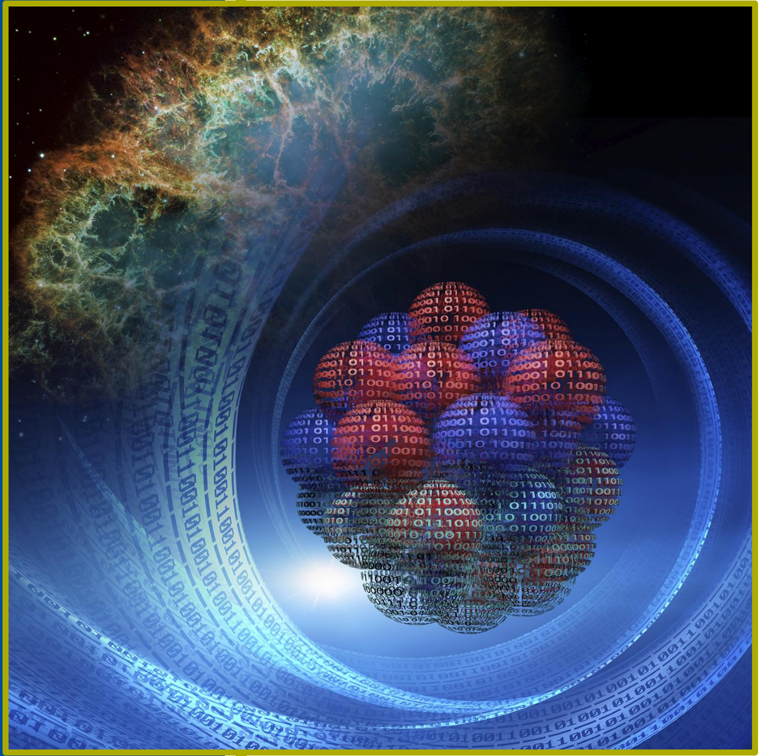
WOUTER RYSSENS



Andy Sproles, ORNL

Microscopic models of nuclear structure for applications

March 26th 2023

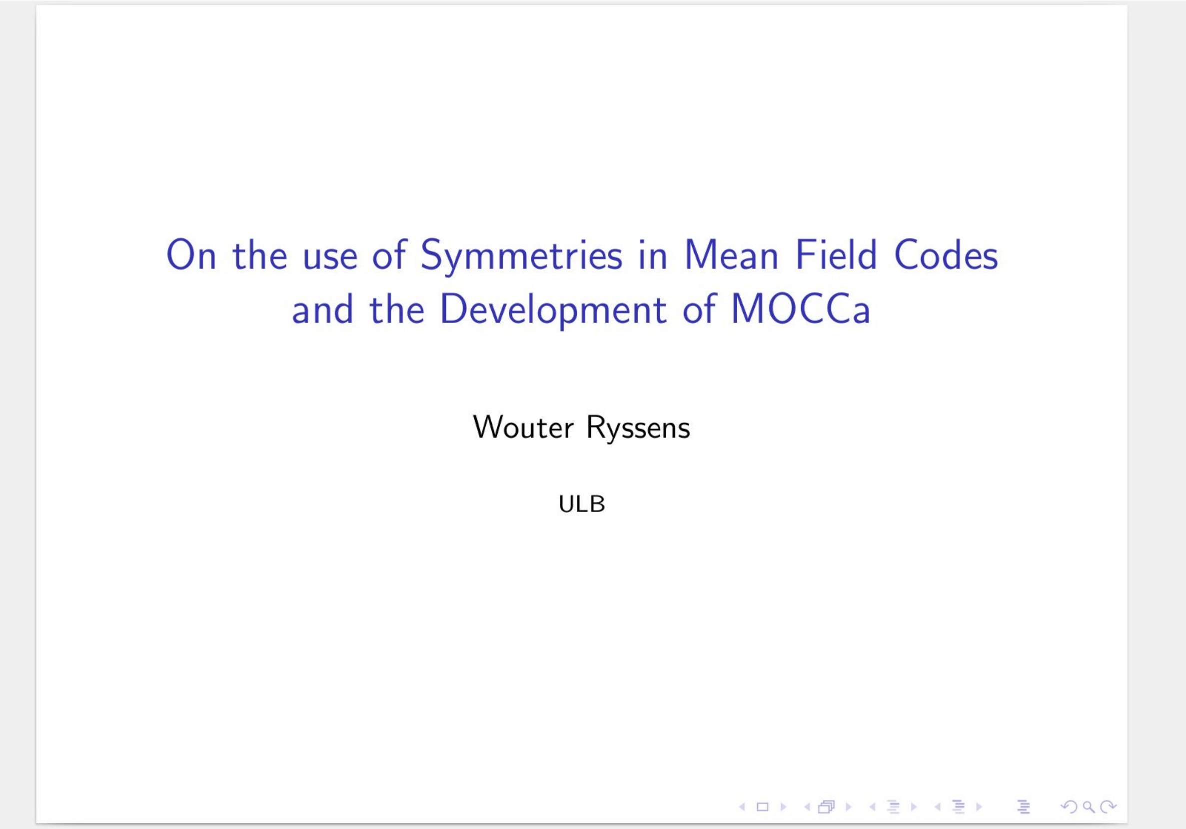
wryssens.com

wryssens@ulb.be

ULB

fnrs LA LIBERTÉ DE CHERCHER

May 2013: a young Belgian arrives in Bordeaux.....



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I. Nuclear theory for applications

The challenge for nuclear theory: extrapolation!

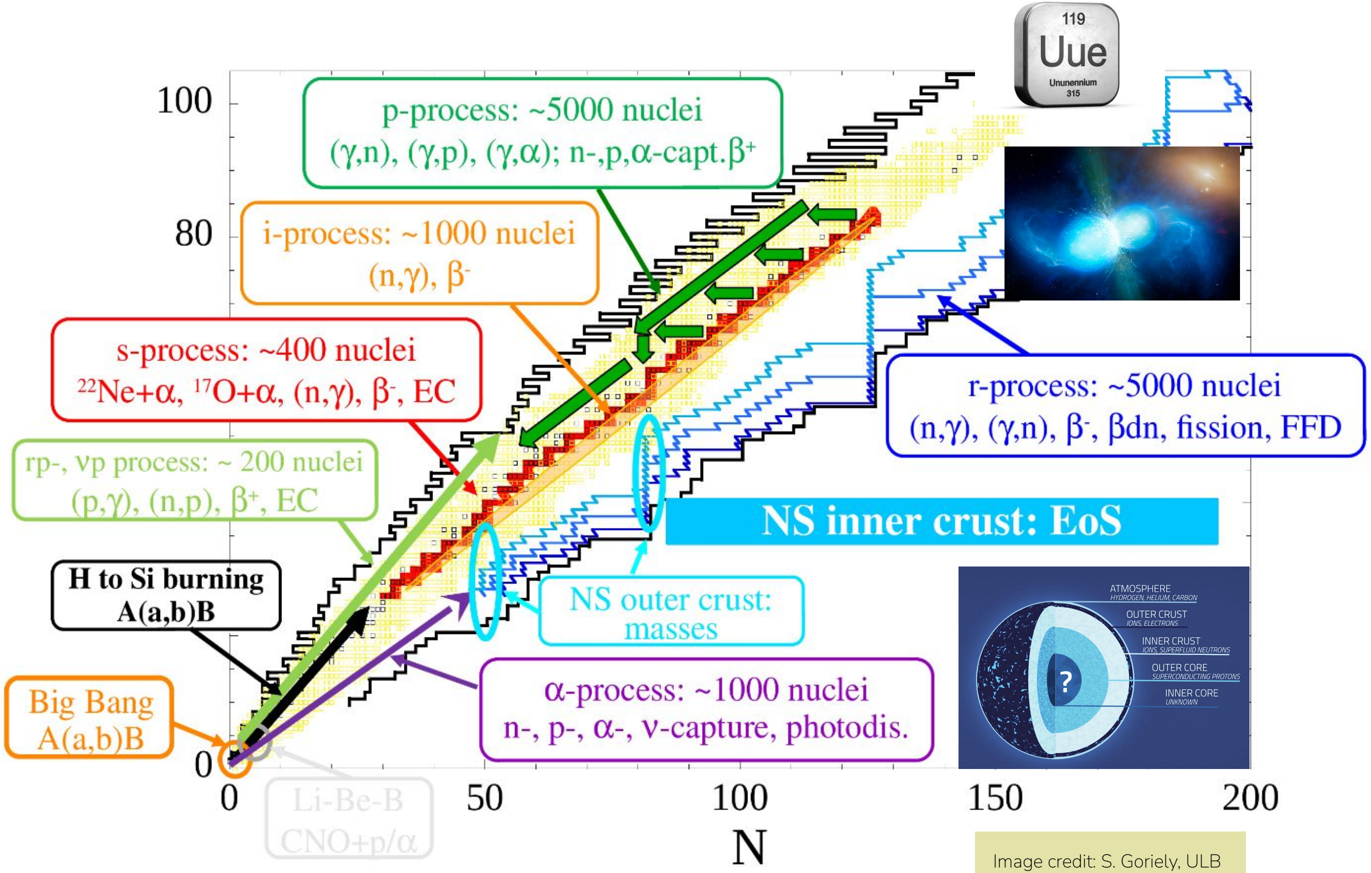


Image credit: S. Goriely, ULB

The challenge for nuclear theory: extrapolation!

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

and all of that for
- **~6k** nuclei
- **many** channels

what we need is theory with **predictive power!**

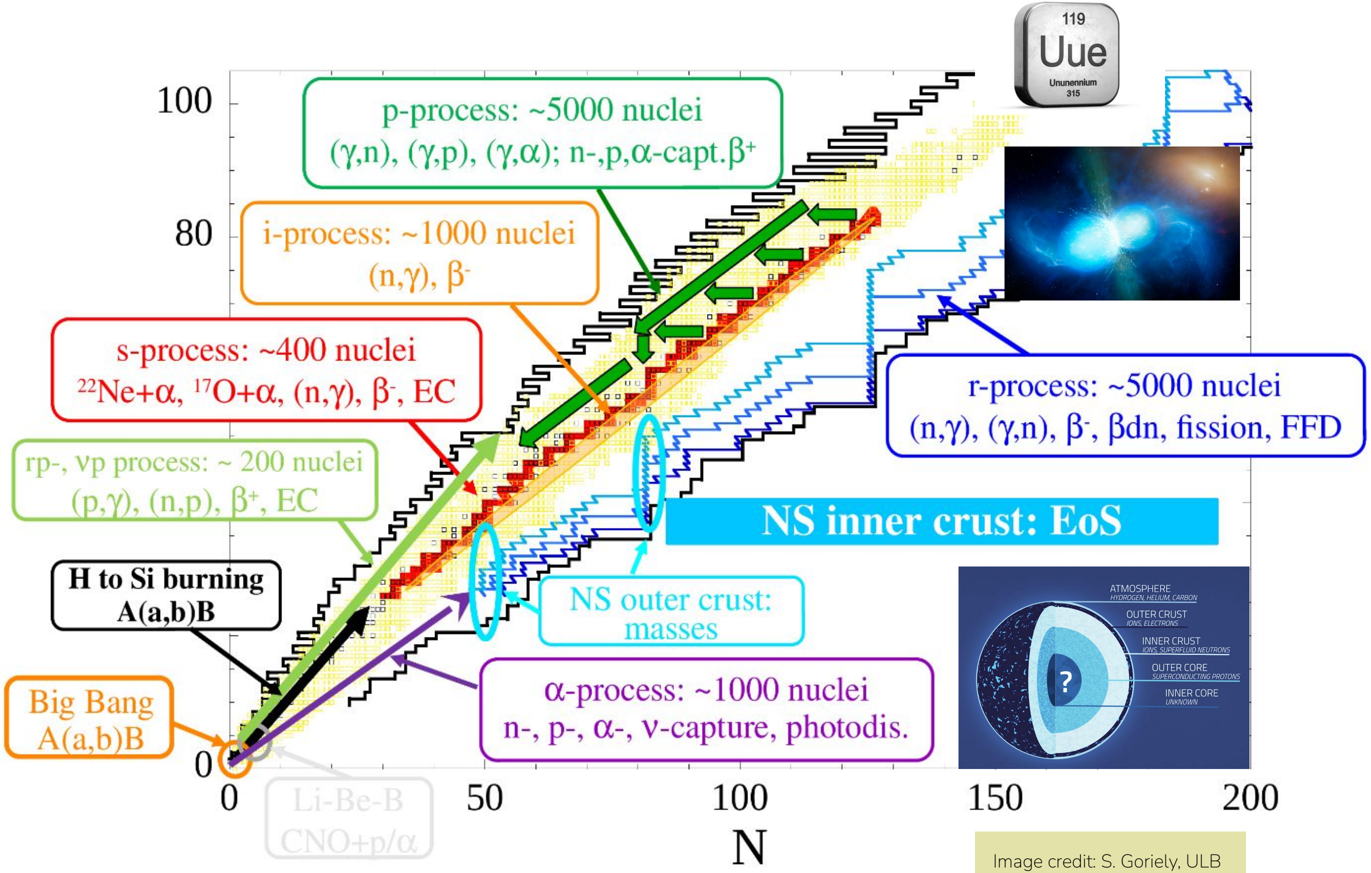
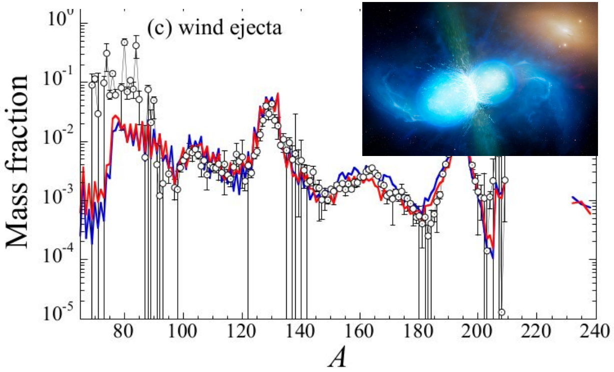


Image credit: S. Goriely, ULB

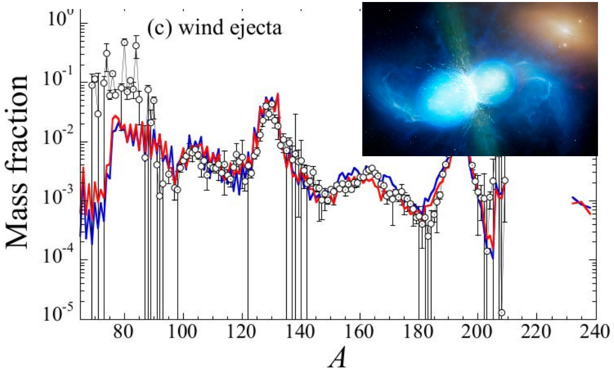
structure models

Nucleosynthesis



Large-scale, microscopic structure models

Nucleosynthesis



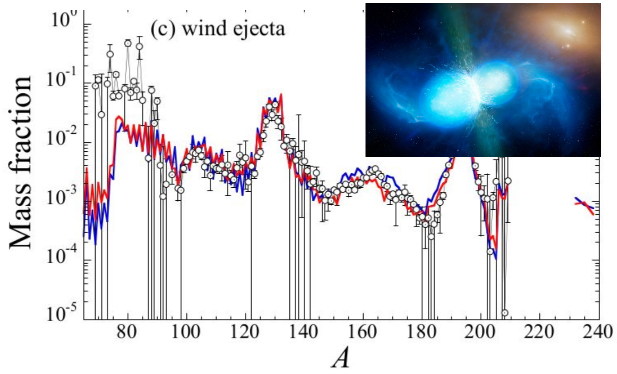
Large-scale, microscopic structure models

Structure details
- deformations
- level schemes
- optical potential

Masses

Nuclear EOS

Nucleosynthesis



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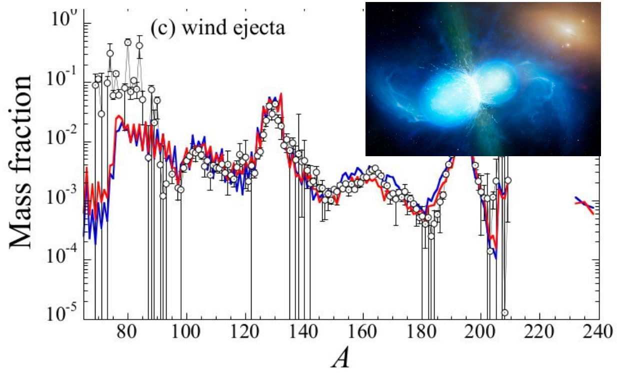

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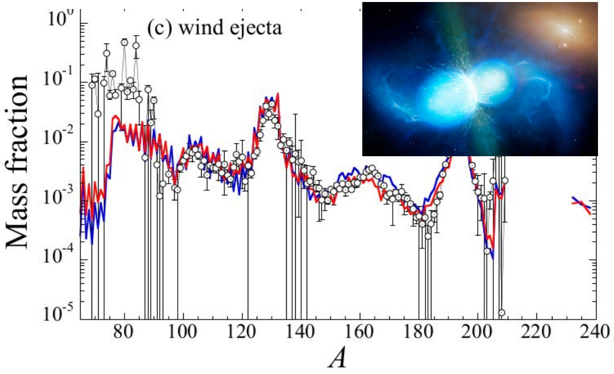

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Structure details
- deformations
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Reaction theory
- reaction rates
- reaction products

Nucleosynthesis

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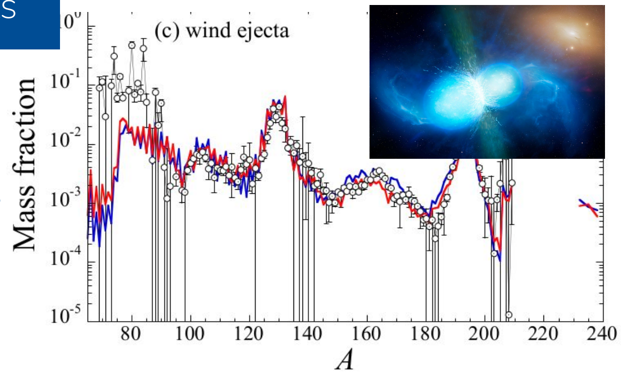

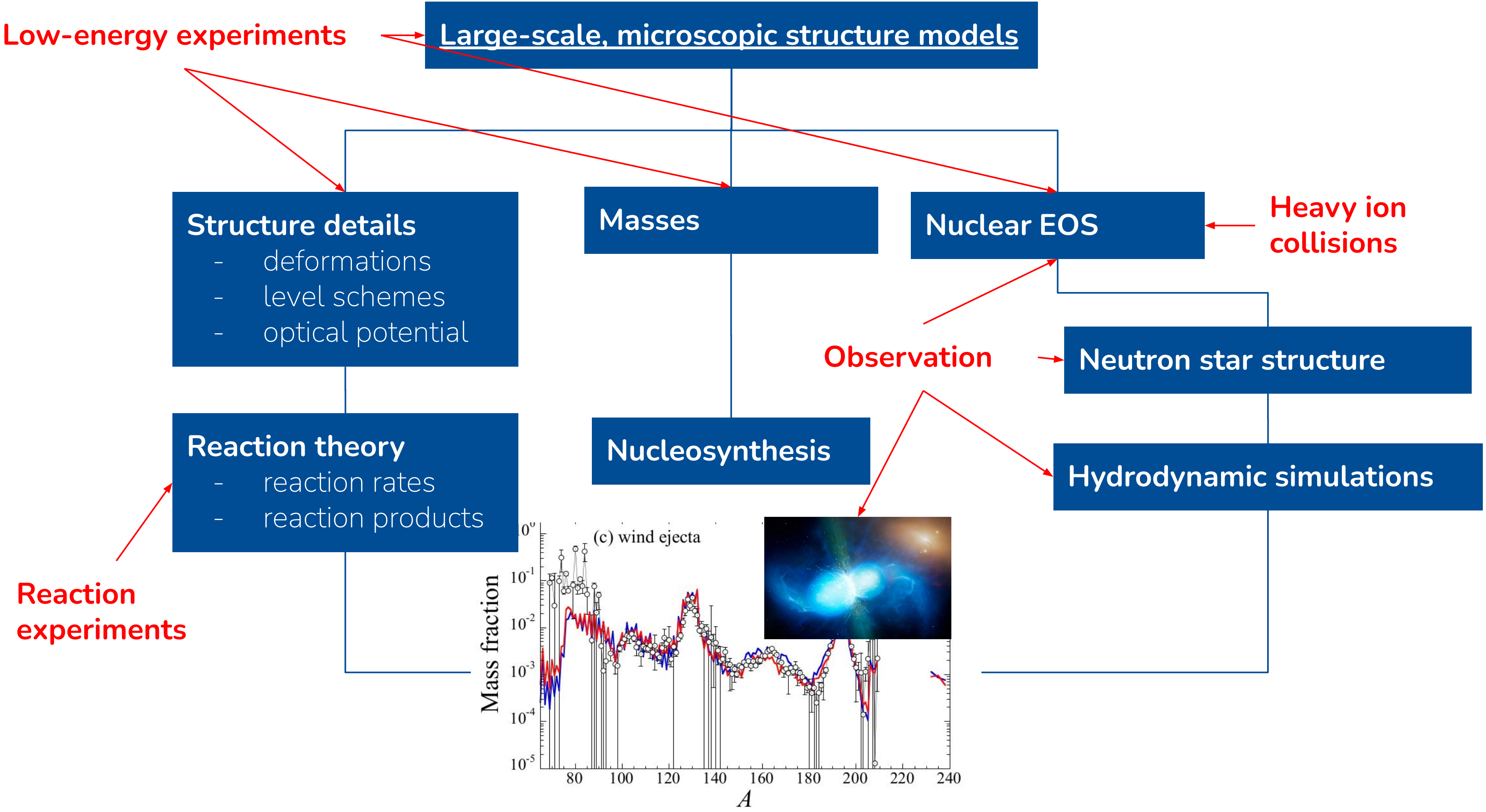
Low-energy experiments
Large-scale, microscopic structure models
Structure details
- deformations
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Masses
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Observation
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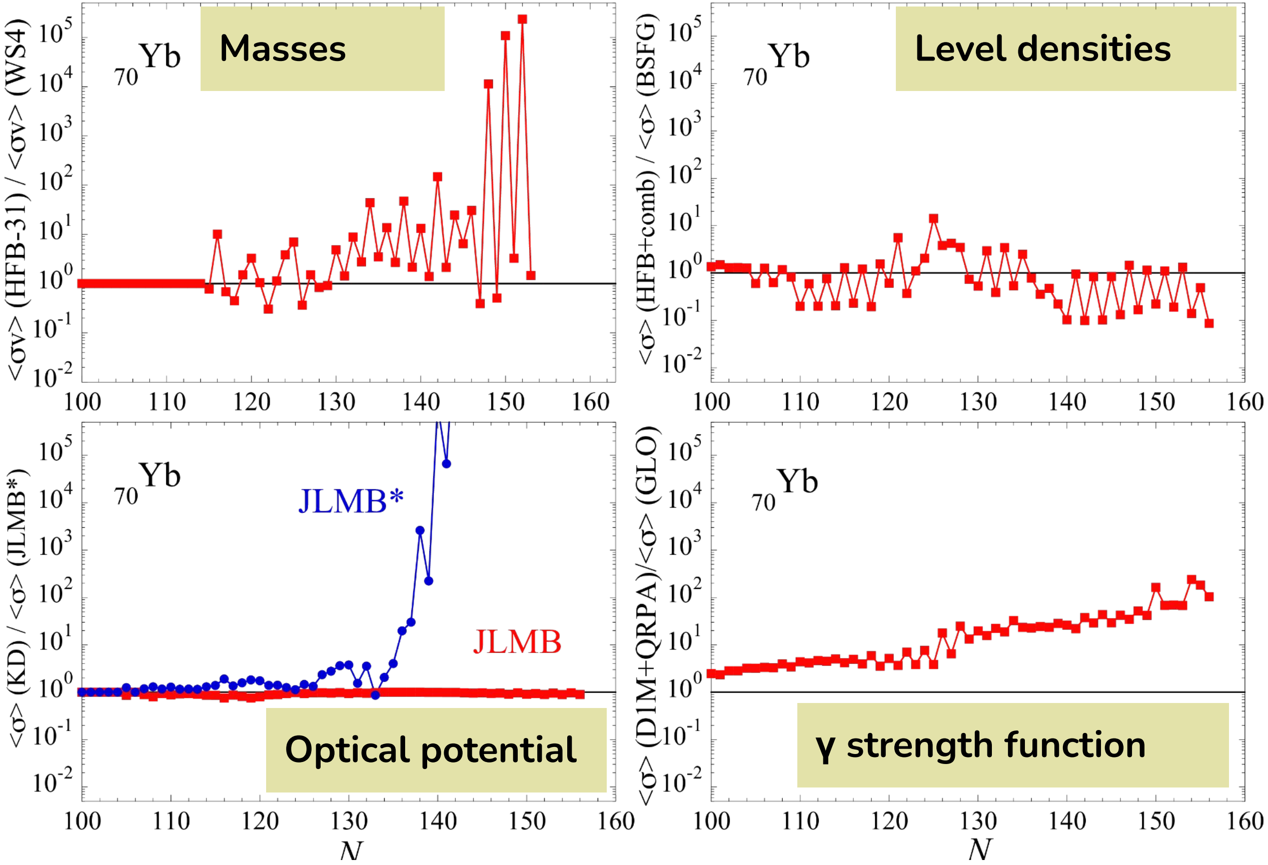
Reaction experiments
(c) wind ejecta
Mass fraction
A
10^-1
10^-2
10^-3
10^-4
10^-5
80
100
120
140
160
180
200
220
240

Models can make all the difference...

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



II. EDFs, deformation and the BSkG models

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

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

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

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- starts from **effective interaction**
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How does experimental data enter this?

1. Selection and weighting of **fitting data**
2. **Functional form** of the EDF
3. Complexity of the **wave function**

Nuclear deformation

- the many-body problem is complex
- look for solutions in a given variational space
  - independent-particle states
  - Hartree-Fock states
  - Hartree-Fock-Bogoliubov states
  - mean-field states
  - .....

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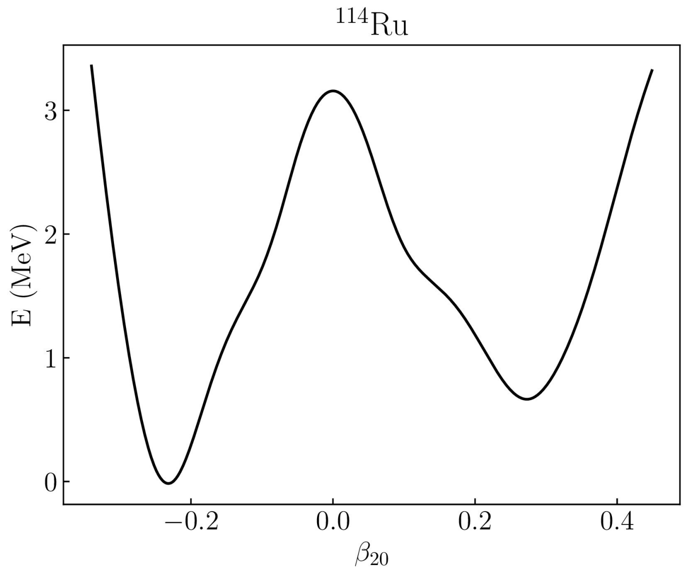
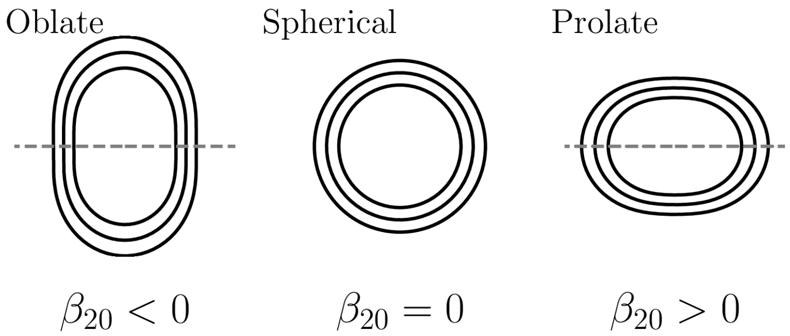
  - ✅ enlarges variational space
  - ✅ grasps sizeable part of correlations
  - ✅ still “in-class” wavefunctions
  - ❌ loses connection to quantum numbers
  - → symmetry-restoration, but expensive!





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Rotational symmetry	Multipole moments
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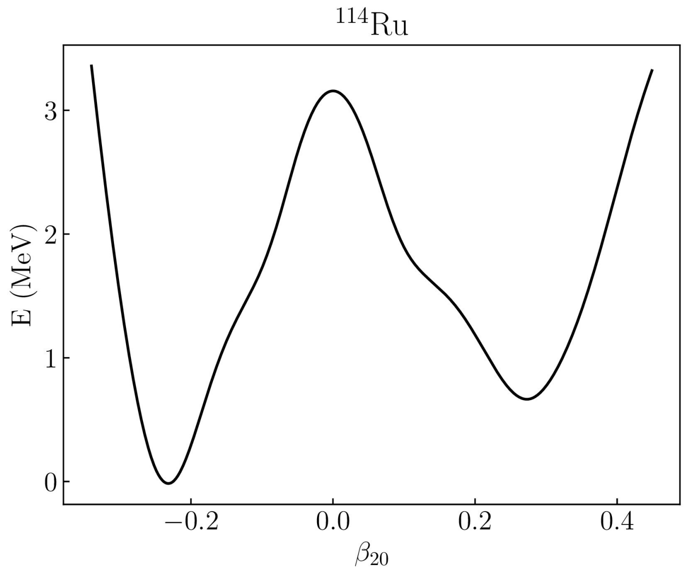
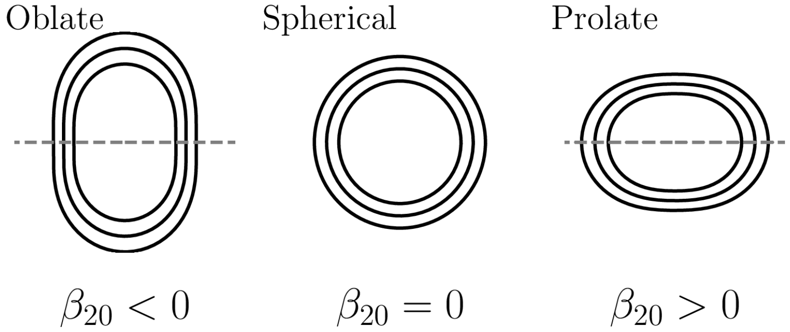
Particle number	Pairing





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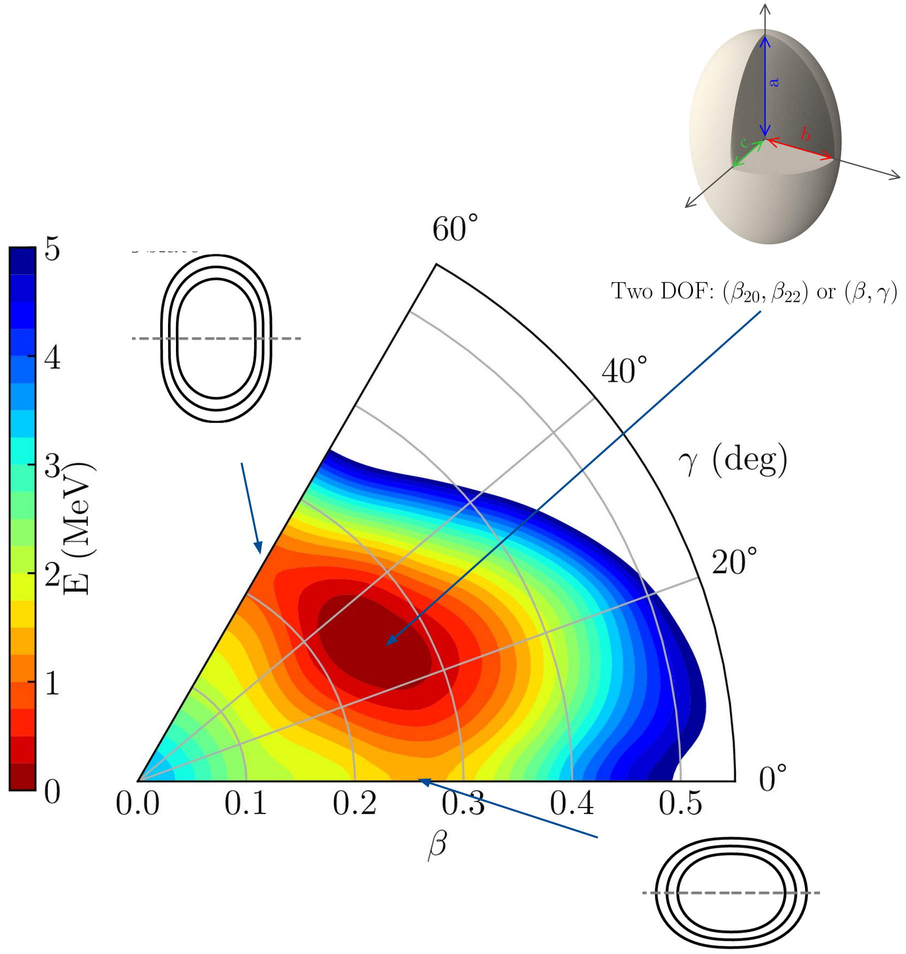

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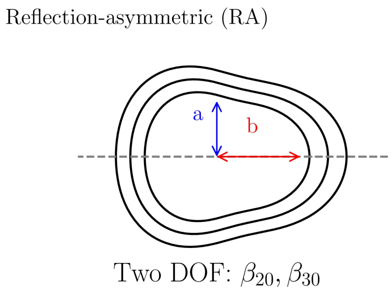

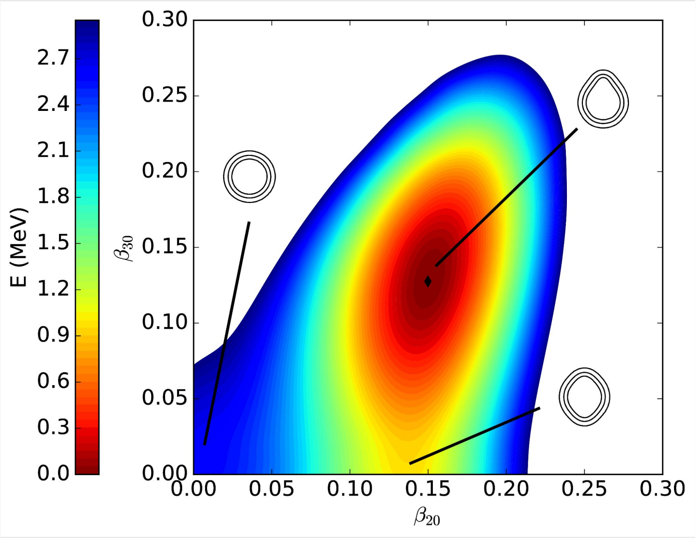

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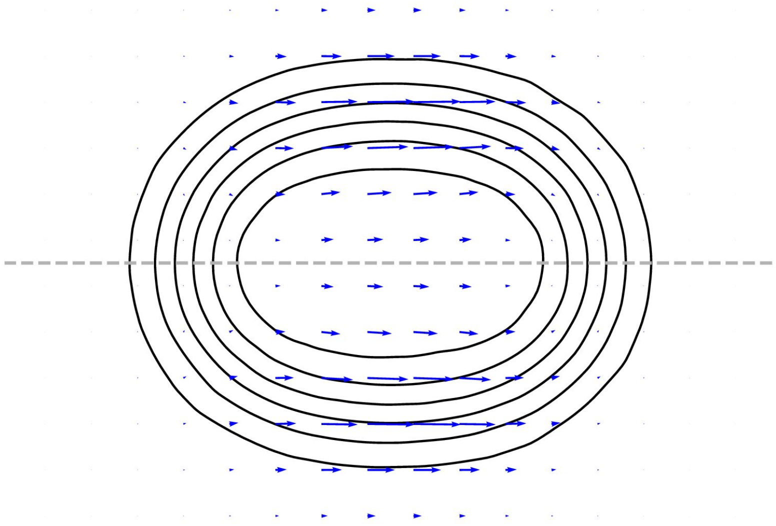

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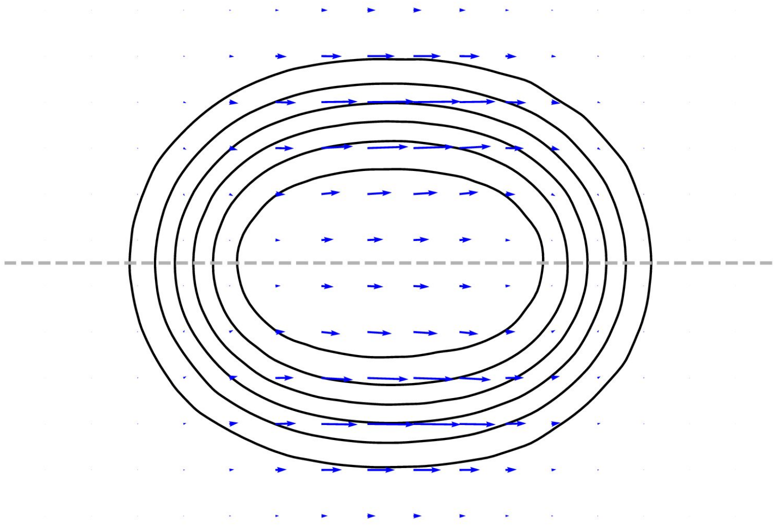
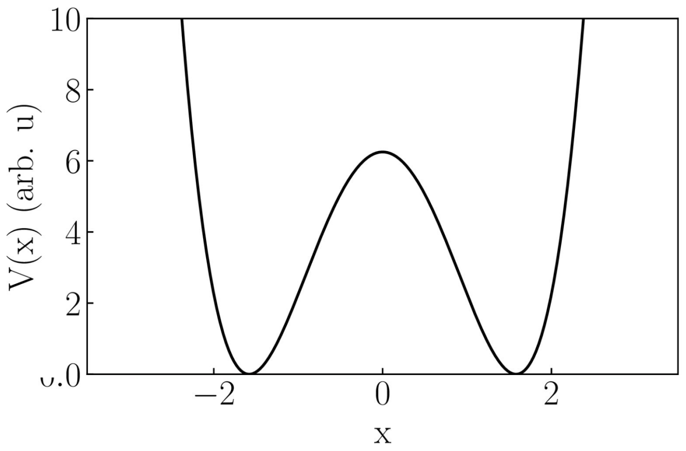
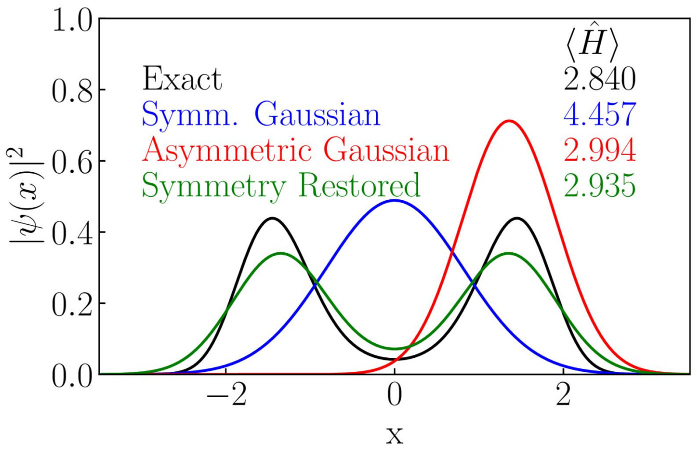


All of these have experimental signatures!

Nuclear deformation





A toy problem

- Gaussians as trial wavefunctions
- Symmetric trial state does badly
- Symmetry-broken solution works!
- …. but misses quantum numbers
- symmetry restoration solves this issue

The Brussels fit strategy

As much **microscopic** physics as possible:

- simple but symmetry-breaking wave functions
- wave functions determined by eff. interaction
- generalized effective interactions
- all ingredients deduced from wave functions
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As much **experimental data** as we can muster:

- ground state properties
  - ❗ **2457** masses of AME20
  - **884** charge radii
  - pairing properties

- fission properties
  - **45** primary & secondary barriers
  - **28** isomer excitation energies

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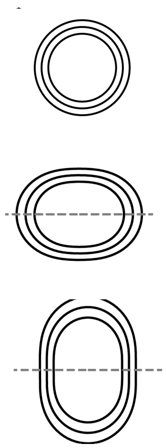

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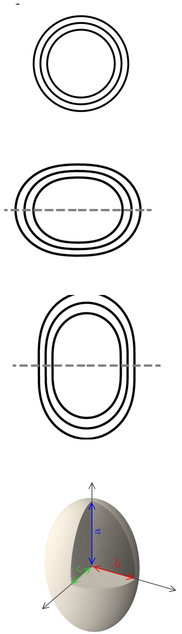
2021	BSkG1	2408	0.741
2022	BSkG2	2457	0.678



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We focus on the masses,
but not at the cost of everything else!

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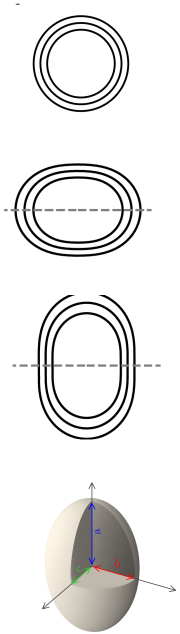
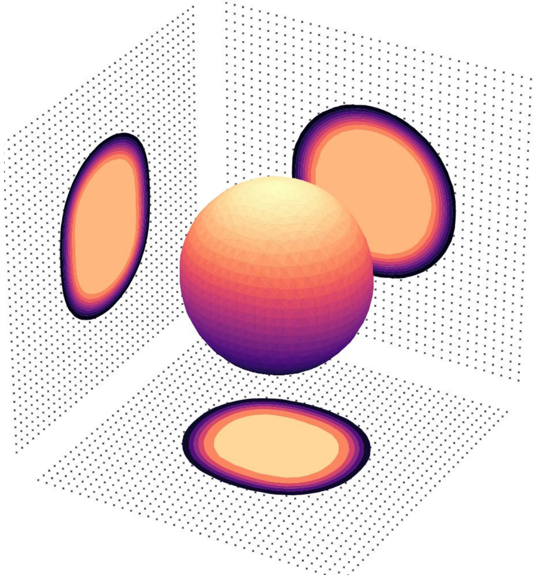


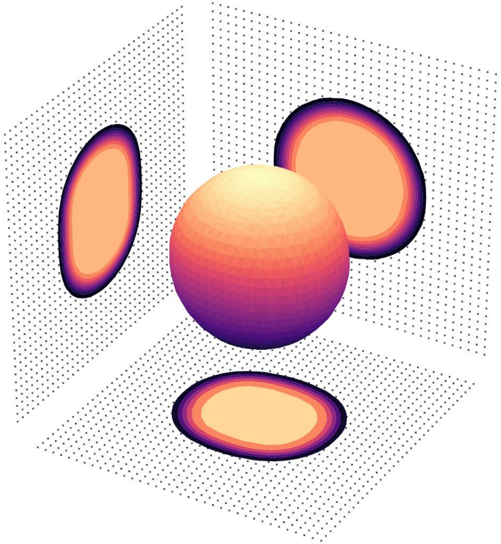
Brussels-**Sk**yrme-on-a-**G**rid: tools



3D coordinate space

- shape-agnostic
- numerical accuracy

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



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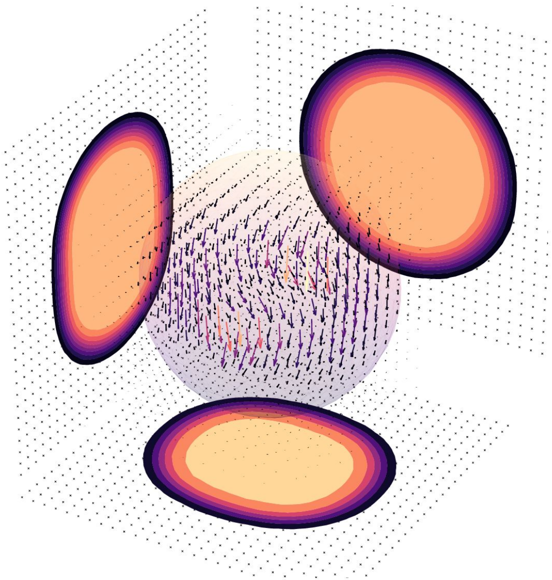
MOCCa

W. R. PhD Thesis, ULB (2016).

- **efficient** and **robust**
- symmetry choices à volonté

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



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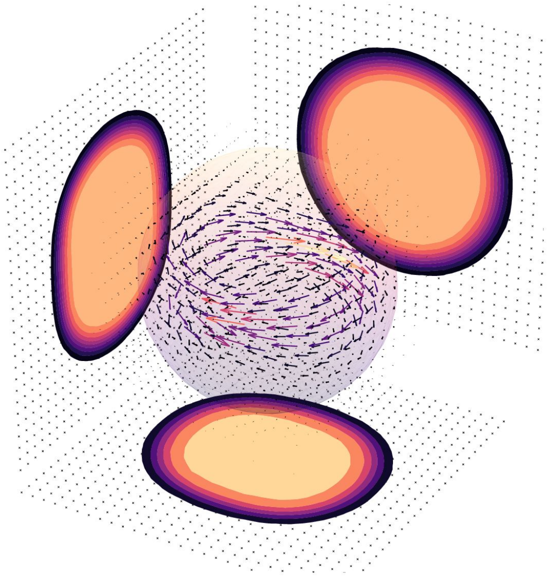

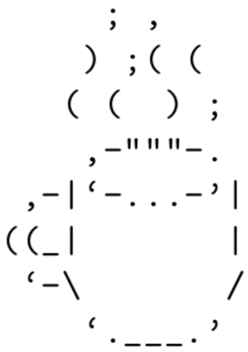

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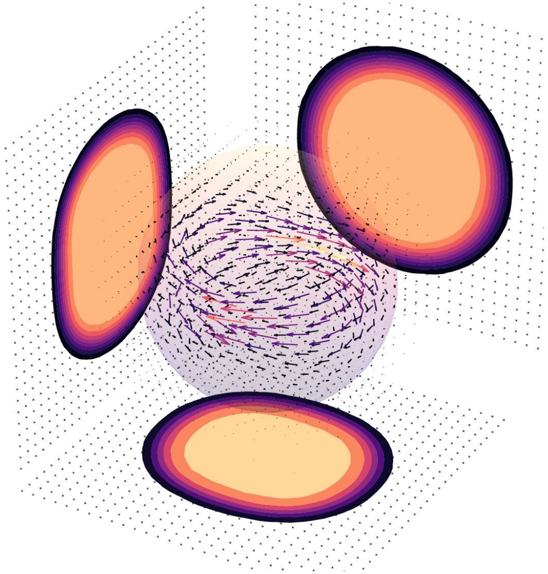
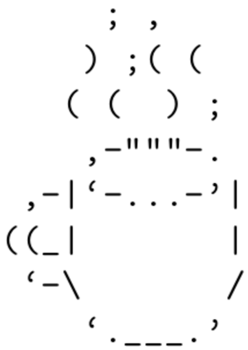
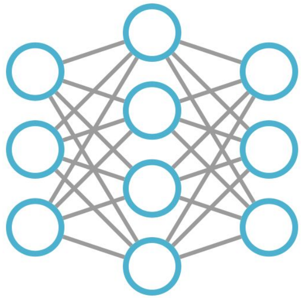
Brussels-Skyrme-on-a-Grid: tools







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W. R. PhD Thesis, ULB (2016).

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ML

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

- emulate MOCCa
- parameter space exploration
- **No actual predictions!**

The BSkG models: the raw numbers

BSkG1

- full 3D representation

BSkG2

- full 3D representation
- time-reversal symmetry breaking
- fission included in the fit

σ (MeV)	BSkG1	BSkG2	HFB-14	FRLDM
2457 masses	**0.741**	**0.678**		
884 charge radii (fm)	0.027	0.027		
45 primary barriers	0.87	0.44		
45 secondary barriers	0.86	0.47		
28 Isomer energies	0.45	0.49		

BSkG2: W. Ryssens et al., EPJA 58, 246 (2022).
BSkG1: G. Scamps et al., EPJA 57, 333 (2021).

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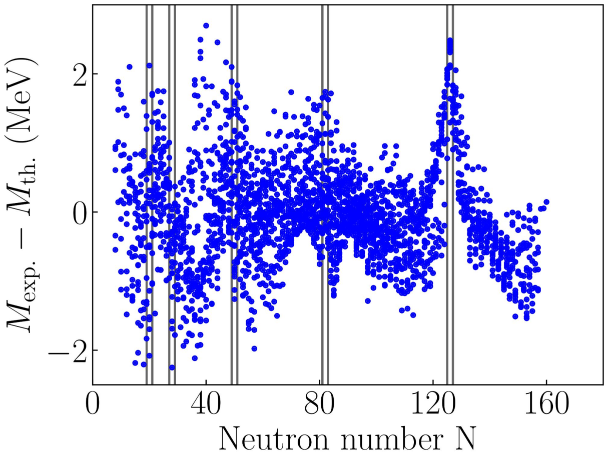


BSkG2: W. Ryssens et al., EPJA 58, 246 (2022).
BSkG1: G. Scamps et al., EPJA 57, 333 (2021).

The BSkG models: the raw numbers

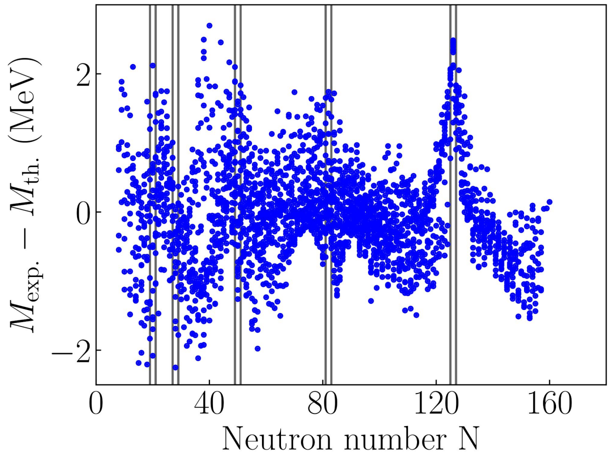
BSkG1

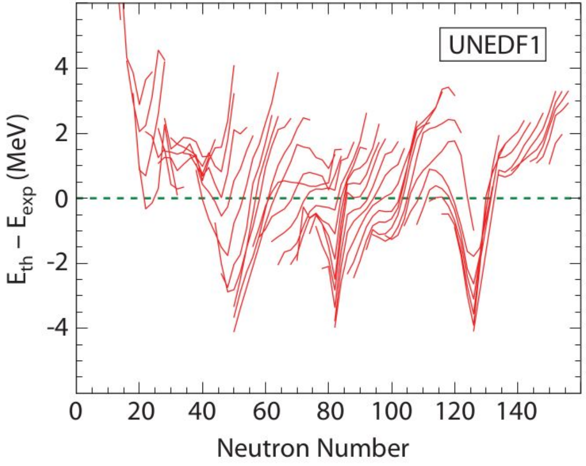
- full 3D representation

BSkG2

- full 3D representation
- time-reversal symmetry breaking
- fission included in the fit

σ (MeV)	BSkG1	BSkG2	HFB-14	FRLDM
2457 masses	**0.741**	**0.678**		
884 charge radii (fm)	0.027	0.027		
45 primary barriers	0.87	0.44		
45 secondary barriers	0.86	0.47		
28 Isomer energies	0.45	0.49		





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The BSkG models: the raw numbers

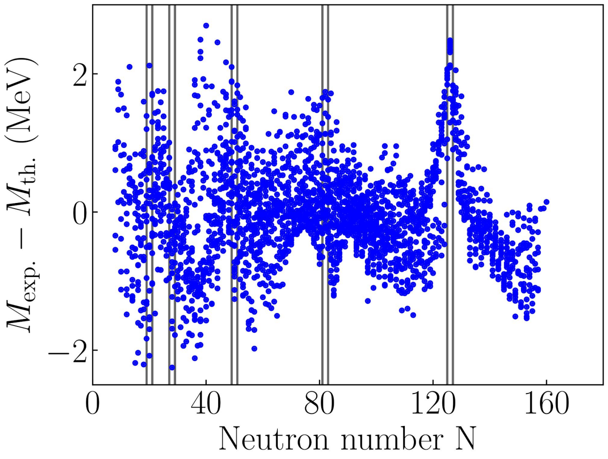
<u>BSkG1</u>

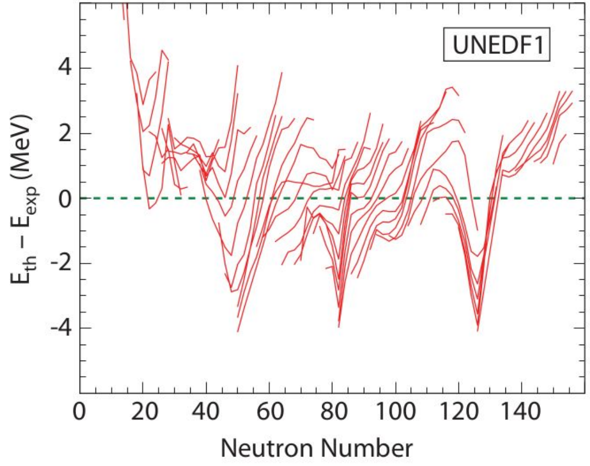
- full 3D representation

BSkG2

- full 3D representation
- time-reversal symmetry breaking
- fission included in the fit

σ (MeV)	BSkG1	BSkG2	HFB-14	FRLDM
2457 masses	**0.741**	**0.678**	**0.729**	**0.808**
884 charge radii (fm)	0.027	0.027	0.039	-
45 primary barriers	0.87	0.44	0.61	0.79
45 secondary barriers	0.86	0.47	0.70	1.35
28 Isomer energies	0.45	0.49	0.93	1.04





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III. Why do we do these complex things?

Interlude: why do we do these complex things?

Mic-mac approaches?

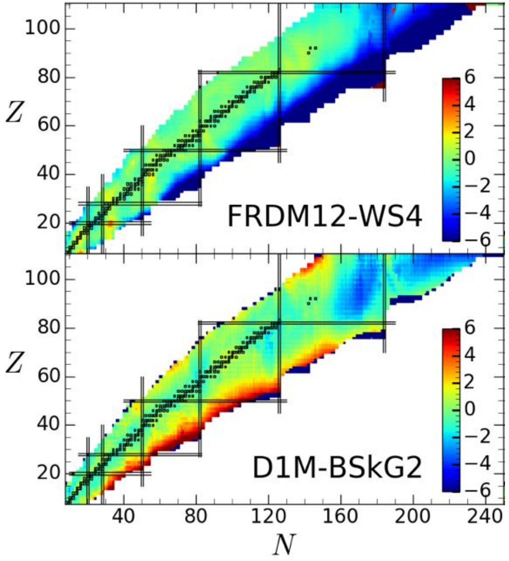
✅ competitive in rms
✅ multiple observables

Machine learning?

Ab Initio?

Interlude: why do we do these complex things?

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



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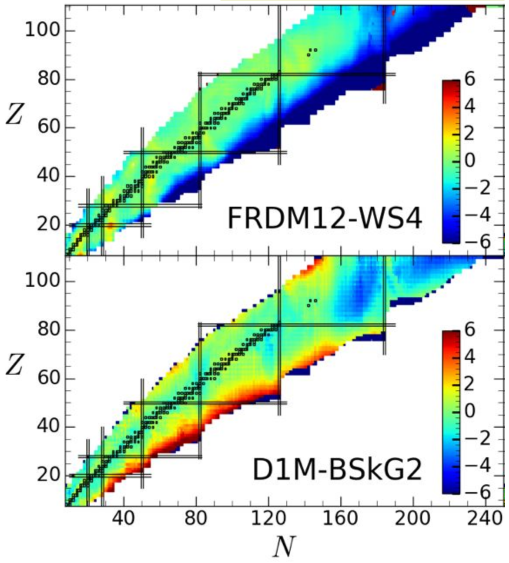

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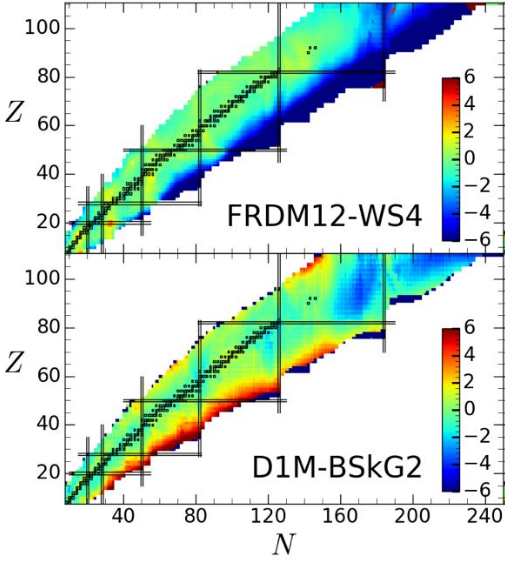

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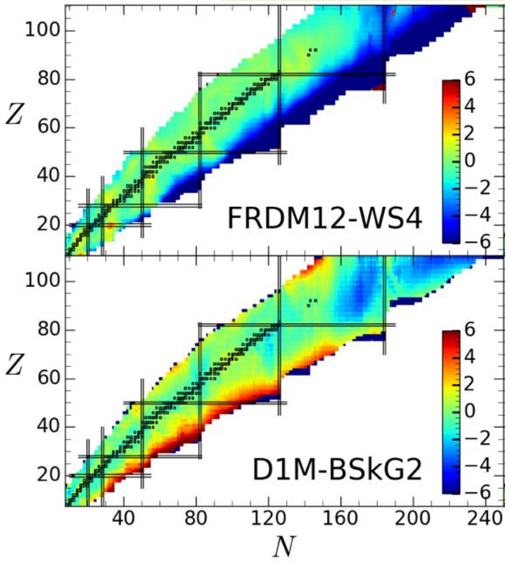
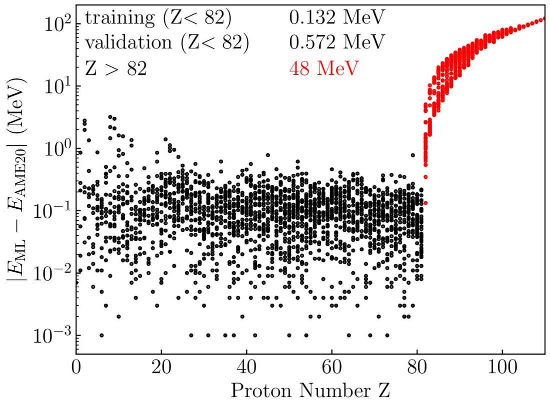


G. Grams, W.R. et al., in preparation



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- ❌ single observable

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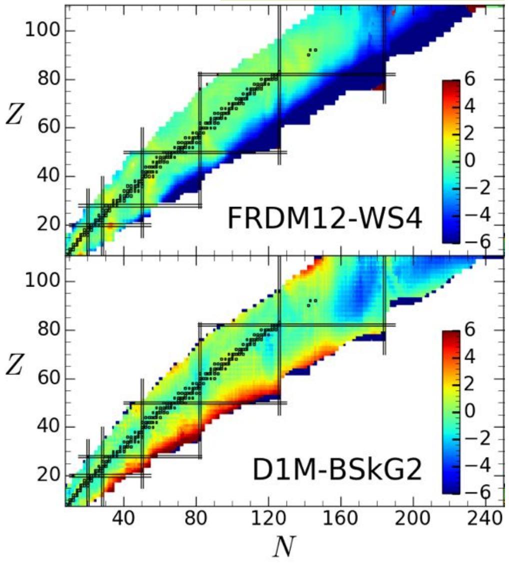

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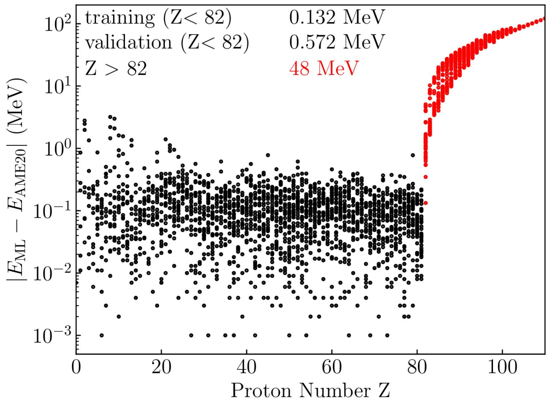

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Ab Initio?

✅ error quantification
✅ “truly” microscopic
✅ multiple observables

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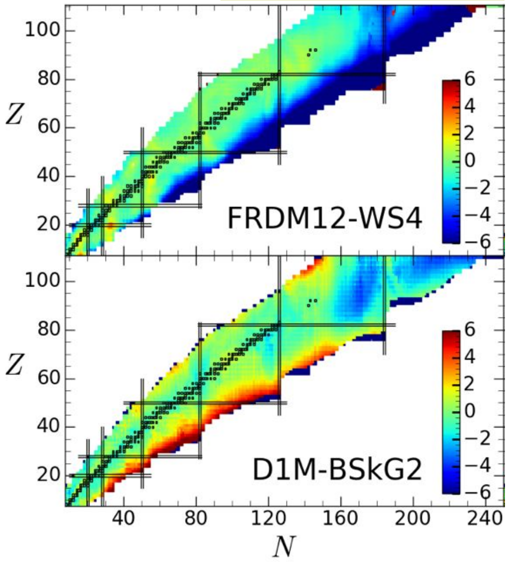

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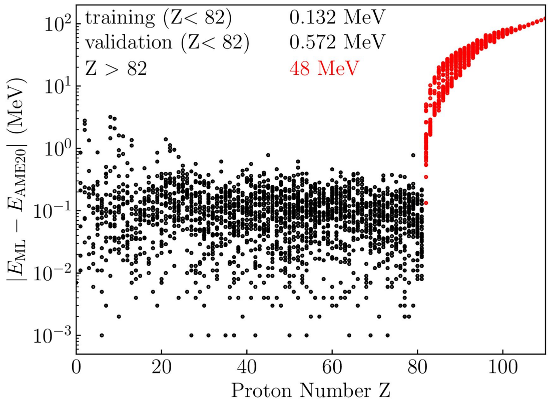

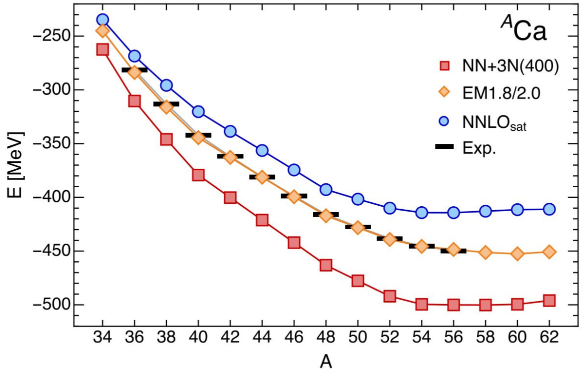

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❌ thousands (?) of parameters
❌ single observable

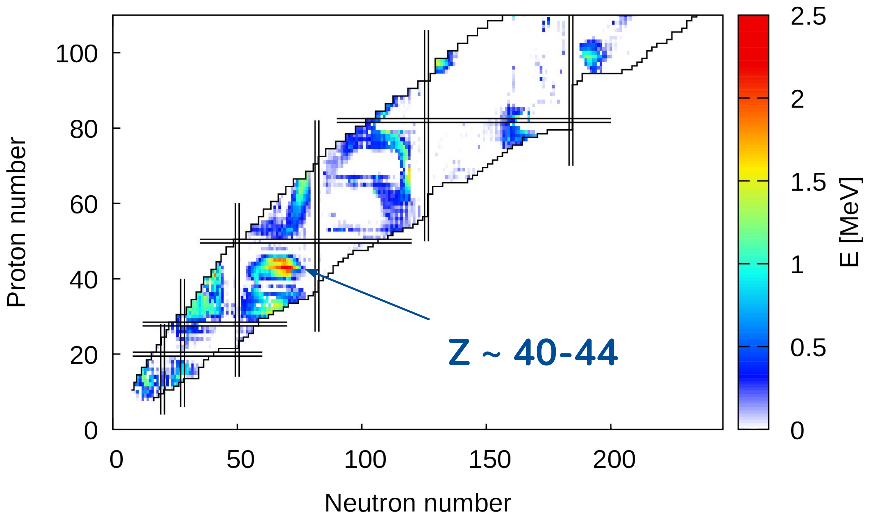
Ab Initio?

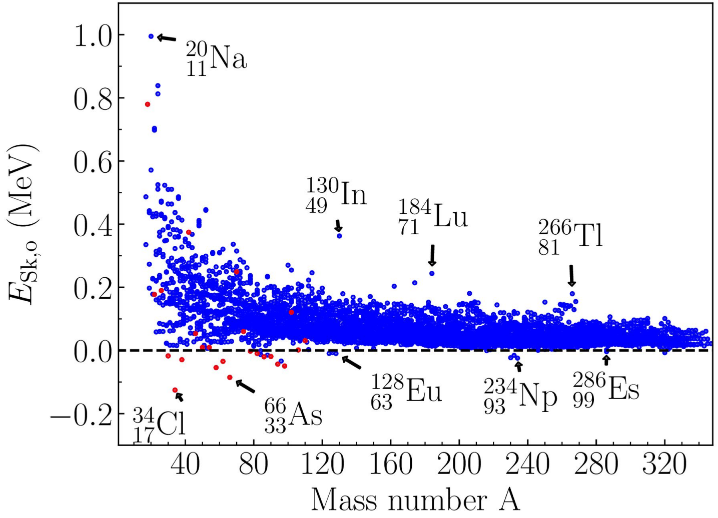
✅ error quantification
✅ “truly” microscopic
✅ multiple observables

❌ infeasible at scale (for now)
❌ not competitive on rms (for now)

IV. Observables

Observables: masses





Triaxial deformation

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

- most nuclei remain axial
- several regions of triaxiality
- large effects from 0.5-2 MeV.

Time-reversal symmetry breaking

W.R. et al., EPJA 58, 246 (2022).

- reduces binding energy
- but small contribution…
- … and grows smaller with system size

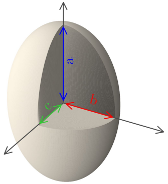
Observables: masses

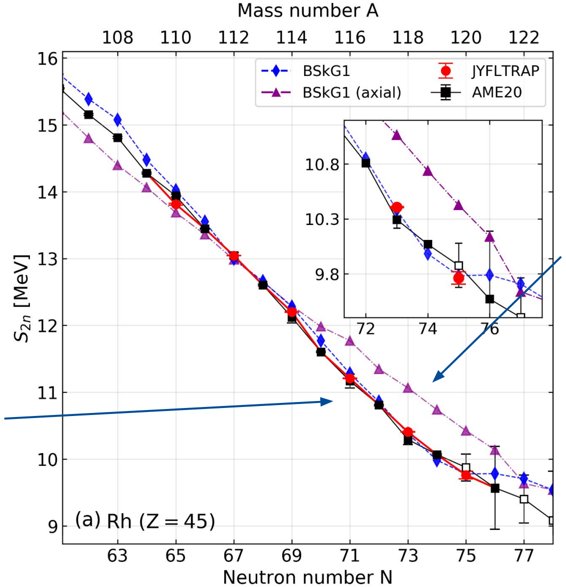
Rh isotopes, nice!

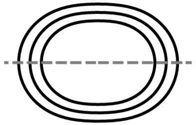
M. Hukkanen et al., PRC 107, 014306 (2023).

- masses of ^{110,112,114,116,118}Rh g.s. measured
- absolute masses within ~ 700 keV

Observables: masses







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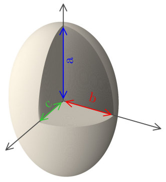

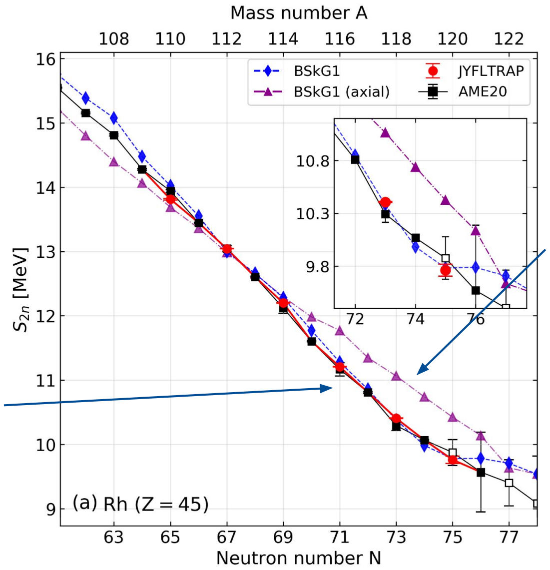

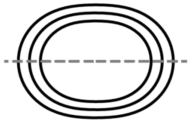

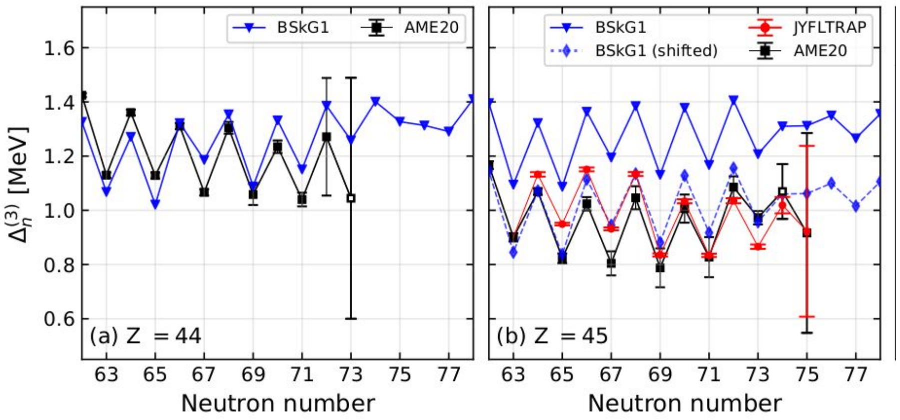

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Rh isotopes, not-so-nice!

W.R. et al., arXiv:2211.03667 [nucl-th].

- total failure to reproduce $\Delta^{(3)}_n$ ....
- ... but works in neighbouring chains!

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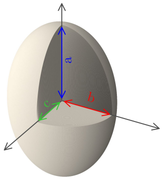

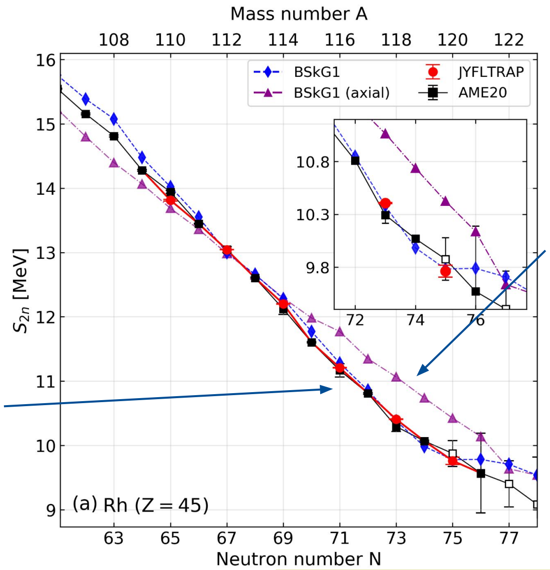

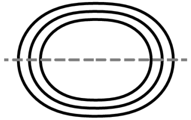

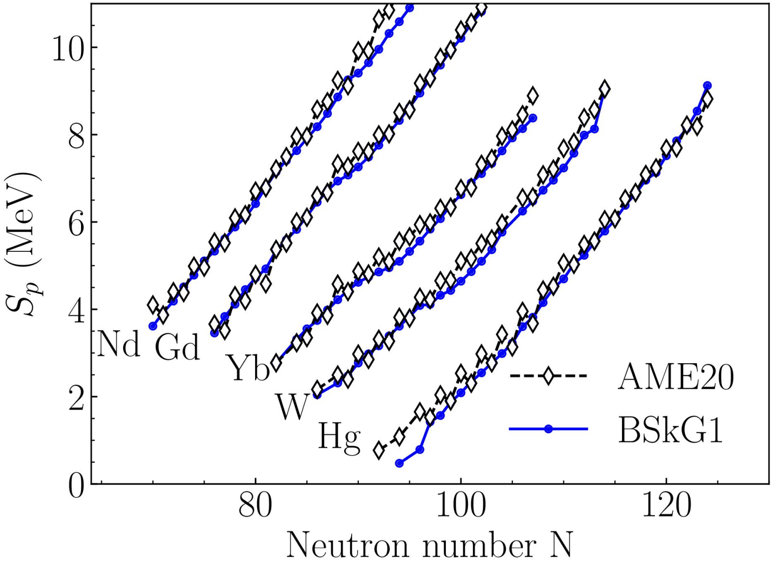

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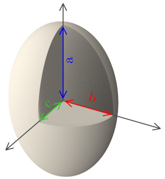
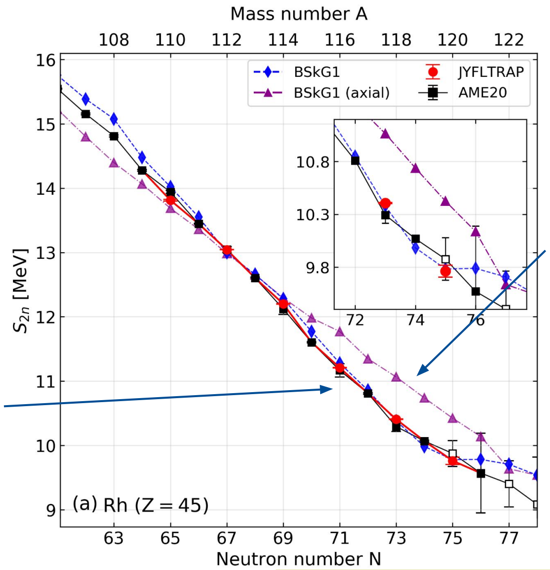
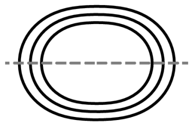
- is linked to interaction odd-n and odd-p?

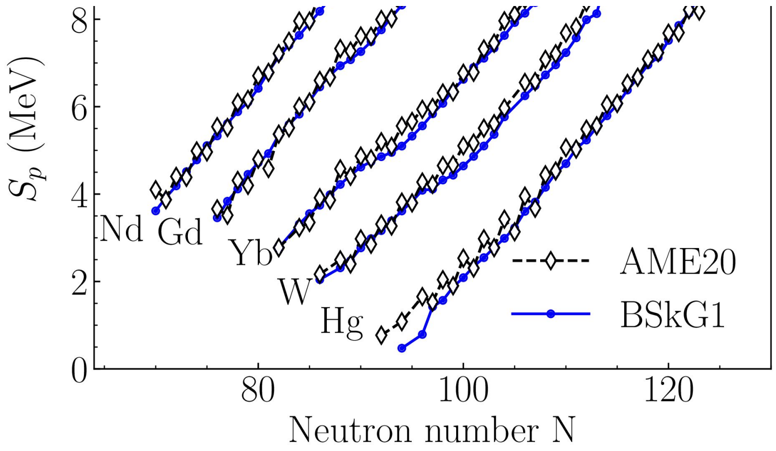
Observables: masses

$$E \sim \int \mathbf{j}_p(\mathbf{r}) \cdot \mathbf{j}_n(\mathbf{r}) + \mathbf{s}_p(\mathbf{r}) \cdot \mathbf{s}_n(\mathbf{r})$$









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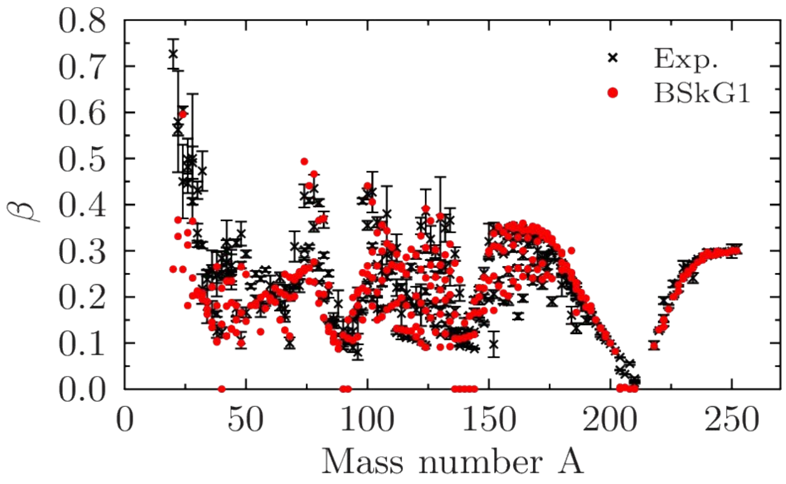
Observables: deformations

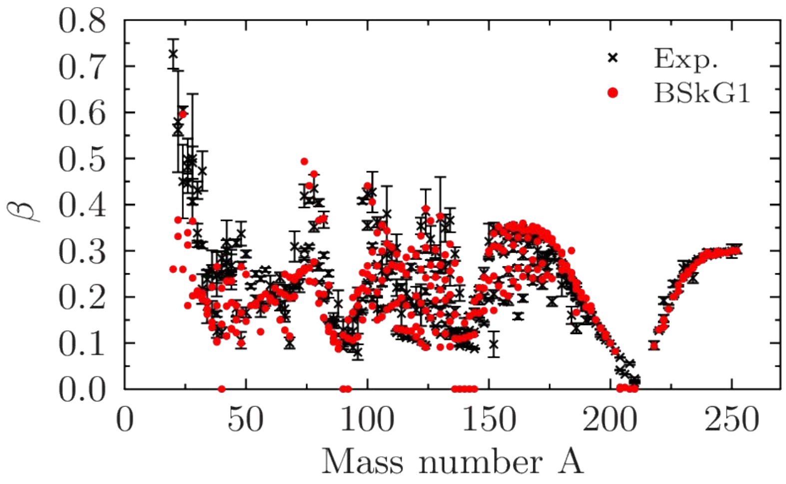


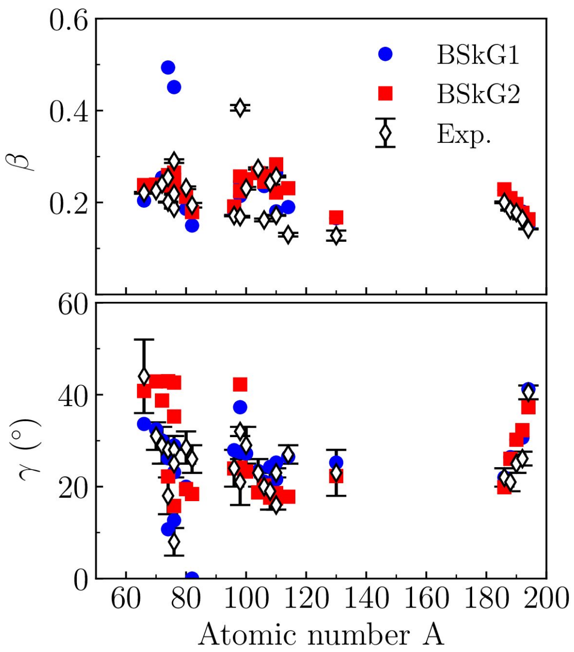
Global systematics

S. Raman, At. Data **78**(1), 1-128 (2001).

- deduced from B(E2) transitions
- good global reproduction
- particularly for heavy nuclei

Observables: deformations





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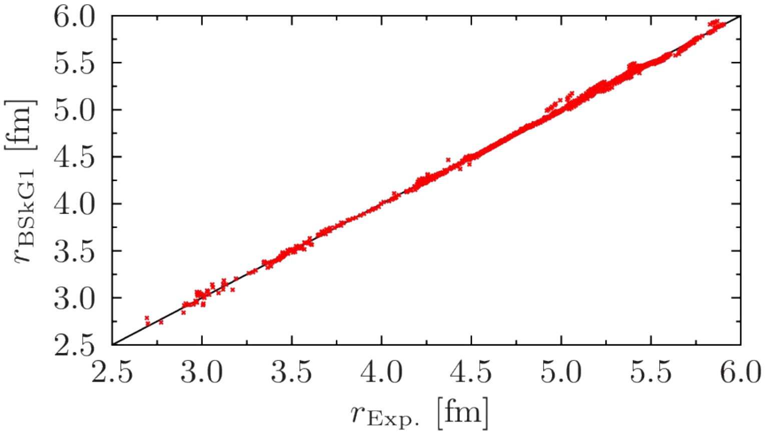
Triaxial deformation?

Thanks to M. Zielinska!

- <u>**ALL**</u> available COULEX data
- very good agreement
  (within model limitations)

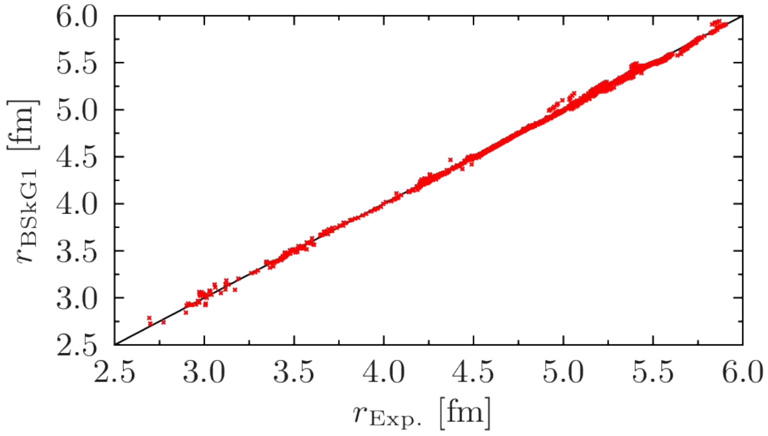
Observables: charge densities/radii

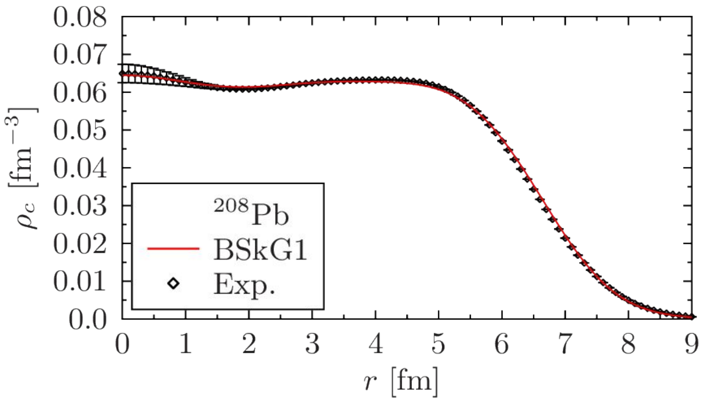


Systematics and details of charge densities

✅ rms (charge radii) ~ 0.027 fm

Observables: charge densities/radii





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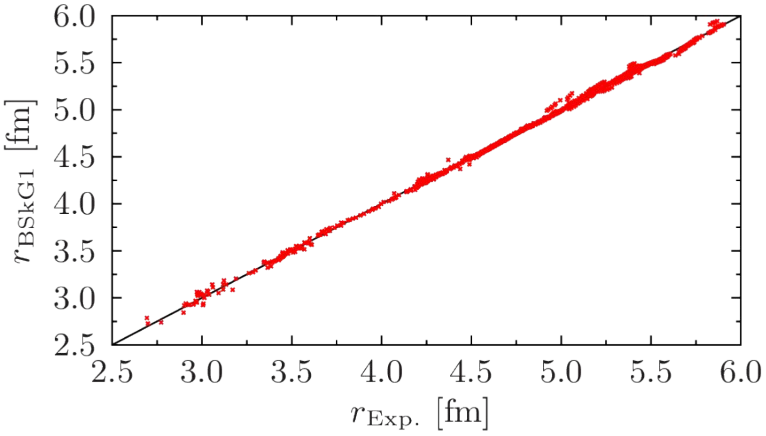
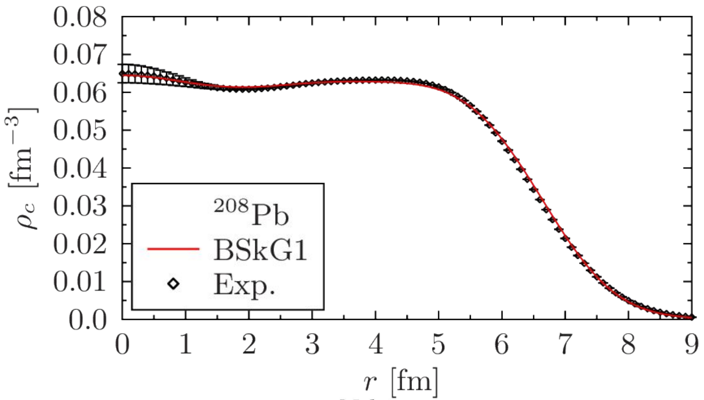
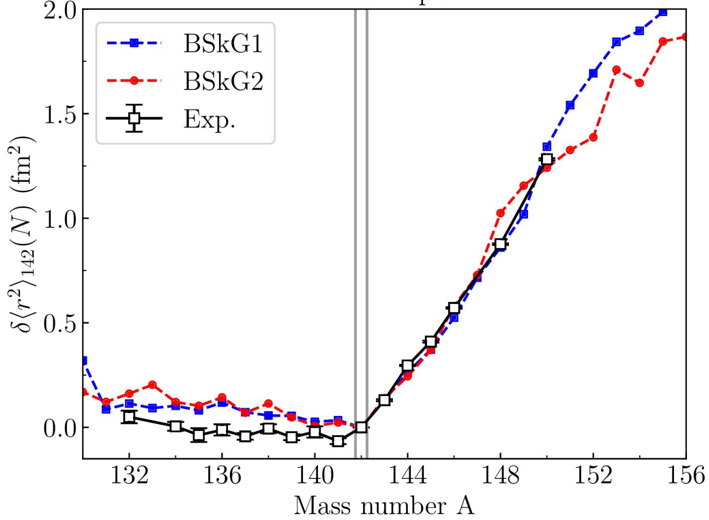




Systematics and details of charge densities

- ✅ rms (charge radii) ~ 0.027 fm
- ✅ complete charge densities
- ✅ dramatic evolution with particle number
  ….. linked to deformation!



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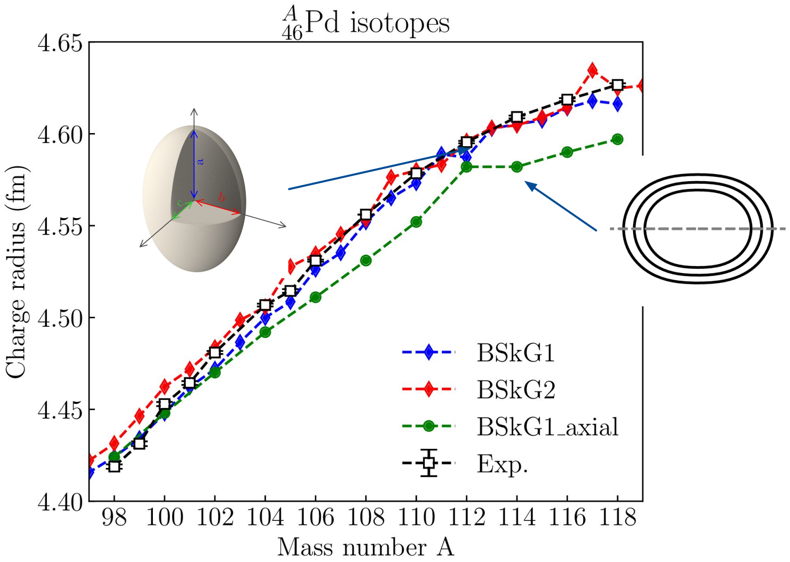
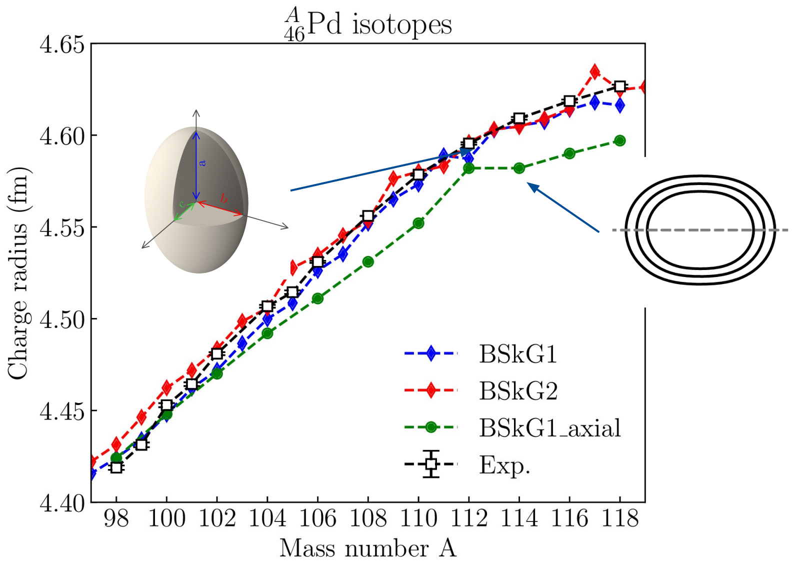


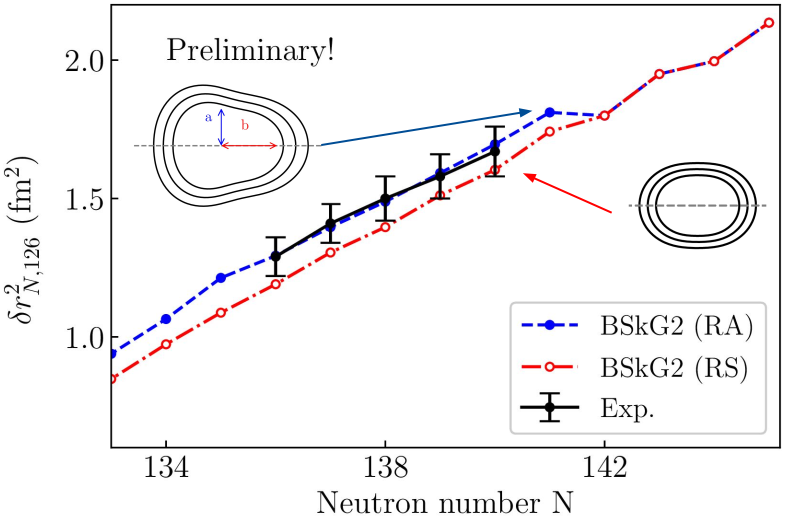
Pd radii

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

- radii are sensitive to ALL deformation
- not just β_{20} , but also β_{22} !

Observables: charge densities/radii





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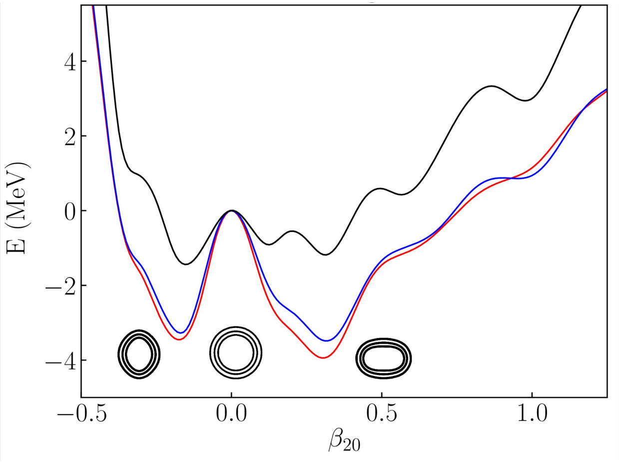
- not just β_{20}, but also β_{22}!

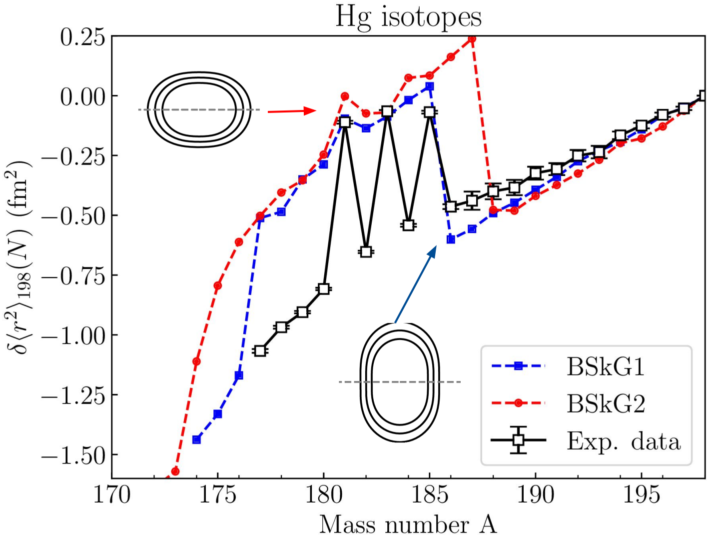
Ac radii

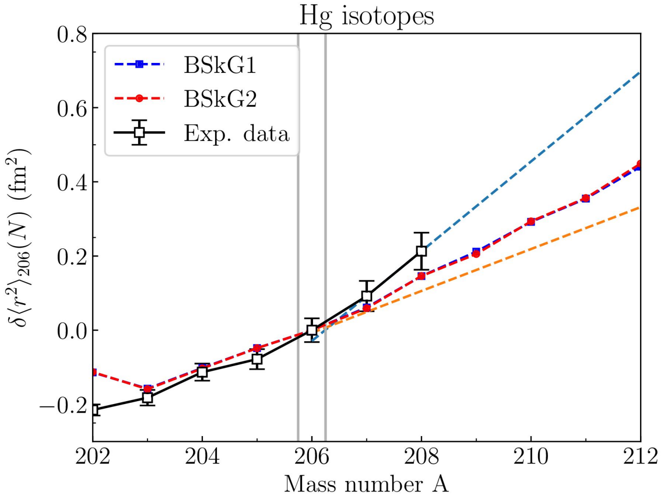
E. Verstraelen et al., PRC 100, 044321 (2019).

- …. and also β_{30}!
- predicted end of octupole region
- New experiment ongoing….

Observables: charge densities/radii







Hg isotopes are hard!

S. Sels et al., Phys. Rev. C 99 (2019).

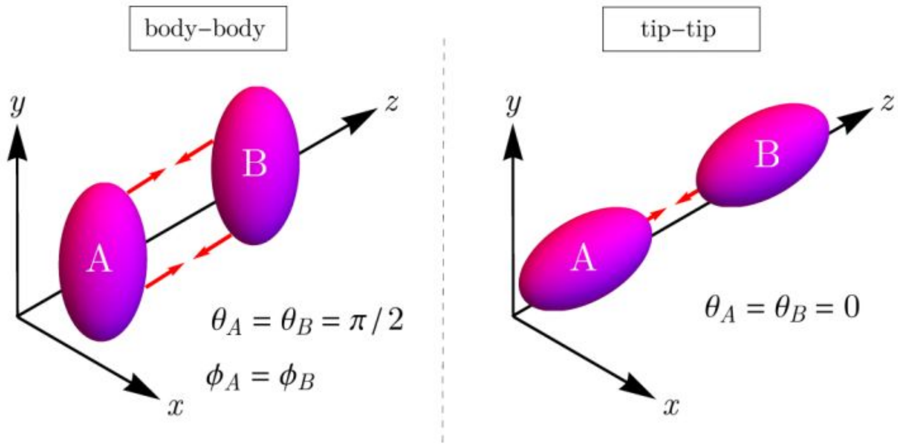
Staggering:

- rapid shape change
- **multiple, competing** minima

Kink at N=126

- no obvious interpretation
- also exists at N=20,50,82!
- my bet: single-particle structure

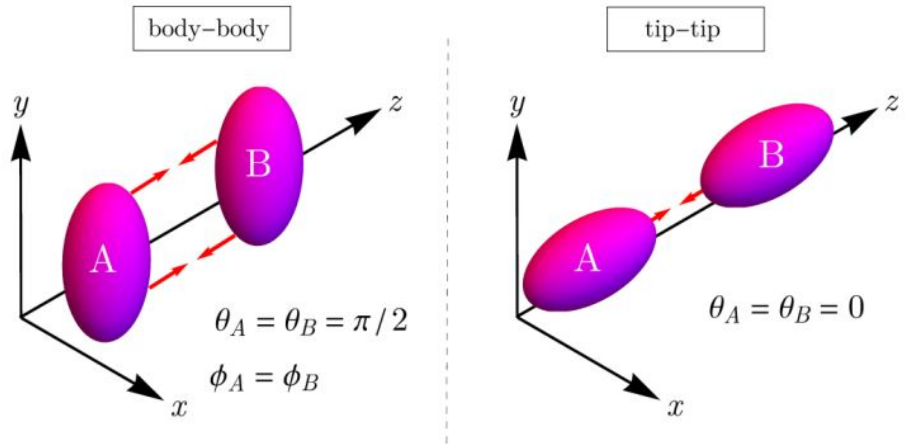
Observables: densities

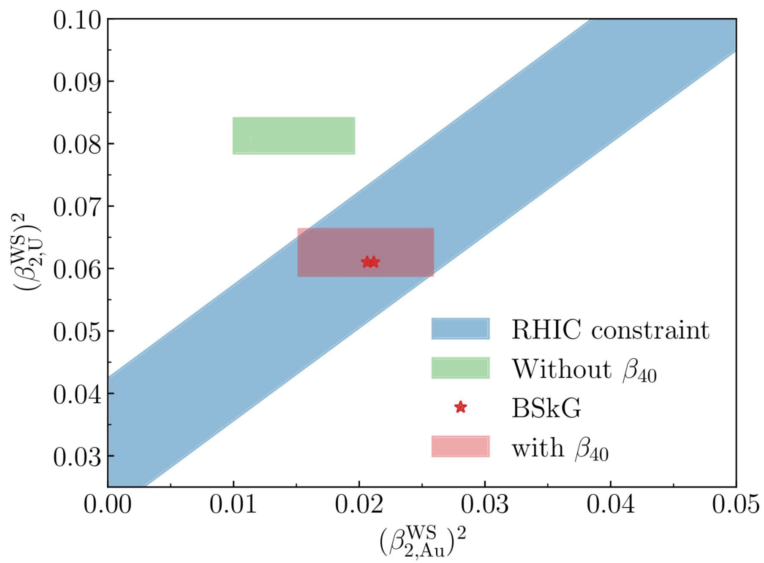


Heavy ion collisions

- shape of the quark-gluon plasma depends on nuclear density
- deformation imprints on the particles detected!

Observables: densities





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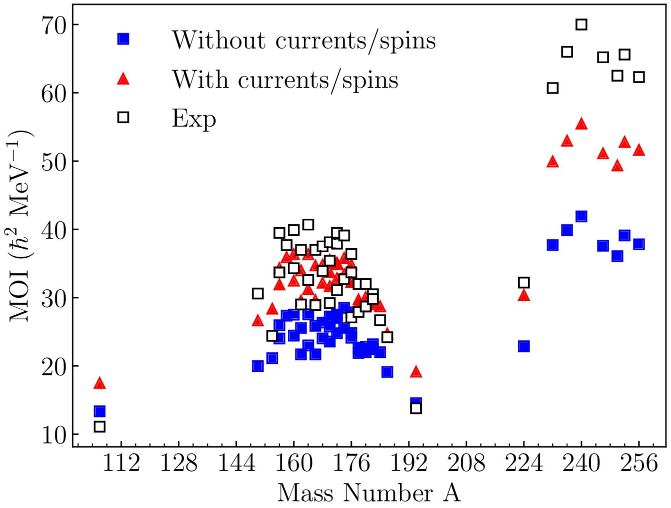
- shape of the quark-gluon plasma depends on nuclear density
- deformation imprints on the particles detected!

Exciting times!

W. R. et al., arXiv:2302.13617 (2023).

- a priori sensitive to ALL aspects
  - exotic multipole moments
  - matter (!) radii
- Au+Au collisions and U+U collisions can only be described by including β_{40}

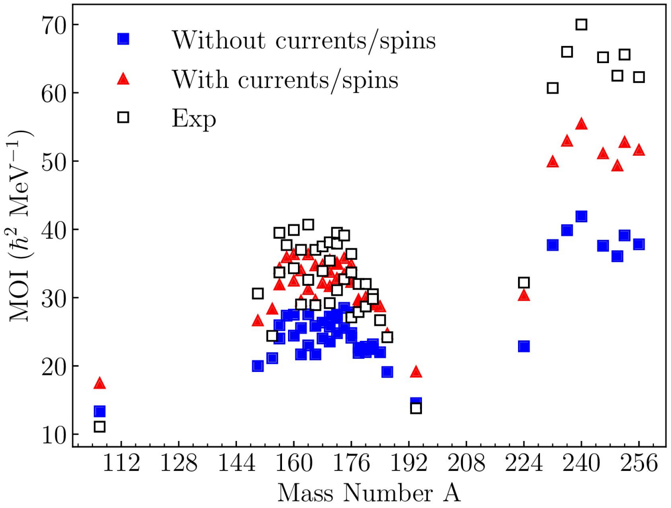
Observables: rotational properties

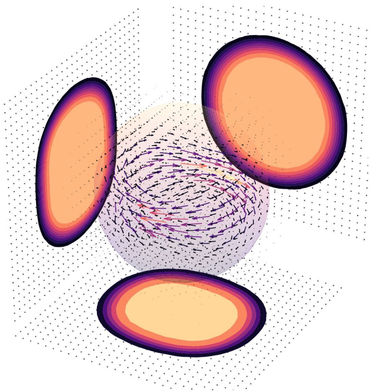


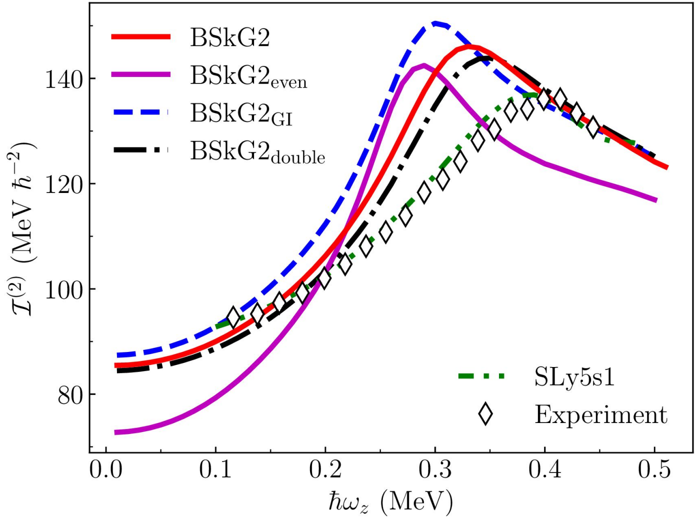
Rotational response of nuclei

- currents and spins contribute to MOI
- ✅ medium-heavy nuclei
- ❌ actinides

Observables: rotational properties







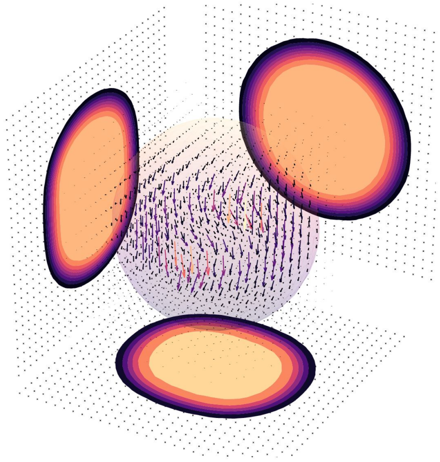
Rotational response of nuclei

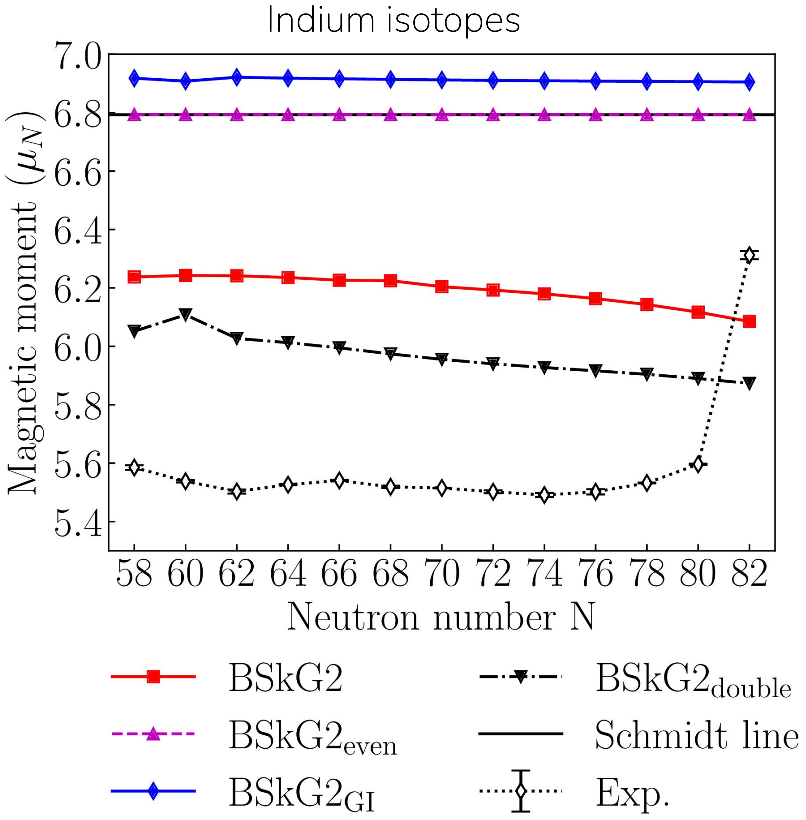
- currents and spins contribute to MOI
- ✅ medium-heavy nuclei
- ❌ actinides

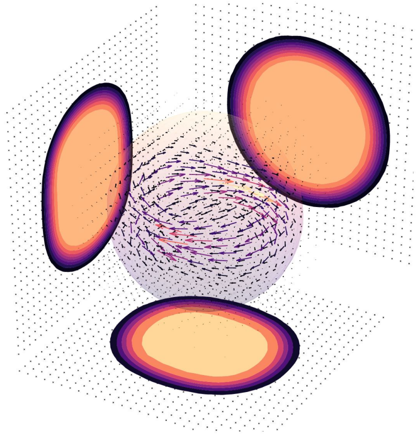
MOI evolve along rotational bands

- top of the peak = “alignment”
- curve sensitive to currents and spins!

Observables: magnetic moments







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

Observables: g.s. spins and parities

Correct spin-parity?	odd-Z	odd-N	odd-odd
Spherical	82%	68%	33%
Transitional	70%	63%	13%
Axial deformation	25%	40%	19%
Triaxial deformation	28%	27%	15%

Perhaps the most basic observable....

- g.s. spin and parities require symmetry restoration
- something "quick-n-dirty"
- J^π enters reaction rate calculations ....

...... but this is "as good" as other models

- **all** other EDF approaches
- mic-mac approaches
- See:

L. Bonneau et al., PRC 76, 024320 (2007)

V. Conclusion, problems and outlook

Conclusion

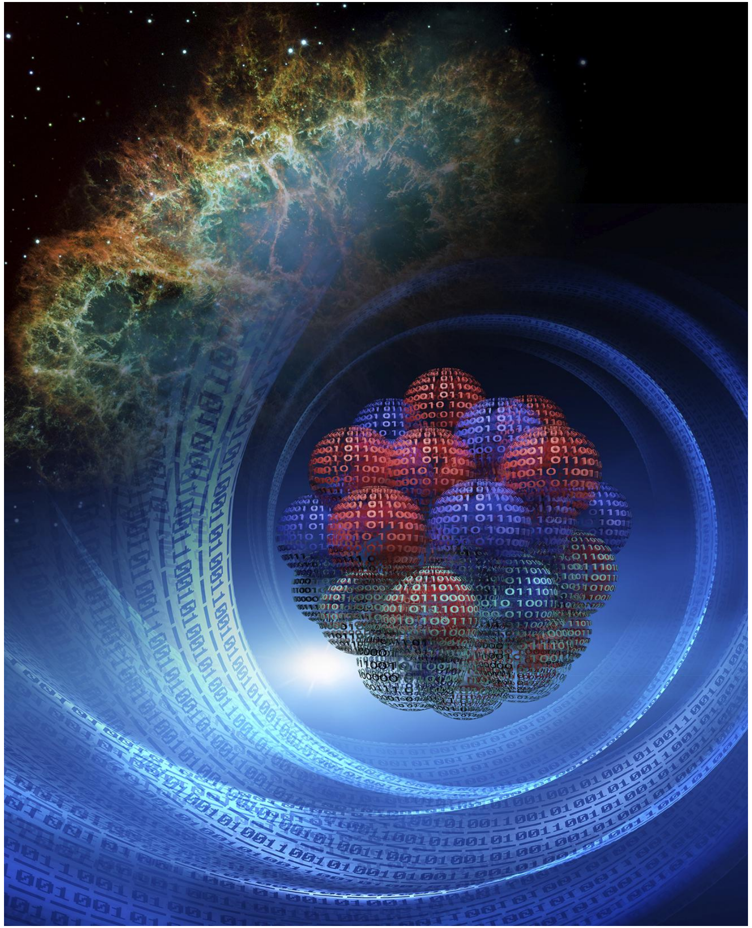
We build **large-scale, microscopic** models of nuclear structure for applications.

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

BSkG1 and **BSkG2** are the latest models

- full three-dimensional representation of nuclei
- includes **triaxial deformation!**
- and **time-reversal** symmetry breaking => new observables!
- data available to all!

BSkG2: W. Ryssens et al. EPJA 58, 246 (2022).
BSkG1: G. Scamps et al., EPJA 57, 333 (2021).



Available:

1. **BSkG2, fission:** W. Ryssens et al., arXiv:2302.03097 [nucl-th].
2. **BSkG2, g.s. properties:** W. Ryssens et al. EPJA 58, 246 (2022).
3. **BSkG1, g.s. properties:** G. Scamps et al., EPJA 57, 333 (2021).

Coming soon(-ish) on http://www.astro.ulb.ac.be/bruslib/

Regular Article - Theoretical Physics | Published: 16 December 2021

Skyrme-Hartree-Fock-Bogoliubov mass models on a 3D mesh: effect of triaxial shape

Guillaume Scamps, Stephane Goriely, Erik Olsen, Michael Bender & Wouter Ryssens

The European Physical Journal A 57, Article number: 333 (2021) | Cite this article

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Abstract

The modelling of nuclear reactions and radioactive decays in astrophysical or earth-based conditions requires detailed knowledge of the masses of essentially all nuclei. Microscopic mass models based on nuclear energy density functionals (EDFs) can be descriptive and used to provide this information. The concept of intrinsic symmetry breaking is central to the predictive power of EDF approaches, yet is generally not exploited to the utmost by mass models because of the computational demands of adjusting up to about two dozen parameters to thousands of nuclear masses. We report on a first step to bridge the gap between what is presently feasible for studies of individual nuclei and large-scale models: we present a new Skyrme-EDF-based model that was adjusted using a three-dimensional coordinate-space representation, for the first time allowing for both axial and triaxial deformations during the adjustment process. To compensate for the substantial increase in computational cost brought by the latter, we have employed a committee of multilayer neural networks to model the objective function in parameter space and guide us towards the overall best fit. The resulting mass model BSkG1 is computed with the EDF model independently of the neural network. It yields a root mean square (rms) deviation on the 2457 known masses of 741 keV and an rms deviation on the 884 measured charge radii of 0.024 fm.

1 Introduction

Z	N	Mexp[MeV]	Mth[MeV]	Err[MeV]	Ebind[MeV]	beta20	beta22	beta2	Erot[MeV]	avgap_uv(n)	avgap_uv(p)	rc[fm]	rc_exp[fm]	rc_err[fm]	MOI[hbar^2/MeV]	par(p)	par(n)
8	8	-4.7370	-4.1901	-0.5469	-127.0704	0.000	-0.000	0.000	0.0000	0.0000	0.0000	2.7266	2.6991	-0.0275	0.0000	+	+
8	9	-0.8090	-0.9512	0.1422	-131.9029	0.355	0.000	0.355	2.7760	0.0000	1.4544	2.7858	2.6932	-0.0926	0.0998	+	+
8	10	-0.7830	-1.6022	0.8192	-140.6252	0.178	0.050	0.192	2.4585	1.8518	0.0000	2.7388	2.7726	0.0338	0.3389	+	+
8	11	3.3330	2.7358	0.5972	-144.3585	0.079	0.097	0.158	1.6723	1.3963	0.0000	2.7359	-	-	0.2793	+	+
8	12	3.7960	3.1735	0.6225	-151.9921	0.183	0.065	0.205	2.6620	1.7800	0.0000	2.7451	-	-	0.5241	+	+
8	13	8.0620	8.6529	-0.5909	-154.5841	0.159	0.003	0.159	1.4940	0.8333	0.0000	2.7403	-	-	0.3898	+	+
8	14	9.2830	10.4998	-1.2168	-160.8085	0.171	0.057	0.189	2.4018	1.2386	0.0000	2.7539	-	-	0.6230	+	+
8	15	14.6210	16.8051	-2.1841	-162.5745	0.000	0.000	0.000	0.0000	0.0000	0.0000	2.7454	-	-	0.0000	+	+
8	16	18.5000	20.5370	-2.0370	-166.9139	0.130	0.060	0.155	1.8336	0.0000	0.0000	2.7660	-	-	0.4630	+	+
8	17	27.3290	28.9738	-1.6448	-166.5485	0.092	0.105	0.175	1.2988	0.0000	0.0000	2.7882	-	-	0.2050	+	+
8	18	34.6610	35.3084	-0.6474	-168.2852	0.150	0.050	0.166	1.7523	1.2426	0.0000	2.8062	-	-	0.4905	+	+
8	19	-	44.5570	-	-167.1079	0.190	0.000	0.190	1.3651	0.6120	0.0000	2.8226	-	-	0.3485	+	+
9	8	1.9520	2.2935	-0.3415	-127.8752	0.364	0.002	0.364	2.4104	1.2662	0.0000	2.9205	-	-	0.0822	+	+
9	9	0.8730	-0.1389	1.0119	-138.3789	0.280	0.000	0.280	0.1621	0.0000	0.0000	2.8478	-	-	0.0019	+	+
9	10	-1.4870	-3.1865	1.6995	-149.4978	0.259	0.065	0.275	2.7934	1.7727	0.0000	2.8434	2.8976	0.0542	0.4522	+	+
9	11	-0.0170	-1.5180	1.5010	-155.9006	0.489	0.002	0.489	3.2871	0.0000	0.0000	2.8913	-	-	0.2465	+	+
9	12	-0.0480	-1.4462	1.3982	-163.9002	0.280	0.084	0.304	3.2772	1.6321	0.0000	2.8493	-	-	0.7712	+	+
9	13	2.7930	2.0138	0.7792	-168.5115	0.345	0.055	0.354	2.4933	0.0000	0.0000	2.8623	-	-	1.1644	+	+
9	14	3.2850	2.8458	0.4392	-175.7508	0.265	0.061	0.279	3.1372	1.1771	0.0000	2.8553	-	-	0.7469	+	+
9	15	7.5450	8.1804	-0.6354	-178.4876	0.147	0.133	0.239	1.8038	0.0000	0.0000	2.8559	-	-	0.1405	+	+
9	16	11.3340	11.1995	0.1345	-183.5397	0.160	0.060	0.181	2.0188	0.6849	0.0000	2.8555	-	-	0.4569	+	+
9	17	18.6750	18.3797	0.2953	-184.4309	0.100	0.122	0.199	1.6036	0.0000	0.0000	2.8775	-	-	0.2710	+	+
9	18	25.1330	23.5360	1.5970	-187.3459	0.210	0.059	0.226	2.4134	1.2867	0.0000	2.9017	-	-	0.6680	+	+
9	19	33.4040	32.0142	1.3898	-186.9390	0.220	0.000	0.220	1.7691	0.7540	0.0000	2.9197	-	-	0.3676	+	+
9	20	40.1500	38.0305	2.1195	-188.9940	0.198	0.003	0.198	1.9242	1.2665	0.0000	2.9302	-	-	0.5259	+	+
9	21	-	47.1069	-	-187.9889	0.402	0.003	0.402	2.0890	1.0768	0.0000	2.9536	-	-	0.3698	+	-
10	8	5.3180	4.3718	0.9462	-133.0851	0.180	0.050	0.193	2.4579	0.0000	1.8801	2.9497	2.9714	0.0217	0.3214	+	+
10	9	1.7520	-0.1333	1.8853	-145.6615	0.265	0.065	0.280	2.8855	0.0000	1.8316	2.9384	3.0082	0.0698	0.4394	+	+
10	10	-7.0420	-6.1786	-0.8634	-159.7782	0.234	0.080	0.260	3.4116	1.7750	1.8580	2.9229	3.0055	0.0826	0.8201	+	+
10	11	-5.7320	-5.8554	0.1234	-167.5262	0.470	0.000	0.470	2.6009	0.0000	1.4667	2.9573	2.9695	0.0122	1.0039	+	+
10	12	-8.0250	-6.8244	-1.2006	-176.5666	0.310	0.083	0.331	3.5051	1.5459	1.6700	2.9294	2.9525	0.0231	1.4351	+	+
10	13	-5.1540	-5.3781	0.2241	-183.1915	0.340	0.090	0.363	3.3549	0.0000	1.5700	2.9403	2.9104	-0.0299	1.8282	+	+
10	14	-5.9520	-5.3020	-0.6500	-191.1868	0.241	0.069	0.260	3.2992	1.0790	1.6624	2.9196	2.9007	-0.0189	1.2786	+	+
10	15	-2.0360	-2.2023	0.1663	-196.1584	0.215	0.081	0.244	3.0053	0.0000	1.6645	2.9272	2.9316	0.0044	0.6141	+	+
10	16	0.4810	0.4184	0.0626	-201.6091	0.160	0.060	0.181	2.6321	0.8412	1.7149	2.9256	2.9251	-0.0005	0.8546	+	+
10	17	7.0510	6.2116	0.8394	-203.8872	0.192	0.000	0.192	2.1195	0.0000	1.6357	2.9453	-	-	0.5457	+	+
10	18	11.3000	10.4928	0.8072	-207.6773	0.180	0.065	0.202	2.7443	1.3111	1.6397	2.9680	2.9642	-0.0038	1.1054	+	+
10	19	18.4000	17.9316	0.4684	-208.3098	0.200	0.000	0.200	2.1420	0.7286	1.5669	2.9876	-	-	0.6574	+	+
10	20	23.2800	23.0699	0.2101	-211.2428	0.178	0.050	0.192	2.5117	1.3606	1.5967	2.9981	-	-	1.0041	+	+
10	21	31.1820	31.2781	-0.0961	-211.1060	0.245	0.005	0.245	2.0820	0.8844	1.5125	3.0162	-	-	0.6319	+	-
10	22	-	37.5498	-	-212.9055	0.215	0.067	0.235	2.6272	1.3669	1.5138	3.0289	-	-	1.6846	+	+
10	23	-	46.0170	-	-212.5097	0.392	0.001	0.392	1.9418	0.0328	1.1161	3.0779	-	-	1.8872	+	-
11	8	12.9290	12.3223	0.6067	-132.4226	0.084	0.102	0.167	1.6694	0.0000	1.4141	3.0313	-	-	0.2937	+	+
11	9	6.8500	5.3716	1.4784	-147.4447	0.481	0.000	0.481	3.0642	0.0000	0.0000	3.0615	2.9718	-0.0897	0.2520	+	+
11	10	-2.1850	-2.0834	-0.1016	-162.9710	0.480	0.003	0.480	2.4773	1.3587	0.0000	3.0343	3.0136	-0.0207	1.1297	+	+
11	11	-5.1810	-8.2693	3.0883	-177.2282	0.570	0.001	0.570	3.8176	0.0000	0.0000	3.0615	2.9852	-0.0763	0.4655	+	+
11	12	-9.5300	-9.5082	-0.0218	-186.5384	0.500	0.065	0.508	3.1638	0.9226	0.0000	3.0442	2.9936	-0.0506	1.7894	+	+
11	13	-8.4180	-9.0454	0.6274	-194.1469	0.460	0.069	0.470	3.6105	0.0000	0.0000	3.0398	2.9735	-0.0663	1.3909	+	+
11	14	-9.3580	-9.7868	0.4288	-202.9597	0.380	0.073	0.394	4.0099	1.2041	0.0000	3.0229	2.9769	-0.0460	1.1758	+	+
11	15	-6.8610	-7.2132	0.3522	-208.4574	0.355	0.066	0.368	3.3054	0.0000	0.0000	3.0251	2.9928	-0.0323	0.4585	+	+
11	16	-5.5180	-5.7986	0.2806	-215.1141	0.215	0.078	0.242	2.9663	1.0290	0.9234	3.0003	3.0136	0.0133	0.9102	+	+
11	17	-0.9880	-1.3869	0.3989	-218.7738	0.300	0.000	0.300	2.5545	0.0000	0.0000	3.0338	3.0400	0.0062	0.5048	+	+
11	18	2.6800	1.7963	0.8837	-223.6619	0.310	0.059	0.321	3.1652	1.4265	0.0000	3.0517	3.0922	0.0405	1.2023	+	+
11	19	8.4750	7.8788	0.5962	-225.6507	0.407	0.053	0.414	3.1618	0.9215	0.0000	3.0897	3.1180	0.0283	1.2829	+	-
11	20	12.2460	11.9322	0.3138	-229.6686	0.350	0.050	0.357	2.8842	1.5311	0.0000	3.0859	3.1704	0.0845	1.6665	+	+
11	21	18.6400	18.5697	0.0703	-231.1024	0.570	0.053	0.575	3.2654	0.0000	0.0000	3.1614	-	-	2.2225	+	-
11	22	23.7800	23.4149	0.3651	-234.3285	0.451	0.006	0.451	2.4898	1.4027	0.0000	3.1369	-	-	2.3669	+	+
11	23	31.6800	30.4369	1.2431	-235.3779	0.411	0.001	0.411	2.7033	0.0000	0.0000	3.1479	-	-	0.8608	+	-
11	24	-	36.5526	-	-237.3335	0.461	0.049	0.466	2.7262	1.2039	0.0000	3.1717	-	-	3.2194	+	+
11	25	-	44.9174	-	-237.0400	0.456	0.054	0.462	2.2789	0.2259	0.0000	3.1827	-	-	4.6060	+	-
11	26	-	51.3995	-	-238.6292	0.442	0.059	0.450	2.6801	1.0647	0.0000	3.1872	-	-	3.4525	+	+
11	27	-	60.2112	-	-237.8889	0.339	0.155	0.403	2.7426	0.9023	0.0000	3.1887	-	-	3.8136	+	-
12	8	17.4780	16.5685	0.9095	-135.4644	0.201	0.075	0.227	2.7749	0.0000	1.7925	3.1206	-	-	0.5521	+	+
12	9	10.9040	9.1280	1.7760	-150.9762	0.293	0.085	0.317	3.3169	0.0000	1.6717	3.0944	-	-	0.7672	+	+
12	10	-0.4000	0.7230	-1.1230	-167.4525	0.350	0.078	0.367	3.4120	1.5221	1.5412	3.0825	-	-	1.6174	+	+
12	11	-5.4740	-5.7646	0.2906	-182.0115	0.500	0.067	0.509	3.3209	0.0000	1.0704	3.1117	-	-	1.7039	+	+
12	12	-13.9340	-12.4522	-1.4818	-196.7704	0.590	0.057	0.595	3.5070	0.0000	0.0000	3.1420	3.0570	-0.0850	3.6693	+	+
12	13	-13.1930	-13.5949	0.4019	-205.9844	0.360	0.110	0.392	3.8541	0.0000	1.3904	3.0765	3.0284	-0.0481	2.1268	+	+
12	14	-16.2150	-14.9807	-1.2343	-215.4415	0.267	0.148	0.339	3.5612	0.0000	1.5820	3.0673	3.0337	-0.0336	2.0362	+	+
12	15	-14.5870	-14.3558	-0.2312	-222.8880	0.241	0.105	0.283	3.6248	0.0000	1.5598	3.0569	-	-	0.9578	+	+
12	16	-15.0200	-13.8893	-1.1307	-230.4928	0.200	0.095	0.241	3.4527	1.1182	1.5914	3.0579	-	-	1.3398	+	+
12	17	-10.6120	-10.4543	-0.1577	-235.1291	0.207	0.085	0.239	2.8012	0.0000	1.5345	3.0727	-	-	1.4210	+	+
12	18	-8.8810	-8.5042	-0.3768	-241.2504	0.189	0.069	0.213	2.9698	1.3487	1.5254	3.0806	-	-	1.4453	+	+
12	19	-3.1220	-3.2515	0.1295	-244.0689	0.165	0.050	0.180	2.1602	0.6025	1.5403	3.0953	-	-	0.7500	+	+
12	20	-0.8290	-0.3484	-0.4806	-249.2372	0.188	0.063	0.208	2.9181	1.4980	1.4876	3.1088	-	-	1.3837	+	+
12	21	4.9630	5.9926	-1.0296	-250.9675	0.223	0.064	0.241	2.7879	1.0737	1.4109	3.1286	-	-	1.2982	+	-
12	22	8.3230	9.7918	-1.4688	-255.2396	0.372	0.070	0.384	3.0862	1.5019	0.9851	3.1725	-	-	3.4412	+	+
12	23	15.6400	16.4728	-0.8328	-256.6300	0.370	0.000	0.370	2.0699	0.0000	0.9605	3.1839	-	-	2.0132	+	-
12	24	20.3800	20.8904	-0.5104	-260.2836	0.479	0.057	0.485	2.9903	1.2820	0.0000	3.2337	-	-	4.8542	+	+
12	25	28.2110	28.2333	-0.0223	-261.0121	0.414	0.066	0.424	2.4869	0.0000	0.5443	3.2275	-	-	5.4832	+	-
12	26	-	33.8556	-	-263.4611	0.447	0.056	0.455	2.8082	1.0653	0.0000	3.2470	-	-	5.1001	+	+
12	27	-	41.9777	-	-263.4103	0.474	0.062	0.483	2.5199	0.0000	0.0000	3.2674	-	-	6.4195	+	-
12	28	-	48.6288	-	-264.8305	0.444	0.063	0.453	2.6728	0.9249	0.0000	3.2657	-	-	5.6170	+	+
12	29	-	57.3936	-	-264.1371	0.302	0.130	0.354	2.5930	0.7479	0.8676	3.2418	-	-	5.1169	+	-
13	8	-	26.2637	-	-133.0570	0.181	0.001	0.181	1.5794	0.0000	0.9543	3.1722	-	-	0.4074	+	+
13	9	-	17.0349	-	-150.3571	0.369	0.062	0.379	2.4846	0.0000	0.0000	3.1696	-	-	1.3760	+	+
13	10	6.7480	6.5772	0.1708	-168.8862	0.343	0.093	0.367	3.2202	1.4794	0.0000	3.1425	-	-	1.9903	+	+
13	11	-0.0490	-0.8824	0.8334	-184.4171	0.465	0.070	0.475	3.5894	0.0000	0.0000	3.1618	-	-	1.4728	+	+
13	12	-8.9160	-9.1454	0.2294	-200.7515	0.365	0.110	0.397	3.7359	1.2693	0.0000	3.1332	-	-	2.2548	+	+
13	13	-12.2100	-14.3105	2.1005	-213.9879	0.365	0.100	0.391	3.7474	0.0000	0.0000	3.1270	-	-	2.0827	+	+
13	14	-17.1970	-17.5805	0.3835	-225.3292	0.307	0.094	0.335	3.8273	0.9111	0.0000	3.1108	3.0610	-0.0498	1.9314	+	+
13	15	-16.8510	-17.0757	0.2247	-232.8956	0.287	0.098	0.318	3.2386	0.0000	0.0000	3.1165	-	-	1.2106	+	+
13	16	-18.2080	-17.8319	-0.3761	-241.7232	0.247	0.098	0.283	3.3949	1.1084	0.0000	3.1178	-	-	1.8421	+	+
13	17	-15.8640	-15.3973	-0.4667	-247.3599	0.228	0.020	0.230	2.2456	0.0000	0.0000	3.1109	-	-	1.0899	+	+
13	18	-14.9510	-14.8907	-0.0603	-254.9246	0.250	0.080	0.274	3.2659	1.4076	0.0000	3.1410	-	-	1.9008	+	+
13	19	-11.0990	-10.5909	-0.5081	-258.6961	0.200	0.000	0.200	2.1029	0.8097	0.0000	3.1390	-	-	0.7082	+	+
13	20	-8.4970	-9.0643	0.5673	-265.2409	0.250	0.070	0.269	3.1429	1.5933	0.0000	3.1633	-	-	1.9722	+	+
13	21	-2.9980	-3.7943	0.7963	-268.0423	0.275	0.067	0.291	2.9838	1.1820	0.0000	3.1814	-	-	1.7456	+	-
13	22	-0.2240	-1.1635	0.9395	-273.4827	0.284	0.071	0.302	3.1212	1.5357	0.0000	3.1951	-	-	2.5278	+	+
13	23	5.9500	4.4965	1.4535	-275.8941	0.342	0.000	0.342	2.5252	0.3205	0.0000	3.2162	-	-	1.1204	+	-
13	24	9.8100	8.2217	1.5883	-280.2402	0.331	0.082	0.351	3.2275	1.3300	0.0000	3.2326	-	-	3.4873	+	+
13	25	-	14.6549	-	-281.8783	0.380	0.060	0.389	2.7360	0.0000	0.0000	3.2552	-	-	4.3431	+	-
13	26	-	19.4976	-	-285.1069	0.324	0.085	0.346	2.9738	1.1012	0.0000	3.2528	-	-	4.1523	+	+
13	27	-	27.1074	-	-285.5685	0.358	0.090	0.380	2.7533	0.6320	0.0000	3.2735	-	-	3.1638	+	-
13	28	-	32.4018	-	-288.3454	0.295	0.109	0.333	3.0548	1.1175	0.0000	3.2708	-	-	3.9208	+	+
13	29	-	40.5826	-	-288.2359	0.285	0.107	0.322	2.6037	0.6336	0.0000	3.2739	-	-	2.9104	+	-
13	30	-	46.9445	-	-289.9454	0.254	0.107	0.296	2.5013	0.9251	0.0000	3.2763	-	-	4.2210	+	+
13	31	-	55.4675	-	-289.4937	0.248	0.142	0.319	2.0671	0.0000	0.0000	3.2925	-	-	5.1489	+	-
14	9	-	22.2155	-	-152.4642	0.273	0.066	0.288	3.0989	0.0000	1.2560	3.2272	-	-	0.7449	+	+
14	10	10.7450	11.1321	-0.3871	-171.6190	0.254	0.081	0.279	3.3129	1.5626	1.1637	3.1881	-	-	1.3895	+	+
14	11	3.8270	2.8585	0.9685	-187.9639	0.400	0.076	0.414	4.0714	0.0000	1.3292	3.2157	-	-	1.1937	+	+
14	12	-7.1410	-6.0241	-1.1169	-204.9178	0.270	0.111	0.312	3.5252	1.4441	0.8952	3.1641	-	-	1.8914	+	+
14	13	-12.3850	-13.0554	0.6704	-220.0204	0.320	0.095	0.347	3.9528	0.0000	1.1049	3.1720	-	-	1.8978	+	+
14	14	-21.4930	-20.4244	-1.0686	-235.4608	0.182	0.223	0.364	2.9857	0.0000	0.0000	3.1850	3.1224	-0.0626	2.3320	+	+
14	15	-21.8950	-21.3579	-0.5371	-244.4655	0.225	0.078	0.251	3.2916	0.0000	0.9098	3.1443	3.1176	-0.0267	0.9639	+	+
14	16	-24.4330	-22.8283	-1.6047	-254.0073	0.181	0.075	0.210	3.0446	1.0441	0.7670	3.1417	3.1336	-0.0081	1.5368	+	+

Conclusion

We build large-scale, microscopic models of nuclear structure for applications.

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

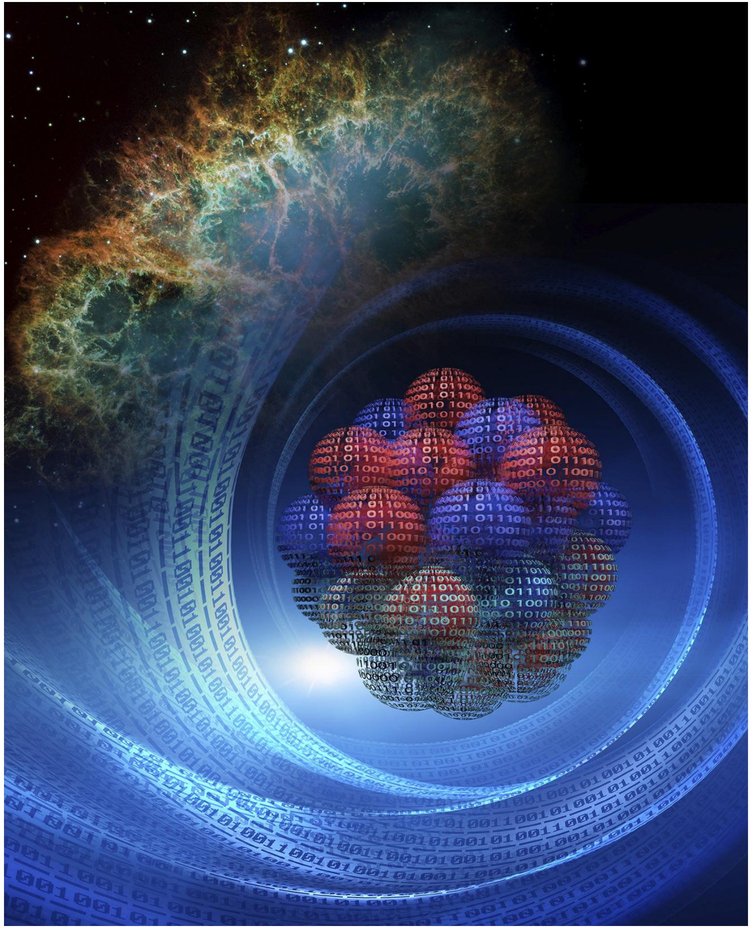
BSkG1 and **BSkG2** are the latest state-of-the art models entries

- full three-dimensional representation of nuclei
- includes **triaxial deformation** !
- **time-reversal** symmetry breaking => new observables!
- data available to all!

BSkG2: W. Ryssens et al. EPJA 58, 246 (2022).
BSkG1: G. Scamps et al., EPJA 57, 333 (2021).

In our project, I hope you want to help with:

1. providing data for our parameter fits
2. telling us where wave functions need refining
3. helping us refine the form of the EDF



Problems: what we cannot do (yet)!

1. "**Single-particle**" properties are deficient
    a. g.s. spins
    b. details of charge radii
    c. magnetic moments

2. The **EDF form** is phenomenological:
    a. no **systematic** improvement possible
    b. no **connection** to the **nucleon-nucleon** interaction
    c. no way to provide **systematic** errors

3. We have no predictions for thousands of nuclei:
    a. β-decay rates
    b. level-schemes + transition rates
    c. magnetic moments

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   c. no way to provide **systematic** errors

3. We have no systematic predictions for
   a. β-decay
   b. level-schemes / transition rates / half-lives
   c. magnetic moments

We need to work on:
1. extendable, non-empirical EDF forms.
2. beyond-mean-field at the scale of the nuclear chart.

Problems: what we cannot do (yet)!

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2. beyond-mean-field at the scale of the nuclear chart.

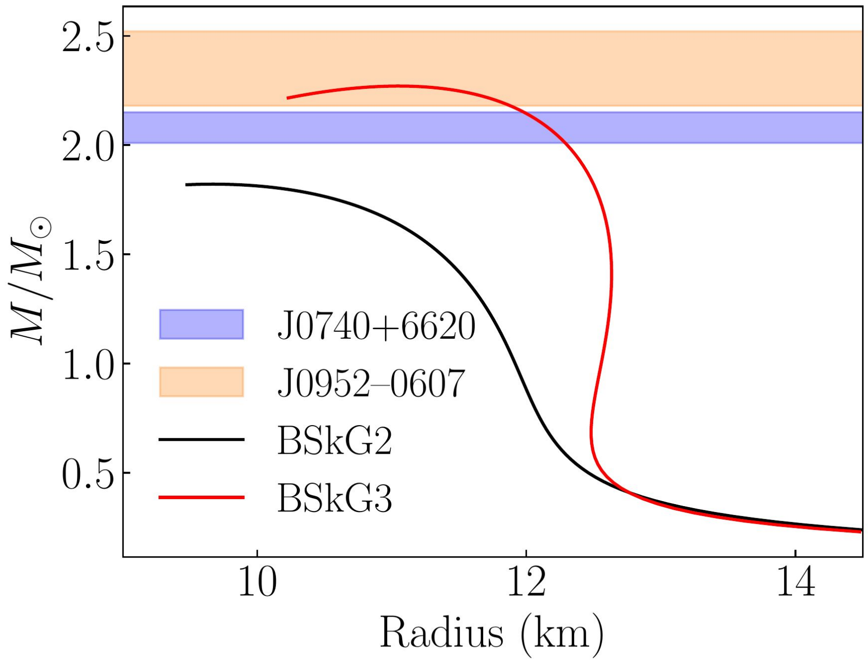
Outlook

BSkG3

- compatible with the existence of heavy pulsars
- without deteriorating structure properties of BSkG1/2

Databases based on BSkG2:

- nuclear level densities
- fission properties
- details of (charge) densities



E. Fonseca *et al.*, ApJL 915, L12 (2021)
R. W. Roman *et al.*, ApJL 934, L17 (2022).

Thank you for...

...... all the wonderful work!

ULB

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

iP2i LES 2 INFINIS LYON

M. Bender
J. Bonnard

UNIVERSITY of WASHINGTON

G. Scamps

JYVÄSKYLÄN YLIOPISTO
UNIVERSITY OF JYVÄSKYLÄ

M. Hukkanen
M. Stryjczyk
A. Kankainen

CENBG

P. Ascher
S. Grévy

KU LEUVEN

S. Sels
E. Verstraelen
T. Cocolios
P. Van Duppen

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

G. Giacalone

Brookhaven National Laboratory

B. Schenke
C. Shen

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iP2i
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J. Bonnard

University of Washington
G. Scamps

Jyväskylän Yliopisto / University of Jyväskylä
M. Hukkanen
M. Stryjczyk
A. Kankainen

CENBG
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...... the computing time!

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...... the funding!

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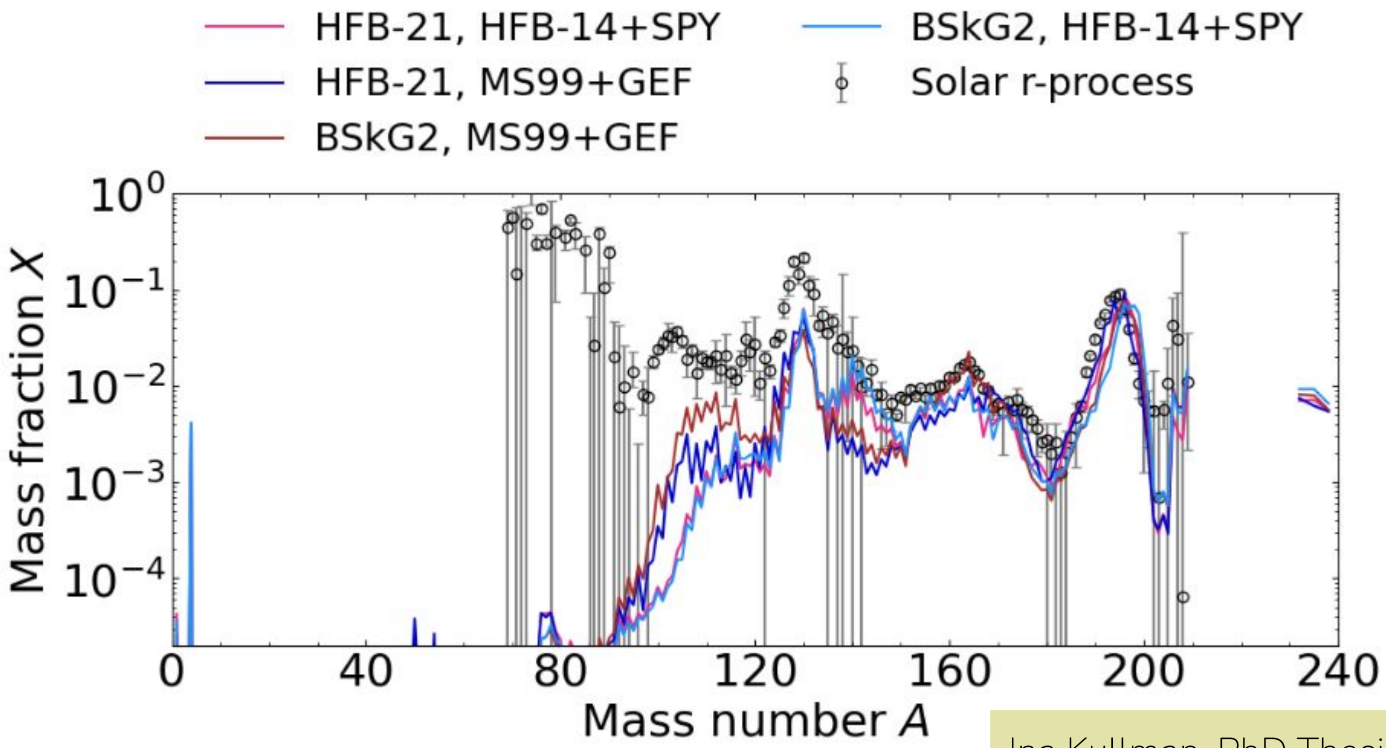
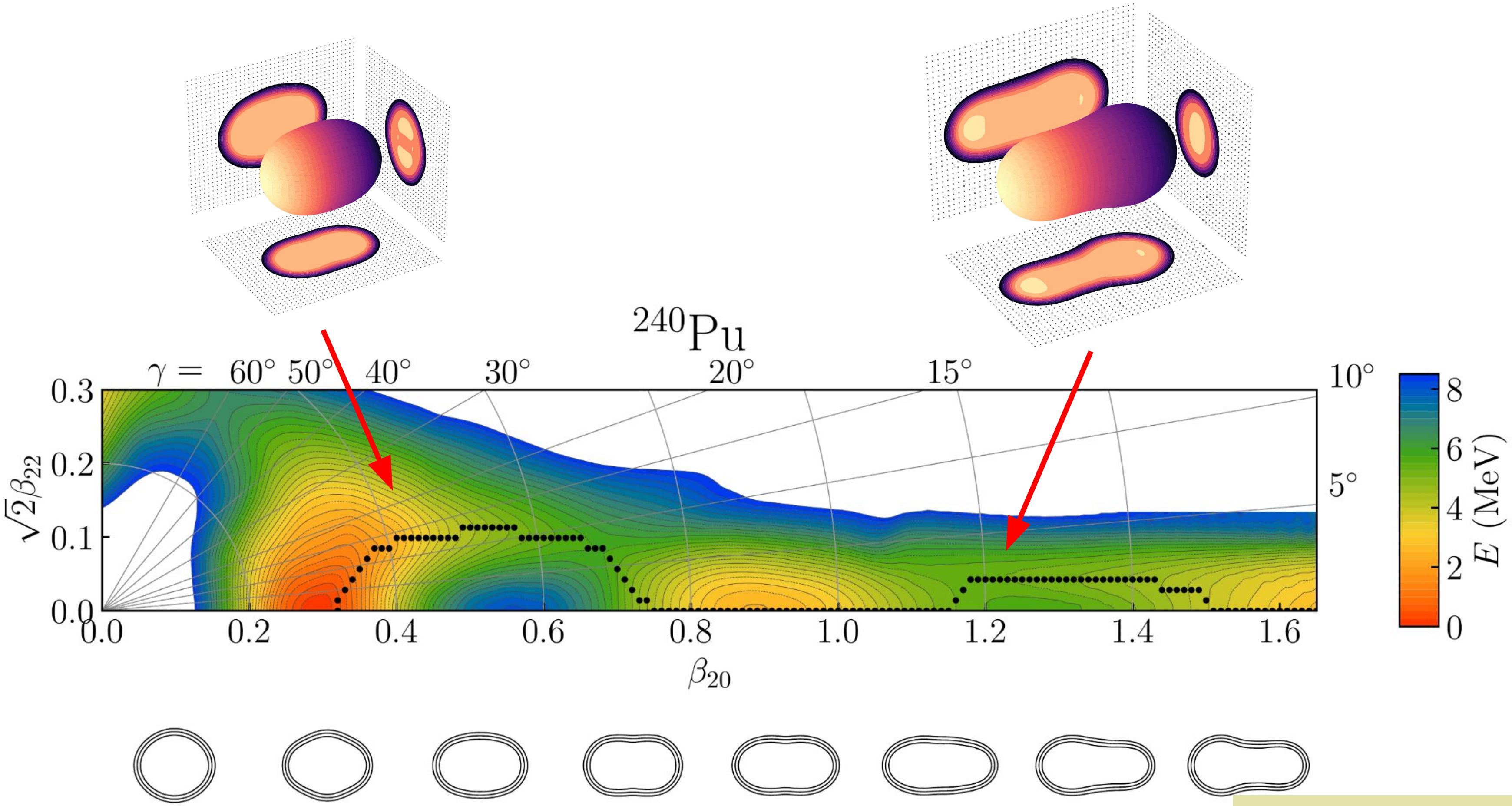
...... your attention!

Bonus!



Ina Kullman, PhD Thesis (2022)

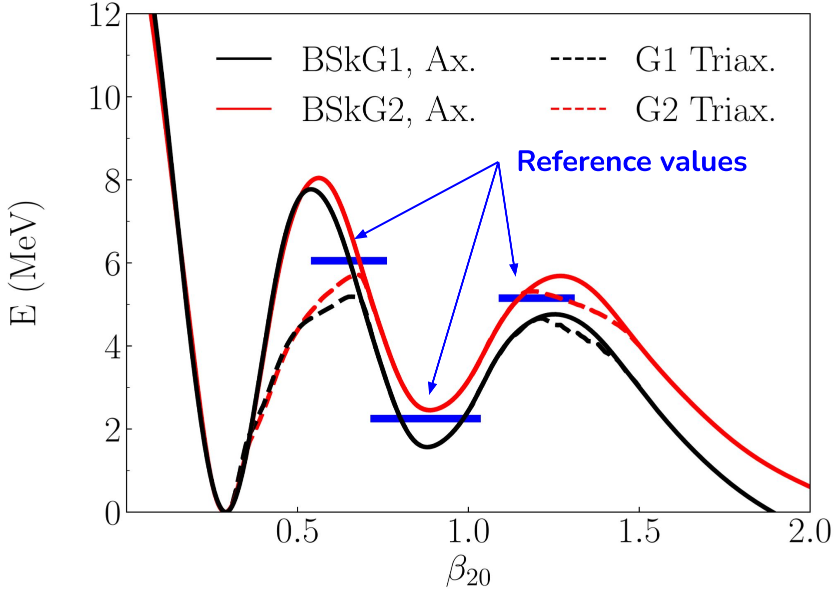
Observables: fission

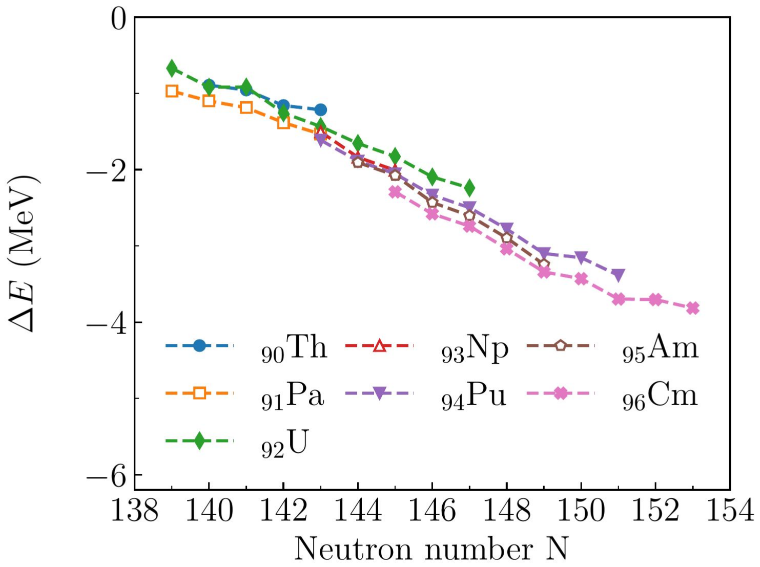


W. Ryssens et al., in preparation.

Observables: fission

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



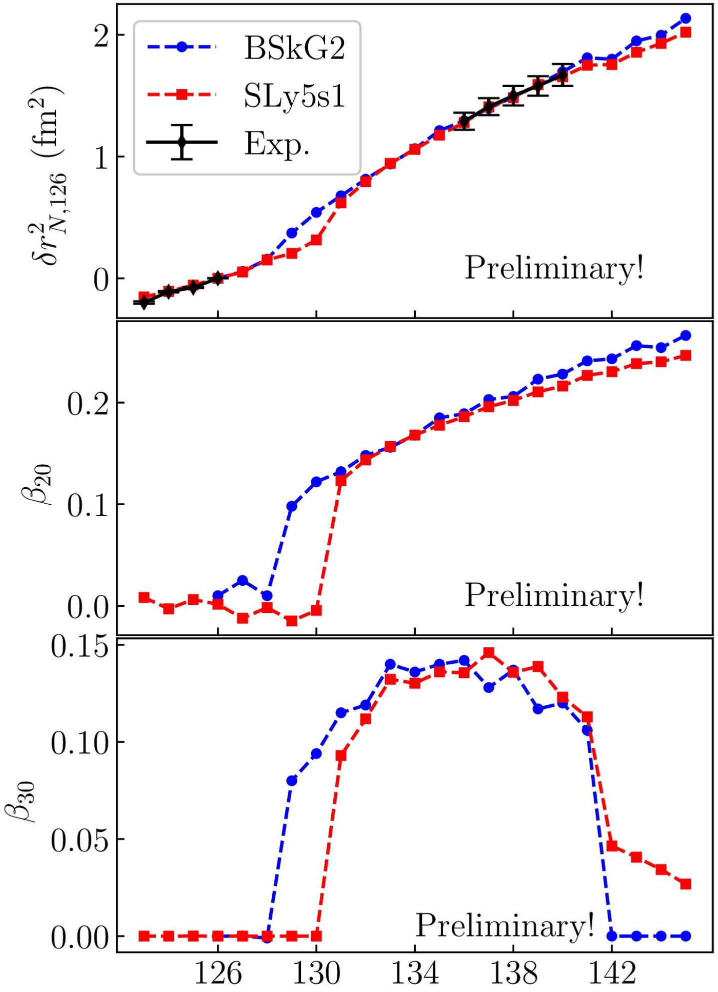


Triaxial deformation for 240Pu

- 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?



BSkG2
SLy5s1
Exp.
$\delta r^2_{N,126}$ (fm^2)
Preliminary!
β_{20}
Preliminary!
β_{30}
Preliminary!
126
130
134
138
142