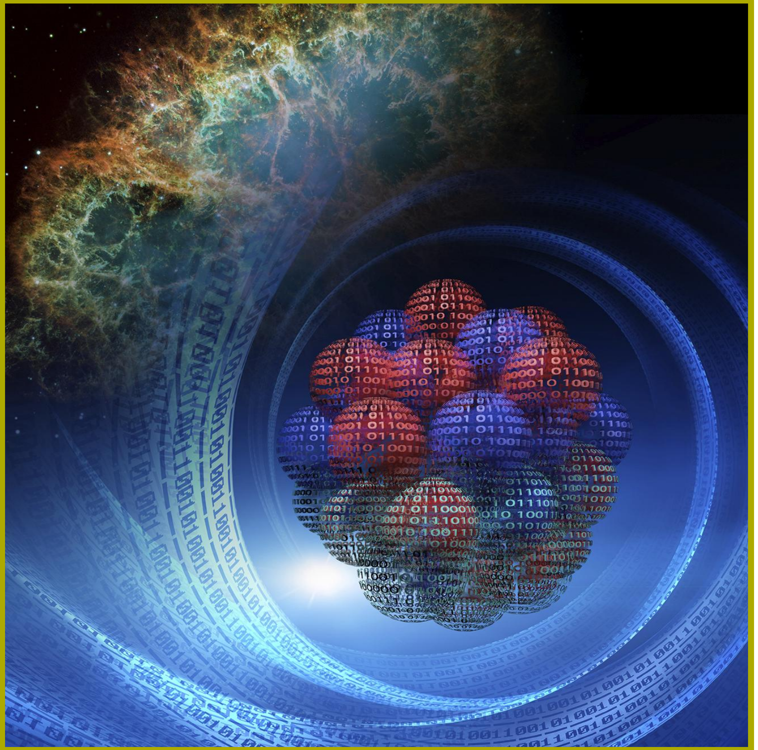
WOUTER RYSSENS



Andy Sproles, ORNL

Microscopic models of nuclear structure: from dripline to dripline

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

3th of July 2023

wryssens.com

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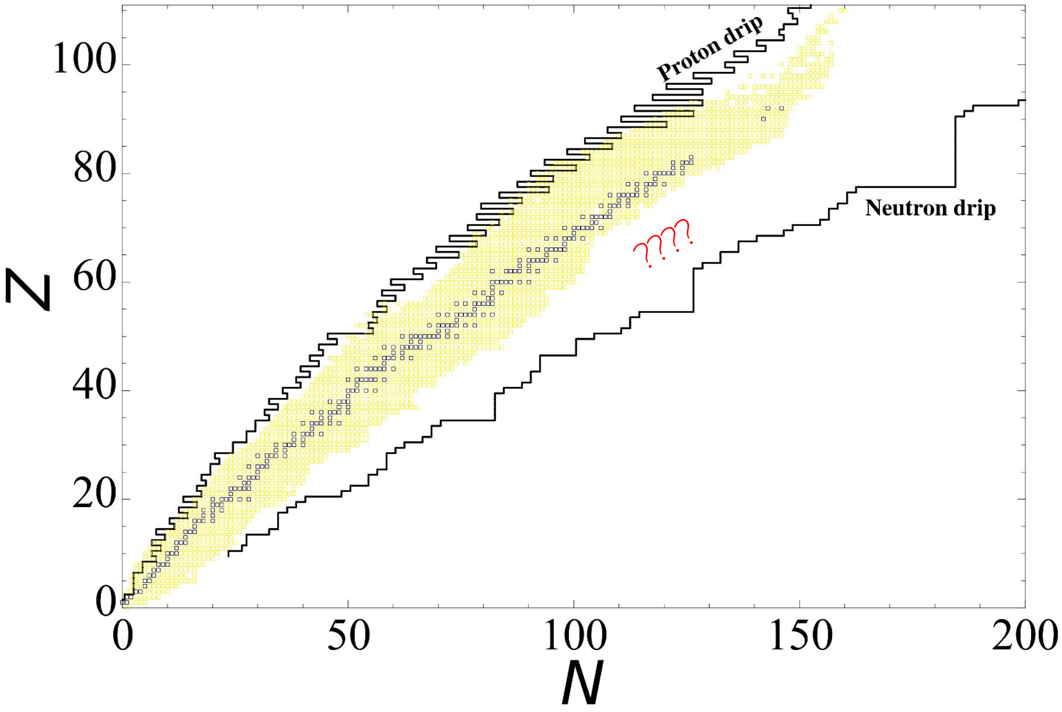
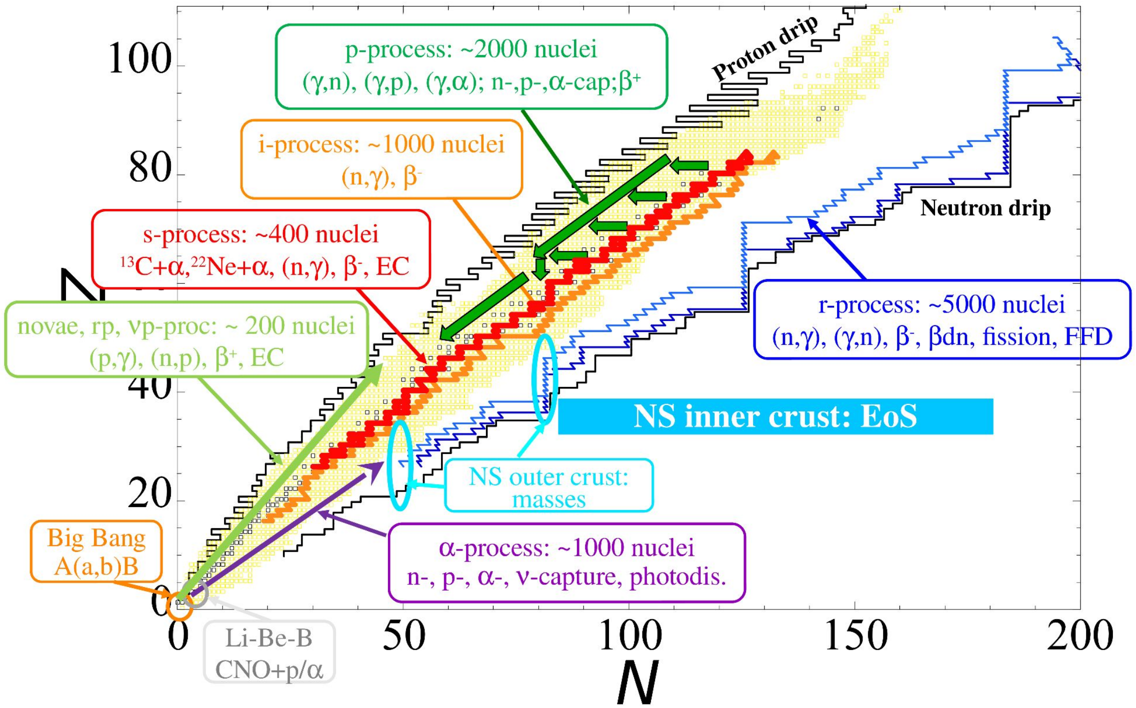
EOS THE EXCELLENCE OF SCIENCE

The nuclear chart...



The nuclear chart and the processes traversing it



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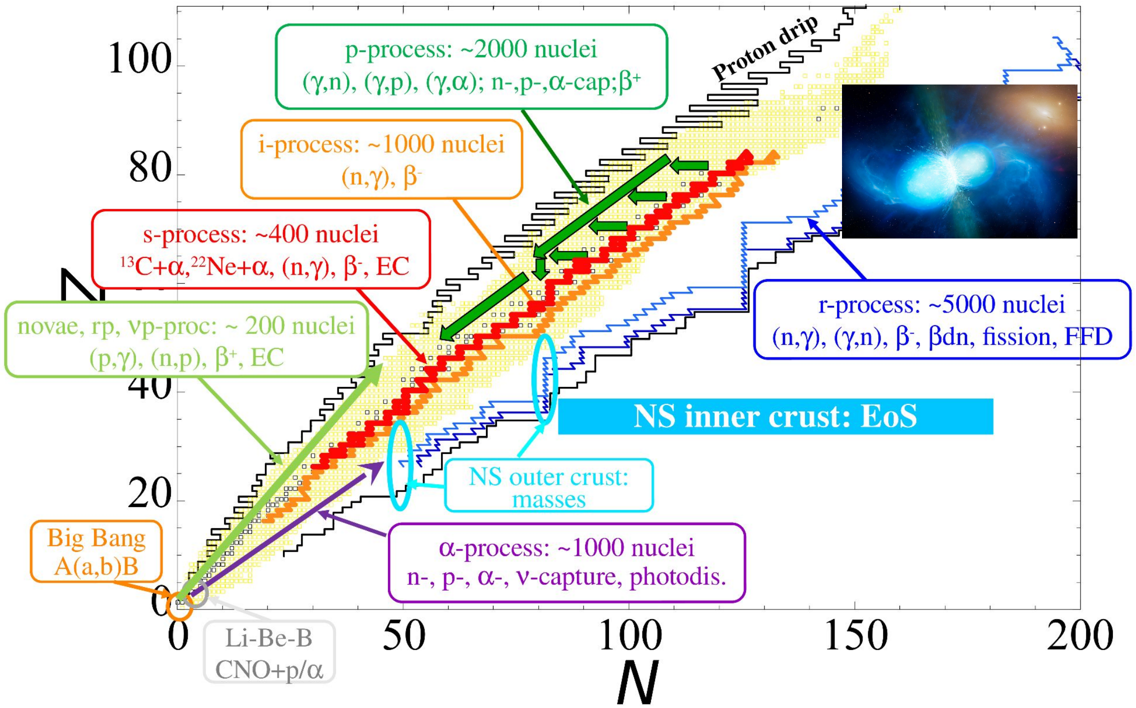
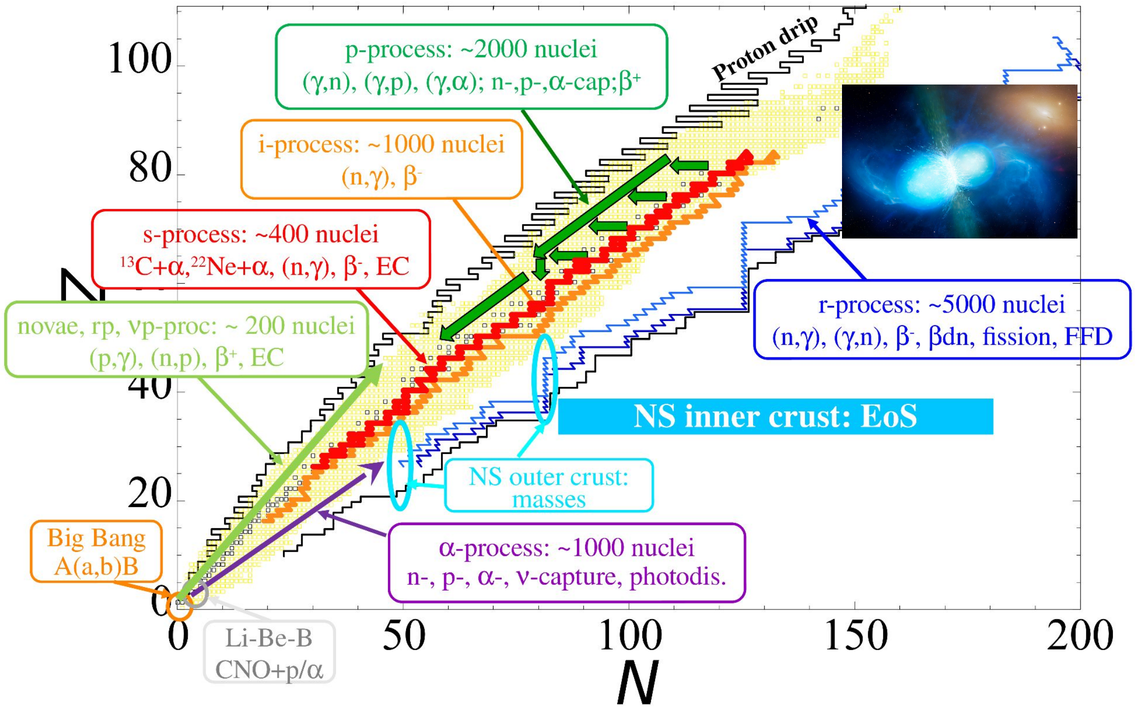


The nuclear chart and the processes traversing it

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



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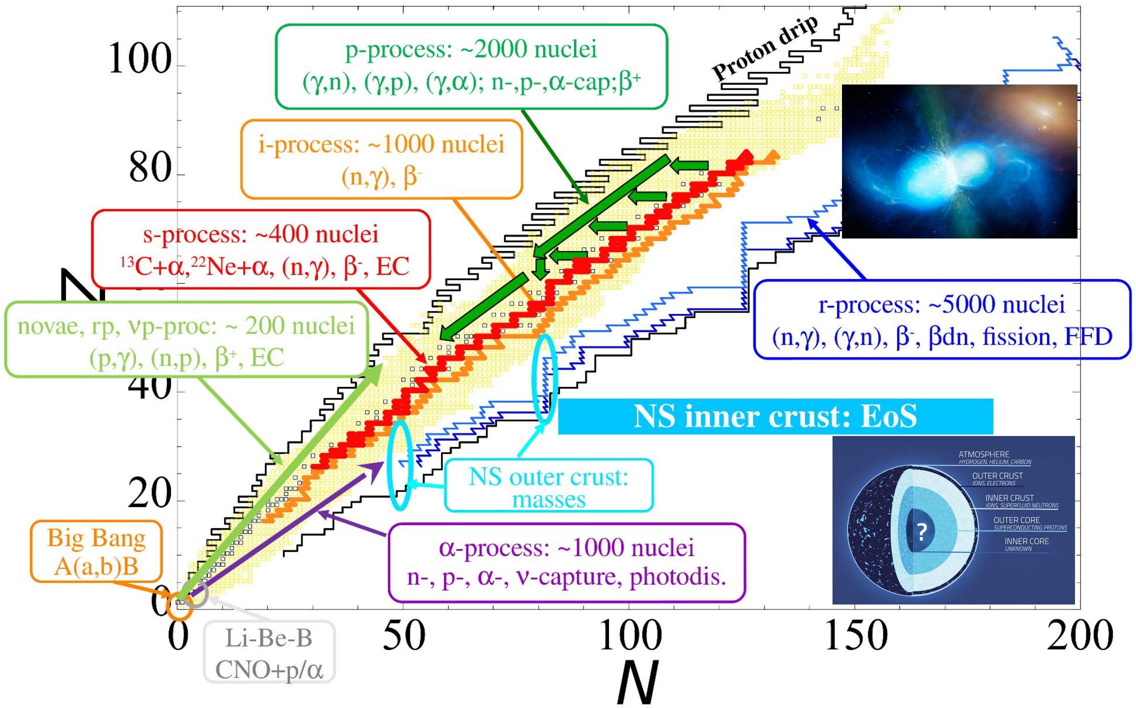

The nuclear chart and the processes traversing it

Extrapolations in
- nucleon number
- energy
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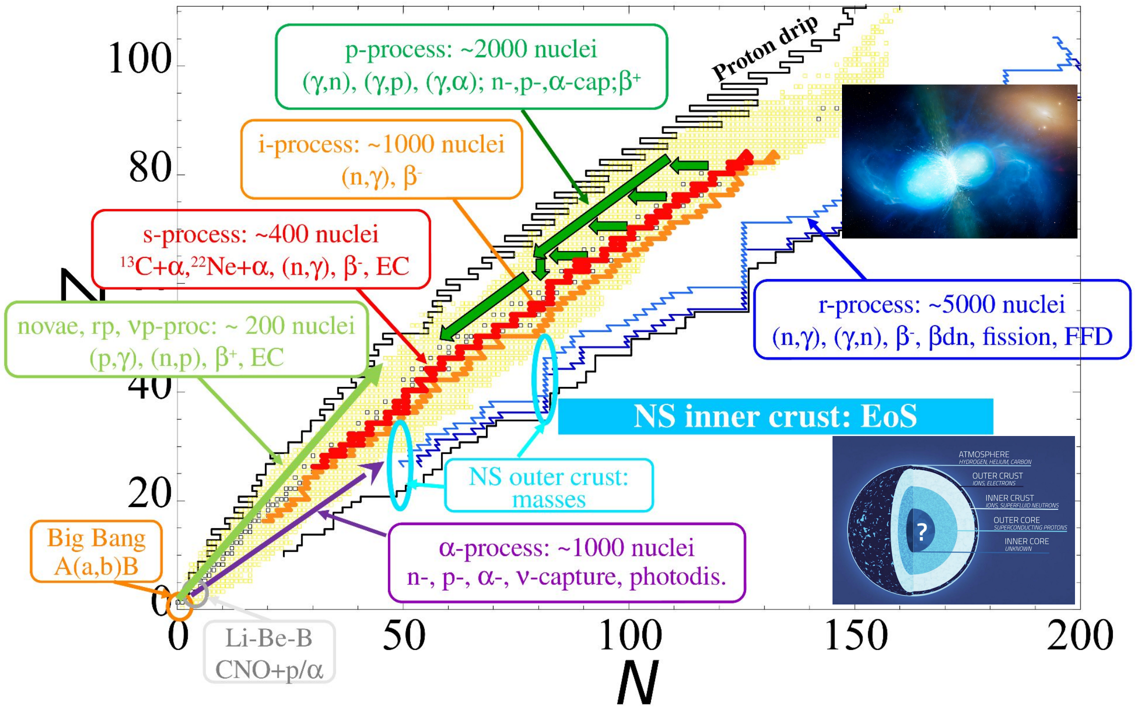
- ……

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



The nuclear chart and the processes traversing it

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

and all of that for
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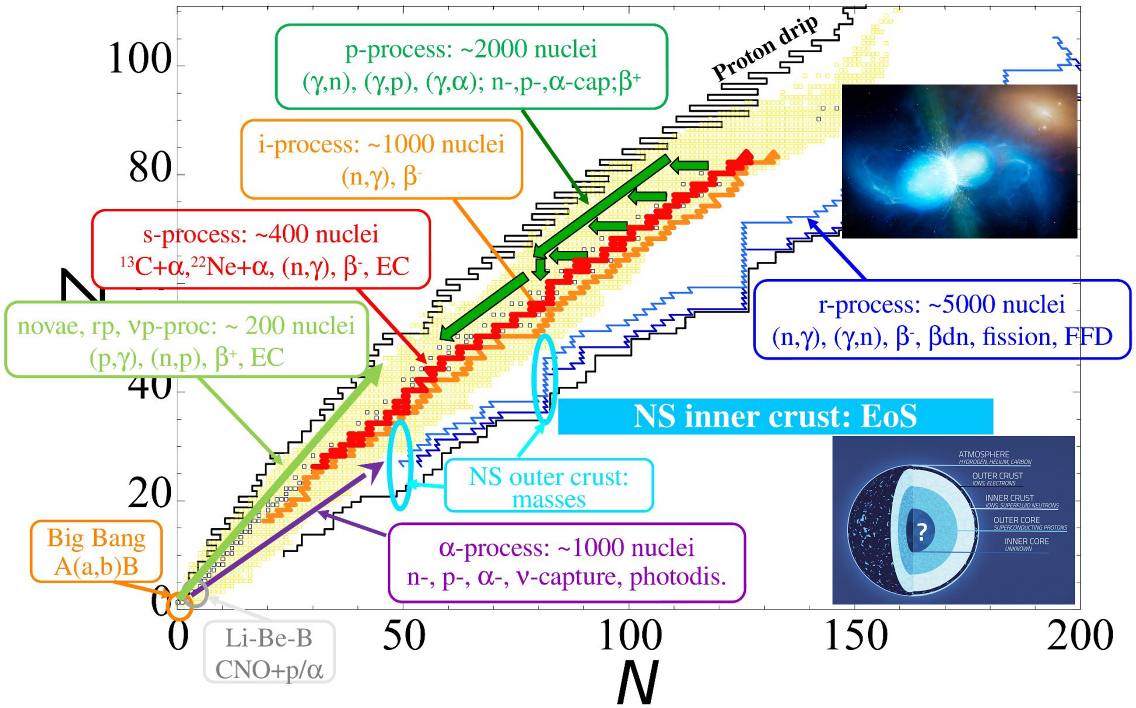
- **many** reactions

what we need is models that should be

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



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

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

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Local densities and currents of a wavefunction

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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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Local densities and currents of a wavefunction

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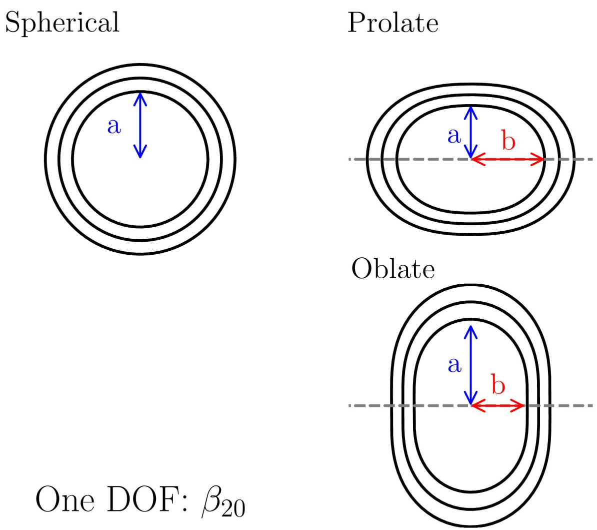
- wavefunctions with individual nucleons
- based on “in-medium” N-N interaction
- many observables accessible
- Feasible for ~**7000** nuclei

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

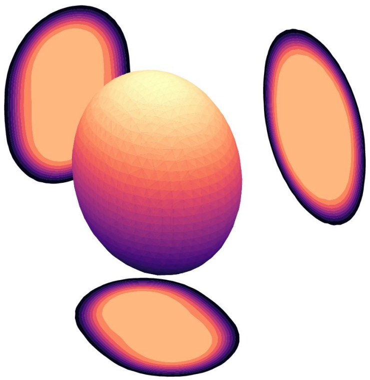


Nuclear deformation

- 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

- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
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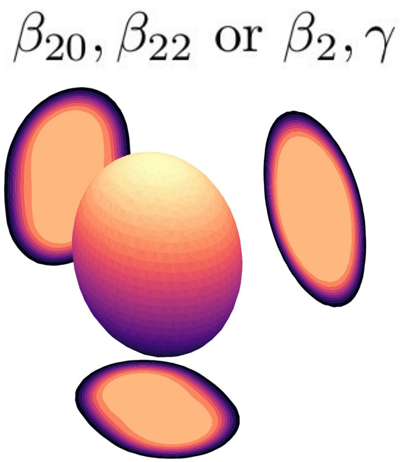
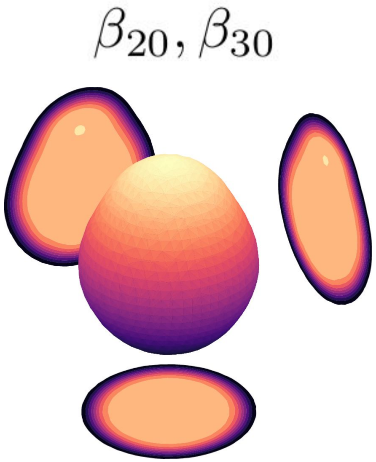
More general configurations

- triaxial shapes

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





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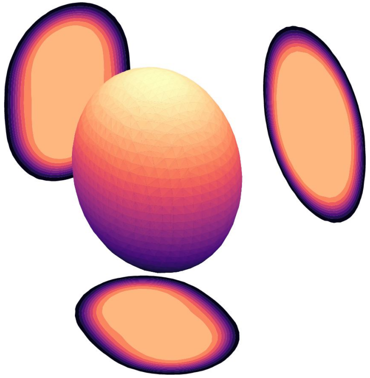
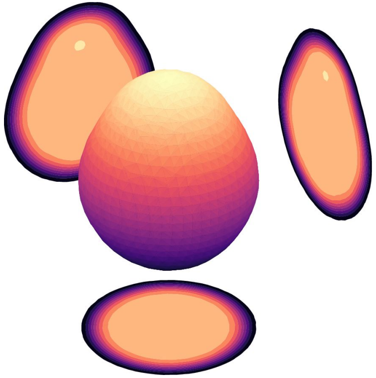
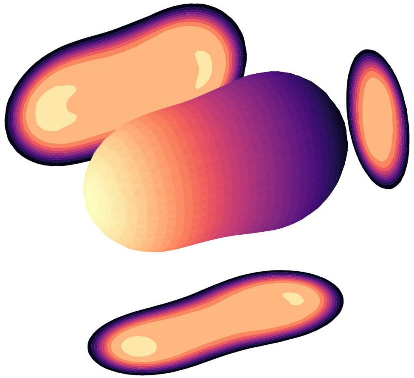


β_{20}, β_{30}



β_{20}, β_{22} **and** β_{30}



Symmetry breaking leads to deformation

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More general configurations

- triaxial shapes
- reflection asymmetry
- elongated shapes

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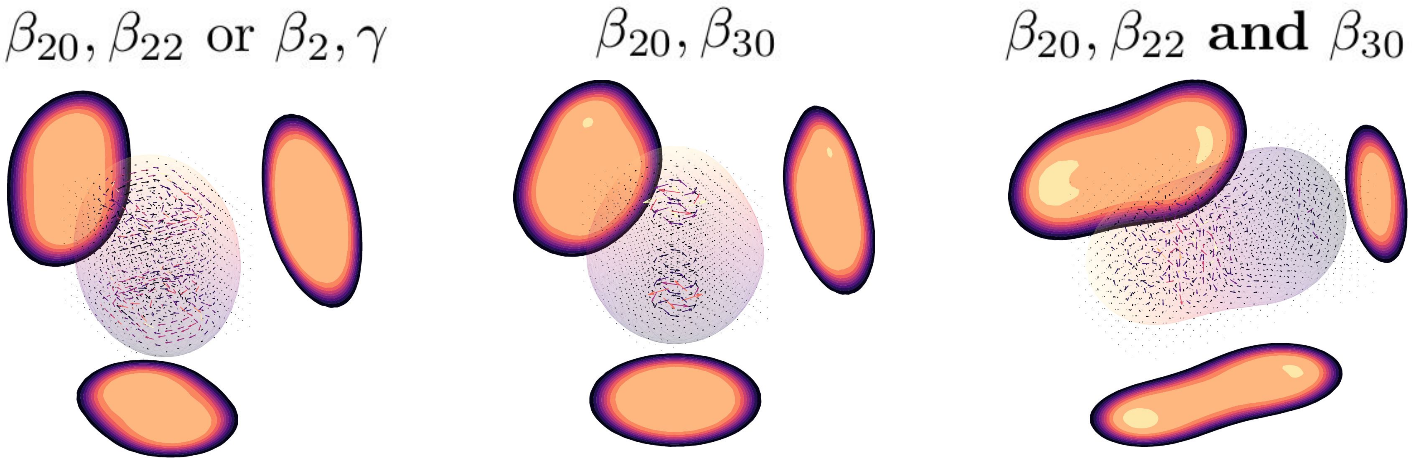


Symmetry breaking leads to deformation

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

More general configurations

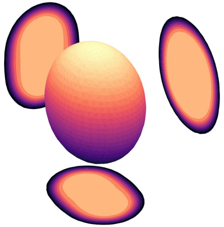
- triaxial shapes
- reflection asymmetry
- elongated shapes
- spin densities and currents

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.

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

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		

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

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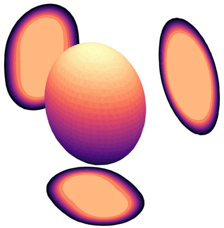

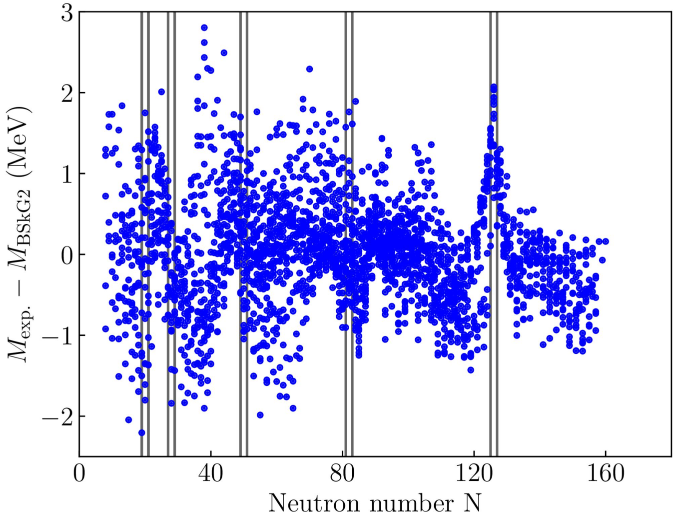

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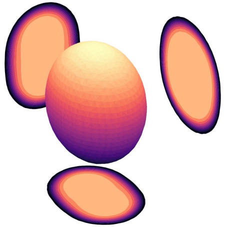
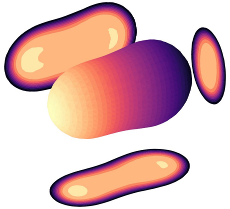
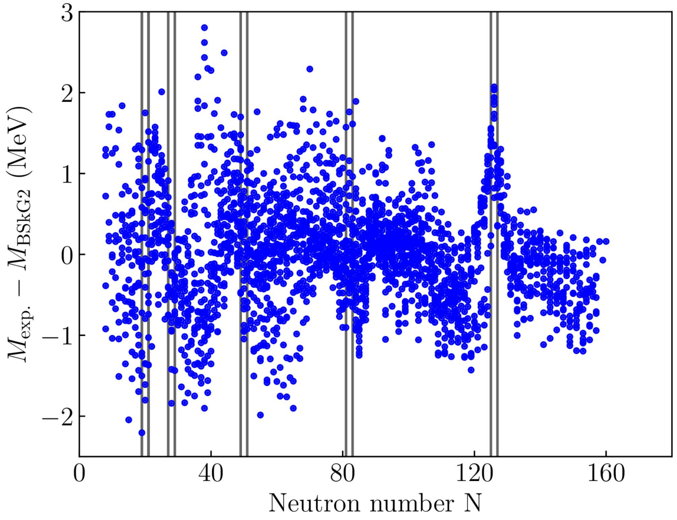


BSkG2 (2022)

- 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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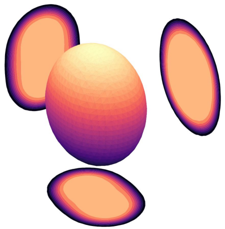
BSkG1 (2021)

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



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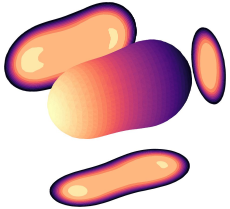
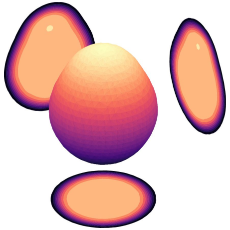
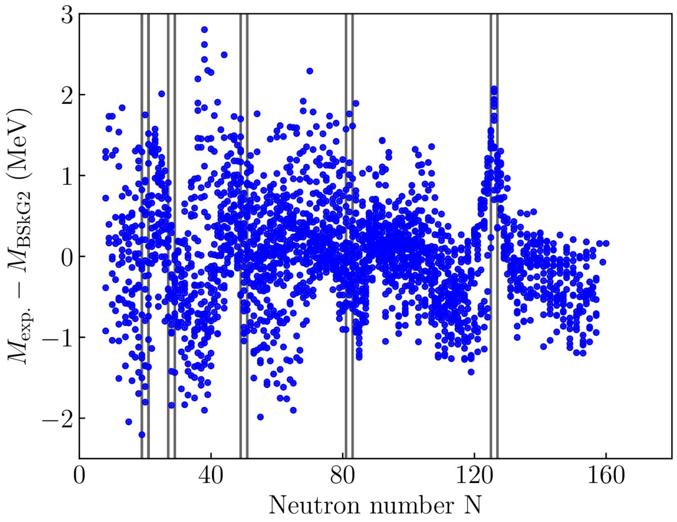


BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation

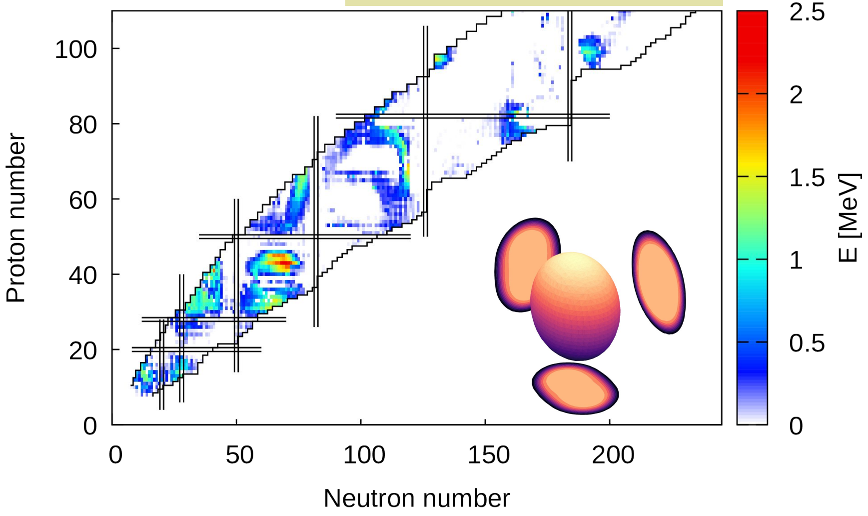




Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
Prim. barriers [MeV]	0.88	0.44	0.33
Secon. barriers [MeV]	0.87	0.47	0.51
Fission isomers [MeV]	1.0	0.49	0.34
Max. NS mass [$M_\odot$]	1.8	1.8	2.3

Masses

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

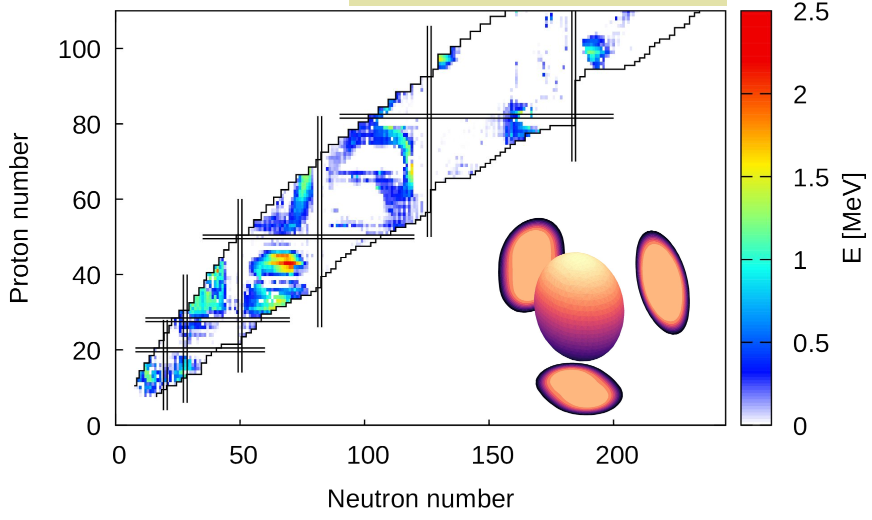


Triaxial deformation

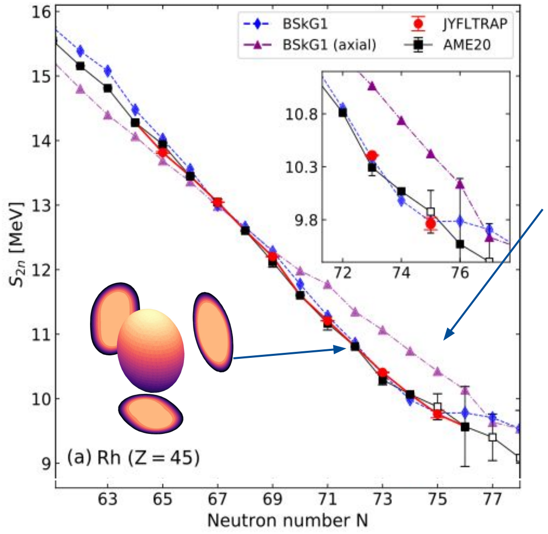
- many nuclei are affected
- effects up to 2.5 MeV near Z~44

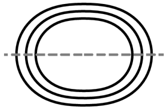
Masses

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



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

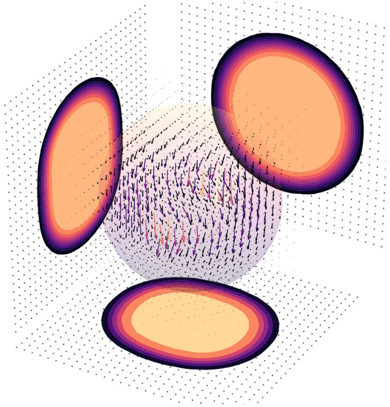


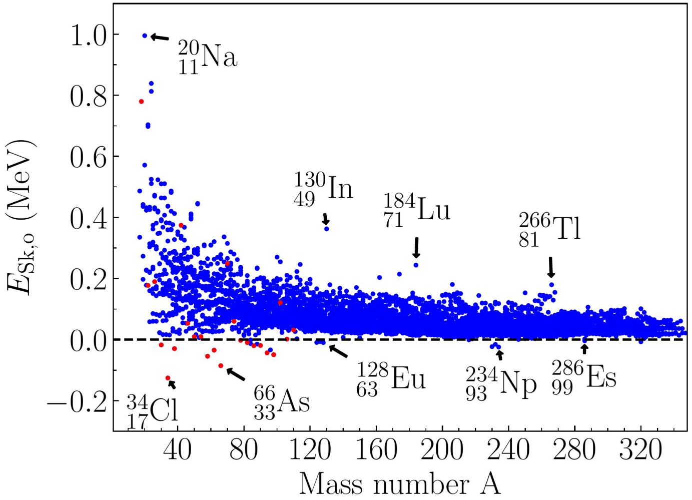


Triaxial deformation

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

Masses



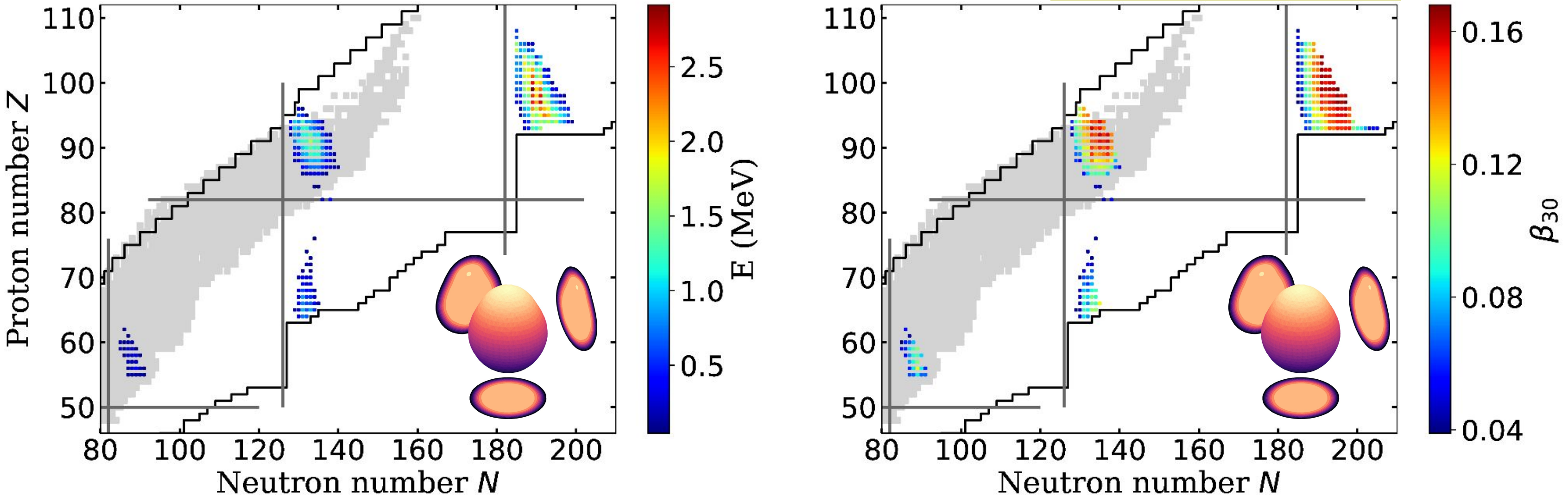


Time-odd terms

- 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.



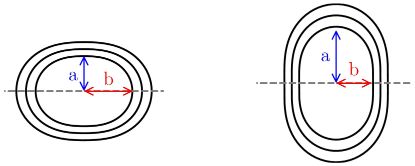
Reflection asymmetry

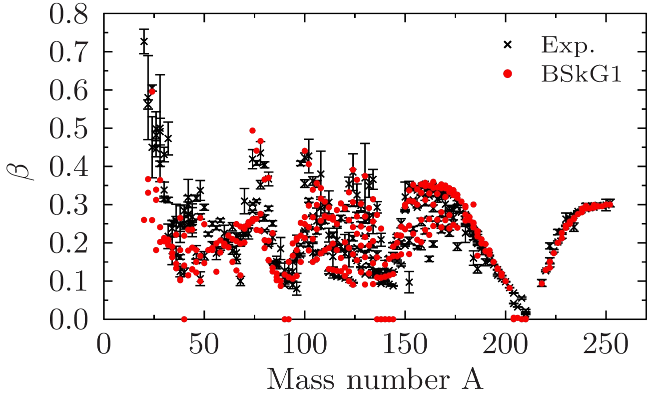
- small number of known nuclei affected
- Near N=184:
  - large effect up to 3 MeV
  - dripline modified
  - fission properties modified

Deformations

Deformations

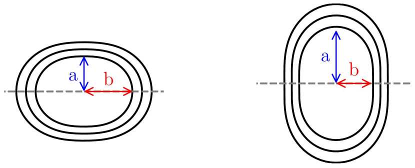
“Ordinary” quadrupole deformation

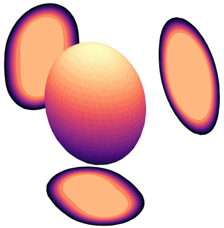


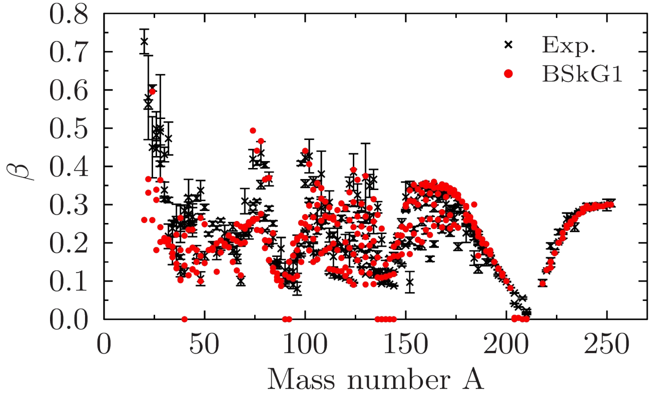


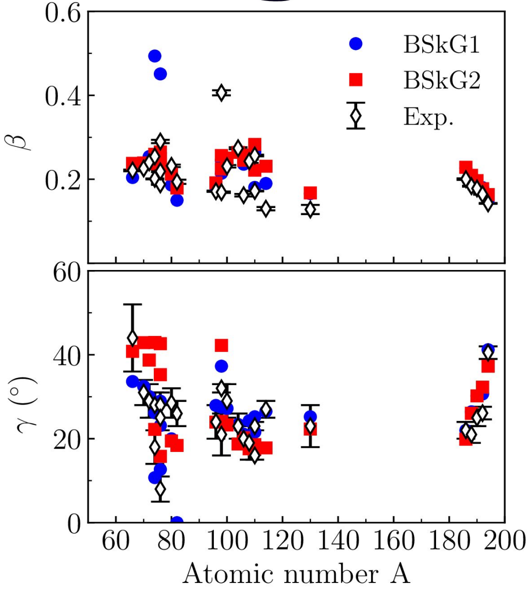
Deformations

"Ordinary" quadrupole deformation ... and triaxial deformation ...



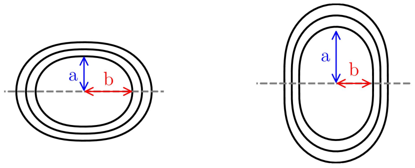


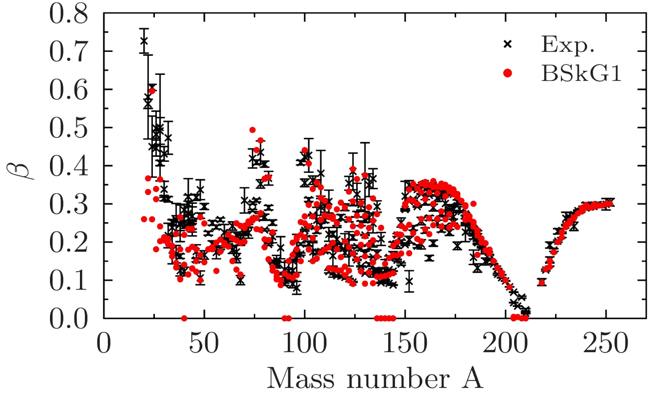




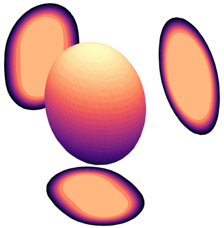
Deformations

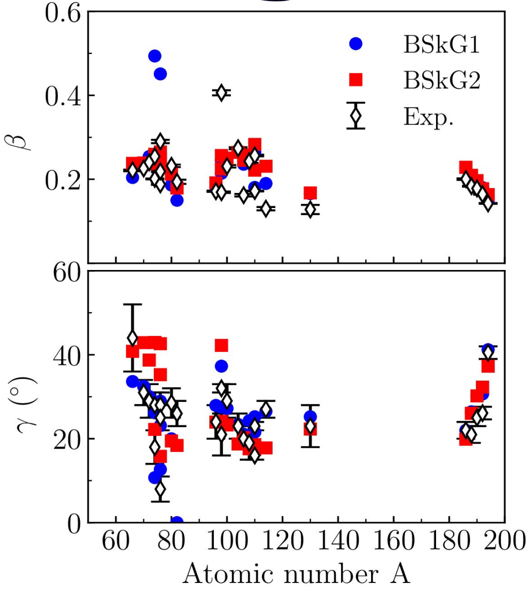
“Ordinary” quadrupole deformation



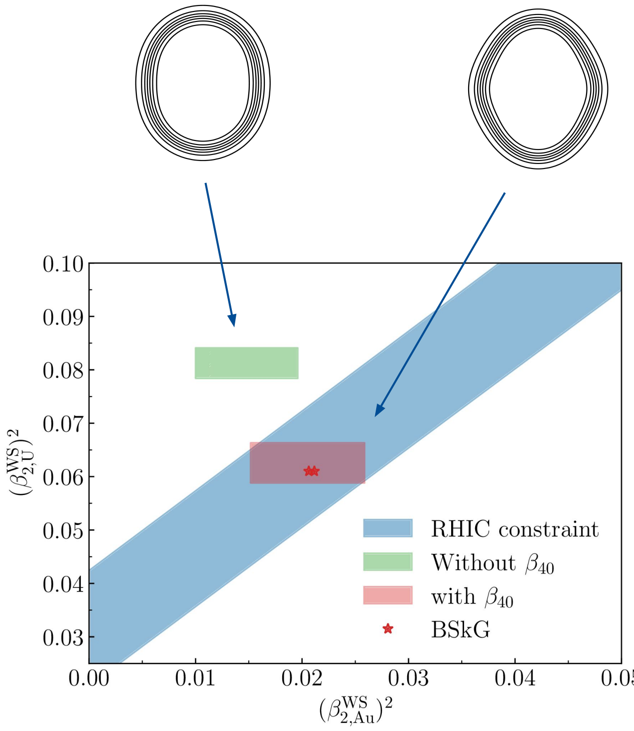


… and triaxial deformation …





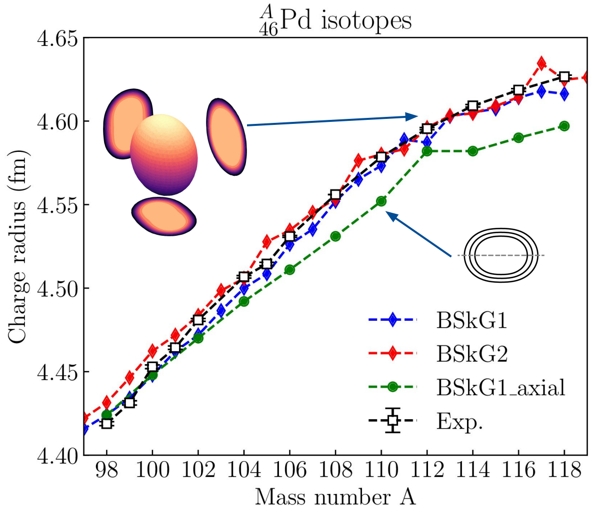
… and even hexadecapole!



W.R. et al., Phys. Rev. Lett. **130**, 212302

Radii

S. Geldhof, PRL **128**, 152501 (2022).



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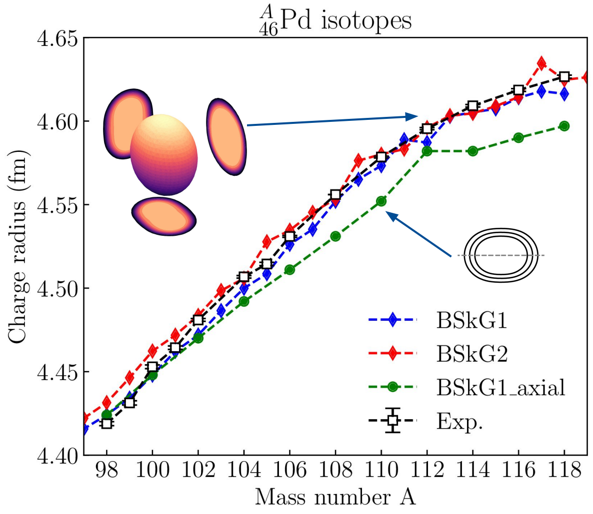
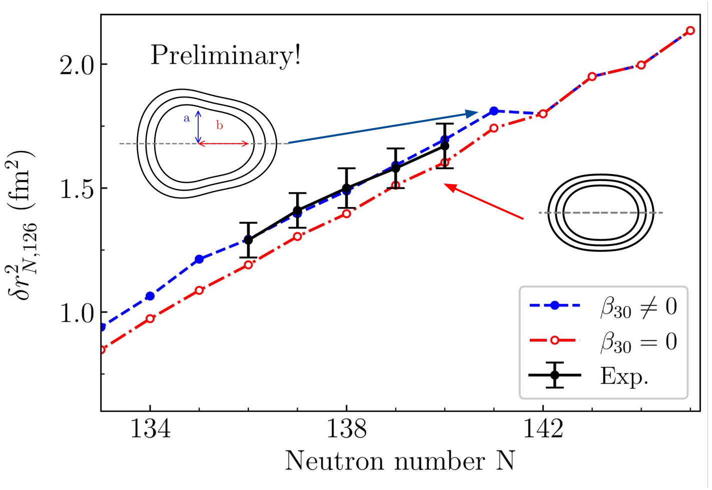
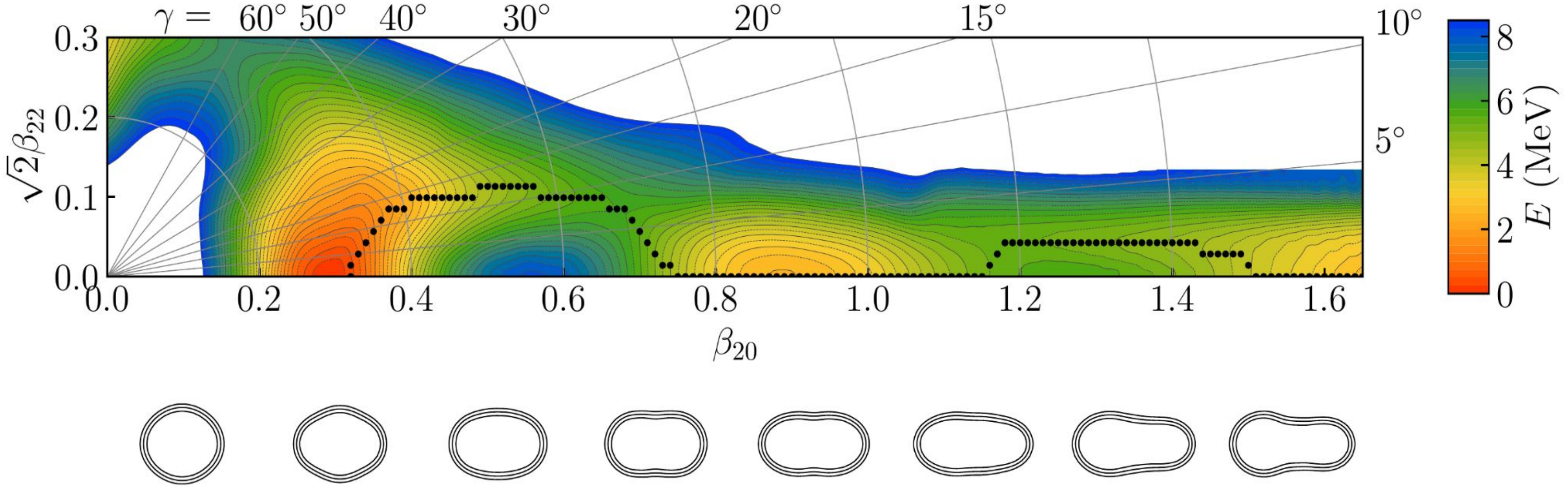


E. Verstraelen, PRC 100, 044321 (2019)



Fission barriers

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



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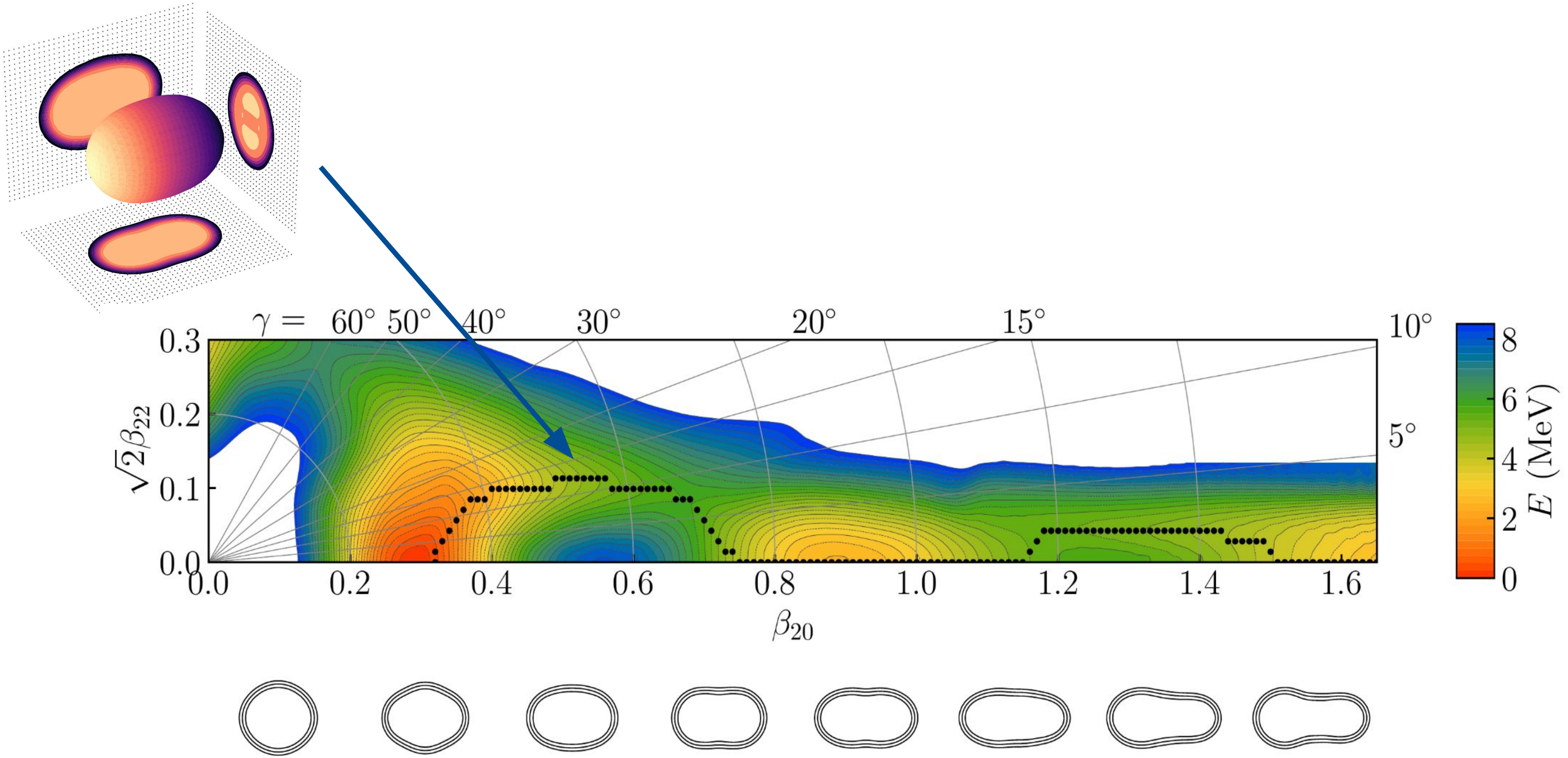

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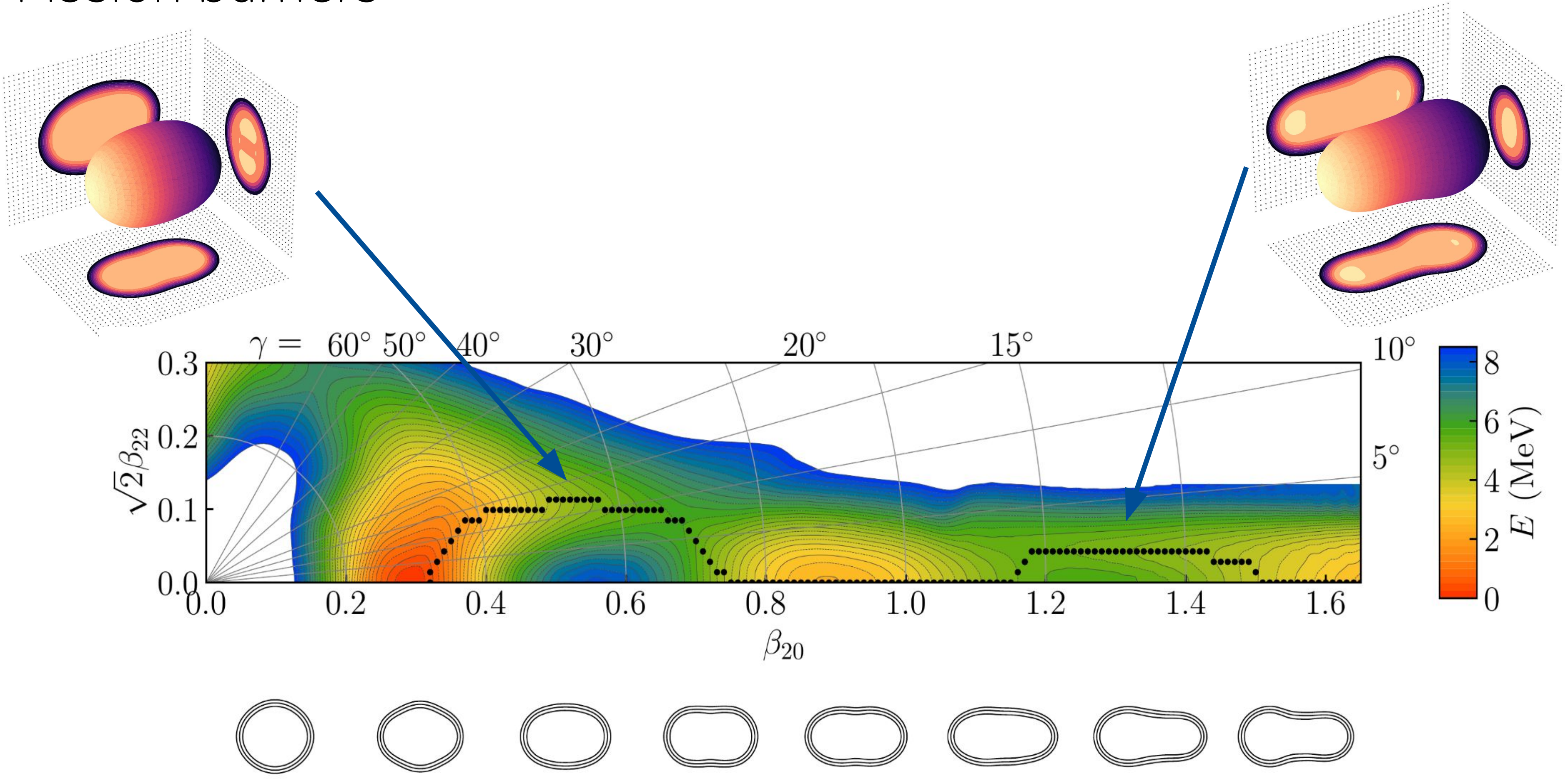

Fission

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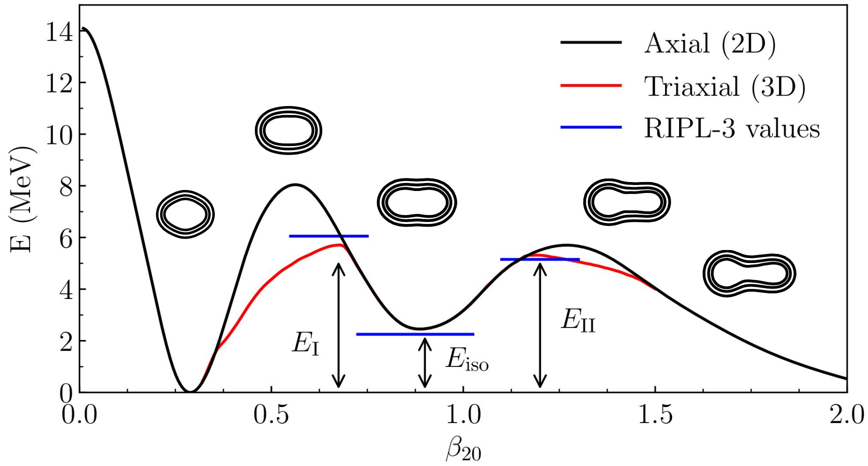

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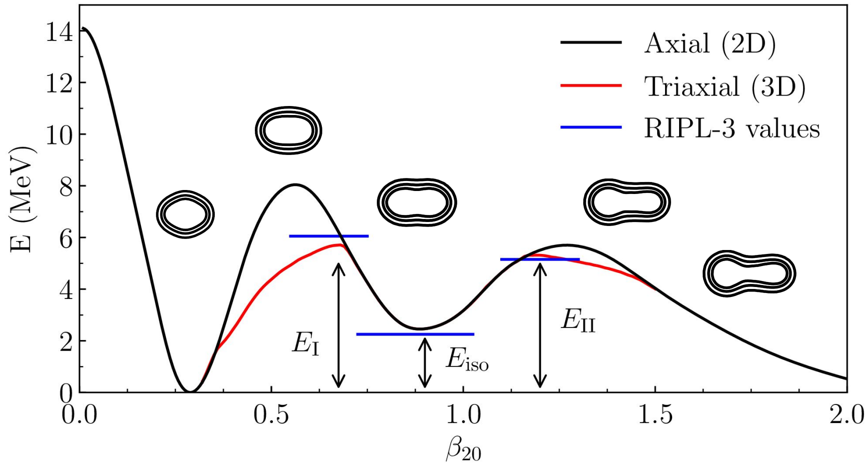
W. R. et al., EPJA **59**, 96 (2023).



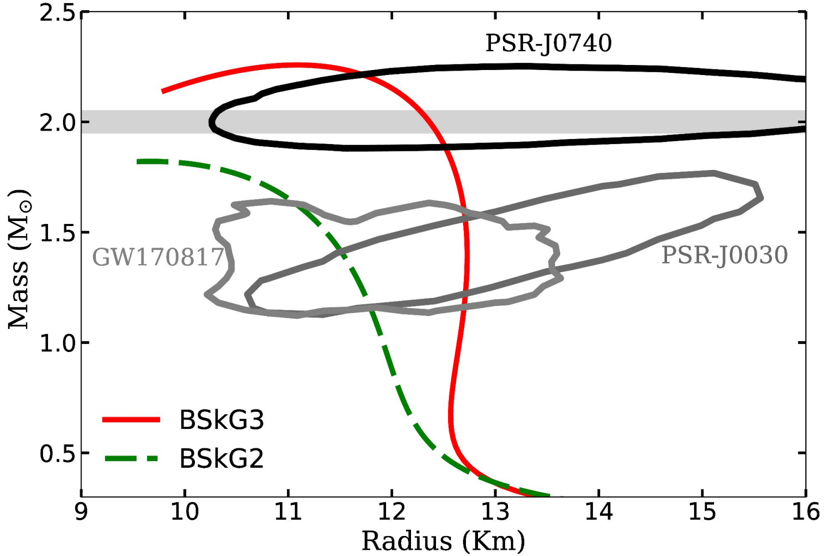
Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
Prim. barriers [MeV]	0.88	0.44	0.33
Secon. barriers [MeV]	0.87	0.47	0.51
Fission isomers [MeV]	1.0	0.49	0.34
Max. NS mass [$M_\odot$]	1.8	1.8	2.3

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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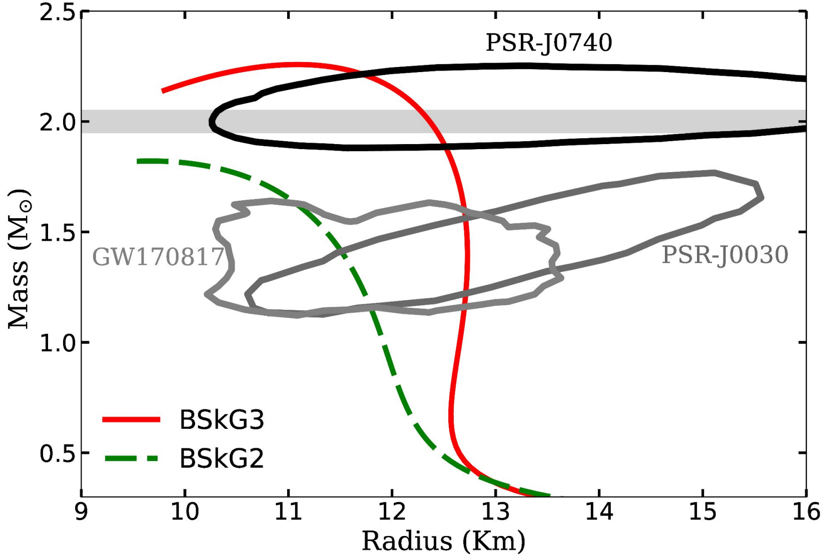
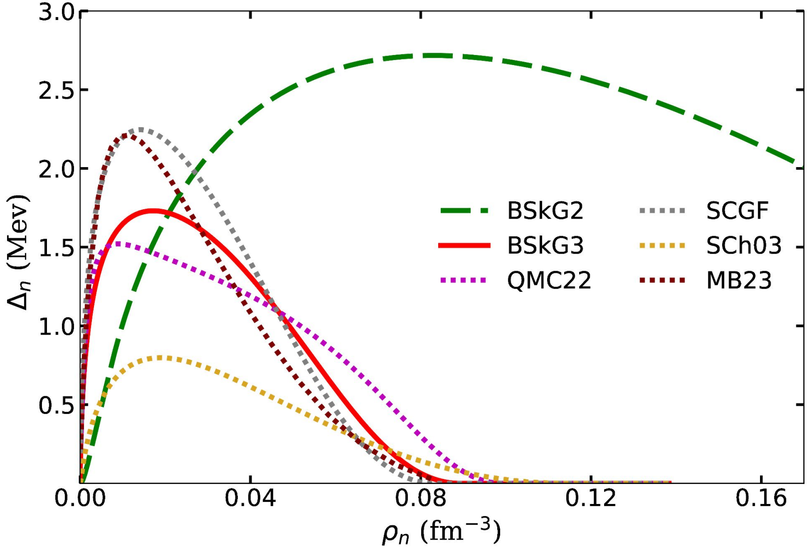
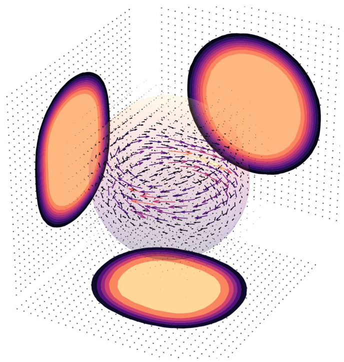




More realistic NS predictions:

- 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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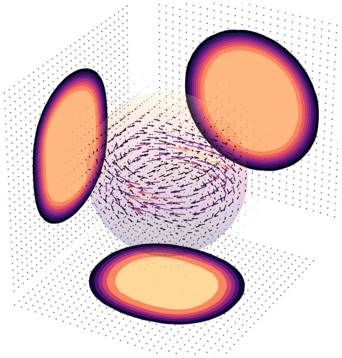

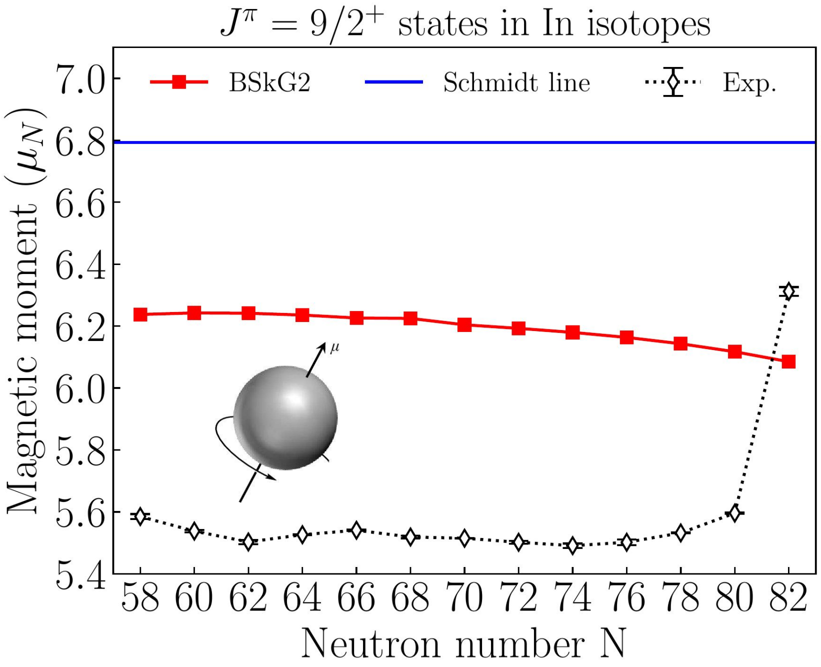

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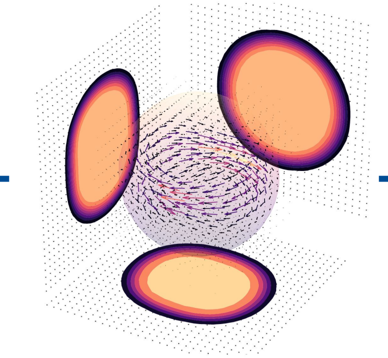
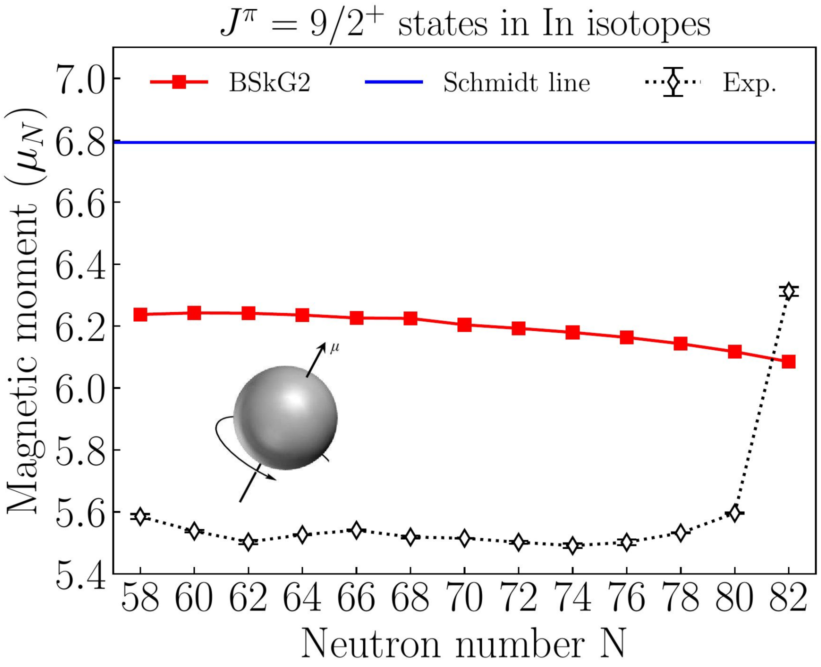
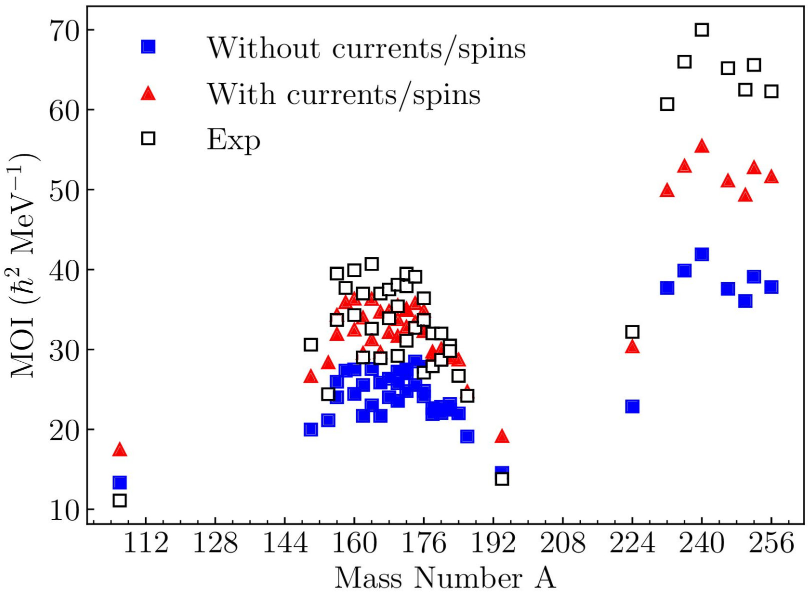
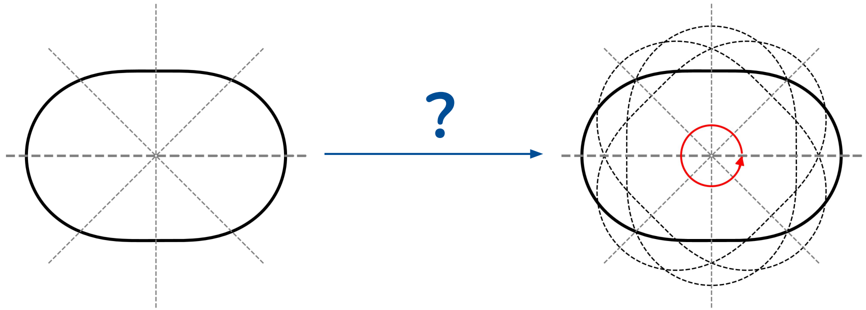






Challenges: less phenomenology

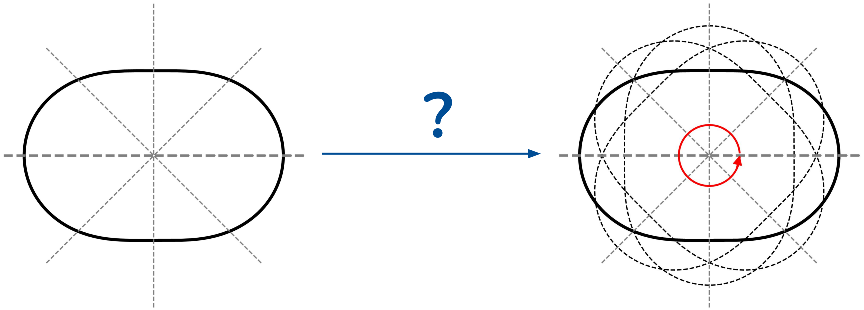


Leave the mean-field picture behind

- techniques exist
- ... but remain extremely costly

Challenges: less phenomenology

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



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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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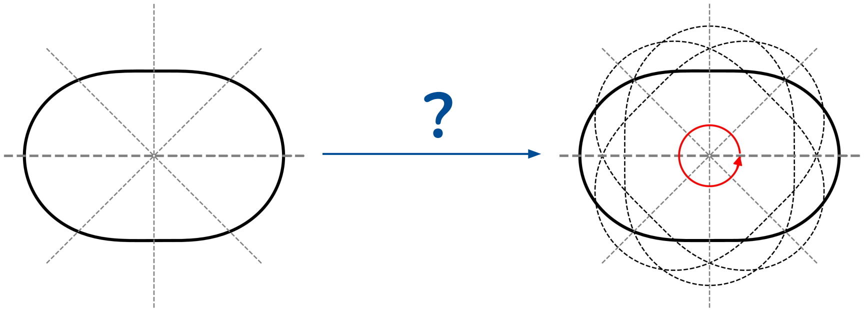

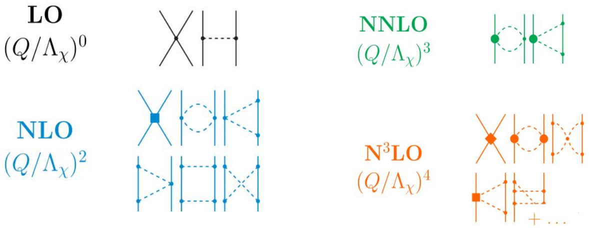

Adapted from H. Hergert, Front. Phys. 8:379 (2020).

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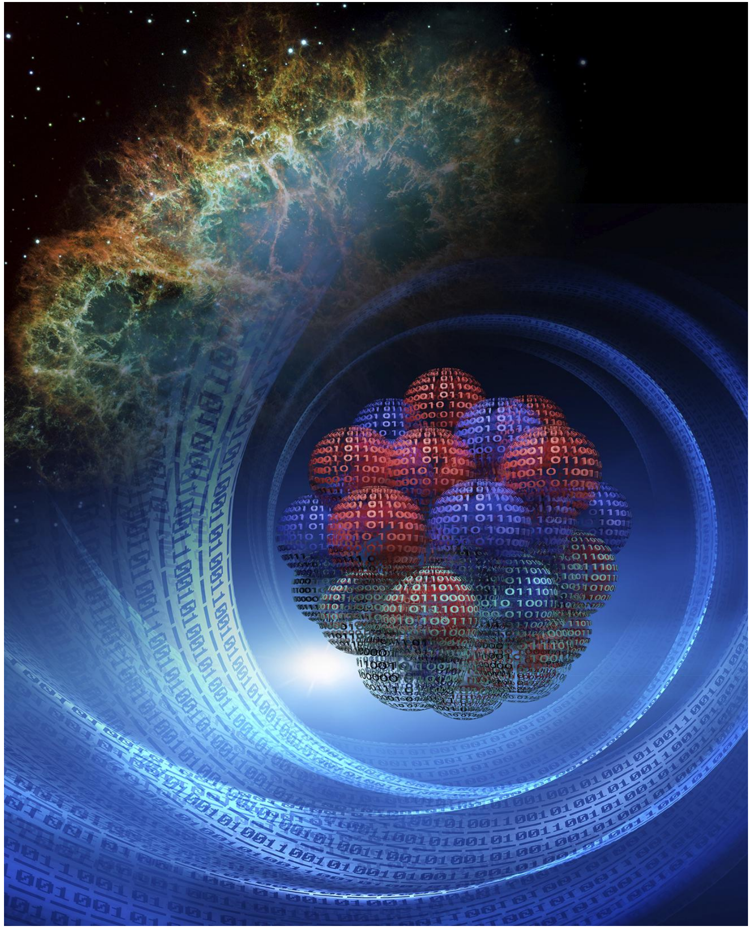
We build **large-scale**, **microscopic** models for (astro) applications.



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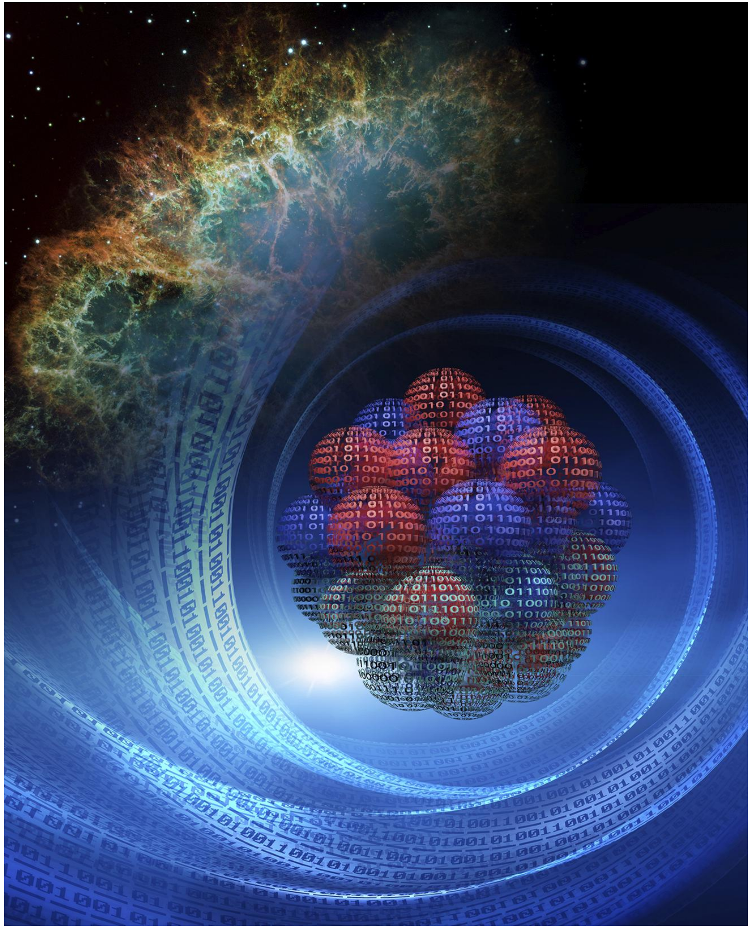

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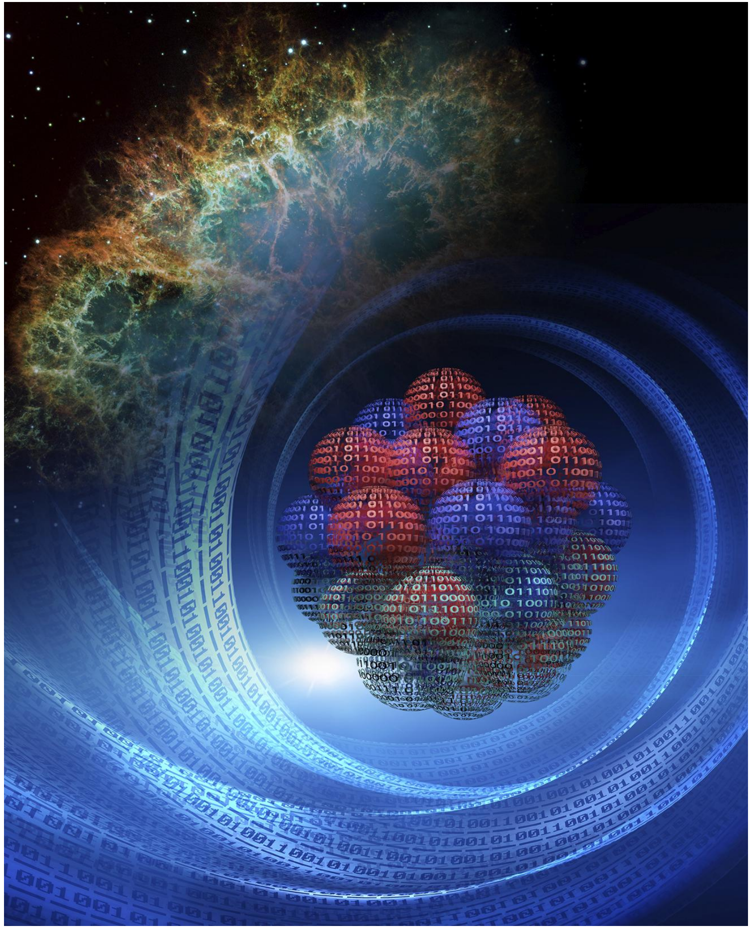

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BSkG3

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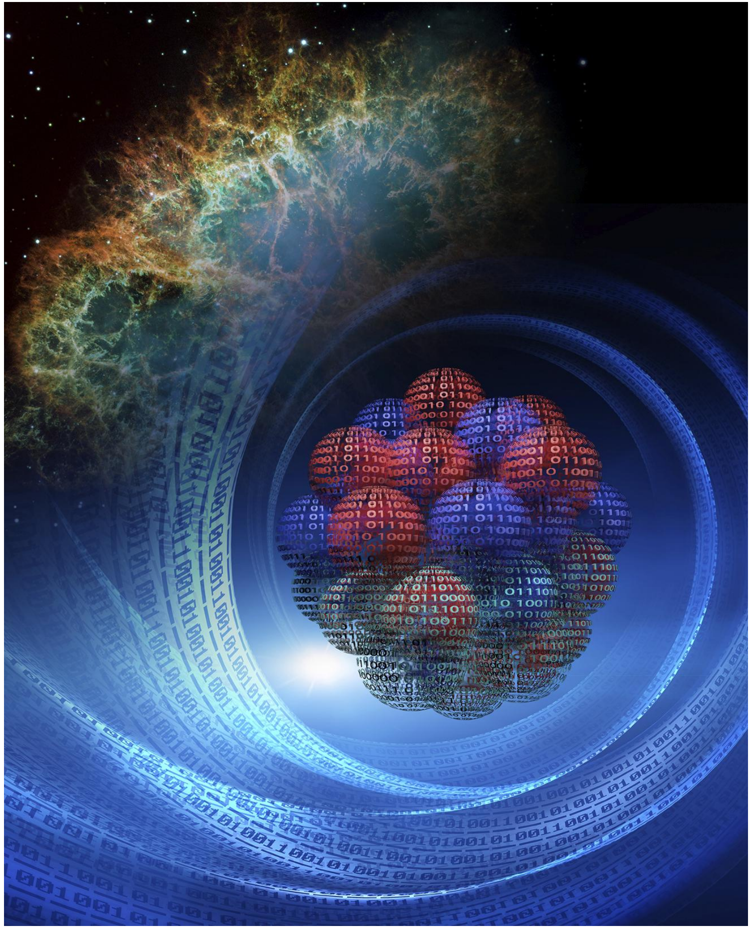
  - time-reversal breaking
  - octupole deformation

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



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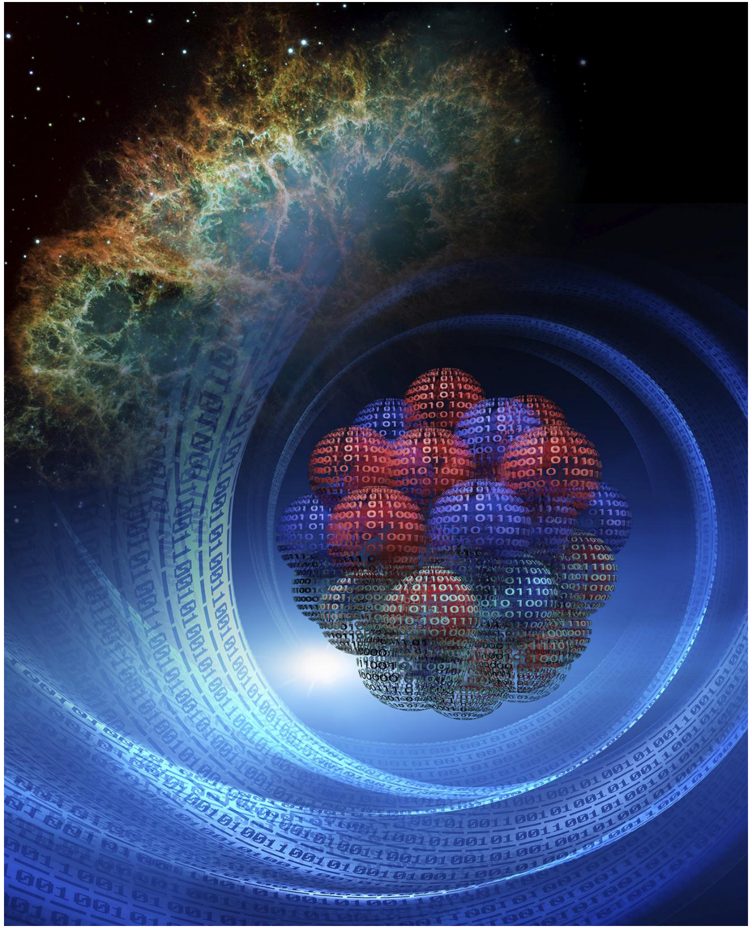
Coming up from the Brussels group:

- 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

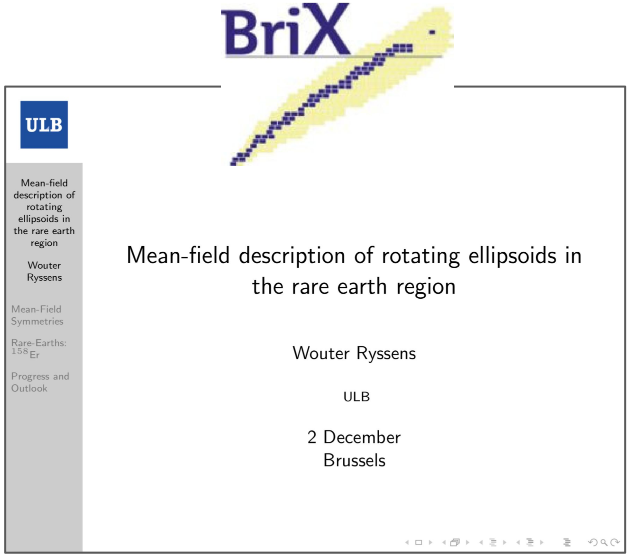
S. Hilaire

...... the computing time!

...... the funding!

...... your attention!

2013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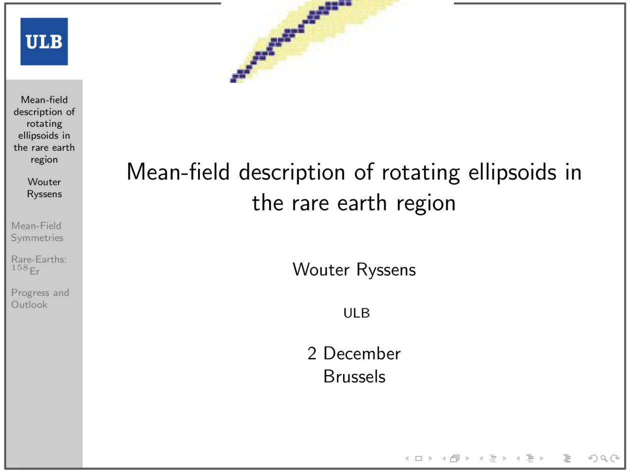
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2023


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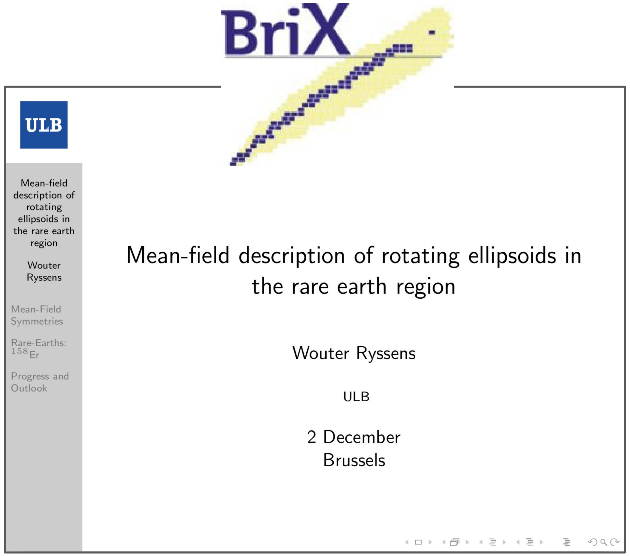
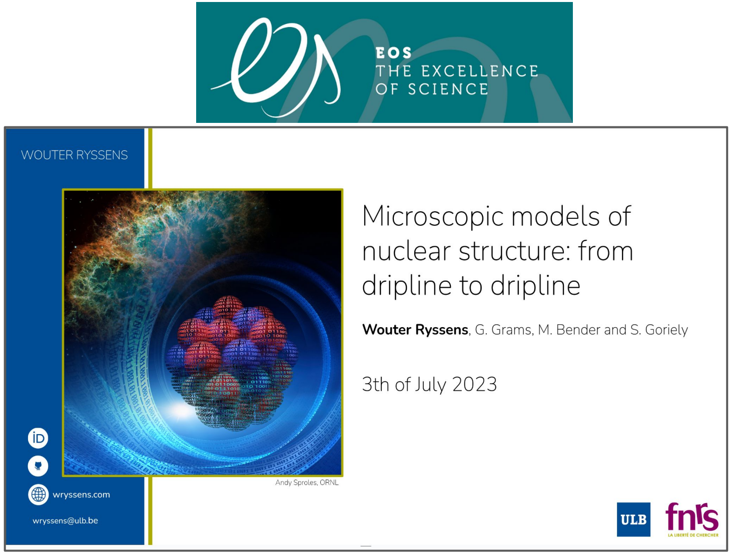
Andy Sproles, ORNL
Microscopic models of nuclear structure: from dripline to dripline
Wouter Ryssens, G. Grams, M. Bender and S. Goriely
3th of July 2023
ULB
fnrs

Thank you for **a decade** of support!

2013



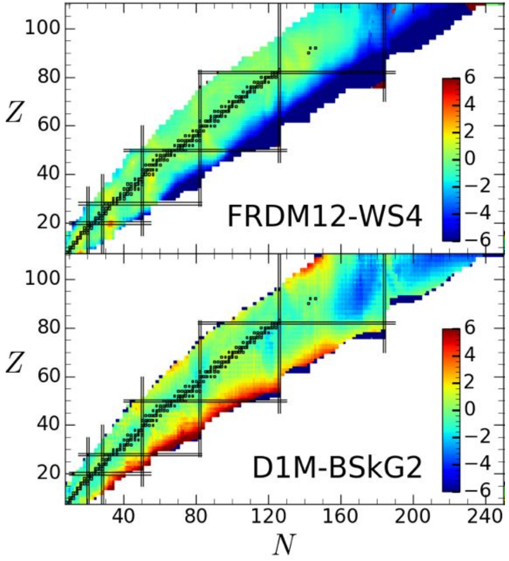
2023



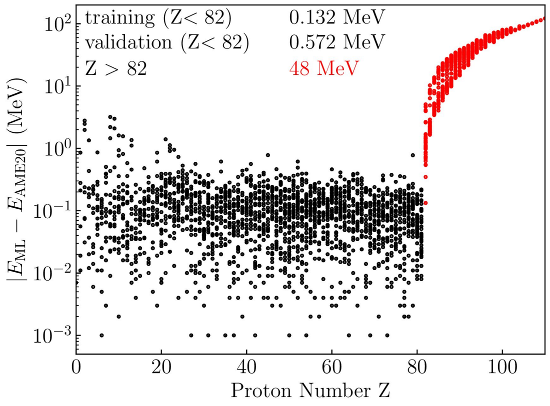
Bonus!

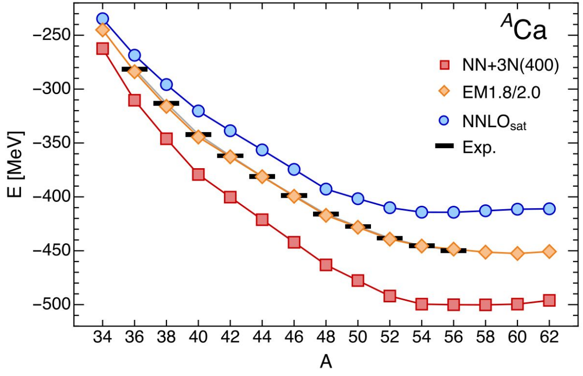
Interlude: why do we do these complex things?

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?

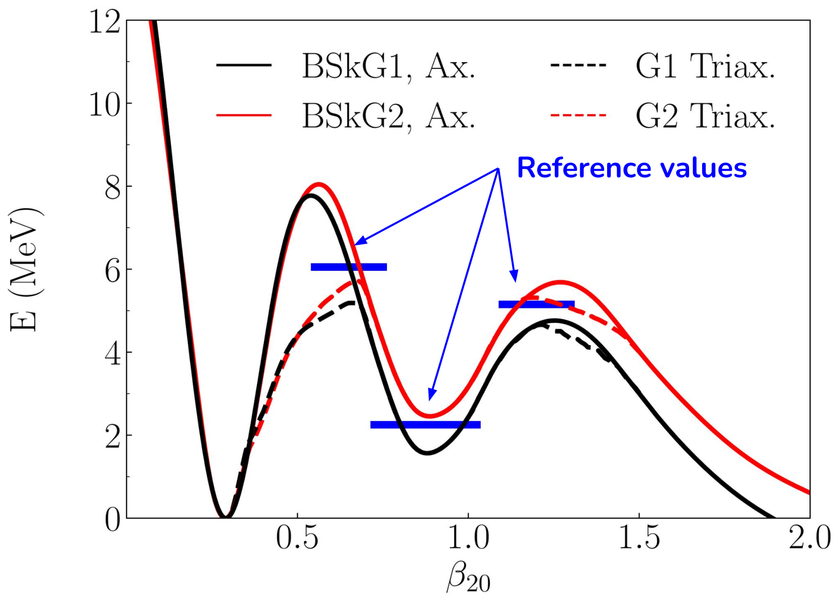
- ✅ absolute champion in rms
- ✅ ridiculously easy
- ❌ thousands (?) of parameters
- ❌ single observable

Ab Initio?

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

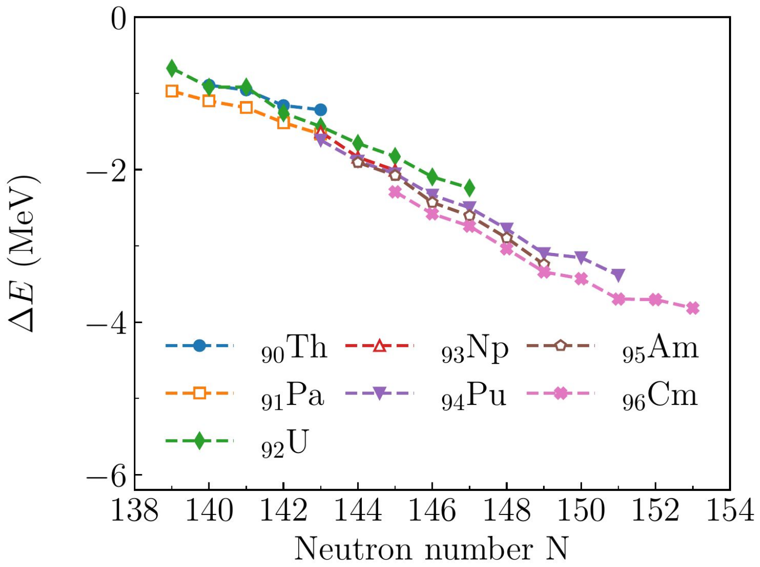
Triaxiality has a **large** effect on barriers

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



Triaxial deformation for 240Pu

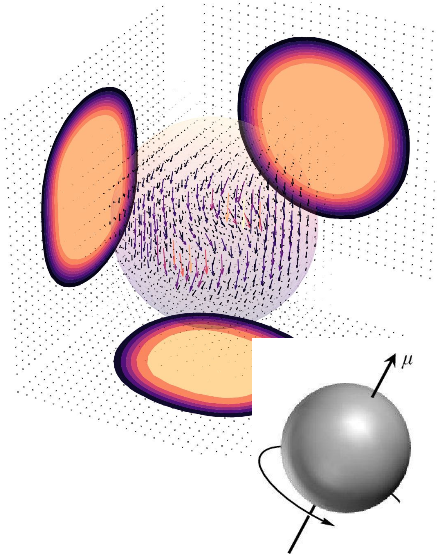
- Large effect on inner barrier
- No effect on isomers
- Modest effect on outer barrier

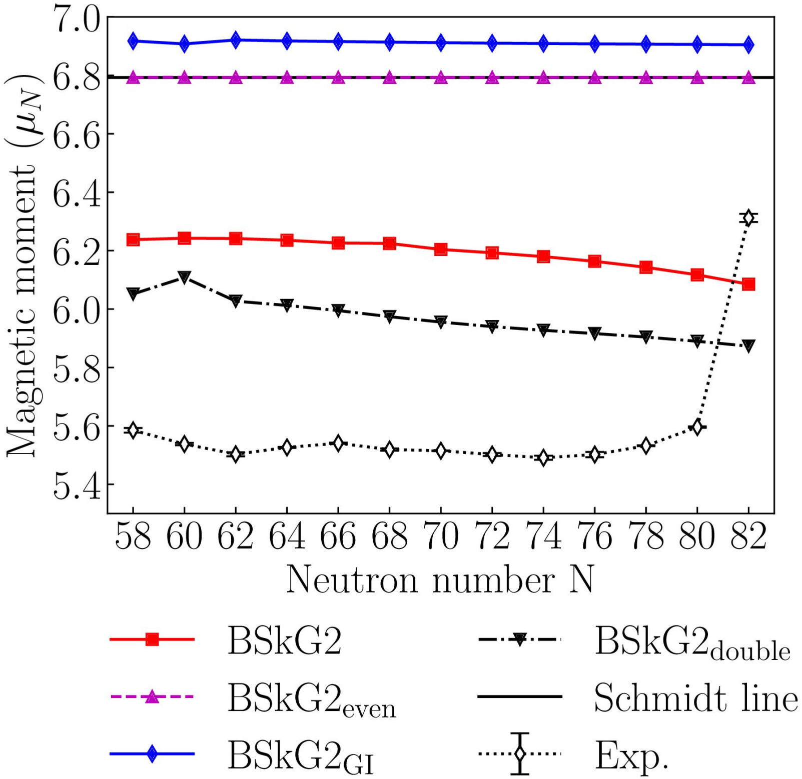


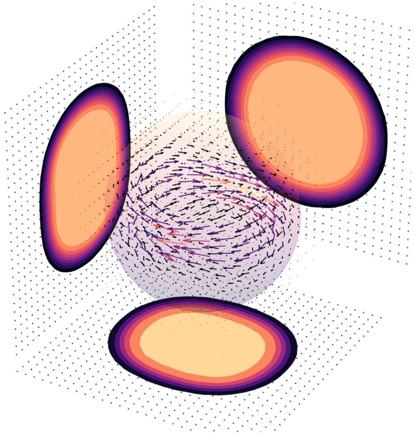
Triaxial deformation for actinides

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

Magnetic moments

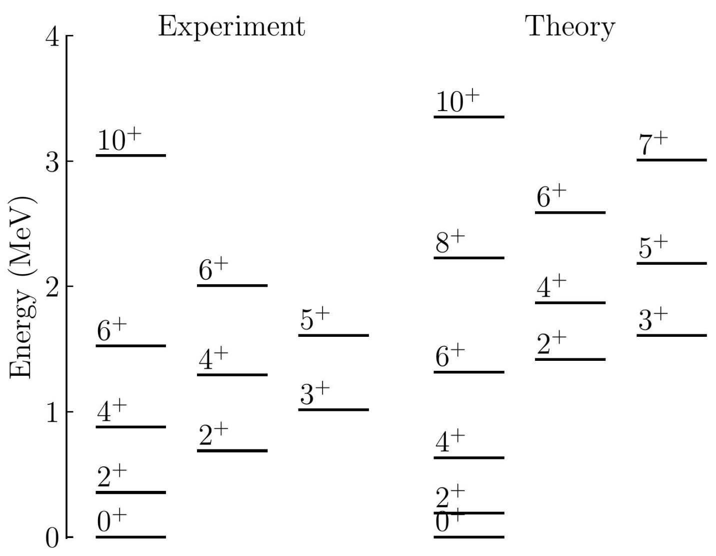


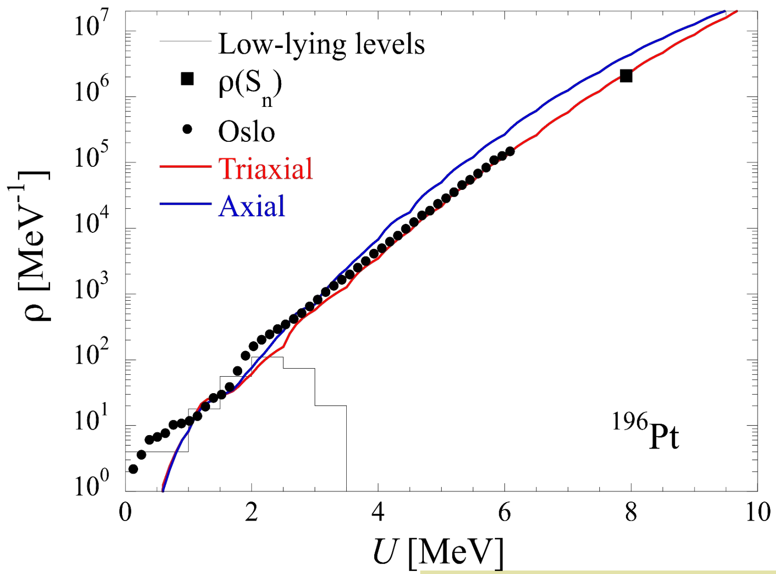




A. R. Vernon et al., Nature 607, 260 (2022).
J. Eberz et al., NPA 464, 9 (1987).

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





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

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

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