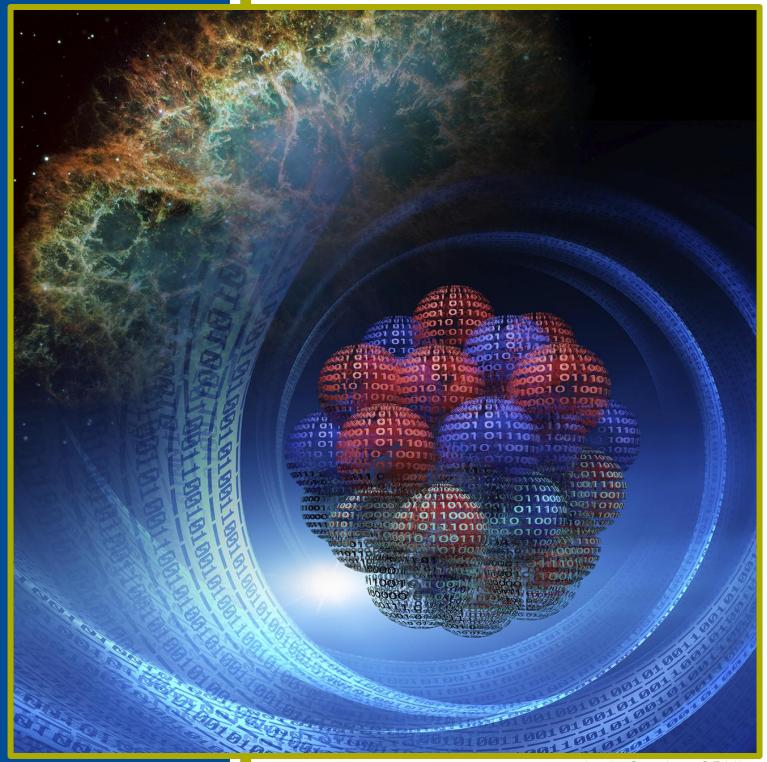
WOUTER RYSSENS



Andy Sproles, ORNL

Microscopic models of nuclear structure at scale

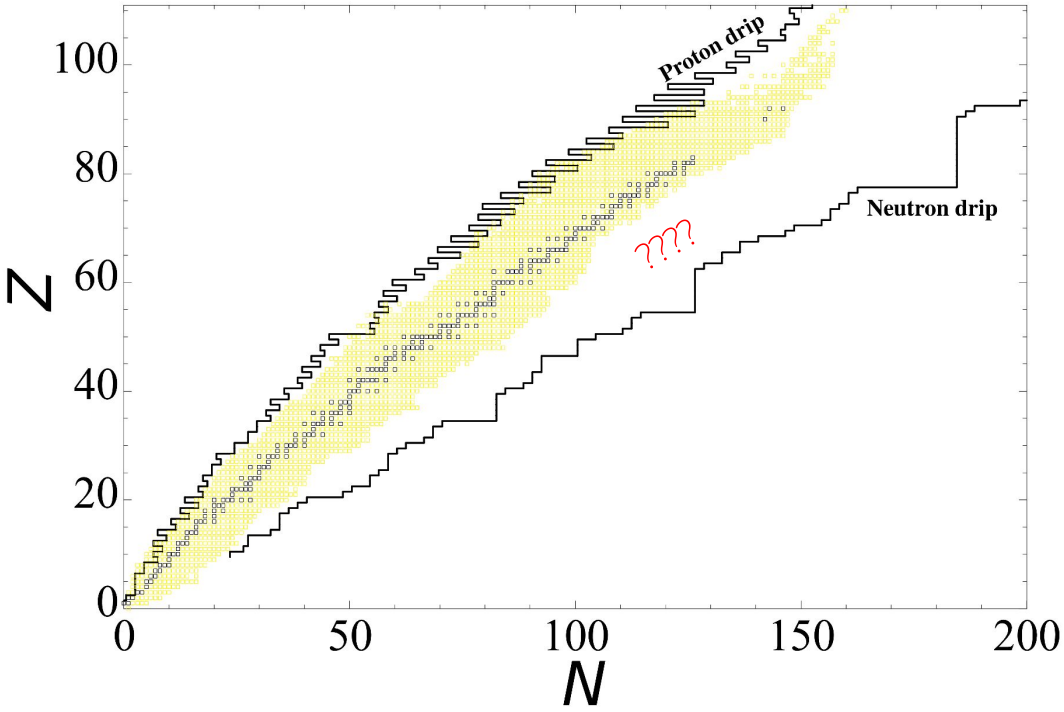
Wouter Ryssens, G. Grams, M. Bender and S. Goriely

5th of June 2023

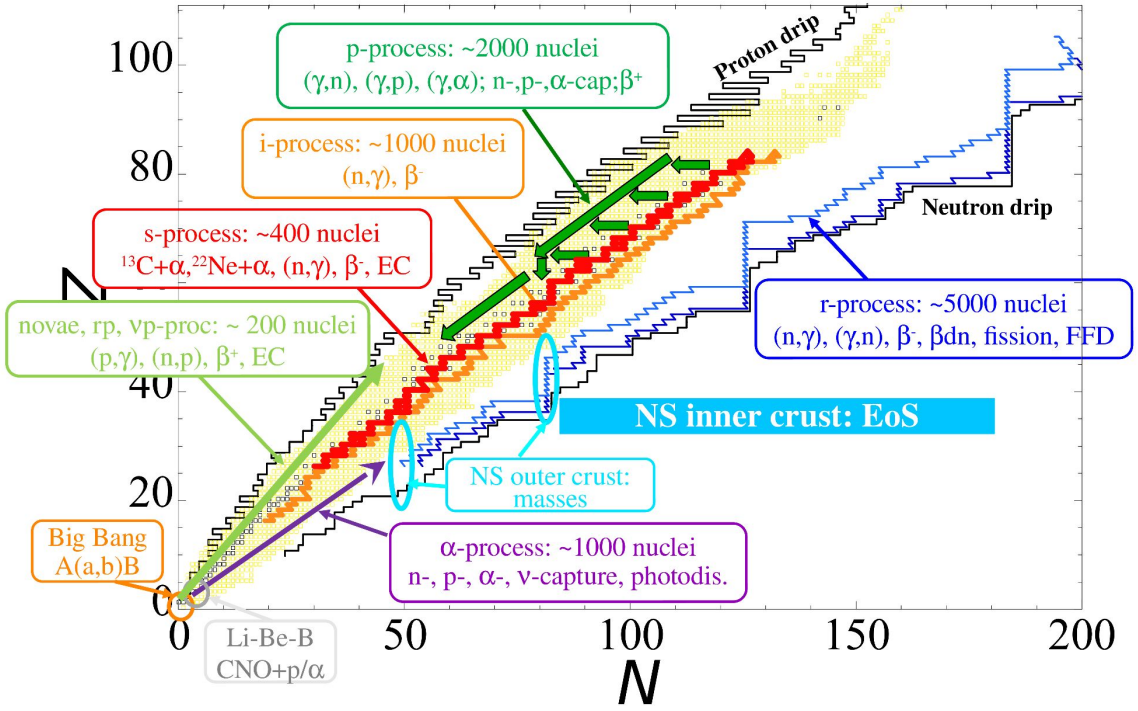
wryssens.com

wryssens@ulb.be

The nuclear chart…



The nuclear chart and the processes traversing it



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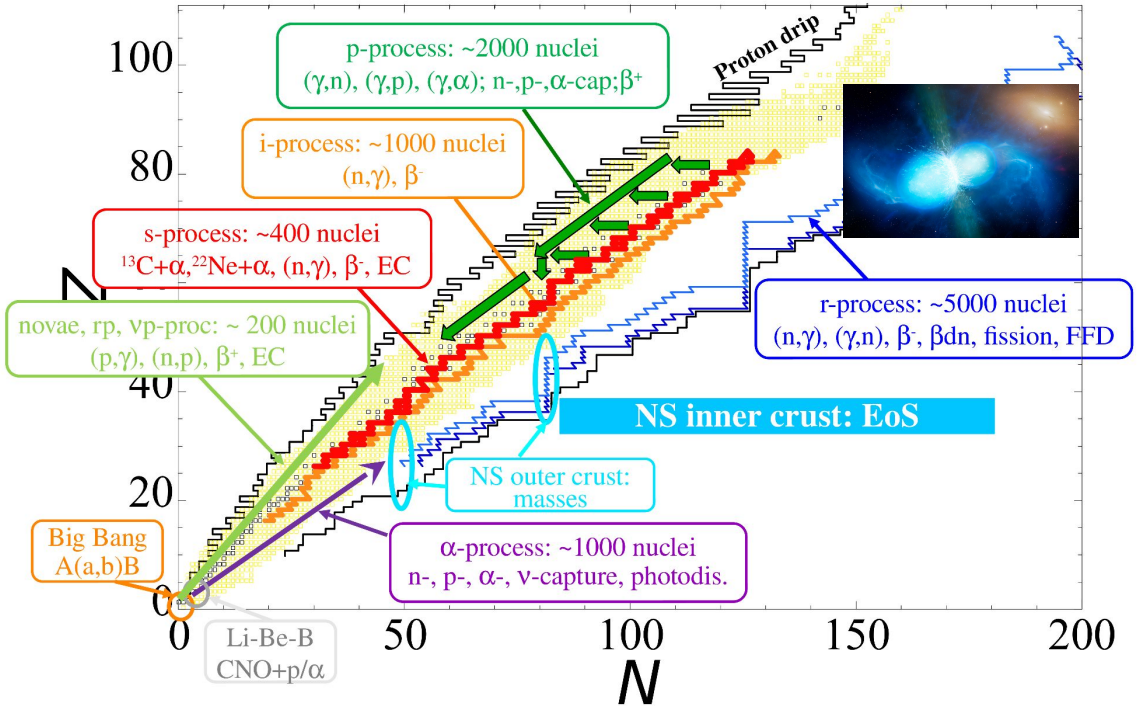
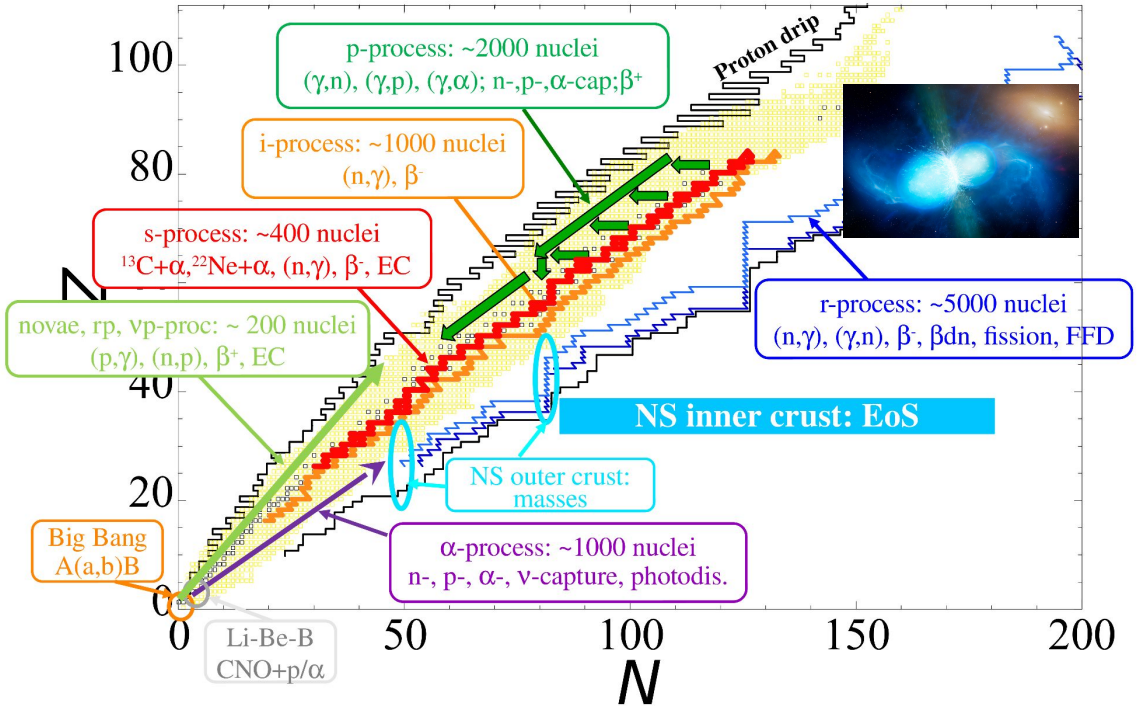


The nuclear chart and the processes traversing it

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



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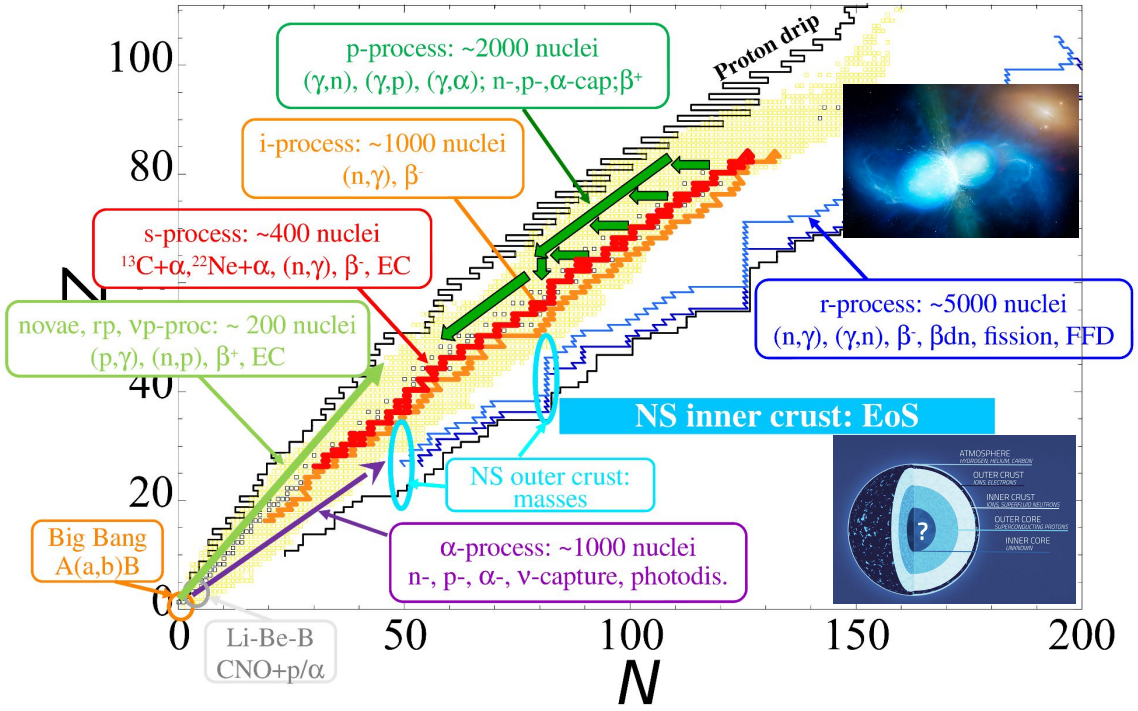

The nuclear chart and the processes traversing it

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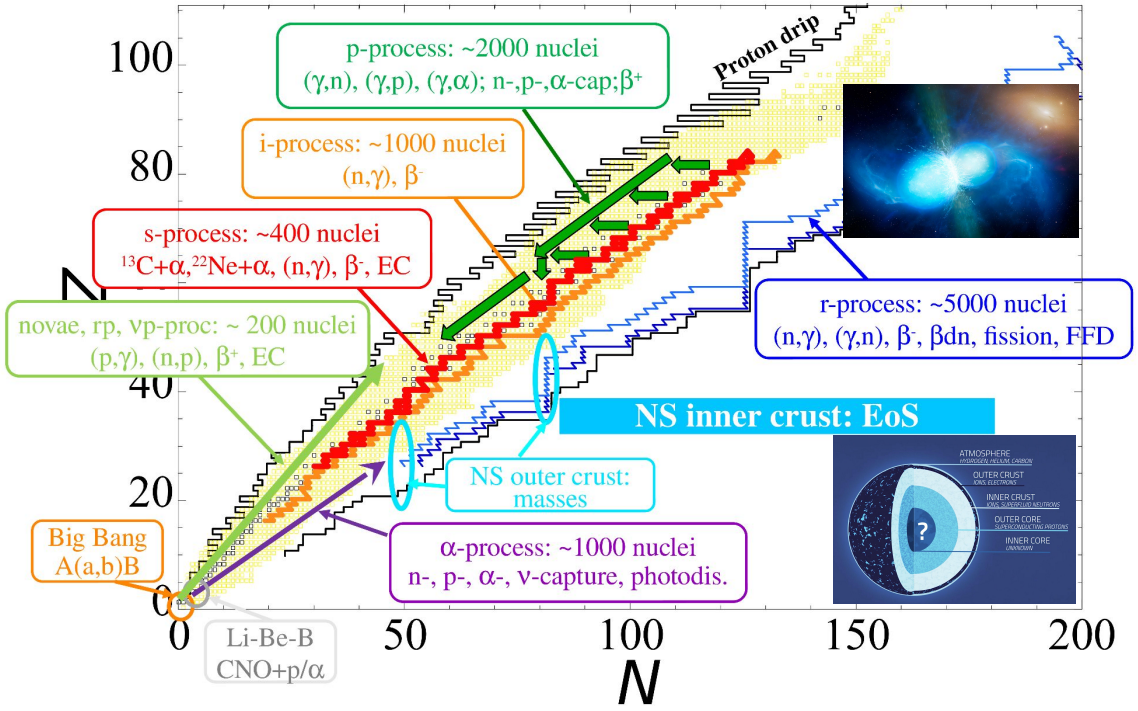
and all of that for
- **~7000** nuclei
- **many** reactions



The nuclear chart and the processes traversing it

Extrapolations in
- nucleon number
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and all of that for
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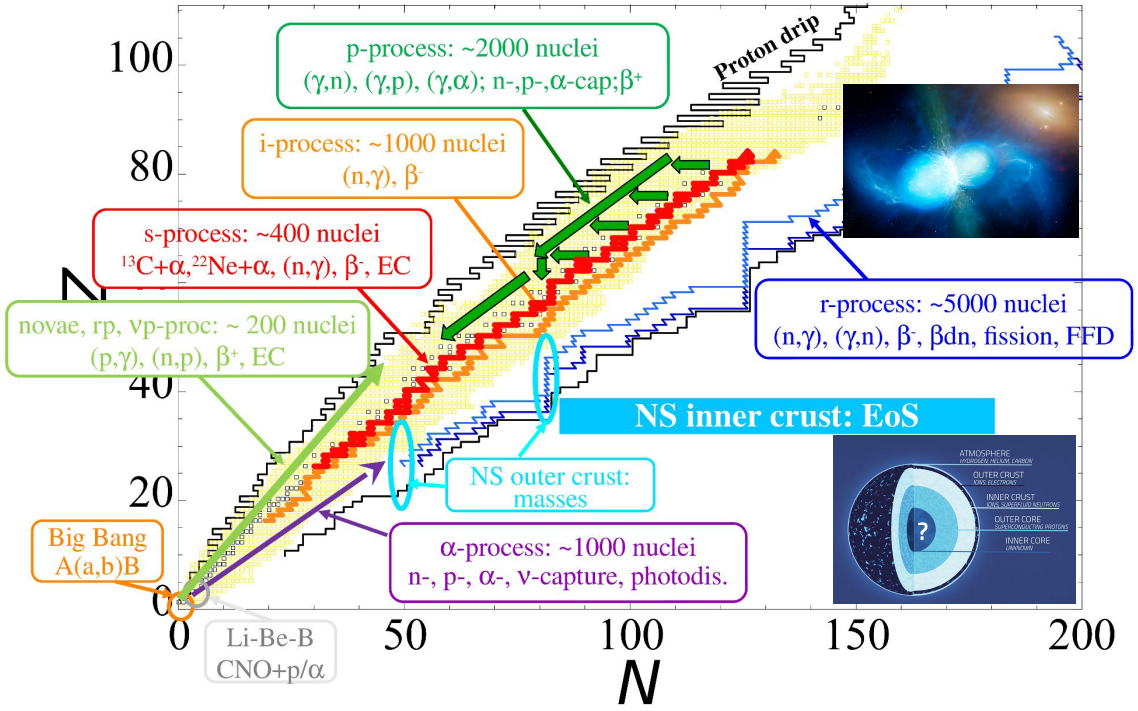
what we need is models that should be

1. **predictive**....
2. but also **complete**



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

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

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

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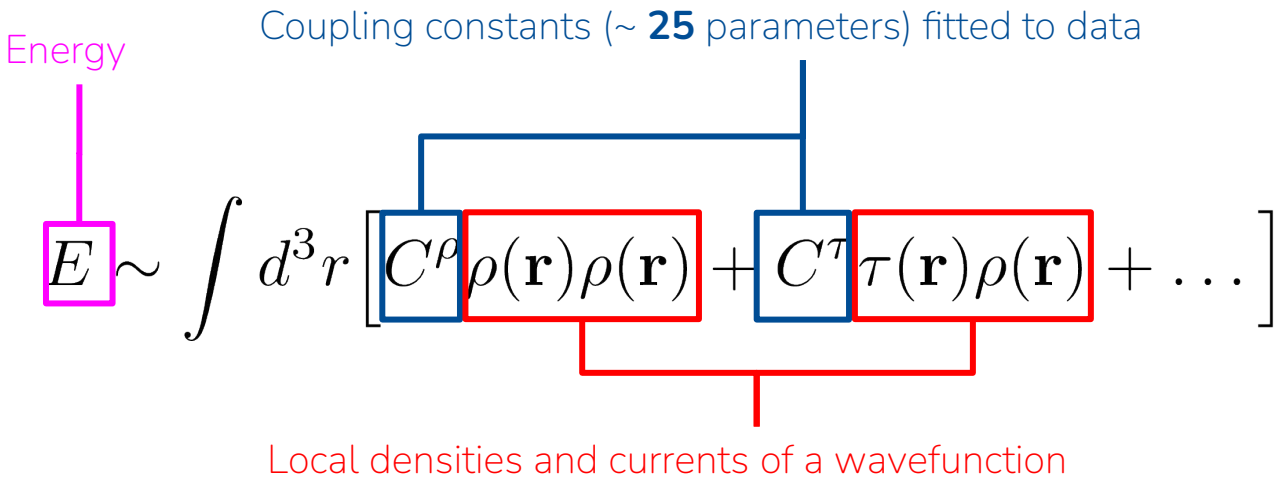

Strong points

- wavefunctions with individual nucleons
- based on “in-medium” N-N interaction
- many observables accessible
- Feasible for ~**7000** nuclei

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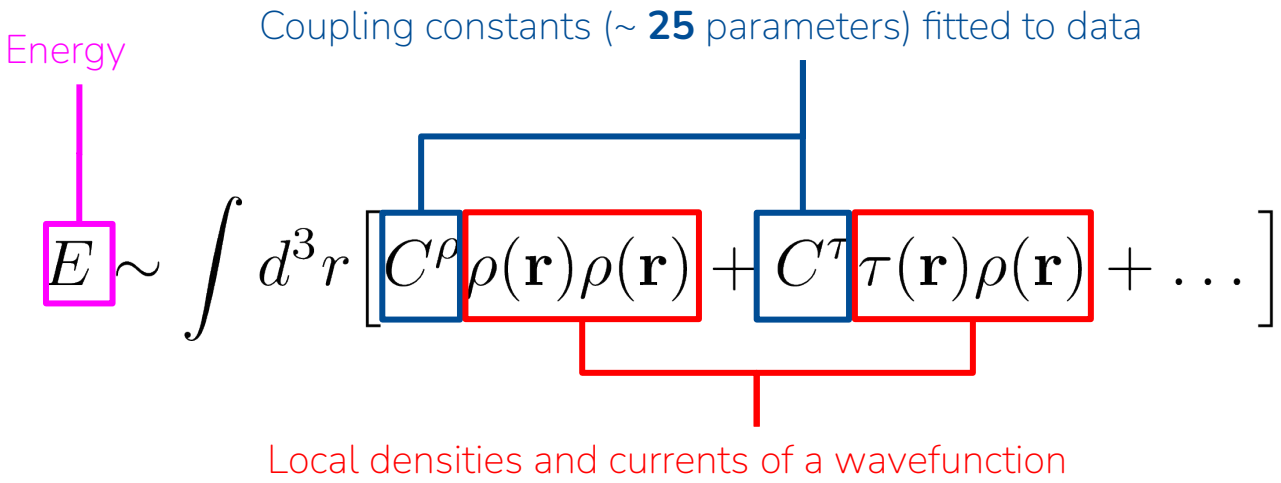

Strong points

- wavefunctions with individual nucleons
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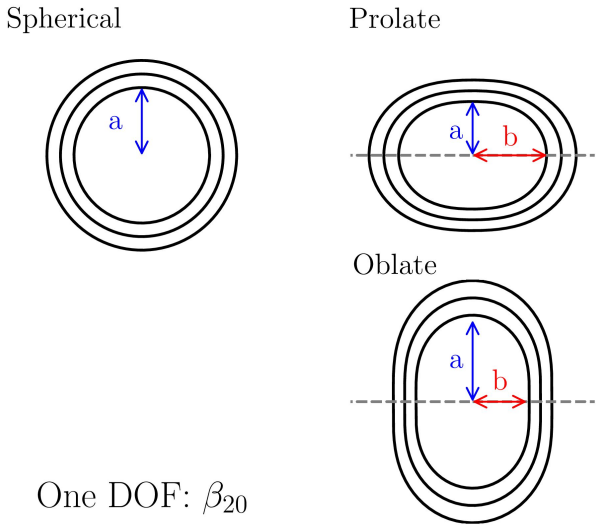
How to move forward?

1. search for a “better” EDF form
2. include more experimental information
3. include more physics in the wavefunction

Large-scale models in 1-2 dimensions

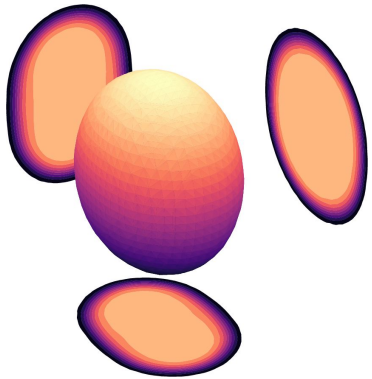


Nuclear deformation

- 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



Symmetry breaking leads to deformation

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More general configurations

- triaxial shapes

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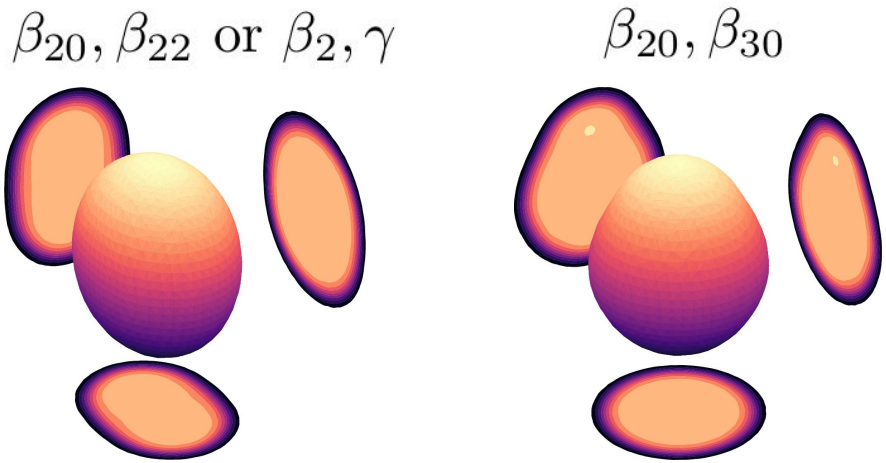

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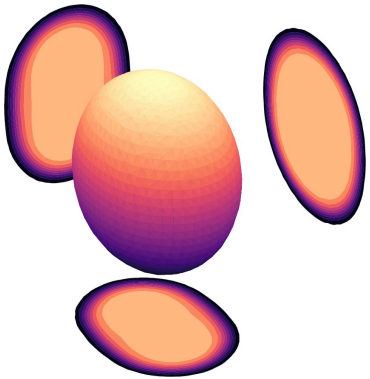
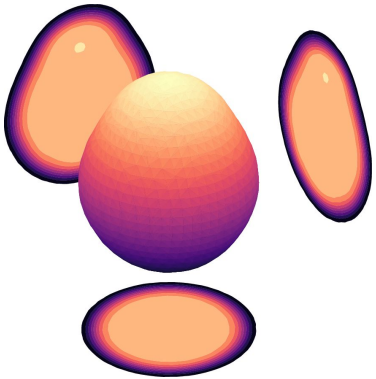
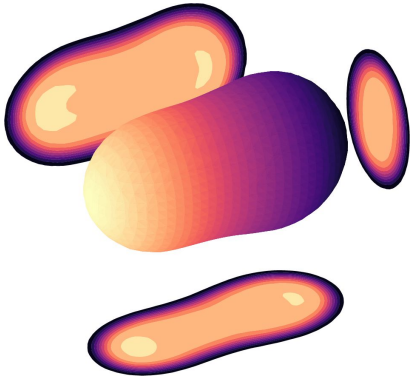


β_{20}, β_{30}



β_{20}, β_{22} **and** β_{30}



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- elongated shapes

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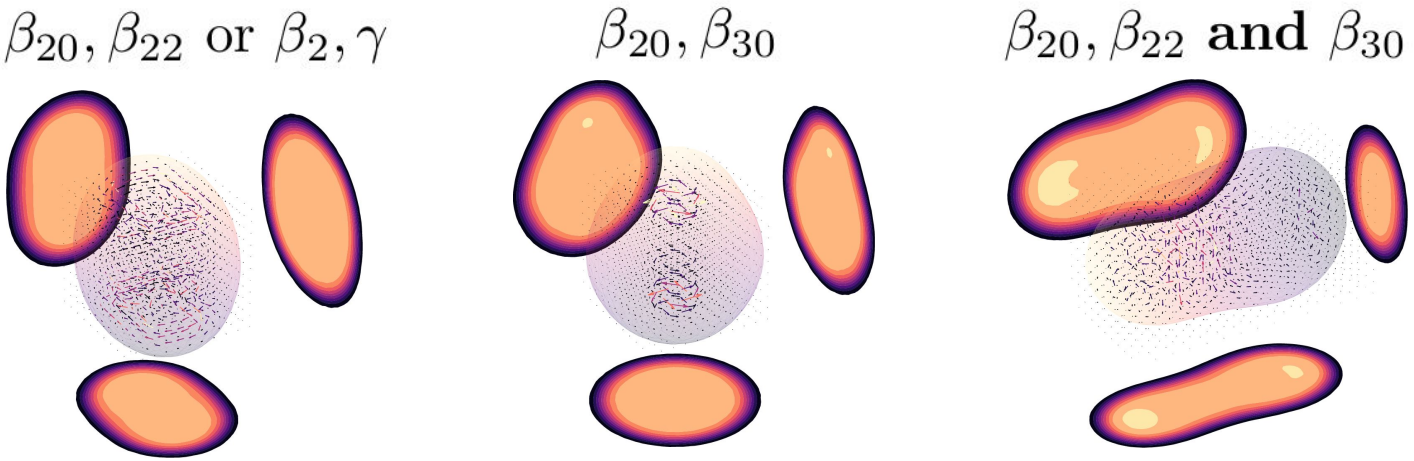

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More general configurations

- triaxial shapes
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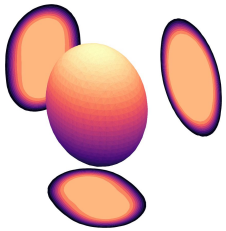
- elongated shapes
- spin densities and currents

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., in preparation.

BSkG1 (2021)

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



Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741		
Radii [fm]	0.024		

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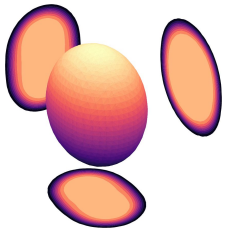

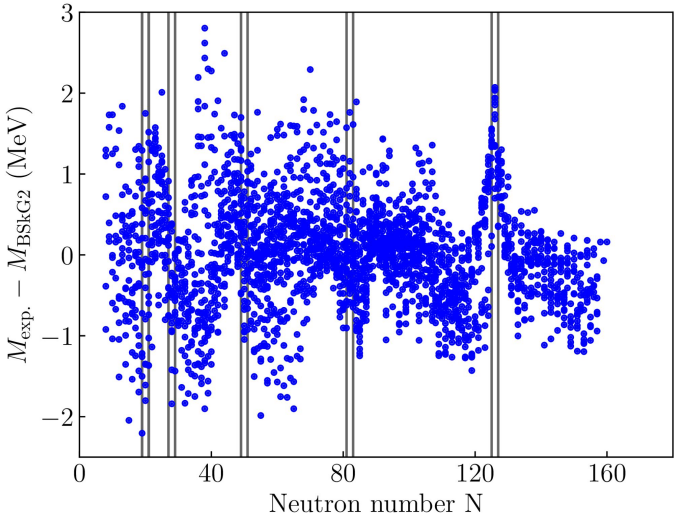

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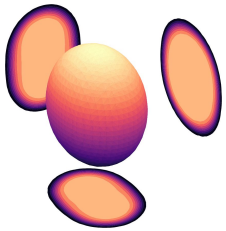
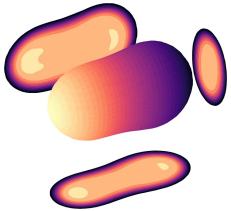
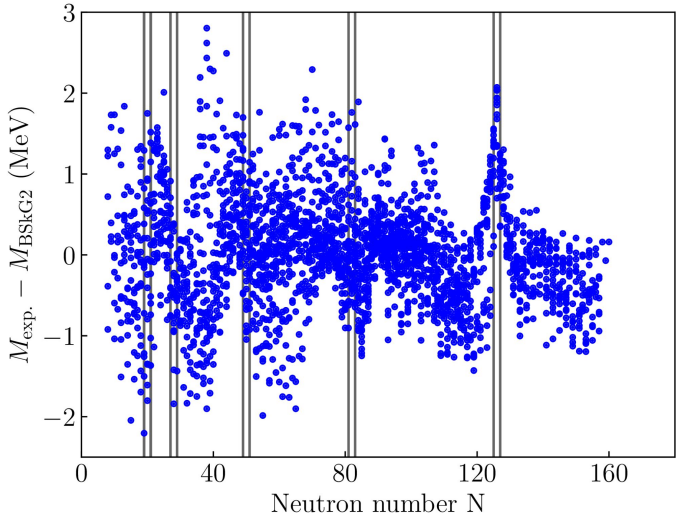


BSkG2 (2022)

- fitted to 45 fission barriers
- includes spins, currents,...





Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	
Radii [fm]	0.024	0.027	
Prim. barriers [MeV]	0.88	0.44	
Secon. barriers [MeV]	0.87	0.47	
Fission isomers [MeV]	1.0	0.49	

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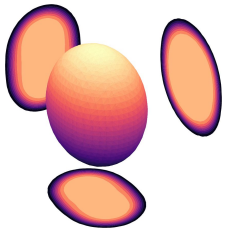

BSkG2 (2022)

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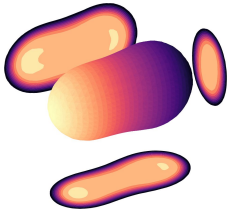
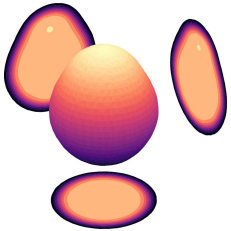
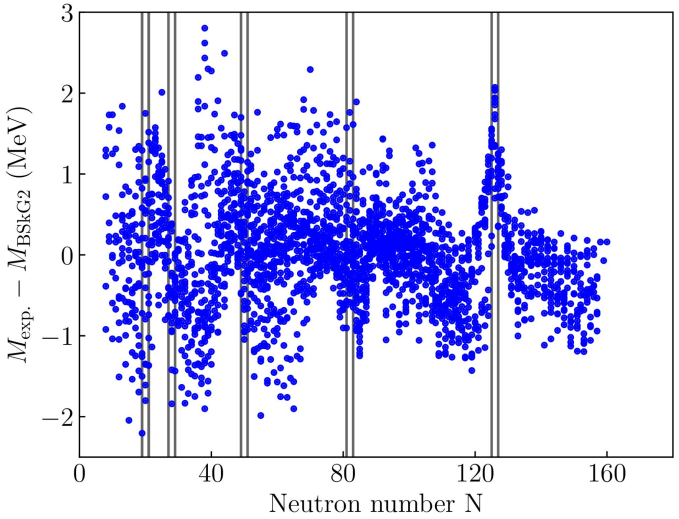


BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation

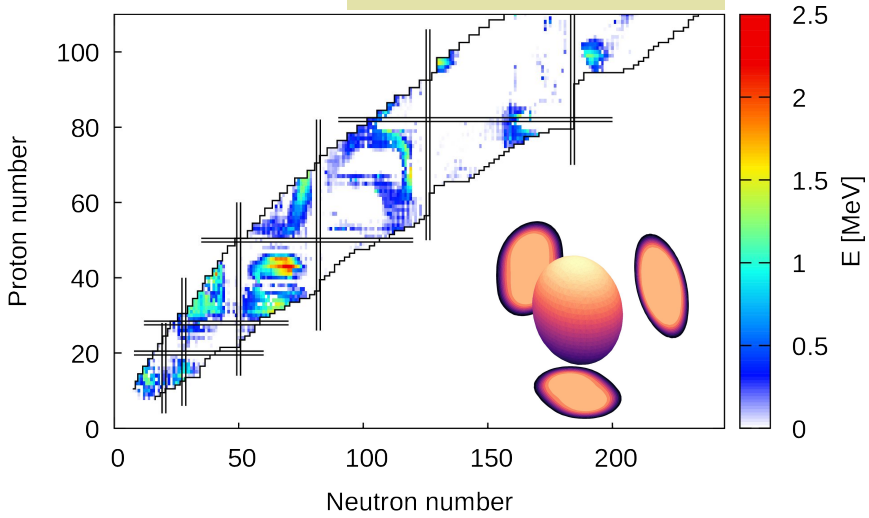




Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
Prim. barriers [MeV]	0.88	0.44	0.33
Secon. barriers [MeV]	0.87	0.47	0.51
Fission isomers [MeV]	1.0	0.49	0.34
Max. NS mass [$M_\odot$]	1.8	1.8	2.3

Masses

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



Triaxial deformation

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

Masses

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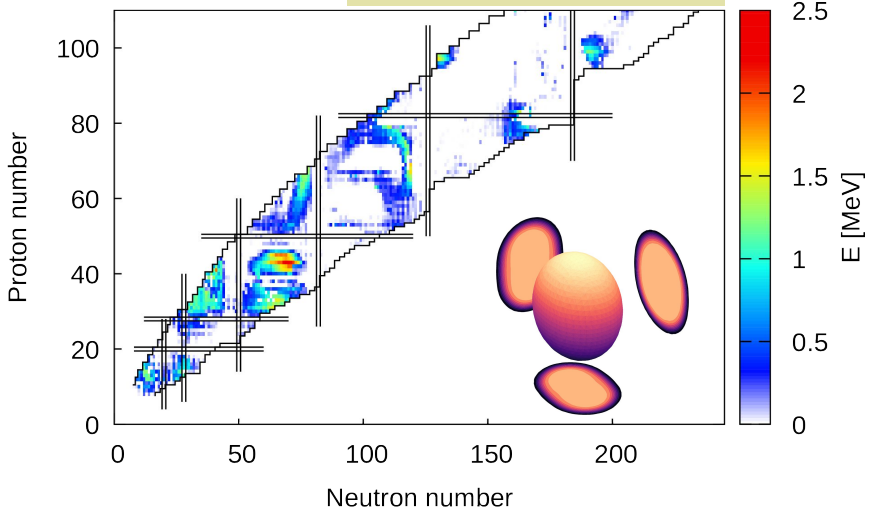
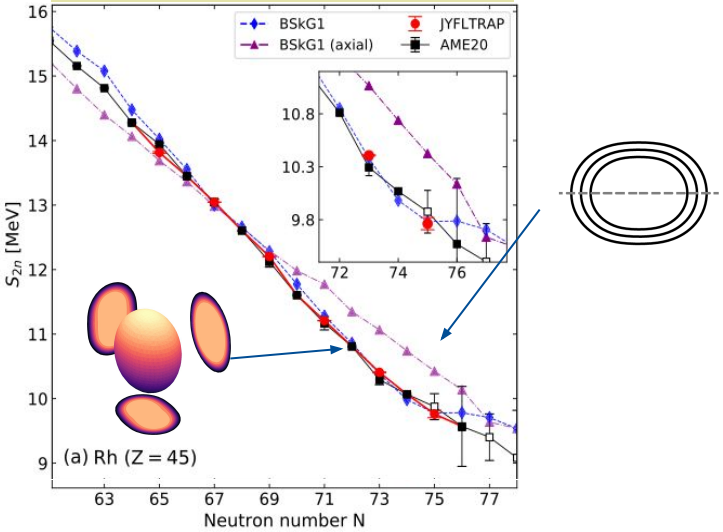


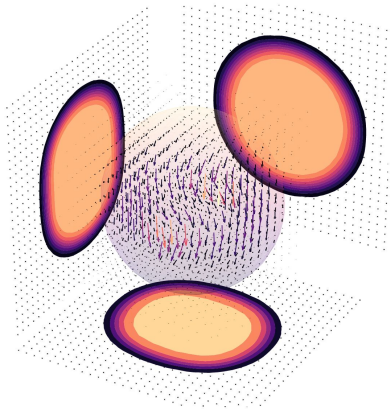
M. Hukkanen, W.R. et al., PRC **107**, 014306 (2023).
Poster by P. Ascher!

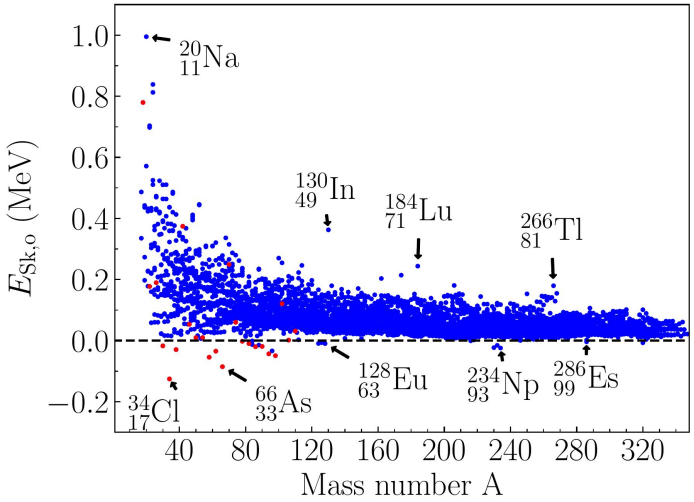


Triaxial deformation

- many nuclei are affected
- effects up to 2.5 MeV near Z~44
- does help reproduce trends, e.g. Rh

Masses



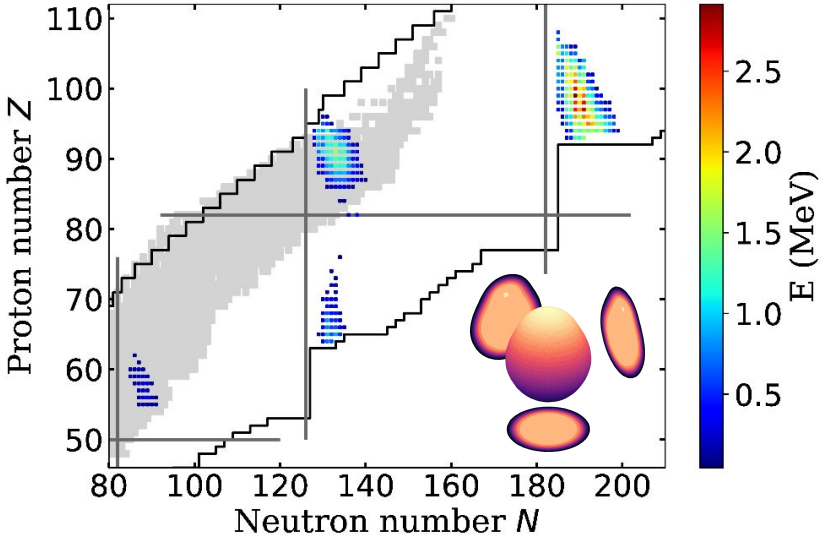


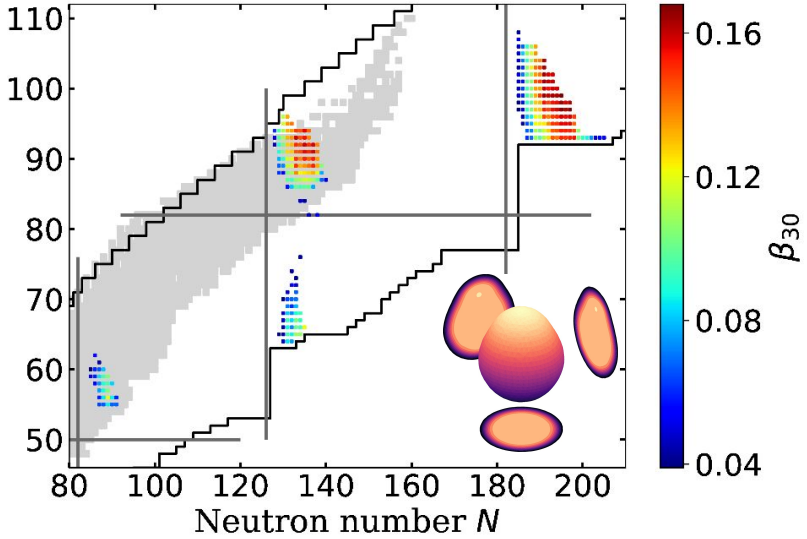
Time-odd terms

- small impact on the masses
- globally repulsive
- first time checked on this scale!
- first step towards other observables

Masses

G.Grams, W.R. et al., in preparation.





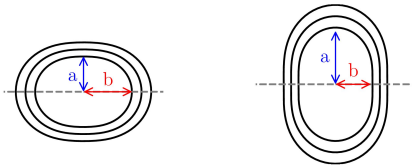
Reflection asymmetry

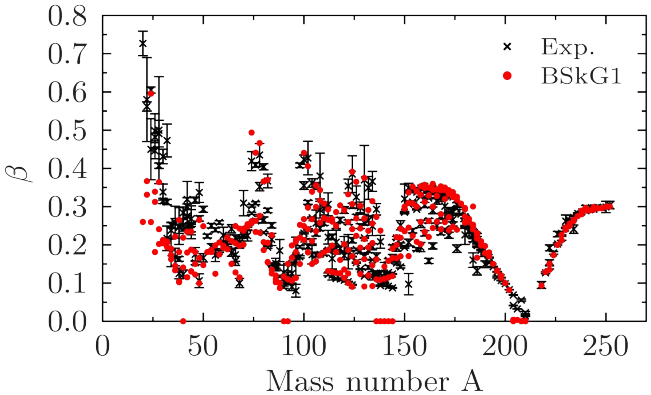
- small number of known nuclei affected
- Near N=184:
  - large effect up to 2.5 MeV
  - dripline modified
  - fission properties modified

Deformations

Deformations

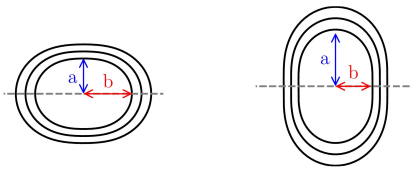
“Ordinary” quadrupole deformation

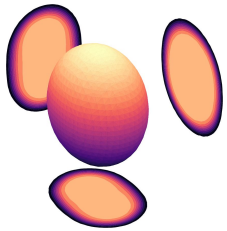


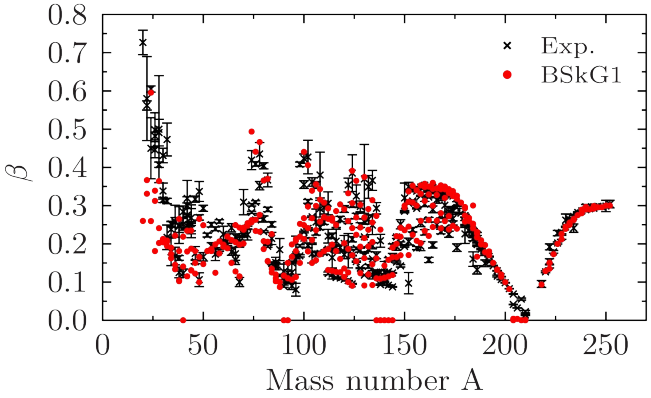


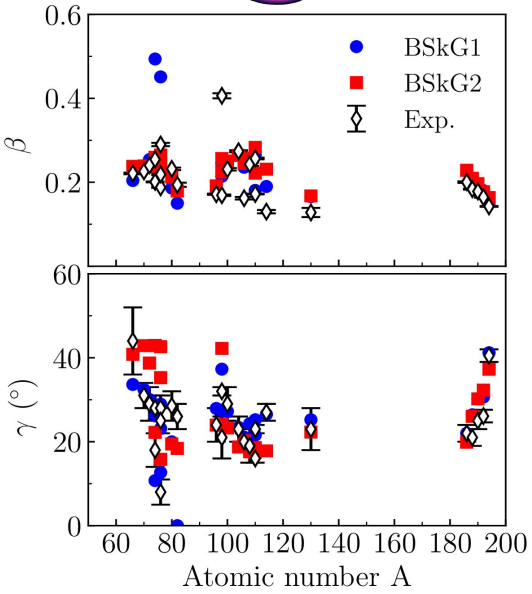
Deformations

“Ordinary” quadrupole deformation … and triaxial deformation …









Deformations

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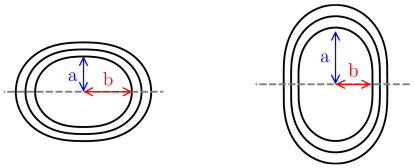
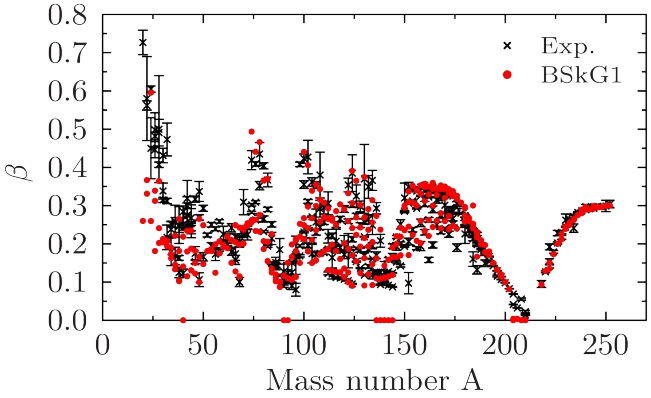
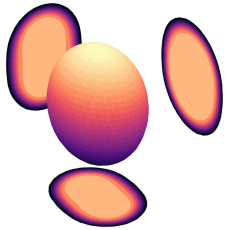
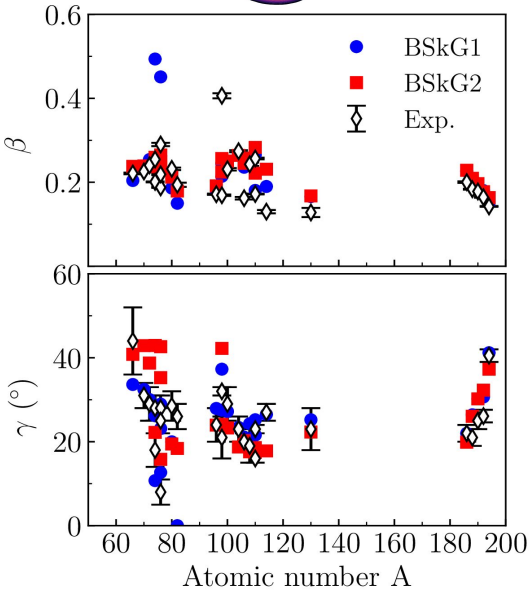


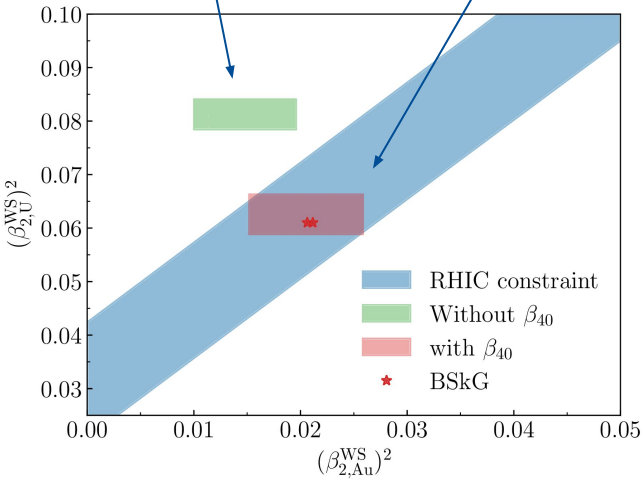


… and triaxial deformation …





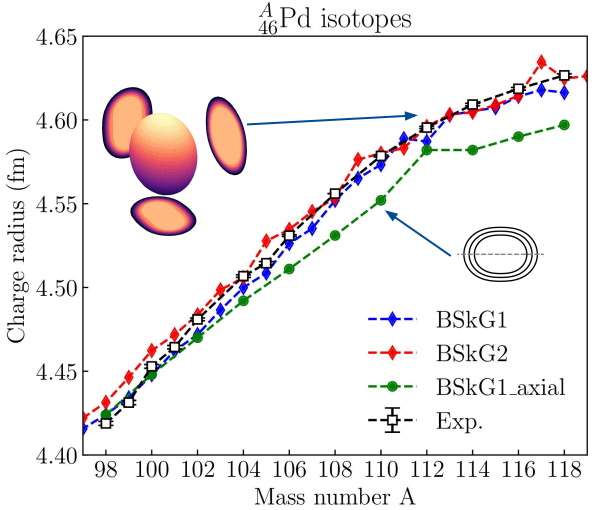
… and even hexadecapole!



W.R. et al., Phys. Rev. Lett. **130**, 212302
Talk by G. Giacalone on Friday!

Radii

S. Geldhof, PRL **128**, 152501 (2022).
Talk by S. Geldhof on Thursday!



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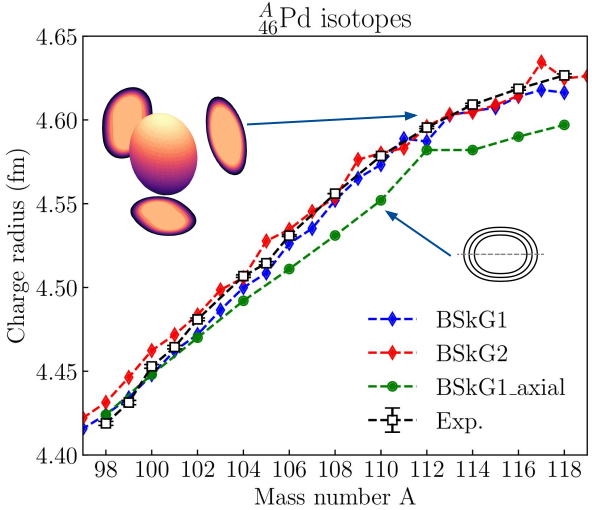
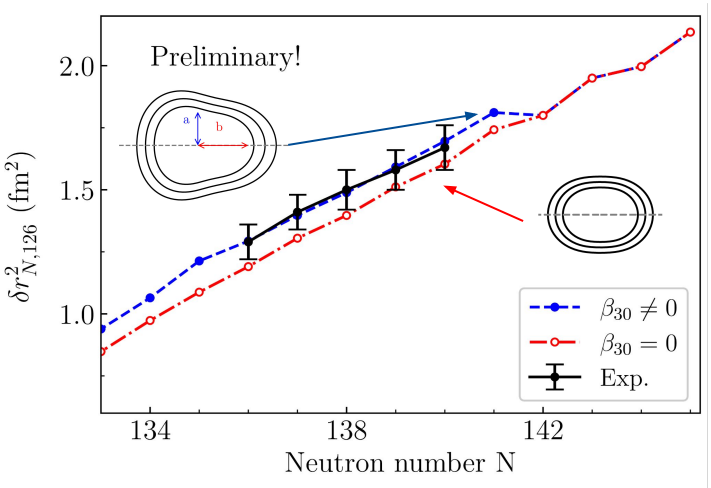
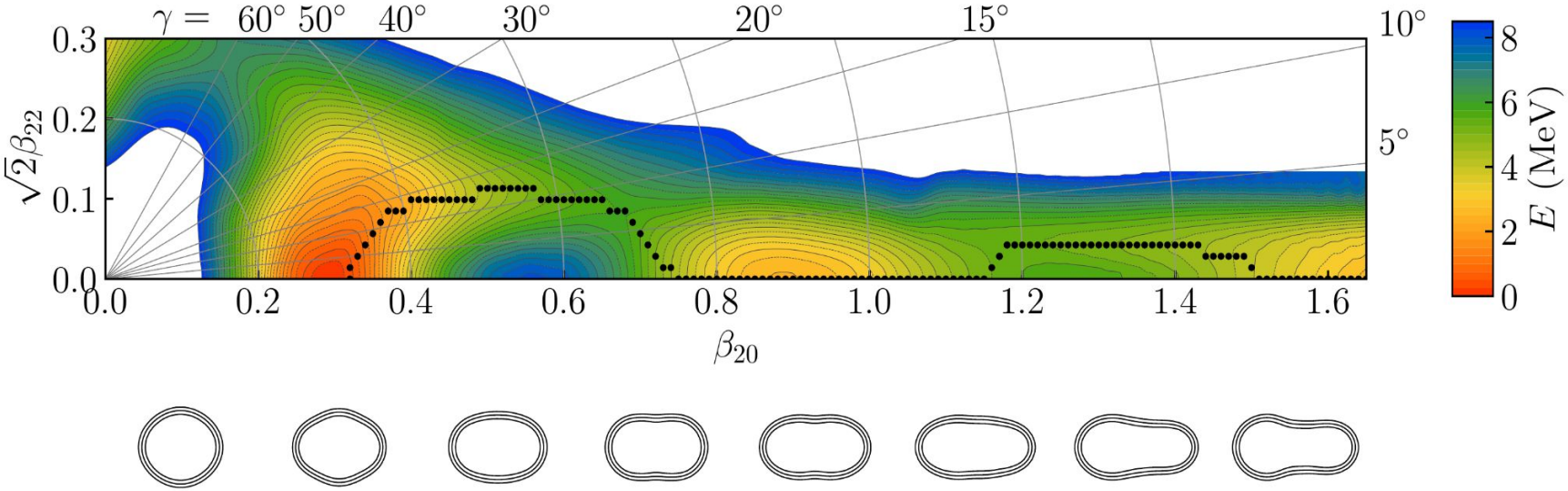


E. Verstraelen, PRC 100, 044321 (2019)



Fission barriers

W. R. et al., EPJA **59**, 96 (2023).



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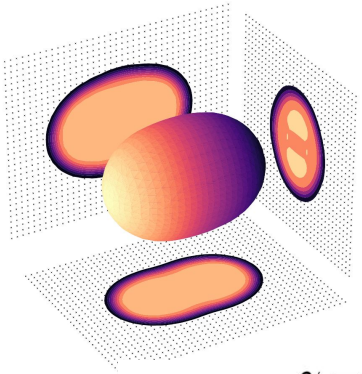

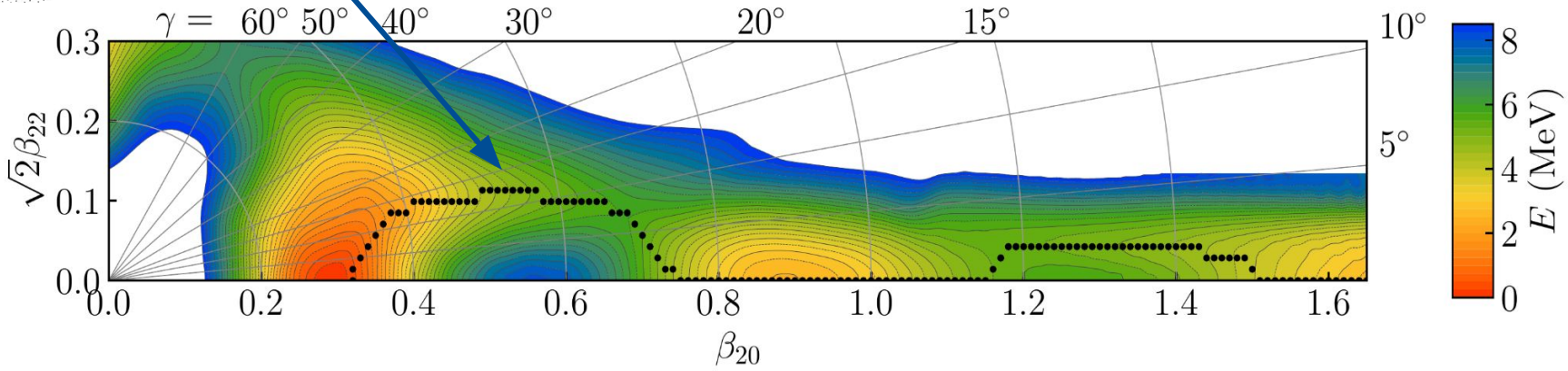

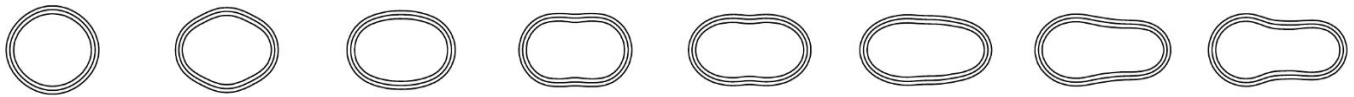

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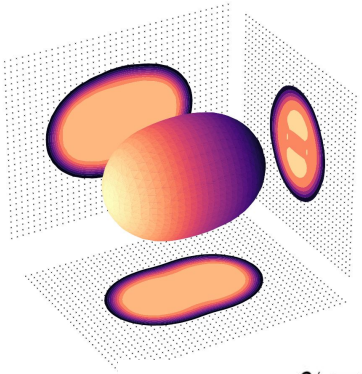

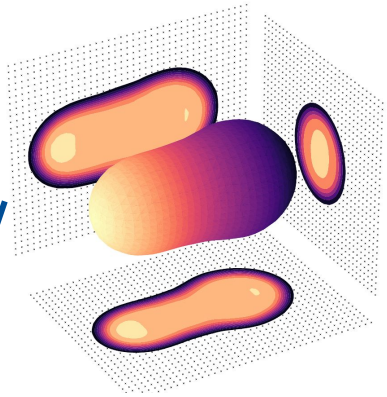

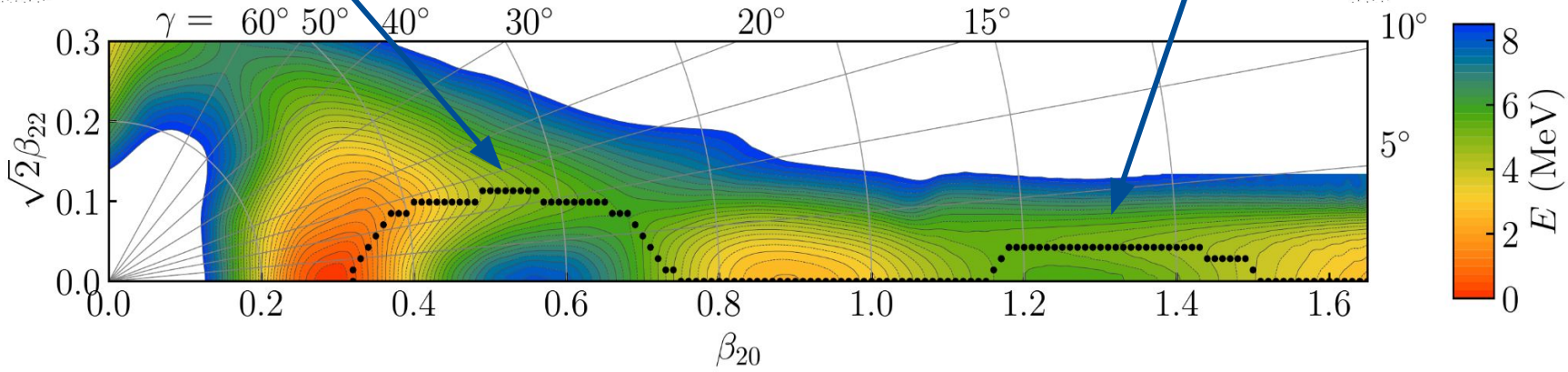

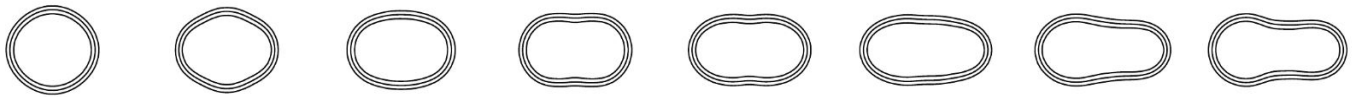

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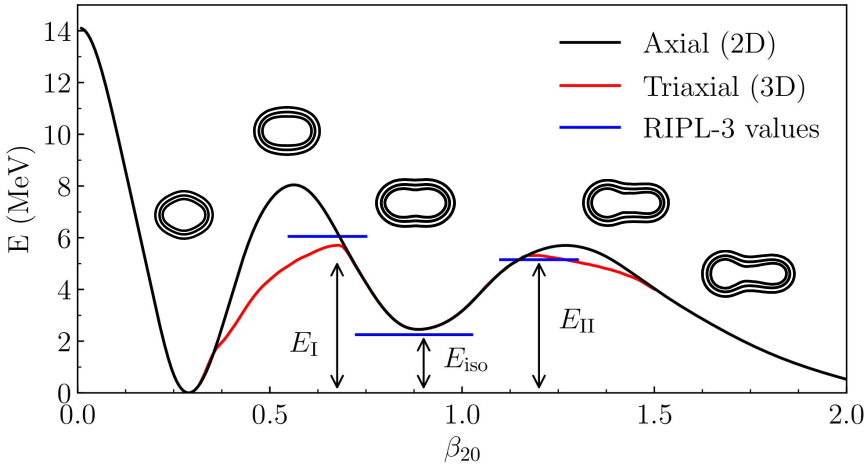

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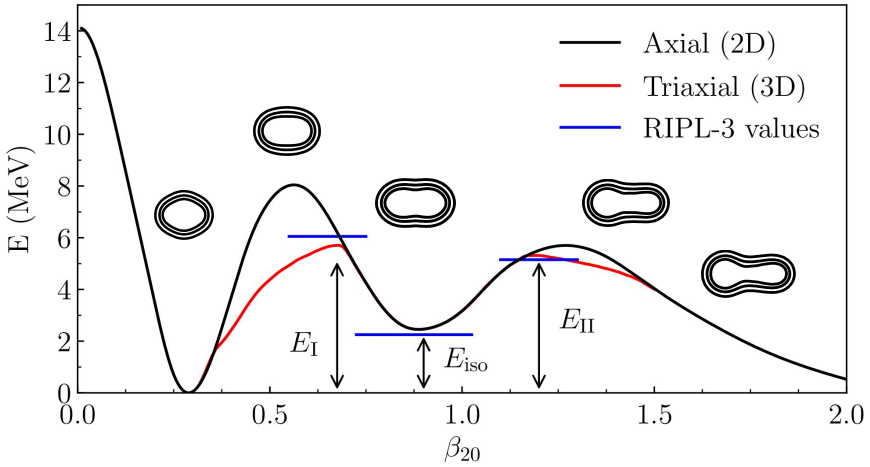


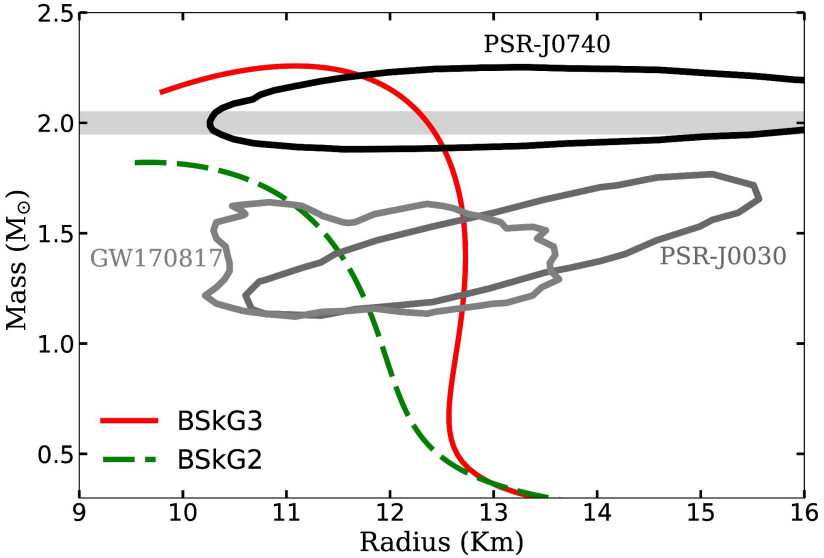
Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
Prim. barriers [MeV]	0.88	0.44	0.33
Secon. barriers [MeV]	0.87	0.47	0.51
Fission isomers [MeV]	1.0	0.49	0.34
Max. NS mass [$M_\odot$]	1.8	1.8	2.3

Fission properties of 45 actinide nuclei

- includes odd-A and odd-odds
- **all** inner barriers exploit triaxiality
- **all** outer barriers exploit
  - octupole deformation
  - triaxial deformation

Neutron stars

G. Grams, W.R. et al., in preparation.



More realistic NS predictions:

- higher maximum mass
  - compatible with NICER
  - compatible with LIGO-VIRGO

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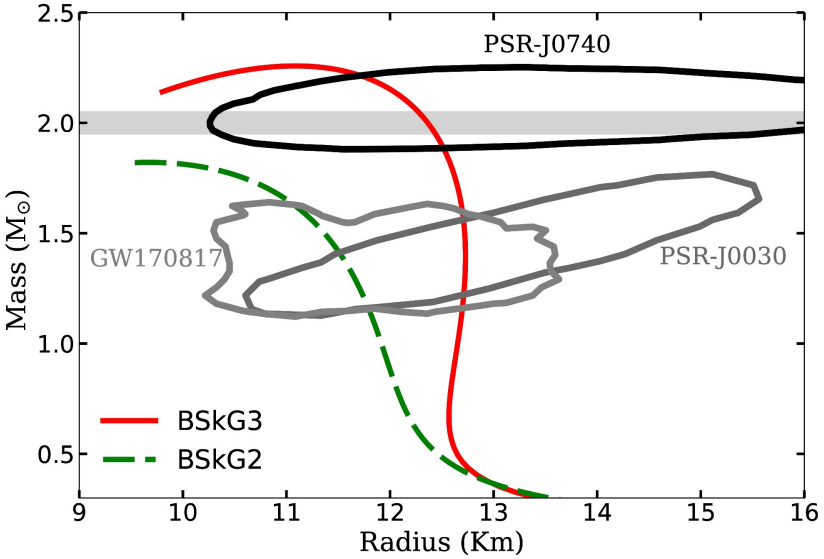
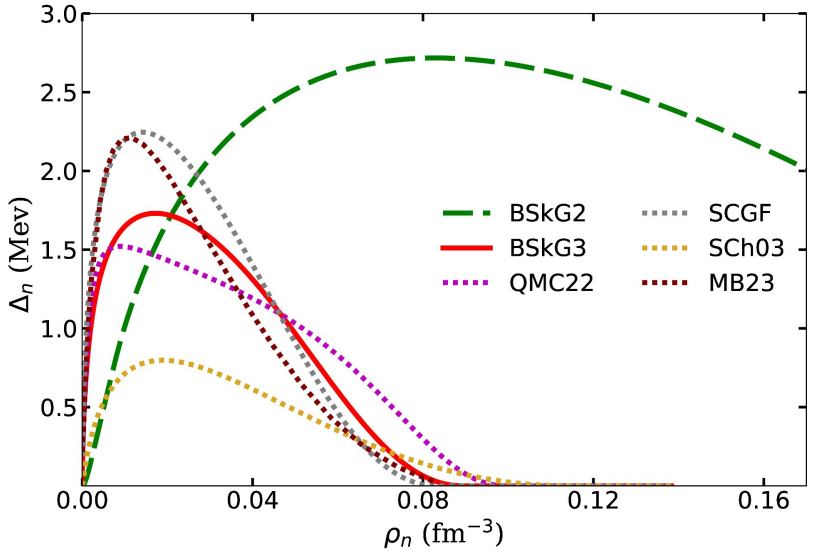
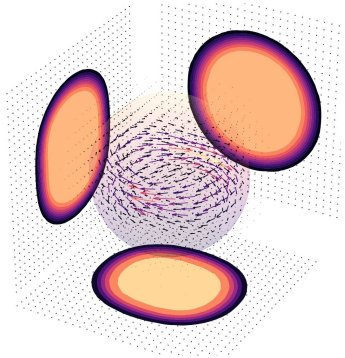




More realistic NS predictions:

- higher maximum mass
  - compatible with NICER
  - compatible with LIGO-VIRGO
- realistic pairing properties in INM
  - constrained to advanced calculations
- .... but not at the cost of finite nuclei!

Additional observables



A. R. Vernon et al., Nature 607, **260** (2022),
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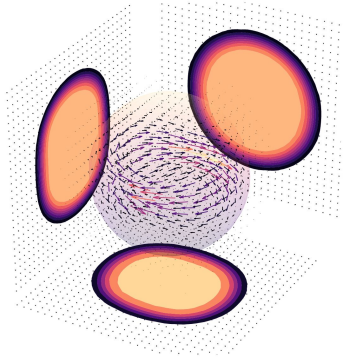

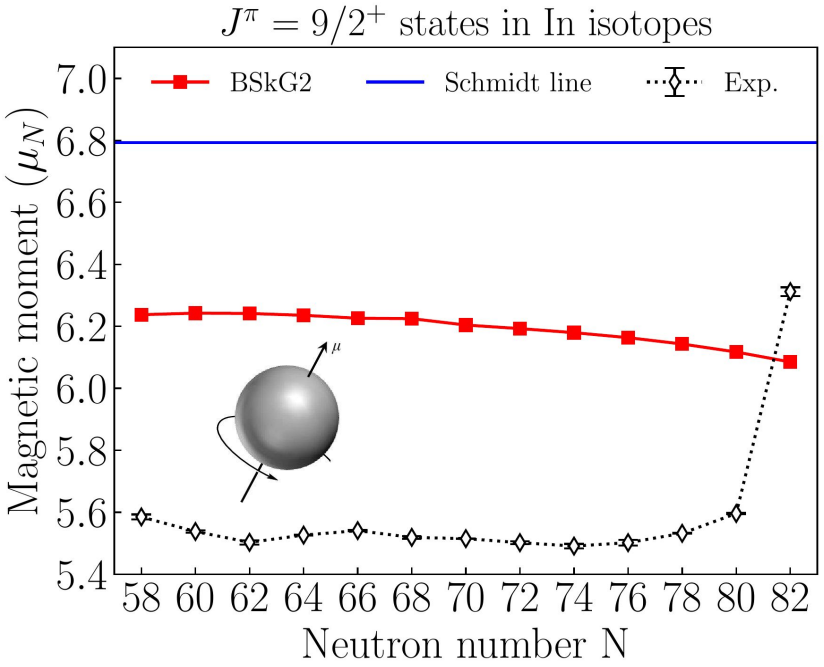

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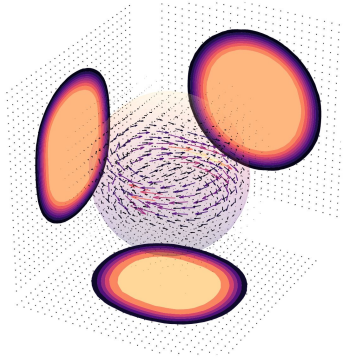
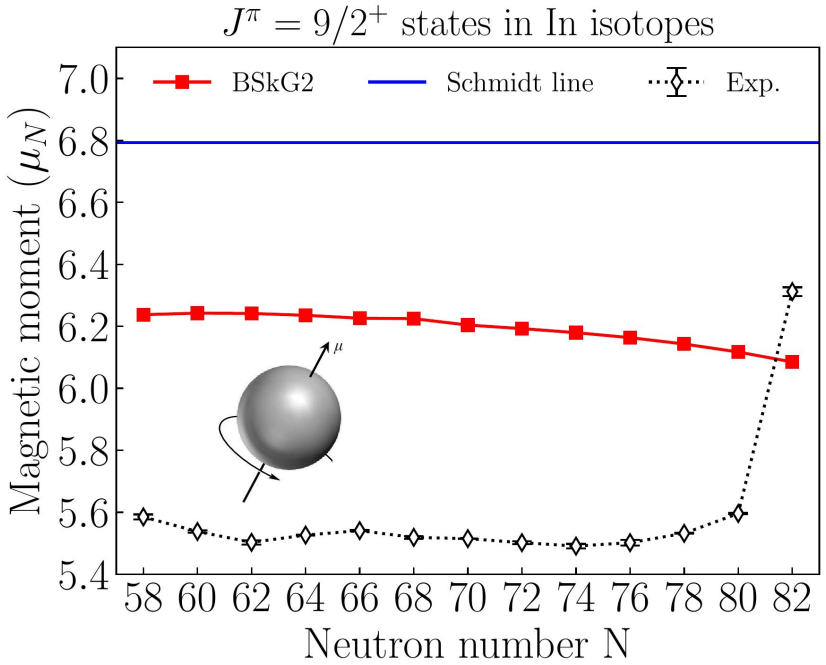
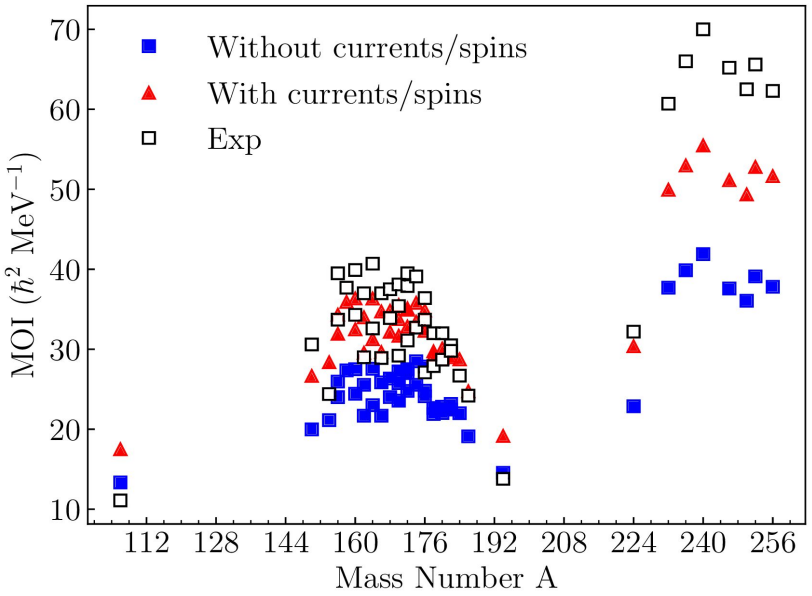
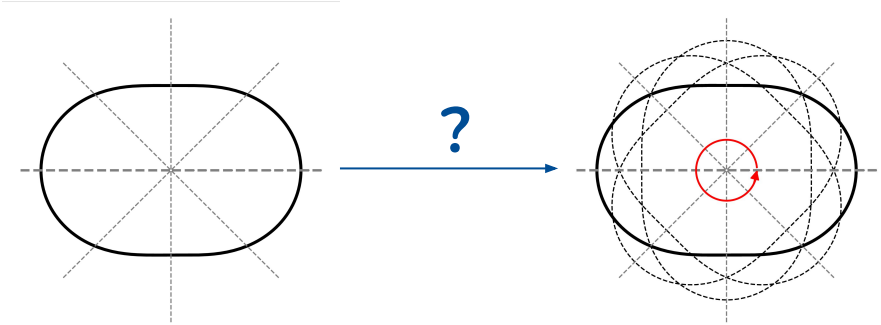






Challenges: less phenomenology



Leave the mean-field picture behind

- techniques exist
- … but remain extremely costly

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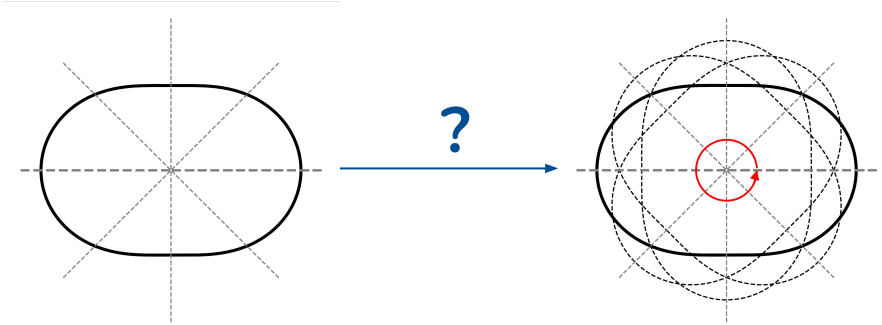

$$E \sim \int d^3r \left[C^\rho \rho(\mathbf{r})\rho(\mathbf{r}) + C^\tau \tau(\mathbf{r})\rho(\mathbf{r}) + \textbf{?}\,. \right]$$

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A “well-founded” functional

- traditional EDF forms are wearing out
- ways for **systematic** construction?
- … perhaps by linking with ab initio?

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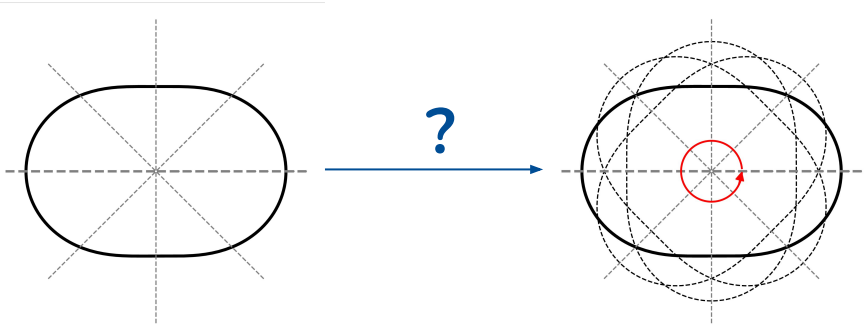

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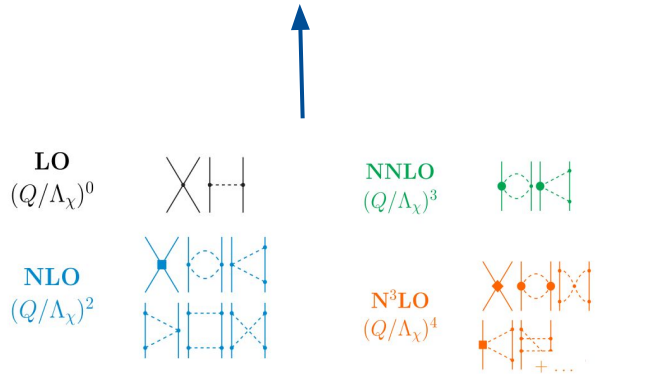

Adapted from H. Hergert, Front. Phys. 8:379 (2020).

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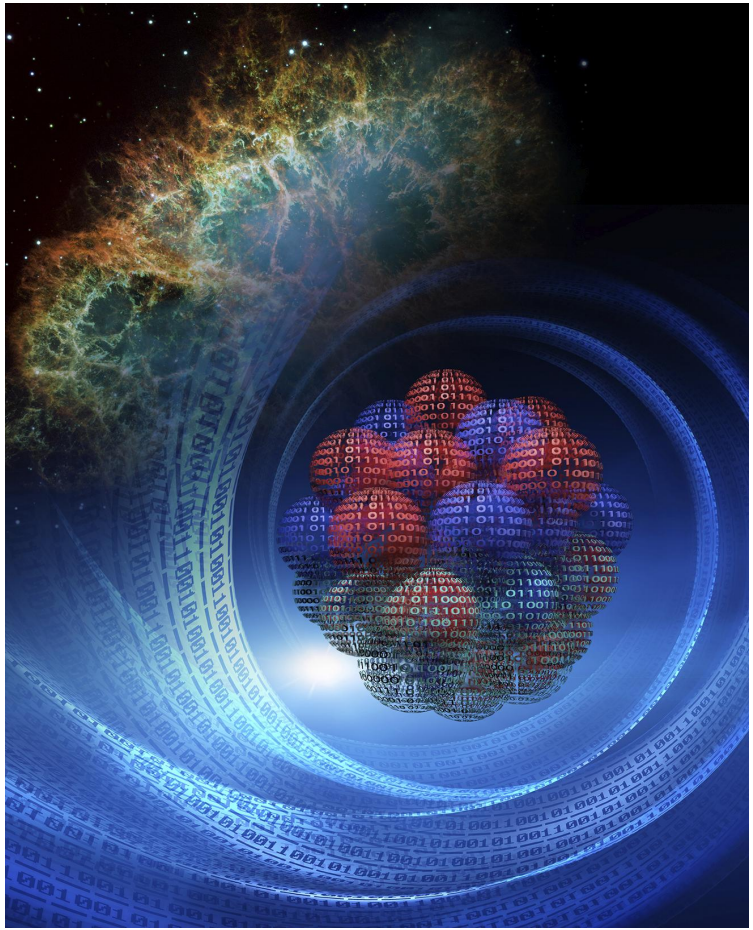

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Large-scale = **thousands** of nuclei and **many observables.**
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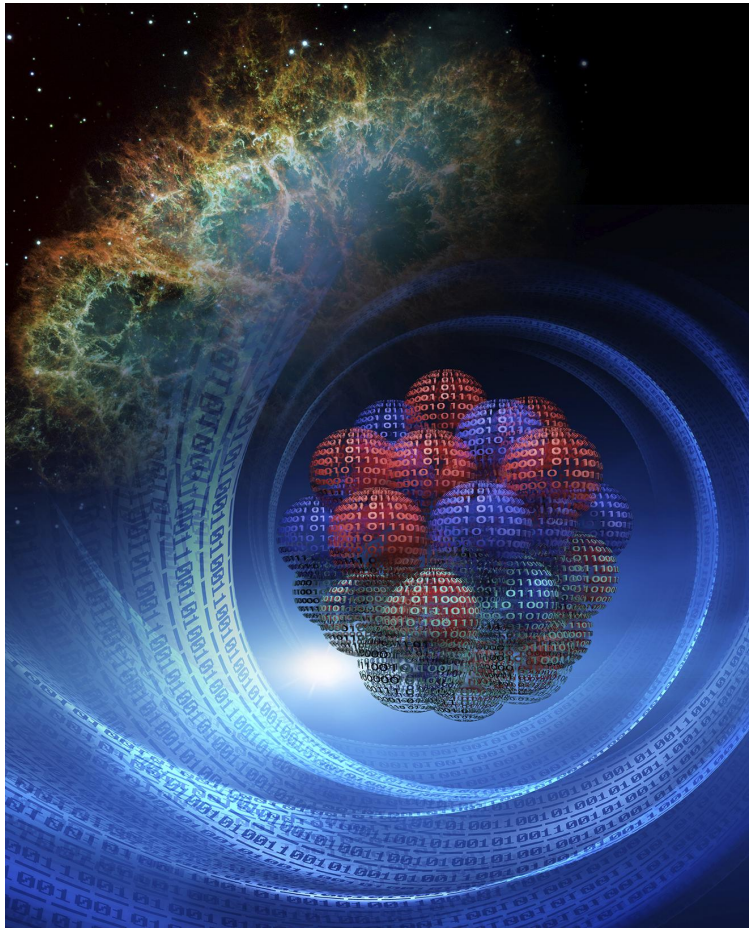

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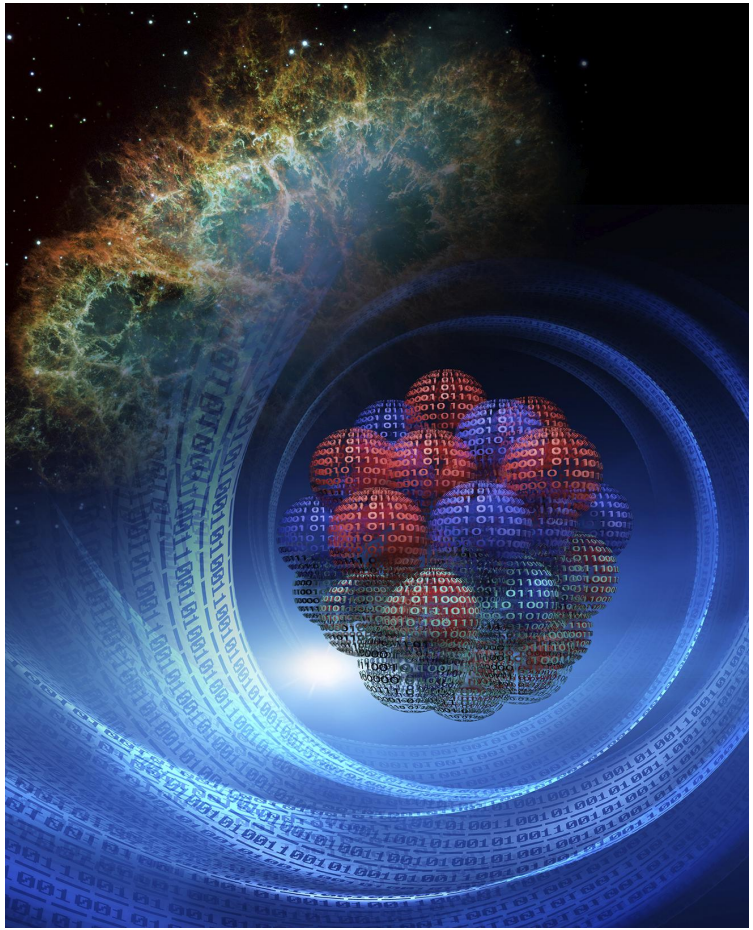

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BSkG3

- global inclusion of
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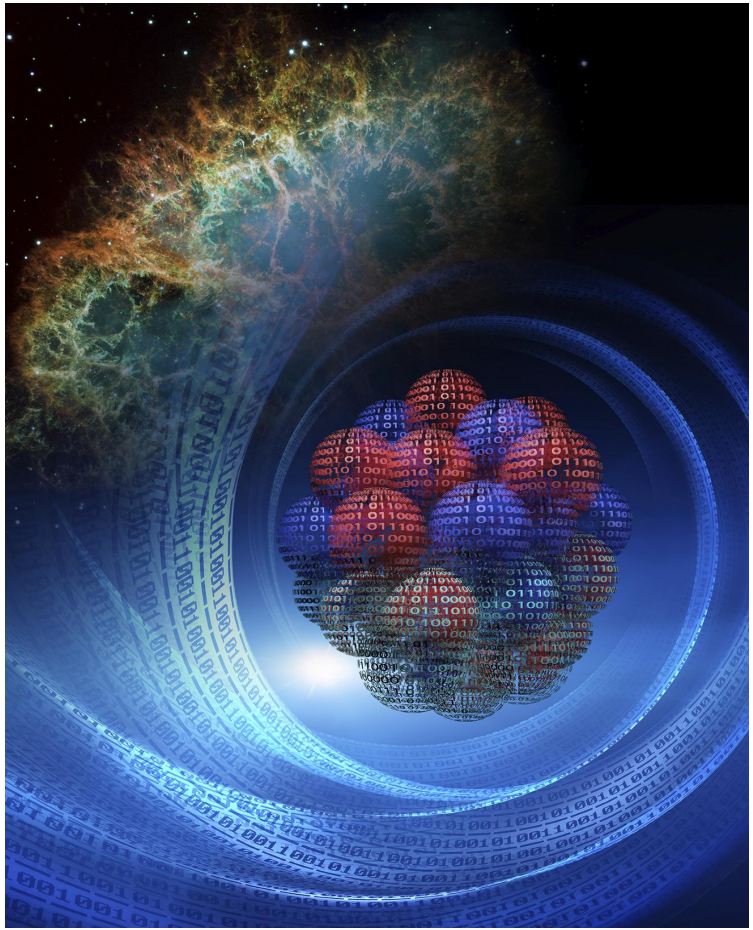
  - time-reversal breaking
  - octupole deformation

- competitive reproduction of masses and charge radii
- best on the market for **fission** properties
- consistent with astrophysical observations



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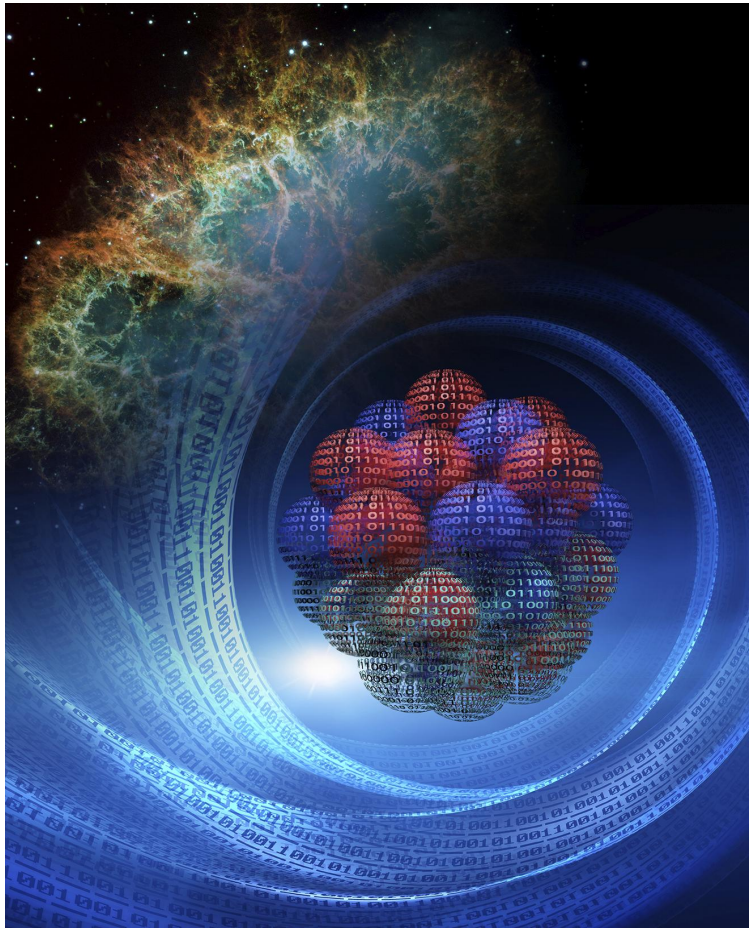
Coming up from the Brussels group:

- all BSkG3 data
- detailed study of ground state densities
- large-scale **fission** and **level density** calculations
- unified Equation of State for neutron star applications



Thank you for...

..... all the wonderful work!

S. Goriely
G. Grams
N. Chamel
N. Shchechilin

M. Bender
J. Bonnard

G. Scamps

M. Hukkanen
M. Stryjczyk
A. Kankainen

P. Ascher
S. Grévy

E. Verstraelen
T. Cocolios
P. Van Duppen

G. Giacalone

B. Schenke
C. Shen

S. Hilaire

..... the computing time!

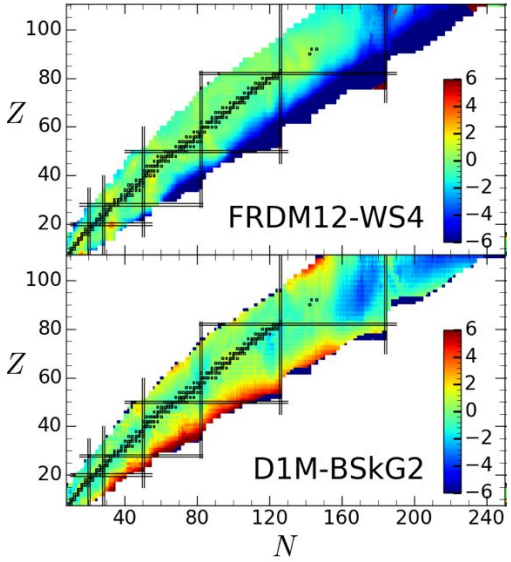
..... the funding!

..... your attention!

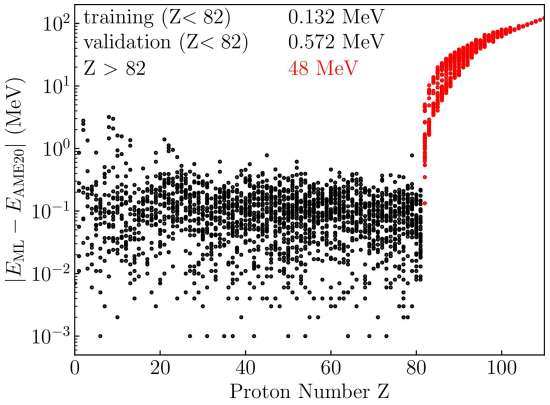
Bonus!

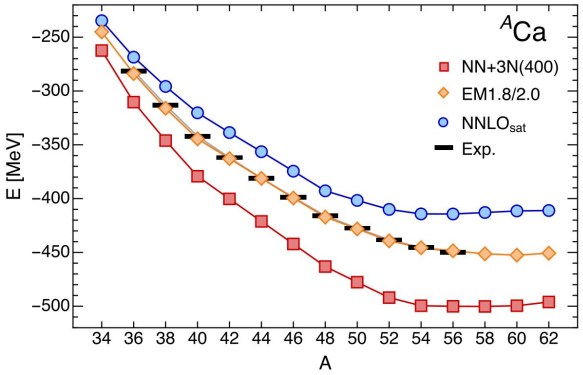
Interlude: why do we do these complex things?

S. Goriely, EPJA 59, **16** (2023).



G. Grams, W.R. et al., in preparation





Mic-mac approaches?

- ✅ competitive in rms
- ✅ multiple observables
- ❌ comparatively unstable
- ❌ no link mic. <-> mac.

Machine learning?

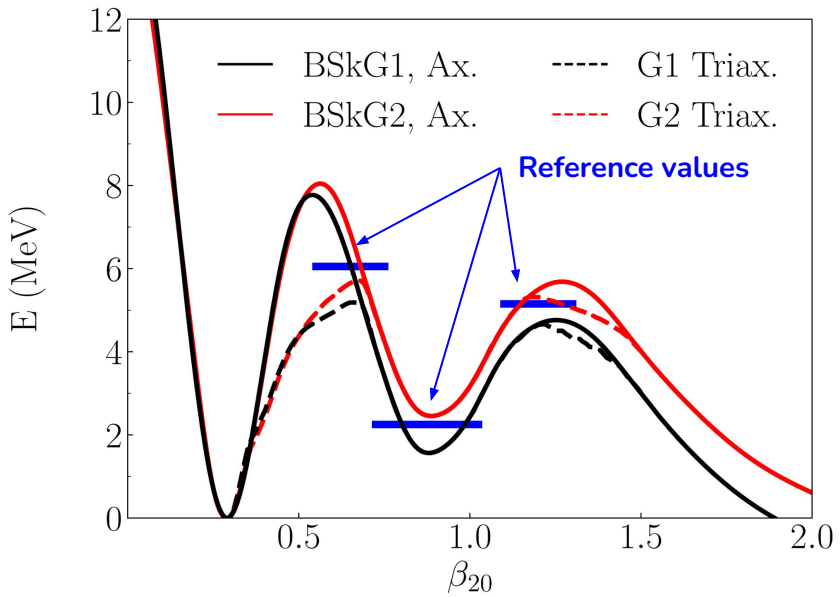
- ✅ absolute champion in rms
- ✅ ridiculously easy
- ❌ thousands (?) of parameters
- ❌ single observable

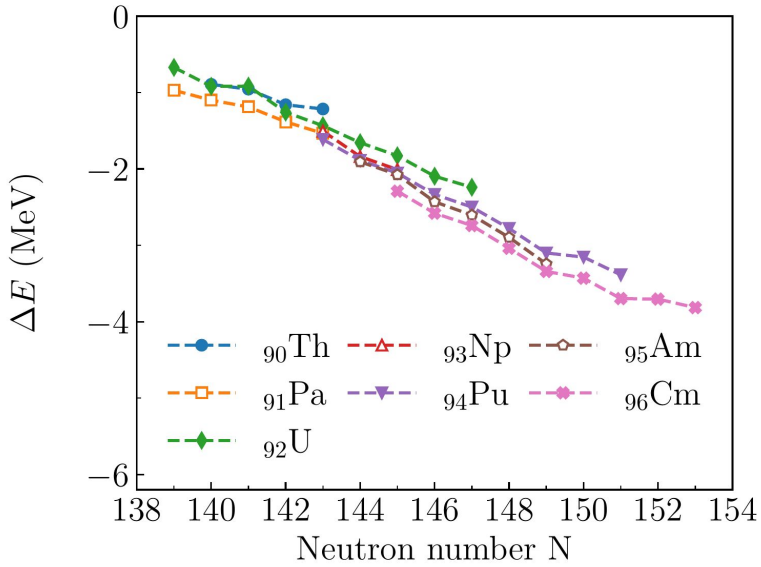
Ab Initio?

- ✅ error quantification
- ✅ “truly” microscopic
- ✅ multiple observables
- ❌ infeasible at scale (for now)
- ❌ not competitive on rms (for now)

Triaxiality has a **large** effect on barriers

Reference values from R. Capote et al.,Nuclear Data Sheets **110**, 3107 (2009).





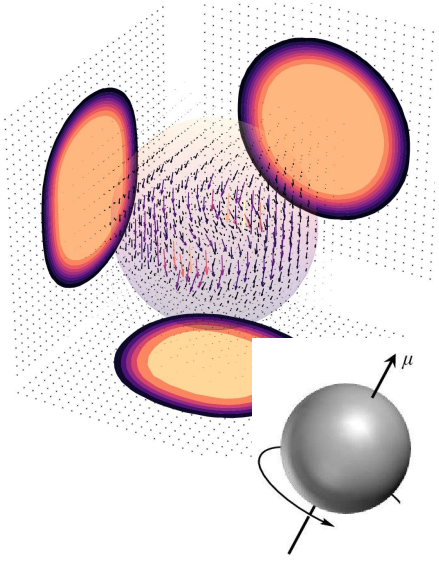
Triaxial deformation for 240Pu

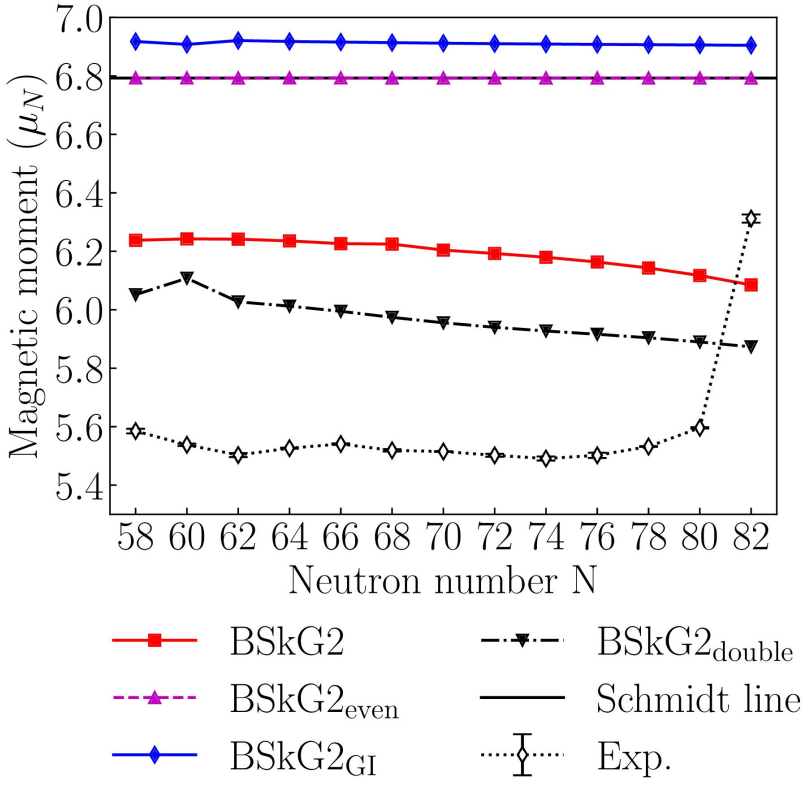
- Large effect on inner barrier
- No effect on isomers
- Modest effect on outer barrier

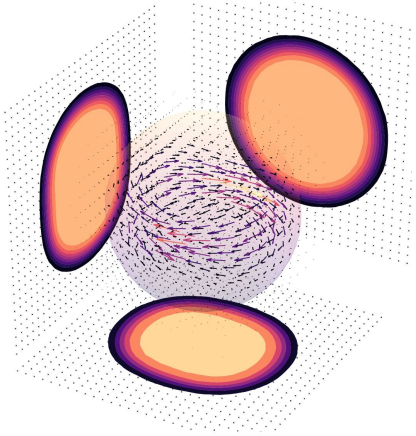
Triaxial deformation for actinides

- Larger effects with growing N
- reminder: **σ(fission) < 0.5 MeV**
- what other regions does it affect?

Magnetic moments

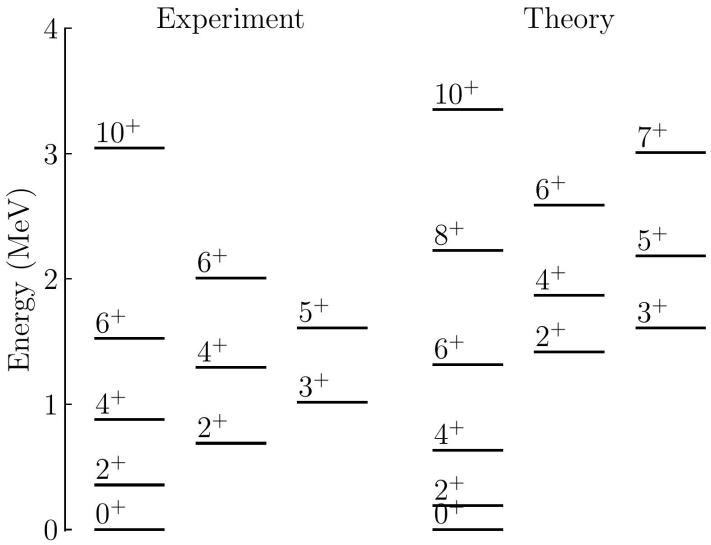


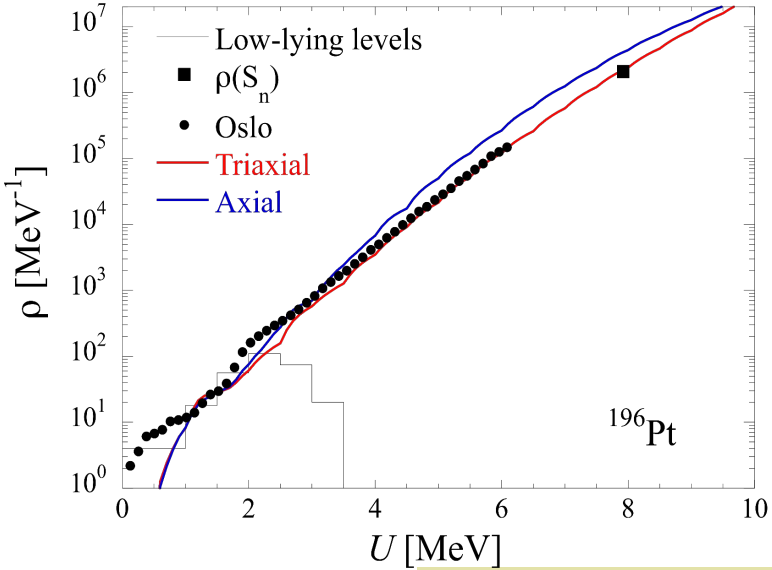




A. R. Vernon et al., Nature 607, 260 (2022).
J. Eberz et al., NPA 464, 9 (1987).

What is the effect on **nuclear level densities?**





Broken symmetries impact NLDs

- **axial** rotors give rise to **sparse** spectra
- **triaxial** rotors have **dense** spectra
- simple models for collective effects

Level densities with BSkG2

F. Giacoppo et al., PRC 90, 054330 (2014).

- not always higher level density
- but a **different energy dependence**!
- systematic calculations underway