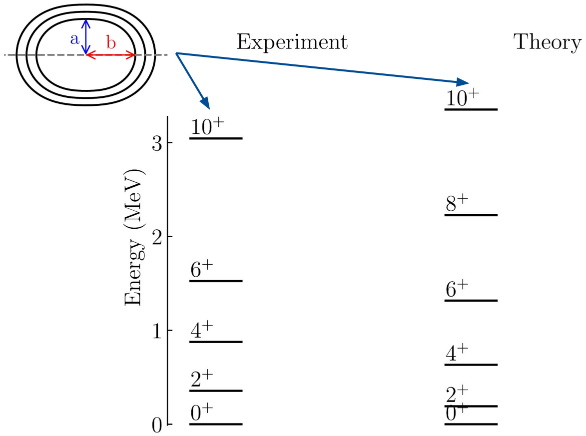
... even with consistent inertia's!

Future

- fission properties for ~3000 nuclei
  - currently ~ 6 nuclei per day
- □df comparison with experiment

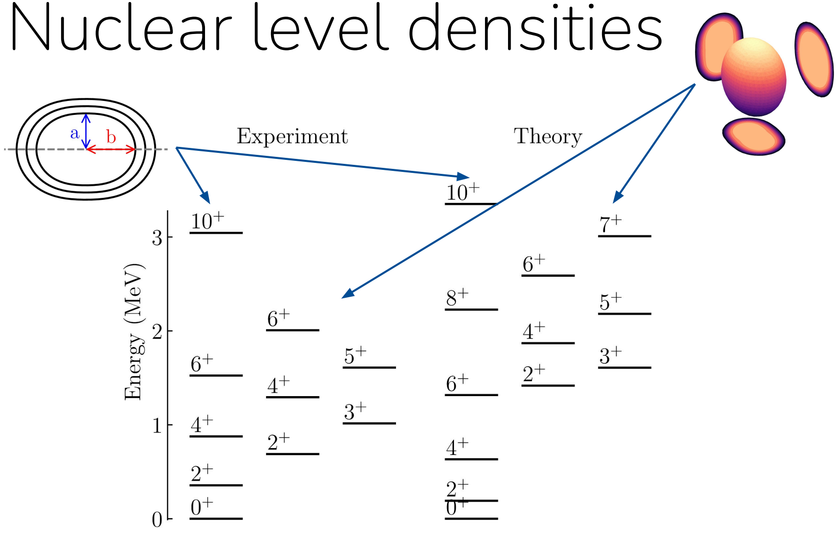
Nuclear level densities



Symmetries dictate NLDs

- larger collective enhancement

Nuclear level densities



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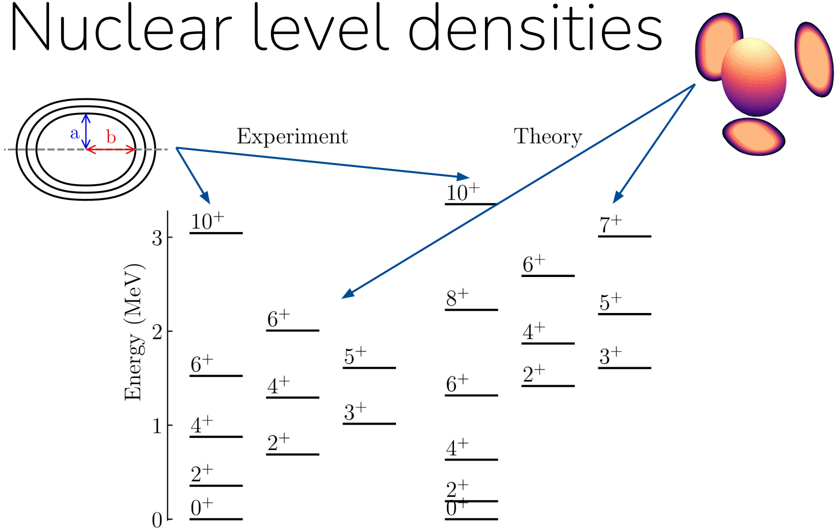
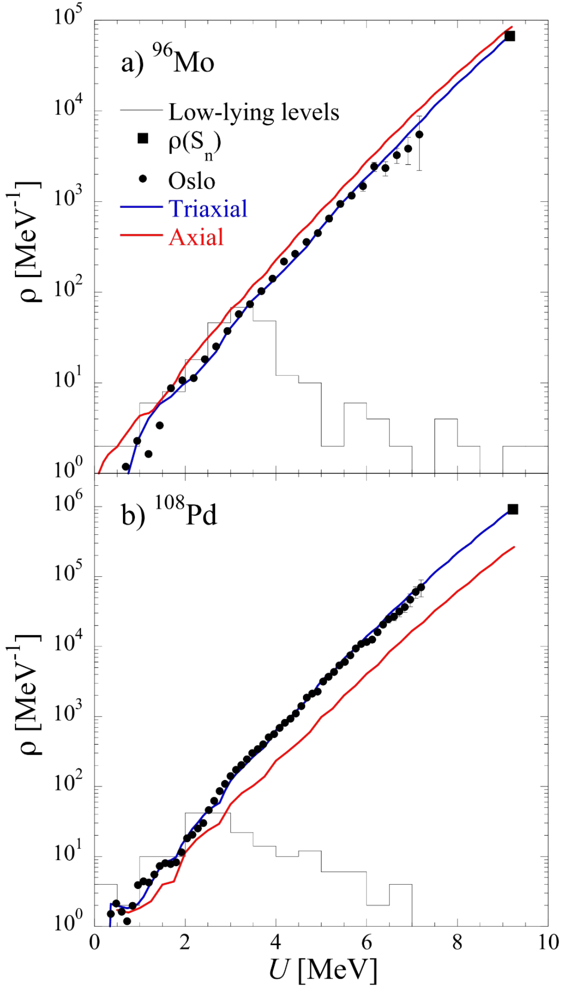
Nuclear level densities



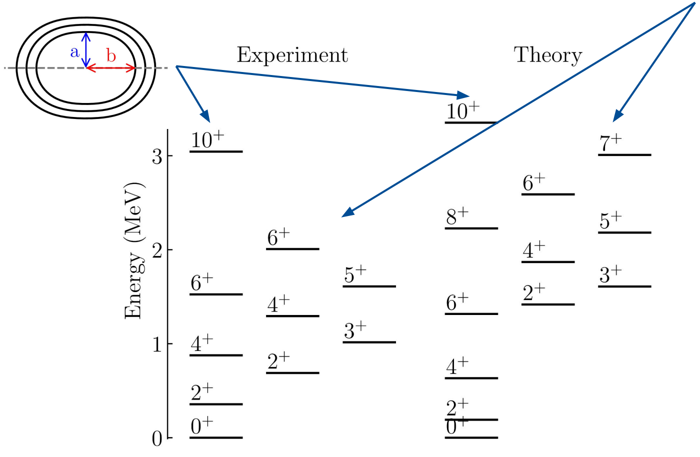


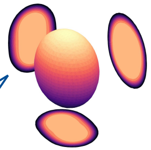
Symmetries dictate NLDs

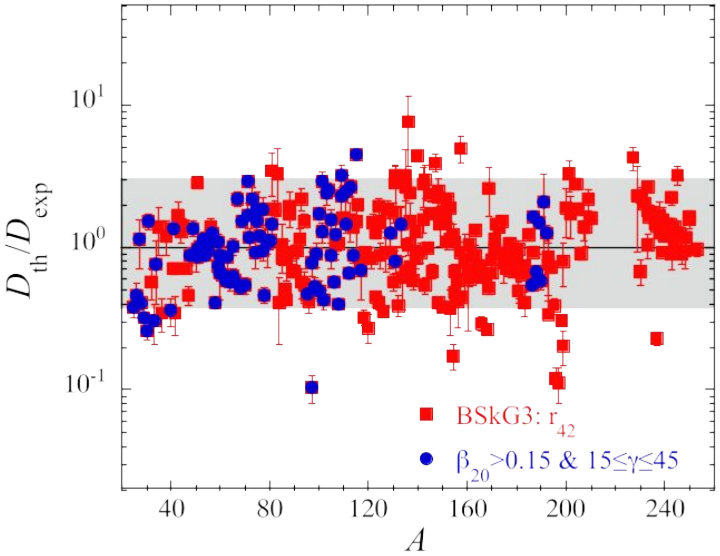
- larger collective enhancement
- combinatorial calculation of NLDs
- … but the story is not so simple!

Nuclear level densities

S. Goriely et al., in preparation.







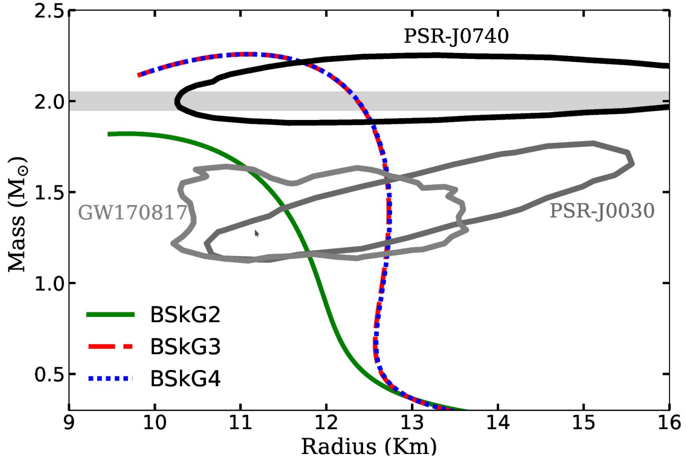
$$f_{\mathrm{rms}} = \exp\left[\frac{1}{N_e}\sum_i^{N_e}(\ln r_i)^2\right]^{1/2} = 1.96\,.$$

Symmetries dictate NLDs

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

Neutron stars

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



Stiffer EoS

- results in higher maximum mass
- usually incompatible with masses

cf. talk by A. Pastore

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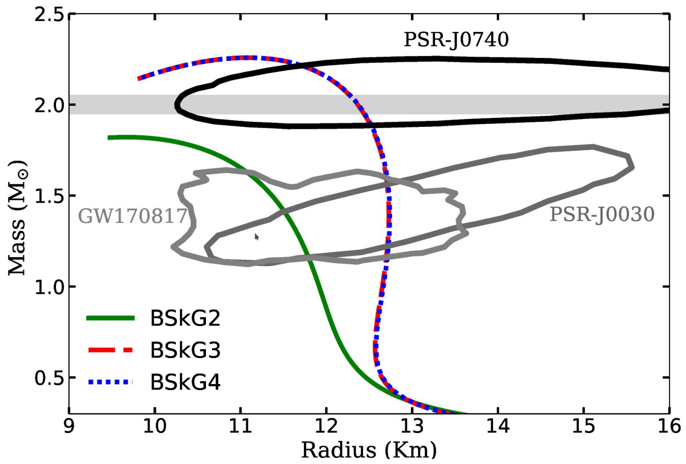

$$
\begin{aligned}
\mathcal{E}_{t,\mathrm{e}}(\mathbf{r}) = {} & C_t^{\rho\rho}(\rho_0)\,\rho_t^2(\mathbf{r}) + \boxed{C_t^{\rho\tau}(\rho_0)}\,\rho_t(\mathbf{r})\,\tau_t(\mathbf{r}) \\
& + C_t^{\rho\nabla J}\,\rho_t(\mathbf{r})\,\nabla\cdot\mathbf{J}_t(\mathbf{r}) \\
& + C_t^{\rho\Delta\rho}\,\rho_t(\mathbf{r})\,\Delta\rho_t(\mathbf{r})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

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Extended density dependencies

- ad-hoc suggestion
- 6 additional parameters

... two are fractional powers!

BSkG5

G. Grams et al., in preparation.

$$
\begin{aligned}
\mathcal{E}^{(0)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1} \Big[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 \Big] , \\
\mathcal{E}^{(2)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1} \Big[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) \Big] , \\
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N2LO EDF

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\end{aligned}
$$

N2LO EDF

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BSkG5

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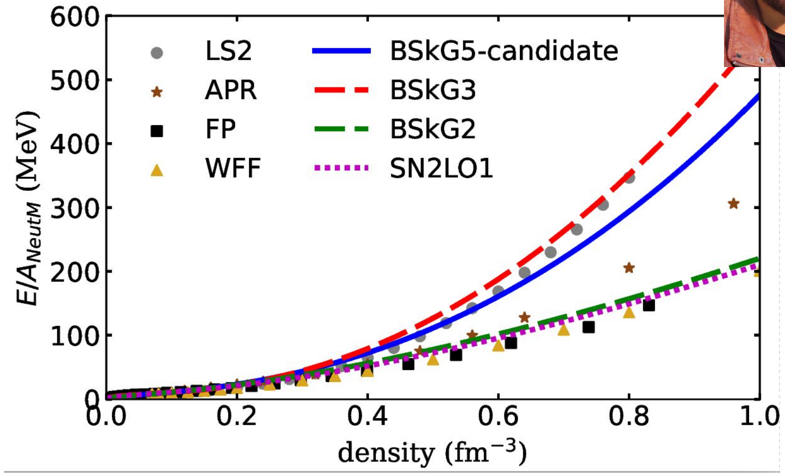

N2LO EDF

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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

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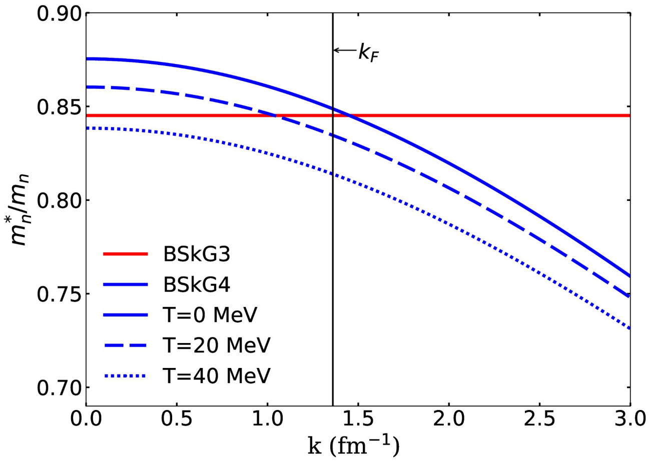
\mathcal{E}^{(4)}_{\mathrm{Sk,o}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(4,1)}_{\mathrm{t,o}}\left(\Delta\vec{D}^{1,\sigma}_t\right)\cdot\left(\Delta\vec{D}^{1,\sigma}_t\right) + A^{(4,2)}_{\mathrm{t,o}}\vec{D}^{1,\sigma}_t\cdot\vec{D}^{\Delta,\Delta\sigma}_t + A^{(4,3)}_{\mathrm{t,o}}\vec{D}^{(\nabla,\nabla)\sigma}_t\cdot\vec{D}^{(\nabla,\nabla)\sigma}_t\\
&\quad + A^{(4,4)}_{\mathrm{t,o}}\sum_{\mu\nu\kappa}D^{\nabla,\nabla\sigma}_{\mu\nu\kappa}D^{\nabla,\nabla\sigma}_{\mu\nu\kappa} + A^{(4,5)}_{\mathrm{t,o}}\sum_{\mu\nu\kappa}D^{\nabla,\nabla\sigma}_{\mu\nu\kappa}\left(\nabla_\mu\nabla_\nu D^{1,\sigma}_\kappa\right),\\
&\quad + A^{(4,6)}_{\mathrm{t,o}}\vec{C}^{1,\nabla}_t\cdot\left(\Delta\vec{C}^{1,\nabla}_t\right) + A^{(4,7)}_{\mathrm{t,o}}\left(\boldsymbol{\nabla}\cdot\vec{C}^{1,\nabla}_t\right)\left(\boldsymbol{\nabla}\cdot\vec{C}^{1,\nabla}_t\right) + A^{(4,8)}_{\mathrm{t,o}}\vec{C}^{1,\nabla}_t\cdot\vec{C}^{\Delta,\nabla}_t\Big],
\end{aligned}
$$



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
- T-dependent effective mass

BSkG5

G. Grams et al., in preparation.

$$
\begin{aligned}
\mathcal{E}^{(0)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1}\Big[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\Big],\\
\mathcal{E}^{(2)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1}\Big[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)\Big],\\
\mathcal{E}^{(4)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(4,1)}_{\mathrm{t,e}}\left(\Delta D^{1,1}_t\right)\left(\Delta D^{1,1}_t\right) + A^{(4,2)}_{\mathrm{t,e}}D^{1,1}_t D^{\Delta,\Delta}_t + A^{(4,3)}_{\mathrm{t,e}}D^{(\nabla,\nabla)}_t D^{(\nabla,\nabla)}_t\\
&\quad + A^{(4,4)}_{\mathrm{t,e}}\sum_{\mu\nu}D^{\nabla,\nabla}_{t,\mu\nu}D^{\nabla,\nabla}_{t,\mu\nu} + A^{(4,5)}_{\mathrm{t,e}}\sum_{\mu\nu}D^{\nabla,\nabla}_{t,\mu\nu}\left(\nabla_\mu\nabla_\nu D^{1,1}_t\right)\\
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\mathcal{E}^{(0)}_{\mathrm{Sk,o}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(0,1)}_{\mathrm{t,o}}\vec{D}^{1,\sigma}_t\cdot\vec{D}^{1,\sigma}_t + A^{(0,2)}_{\mathrm{t,o}}(D^{1,1}_0)^{\alpha}\vec{D}^{1,\sigma}_t\cdot\vec{D}^{1,\sigma}_t\Big],\\
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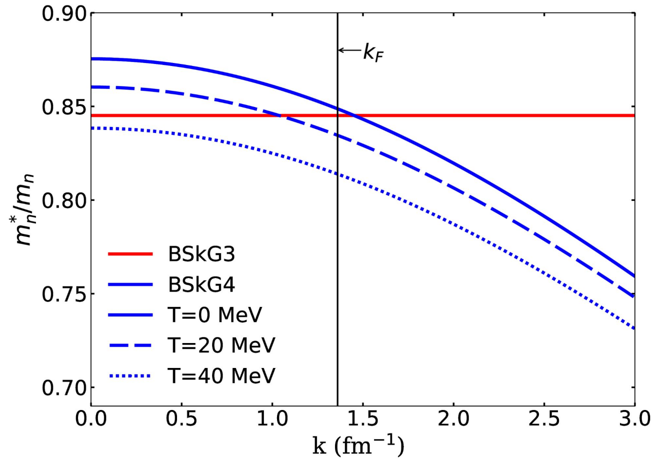

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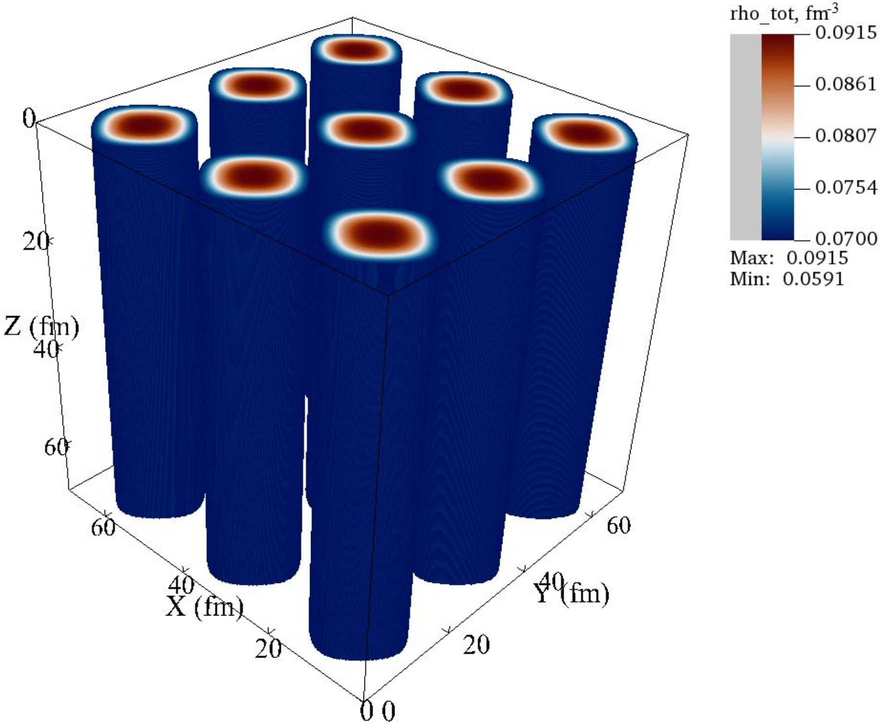
… all with <u>**LESS**</u> parameters!

A complete EoS with the BSkGs

N. Shchechilin et al., in preparation



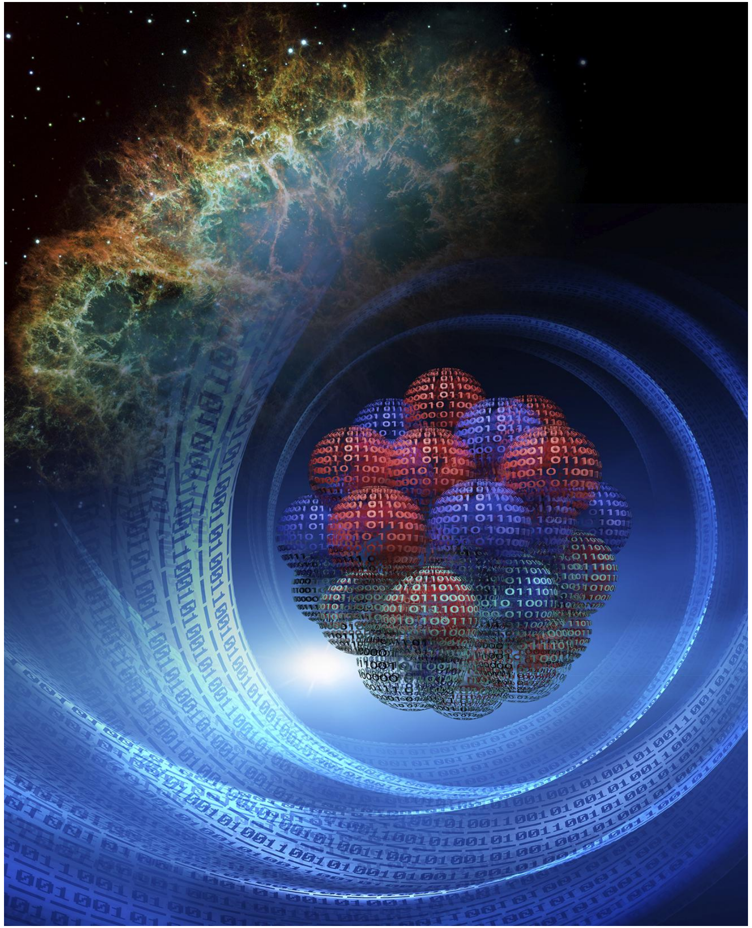
Nuclear pasta

- crystalline structures in NS crust
- impact NS cooling and emitted GW
- QM treatment with NS-appropriate EDFs
- 10^4 - 10^6 particles in large volumes!

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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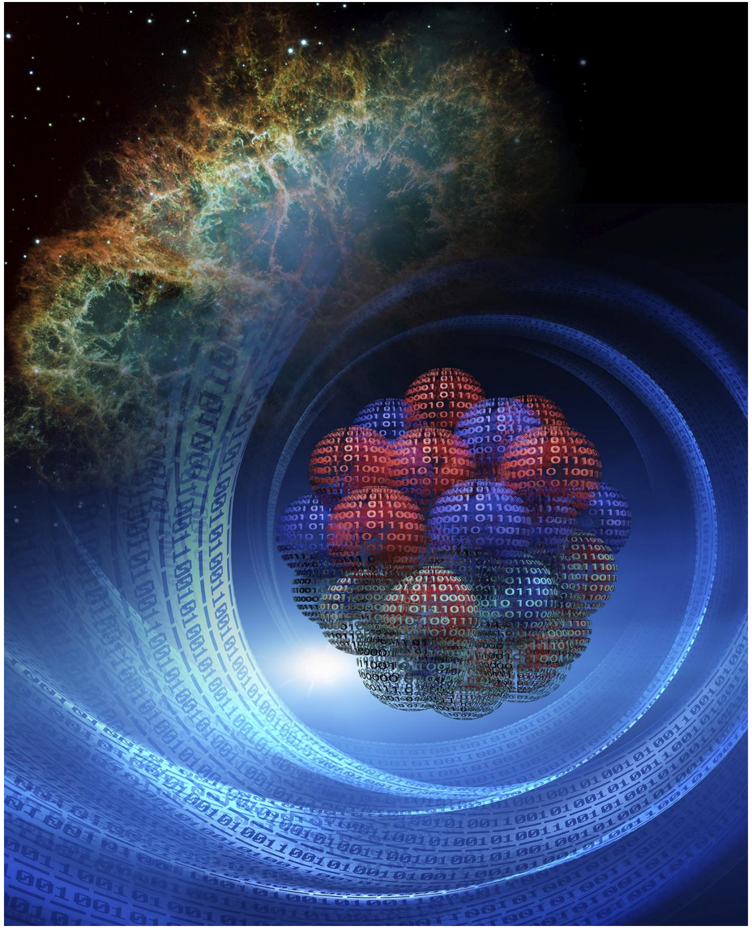
The BSkG models:

- triaxial, octupole and time-reversal deformation
- competitive for masses and charge radii
- unmatched for fission properties
- consistent with NS observations
- masses, densities in TALYS; NLDs soon-to-be



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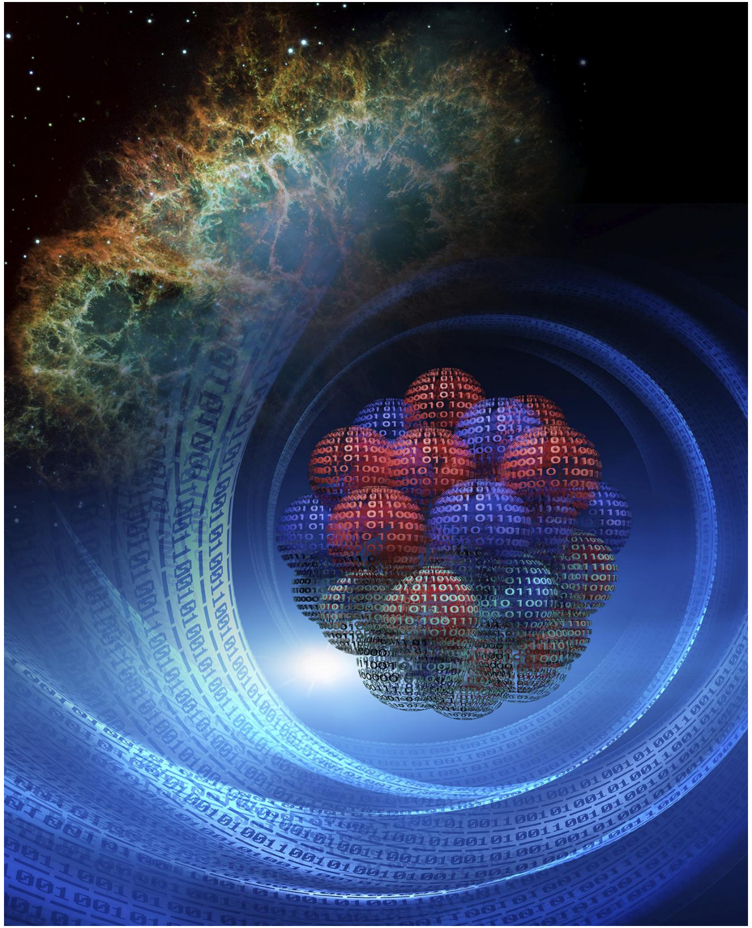
Quite soon:

1. more with less: BSkG5
2. fission properties of ~3000 nuclei
3. a unified neutron star EoS



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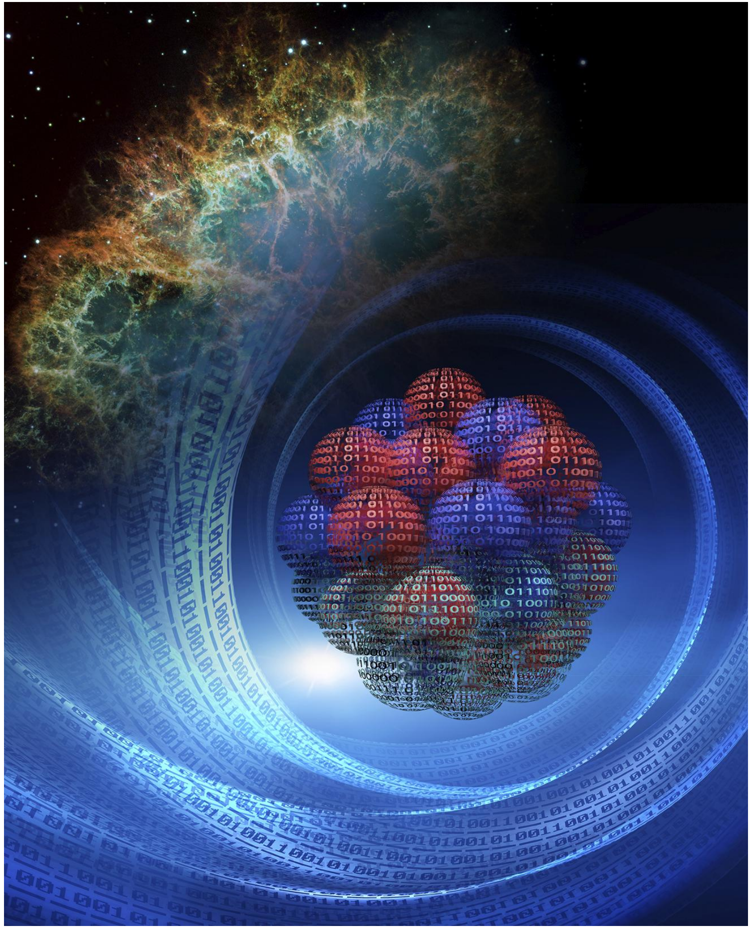
In the coming years:

A consistent set of r-process inputs by adding electroweak transitions.



Thank you for...

...... all the wonderful work!

ULB

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G. Grams
A. Sanchez-Fernandez
N. Shchechilin

cea

S. Hilaire

iP2i LES 2 INFINIS LYON

M. Bender

L2IT

G. Scamps

KU LEUVEN

S. Bara

and several experimental teams!

Thank you for...

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...... the computing time!

...... the funding!

...... your attention!

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CÉCI

Cenaero

EuroHPC Joint Undertaking

...... the funding!

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EOS THE EXCELLENCE OF SCIENCE