

Andy Sproles, ORNL

Microscopic models of nuclear structure at scale

W. Ryssens

N. Chamel, S. Bara, G. Grams, N. Shchepochin,
M. Bender, S. Hilaire and S. Goriely

23rd of April 2024



wryssens.com

wryssens@ulb.be



The nuclear chart and the processes traversing it

Extrapolations in

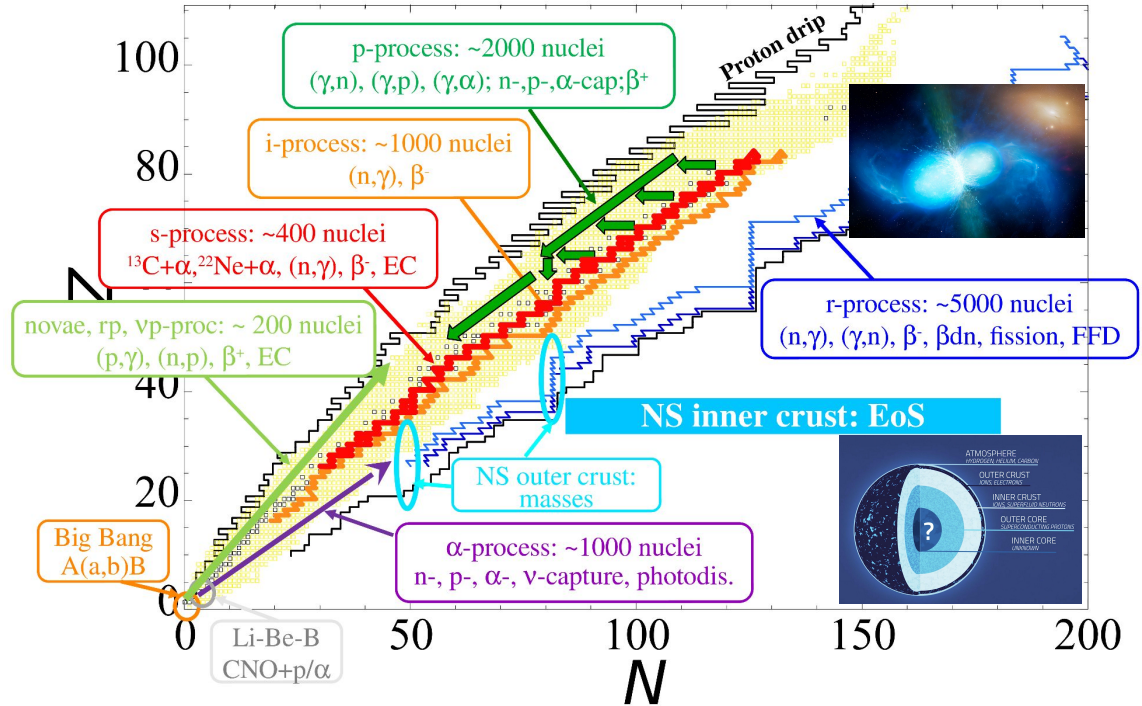
- nucleon number
- energy
- temperature
- density
-

and all of that for

- ~7000 nuclei
- many reactions

what we need is models that should be

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



Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

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



Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

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

Local densities and currents of a wavefunction

Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

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

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

Local densities and currents of a wavefunction

Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

Energy

Coupling constants (~ 25 parameters) fitted to data

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

Local densities and currents of a wavefunction

Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

Energy

Coupling constants (\sim **25** parameters) fitted to data

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

Local densities and currents of a wavefunction

Strong points

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

Skyrme **E**nergy **D**ensity **F**unctionals (**EDFs**)

Energy

Coupling constants (~ 25 parameters) fitted to data

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

Local densities and currents of a wavefunction

Strong points

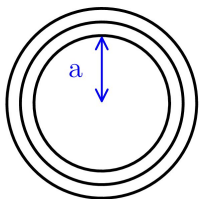
- **simple** wavefunctions but **individual** nucleons
- based on “in-medium” N-N interaction
- many observables accessible
- Feasible for **~7000** nuclei

How to move forward?

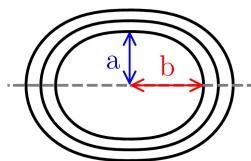
1. search for a “better” EDF form
2. describe more observables simultaneously
3. include more physics in the wavefunction

Large-scale models in 1-2 dimensions

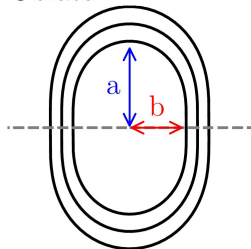
Spherical



Prolate



Oblate



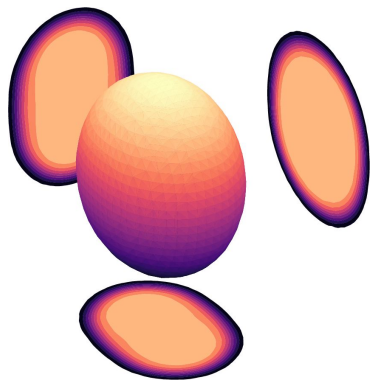
One DOF: β_{20}

Nuclear deformation

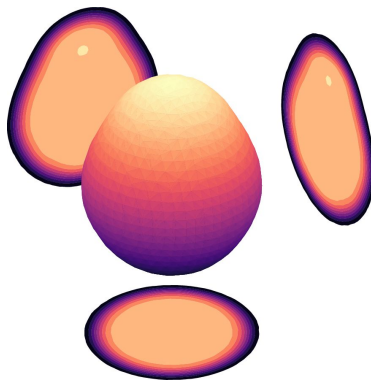
- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
- intuitive interpretation

Large-scale models in 1-2-3 dimensions

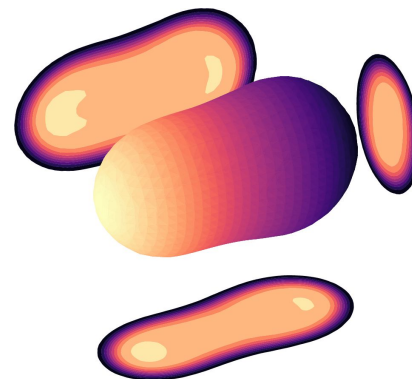
β_{20}, β_{22} or β_2, γ



β_{20}, β_{30}



β_{20}, β_{22} **and** β_{30}



Nuclear deformation

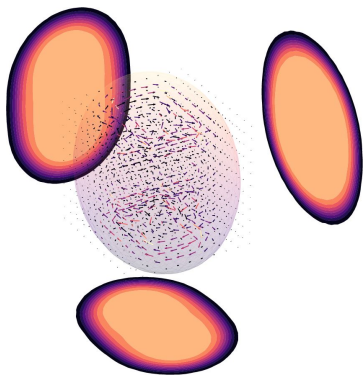
- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
- intuitive interpretation

More general configurations

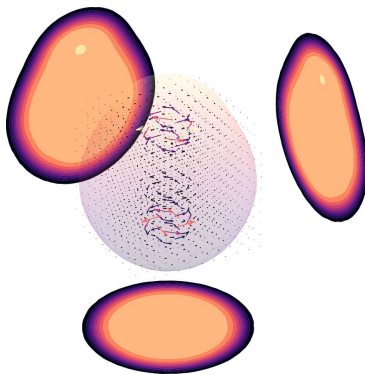
- triaxial shapes
- reflection asymmetry
- elongated shapes

Large-scale models in 1-2-3 dimensions

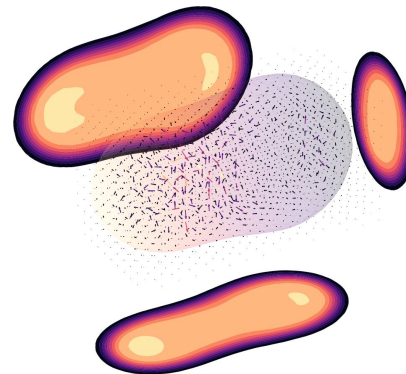
β_{20}, β_{22} or β_2, γ



β_{20}, β_{30}



β_{20}, β_{22} **and** β_{30}



Nuclear deformation

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

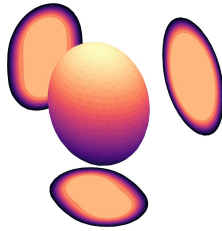
More general configurations

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

Brussels-Skyrme-on-a-Grid: BSkG

BSkG1 (2021)

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



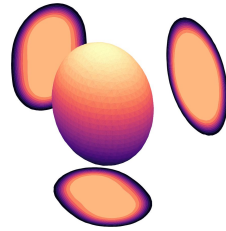
BSkG1: G. Scamps et al., EPJA **57**, 333 (2021).
BSkG2: W. Ryssens et al., EPJA **58**, 246 (2022).
W. Ryssens et al., EPJA **59**, 96 (2023).
BSkG3: G. Grams et al., EPJA **59**, 270 (2023).

Brussels-Skyrme-on-a-Grid: BSkG

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

BSkG1 (2021)

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



BSkG2 (2022)

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

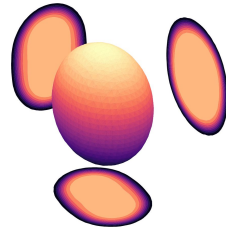


Brussels-Skyrme-on-a-Grid: BSkG

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

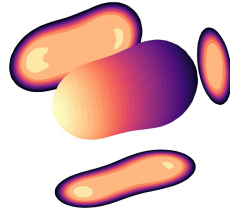
BSkG1 (2021)

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



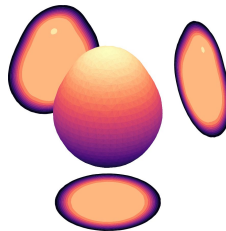
BSkG2 (2022)

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



BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation

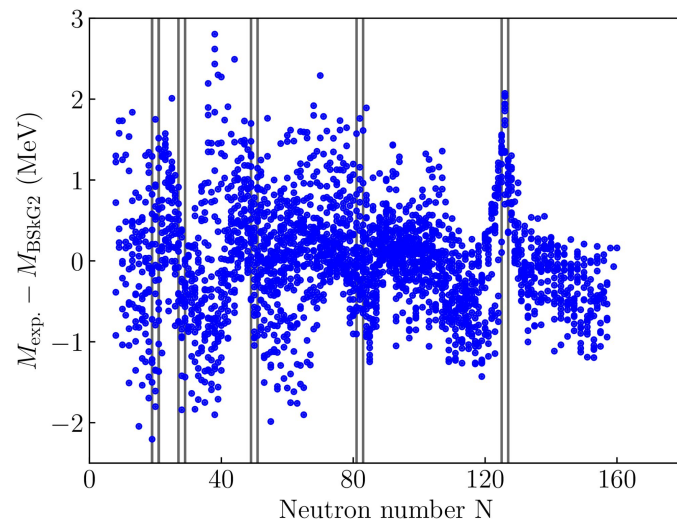
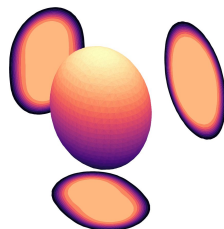


Brussels-Skyrme-on-a-Grid: BSkG

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

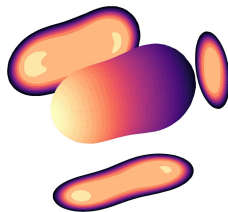
BSkG1 (2021)

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



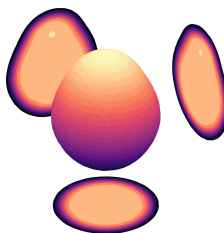
BSkG2 (2022)

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



BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation



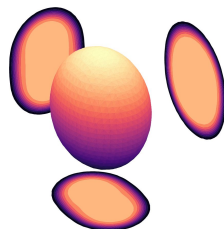
Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]			
Radii [fm]			
Prim. barriers [MeV]			
Secon. barriers [MeV]			
Fission isomers [MeV]			
Max. NS mass [M_{\odot}]			

Brussels-Skyrme-on-a-Grid: BSkG

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

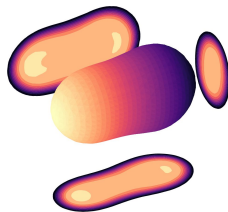
BSkG1 (2021)

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



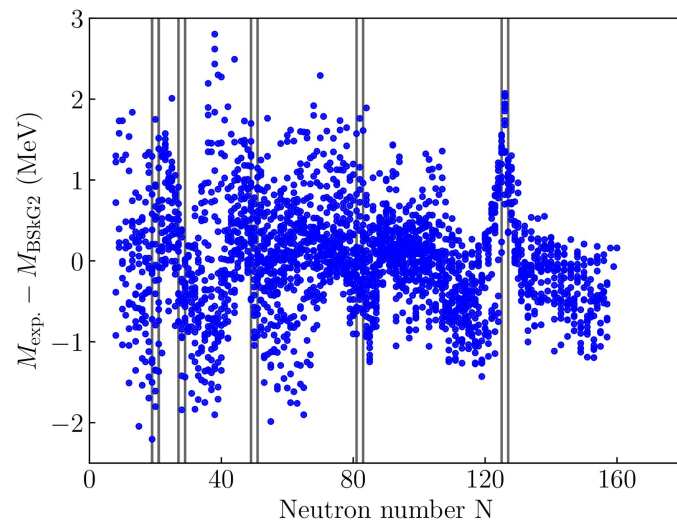
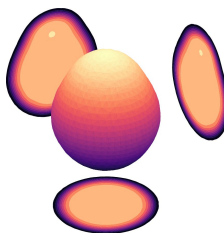
BSkG2 (2022)

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



BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation



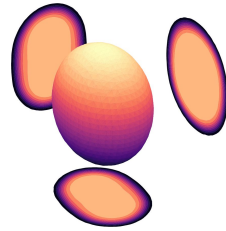
Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
Prim. barriers [MeV]			
Secun. barriers [MeV]			
Fission isomers [MeV]			
Max. NS mass [M_{\odot}]			

Brussels-Skyrme-on-a-Grid: BSkG

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

BSkG1 (2021)

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



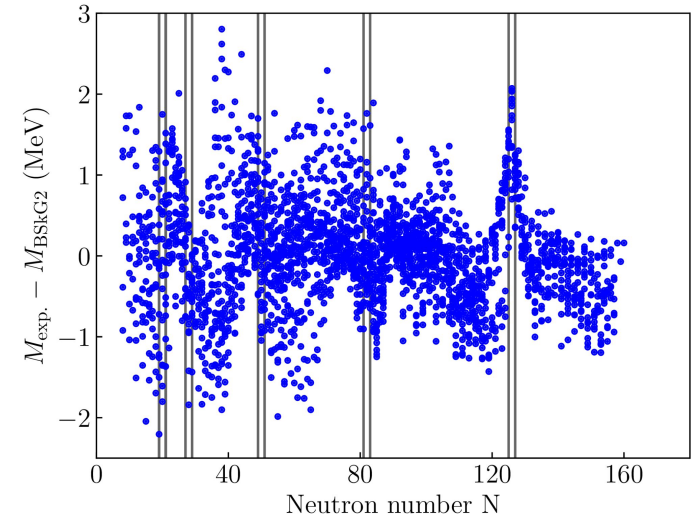
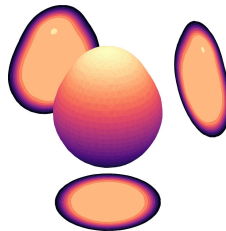
BSkG2 (2022)

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



BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation



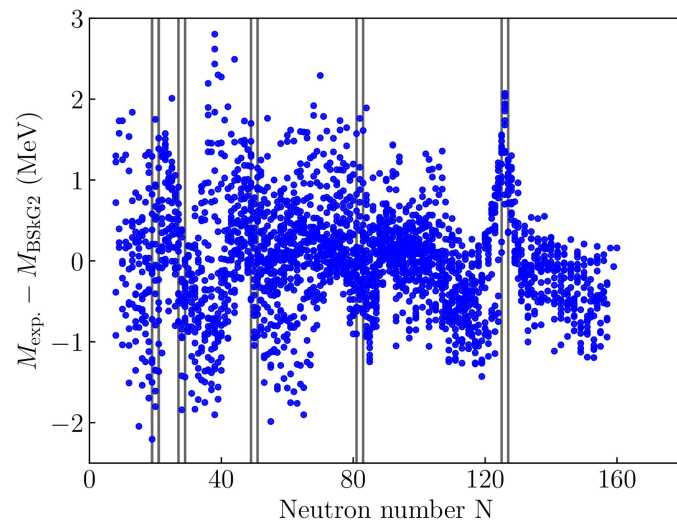
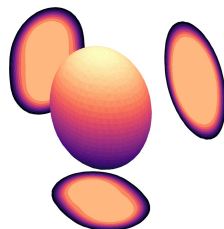
Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
Prim. barriers [MeV]	0.88	0.44	0.33
Secun. barriers [MeV]	0.87	0.47	0.51
Fission isomers [MeV]	1.0	0.49	0.34
Max. NS mass [M_{\odot}]			

Brussels-Skyrme-on-a-Grid: BSkG

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

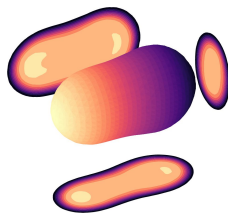
BSkG1 (2021)

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



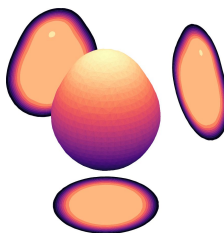
BSkG2 (2022)

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



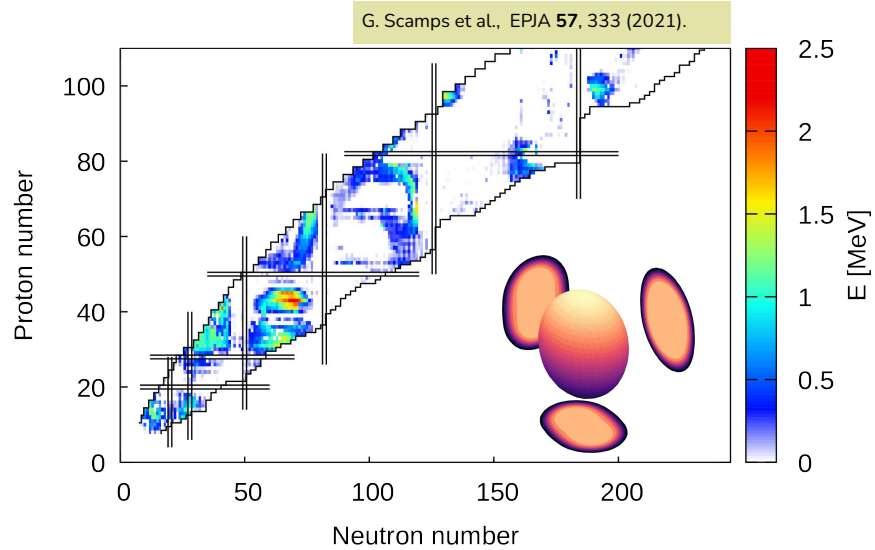
BSkG3 (2023)

- 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
Secun. 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

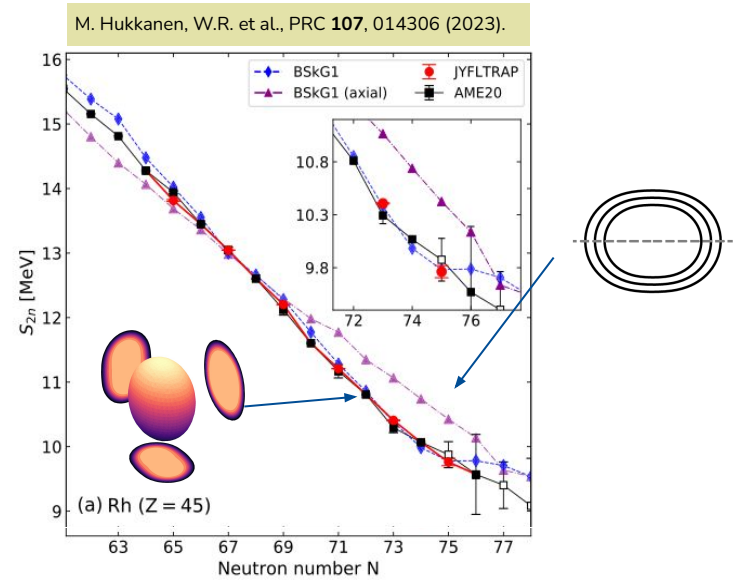
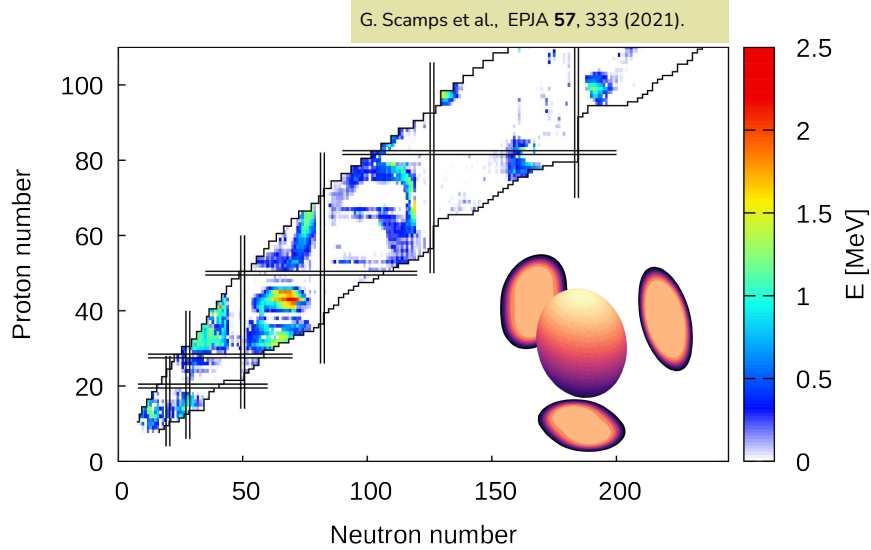
Masses



Triaxial deformation

- many nuclei are affected
- effects up to 2.5 MeV near $Z \sim 44$

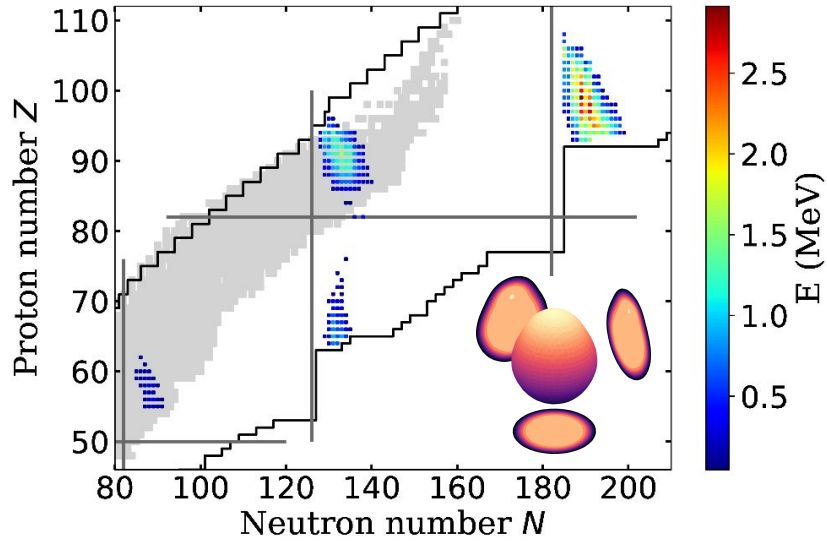
Masses



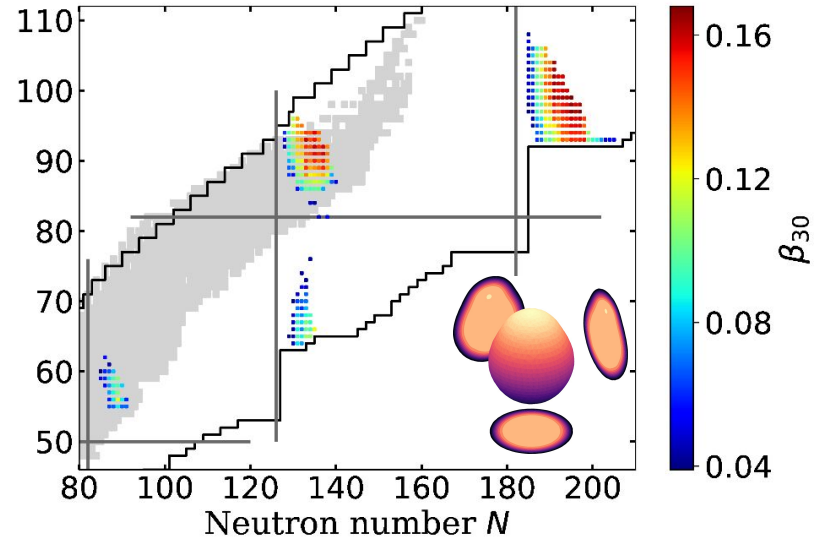
Triaxial deformation

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

Masses



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

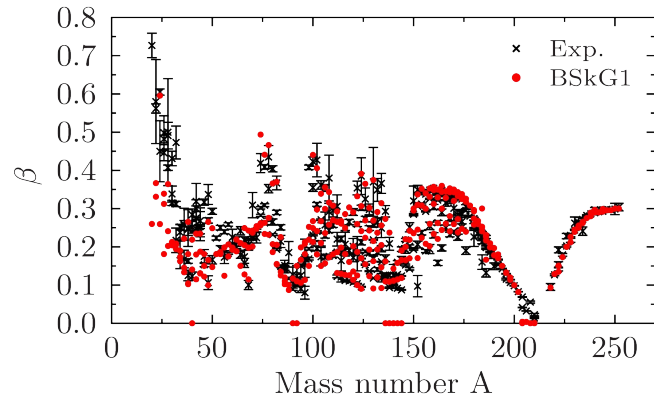
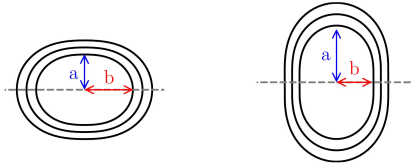


Reflection asymmetry

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

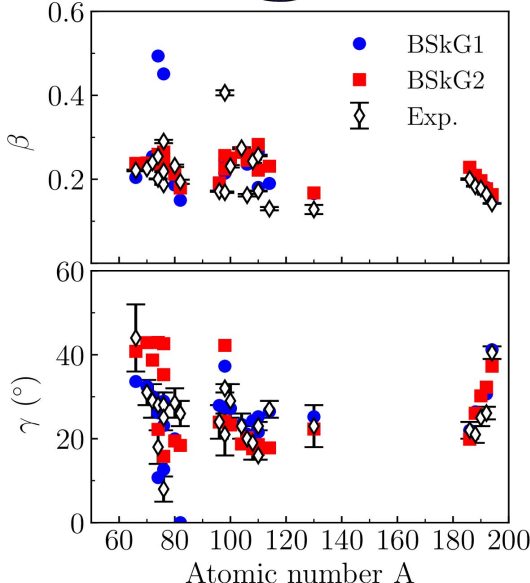
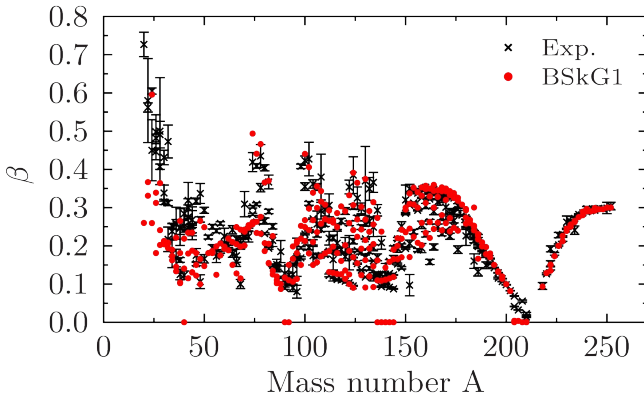
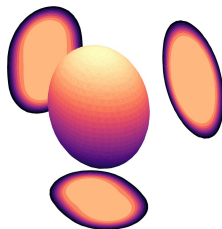
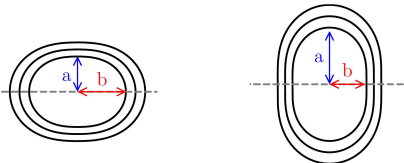
Deformations

“Ordinary” quadrupole deformation



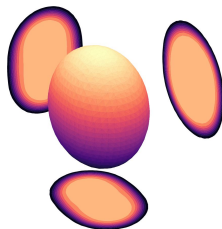
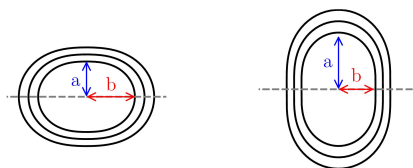
Deformations

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

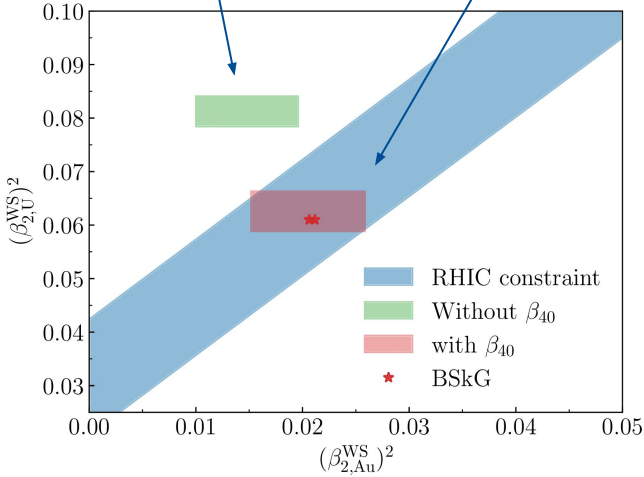
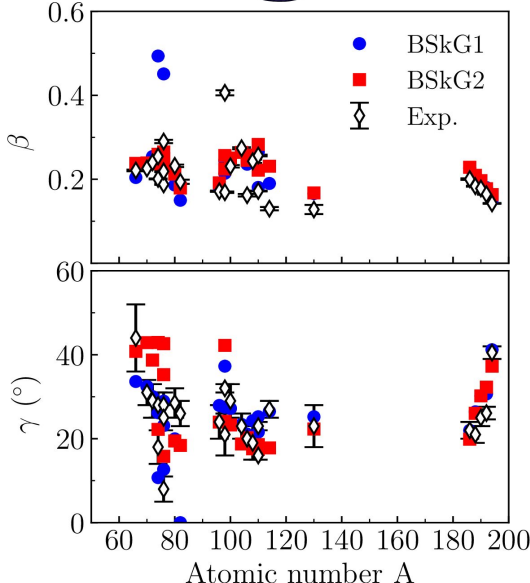
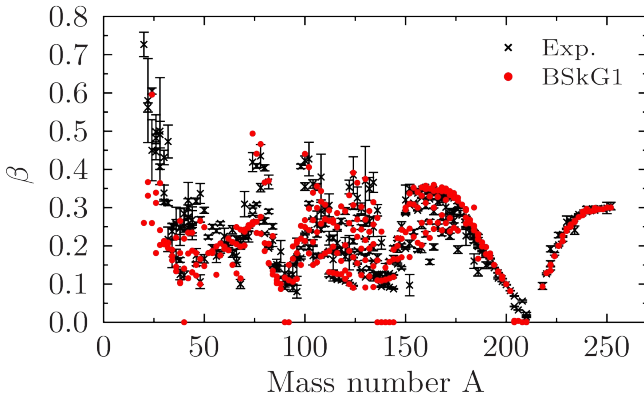


Deformations

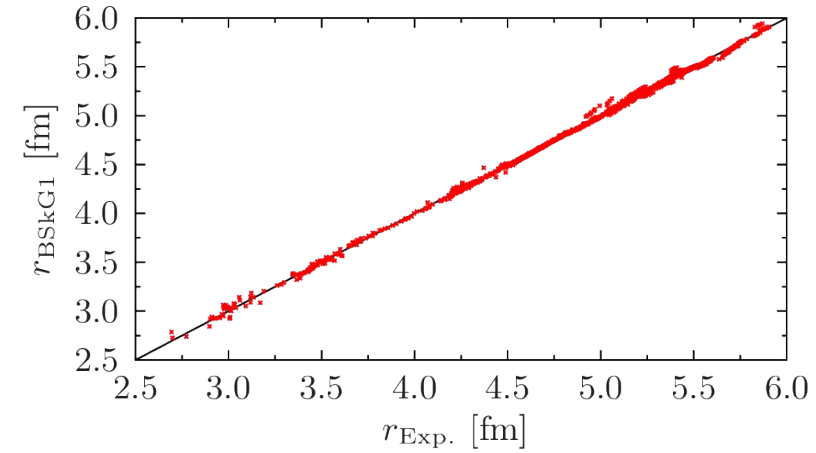
“Ordinary” quadrupole deformation ... and triaxial deformation ...



... and even hexadecapole!



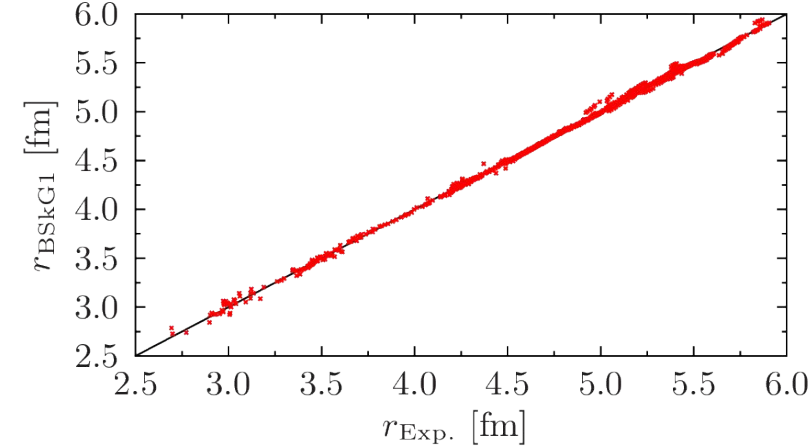
Radii



Systematics and details of charge radii

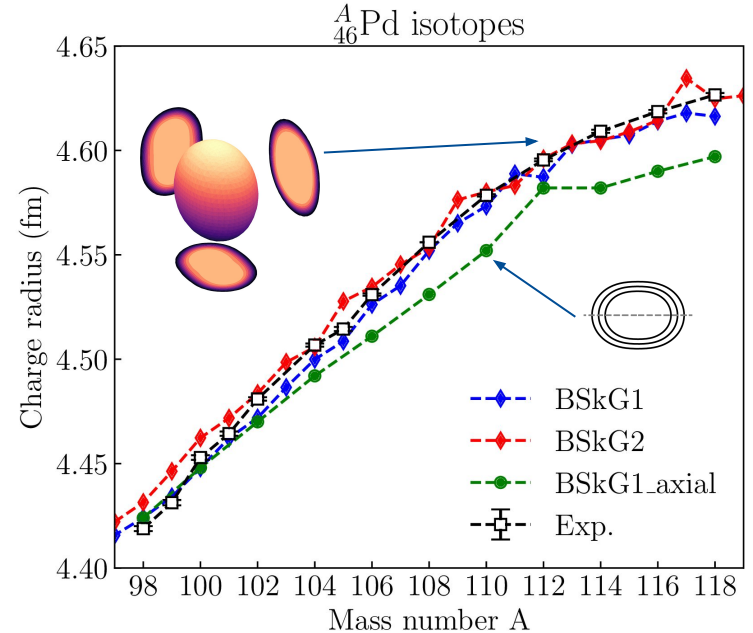
- rms (charge radii) ~ 0.027 fm
- complete charge densities
- ALL deformation affects radii!

Radii



Systematics and details of charge radii

- rms (charge radii) ~ 0.027 fm
- complete charge densities
- ALL deformation affects radii!

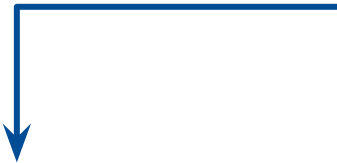
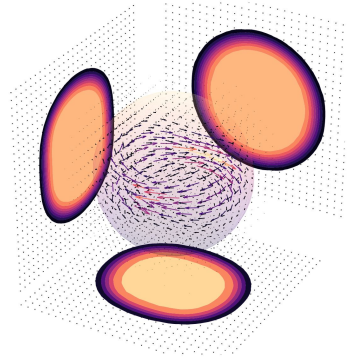


S. Geldhof, PRL **128**, 152501 (2022).

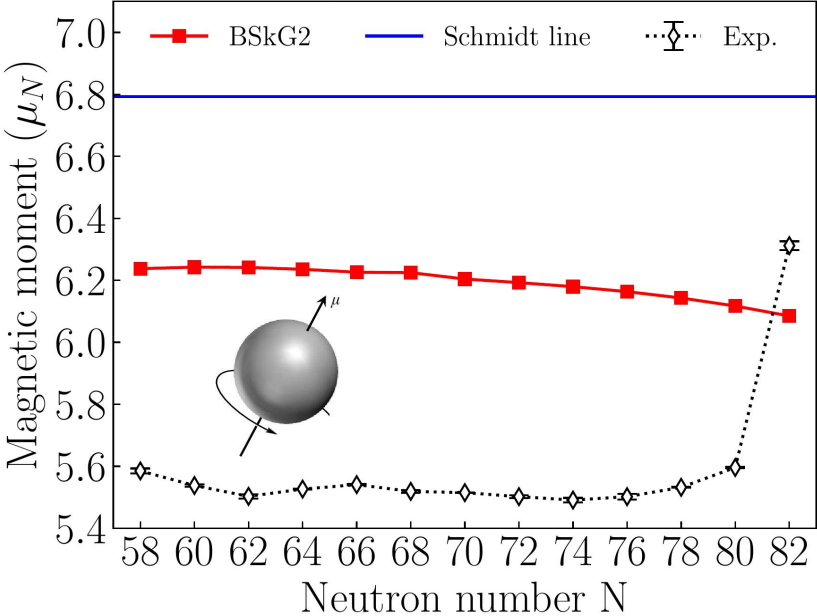
More data on Pd and Ru, coming by the ATLANTIS collaboration!

Additional observables

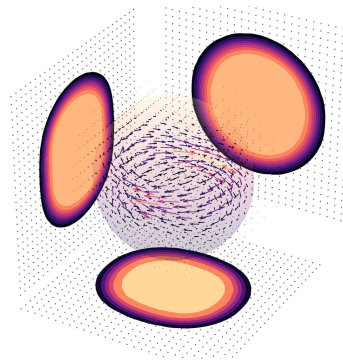
A. R. Vernon et al., Nature 607, 260 (2022),
J. Eberz et al., NPA 464, 9 (1987).
J.Y. Zeng et al. PRC 50, 1388 (1994).



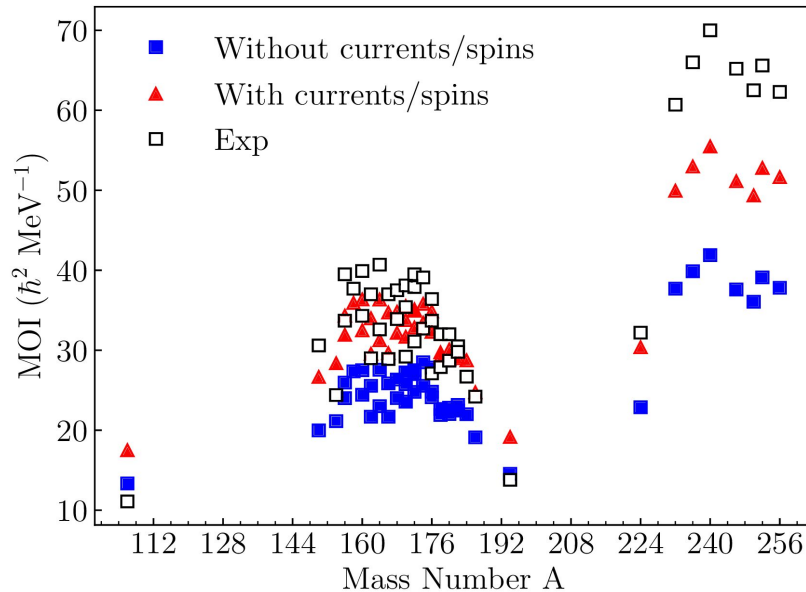
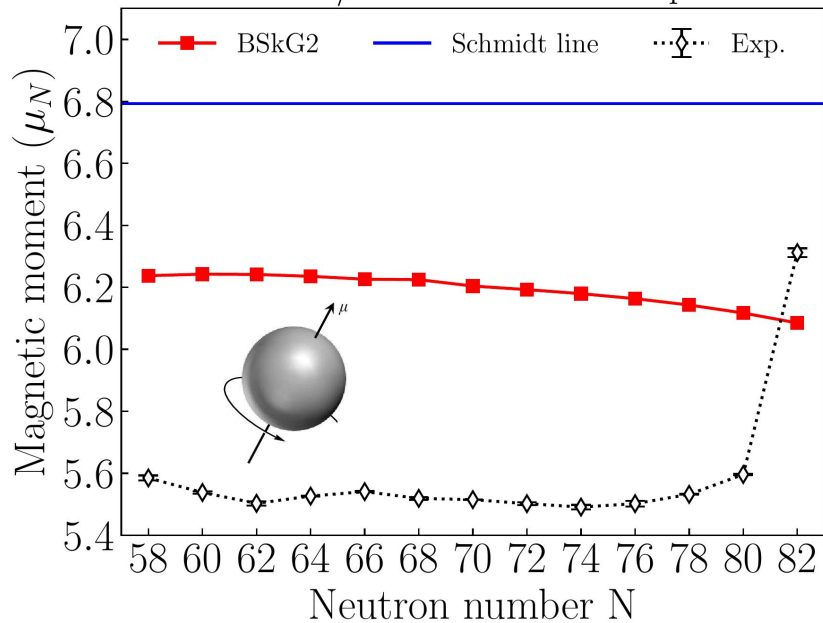
$J^\pi = 9/2^+$ states in In isotopes



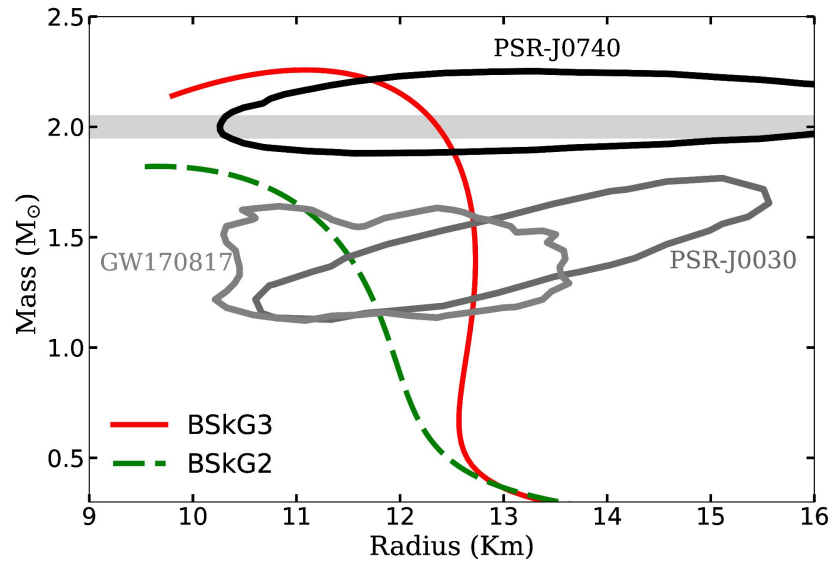
Additional observables



$J^\pi = 9/2^+$ states in In isotopes



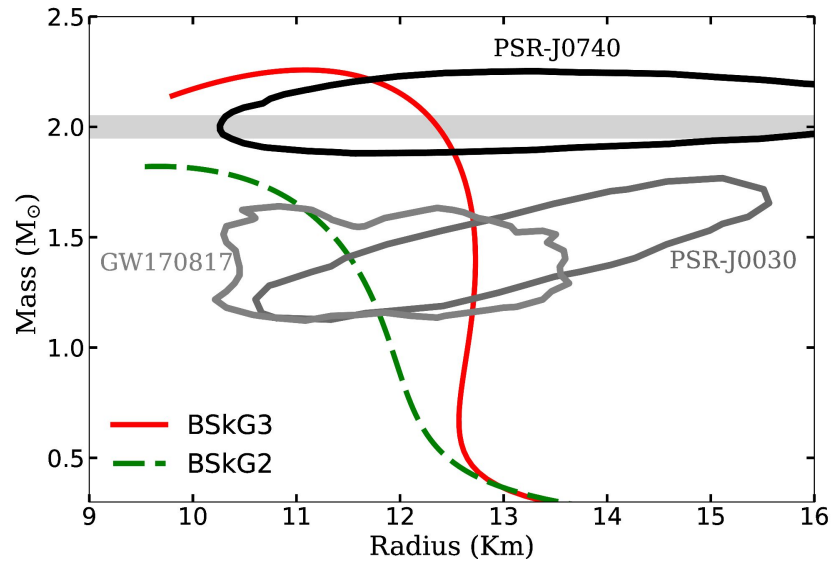
Neutron stars



Stiffer EoS

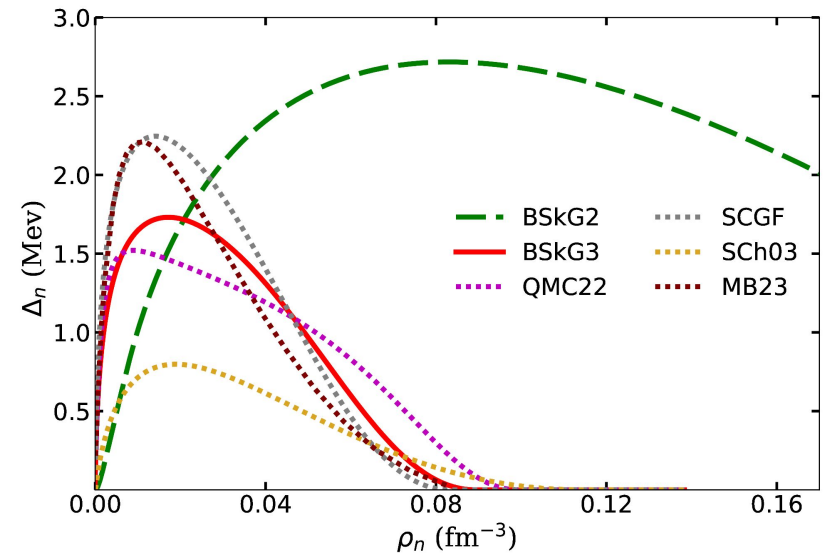
- results in higher maximum mass
- usually incompatible with masses
- we used additional ρ -dependencies

Neutron stars



Stiffer EoS

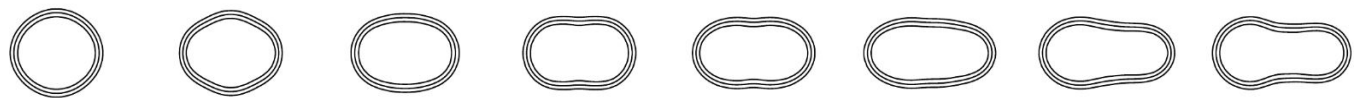
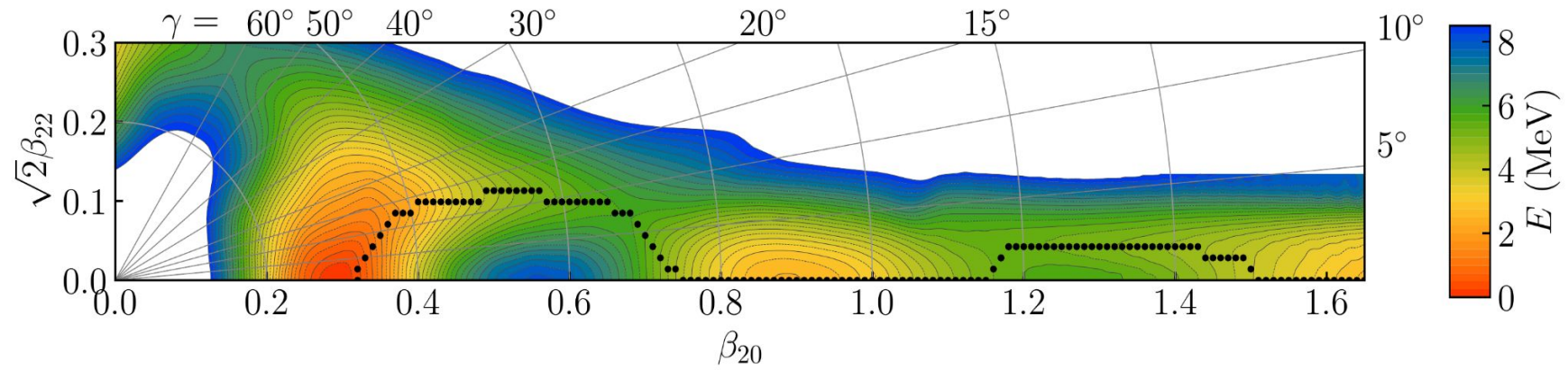
- results in higher maximum mass
- usually incompatible with masses
- we used additional ρ -dependencies



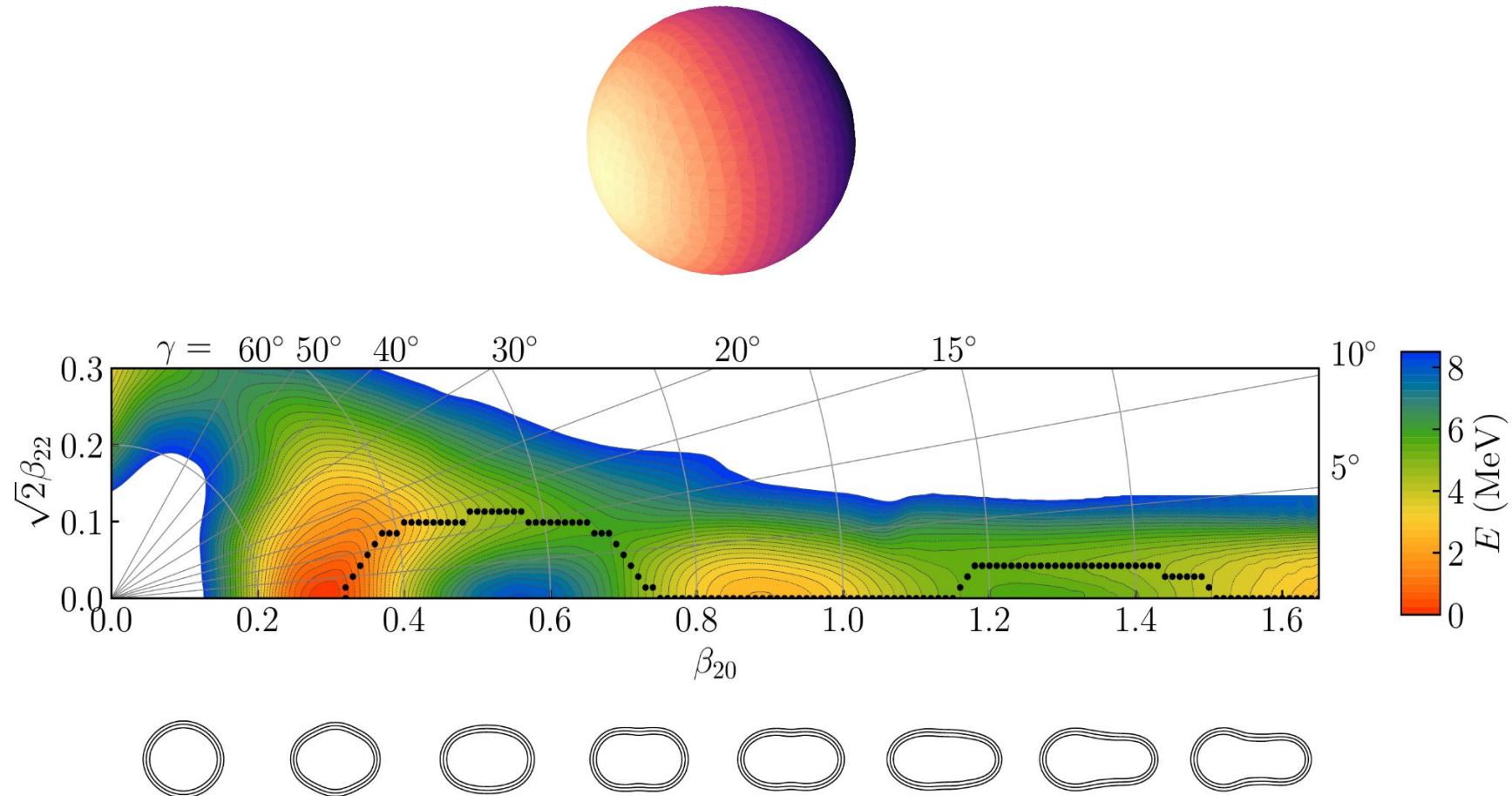
Realistic pairing gaps

- realistic pairing properties in INM
- constrained to advanced calculations

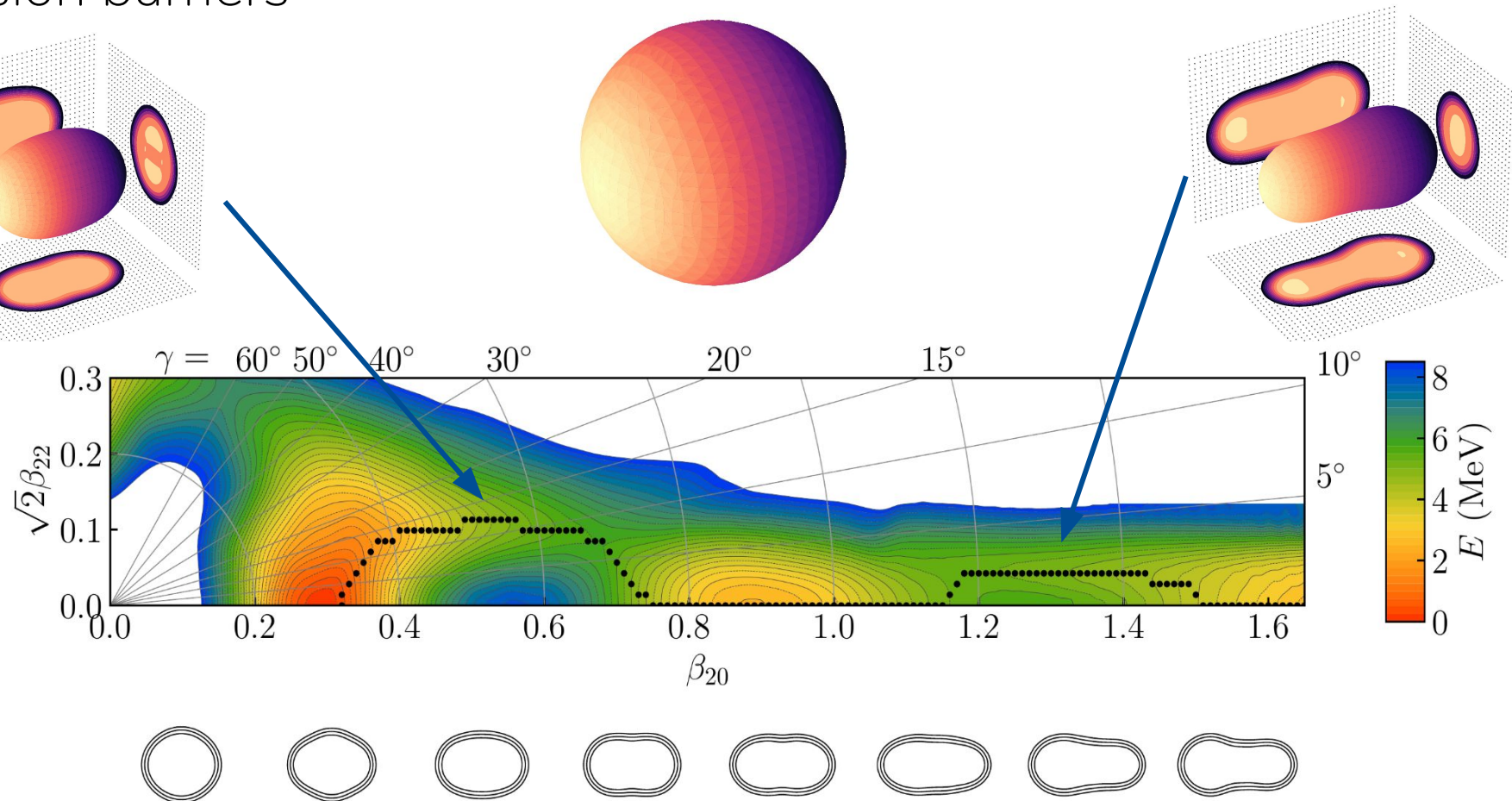
Fission barriers



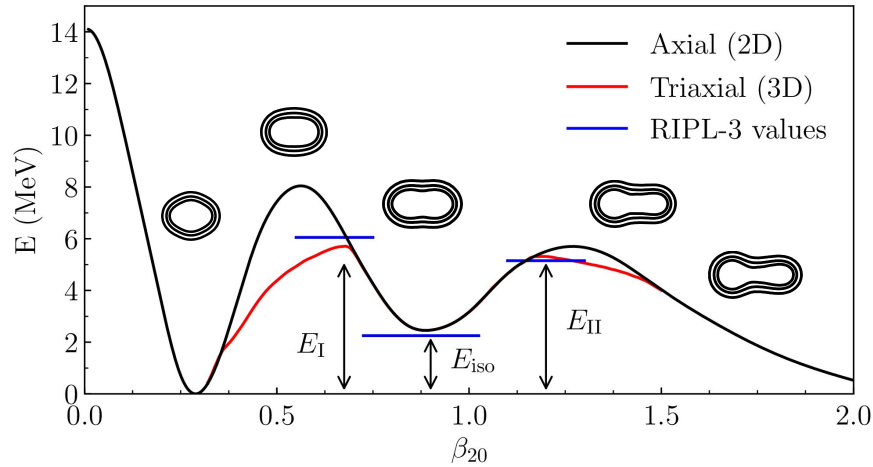
Fission barriers



Fission barriers



Fission

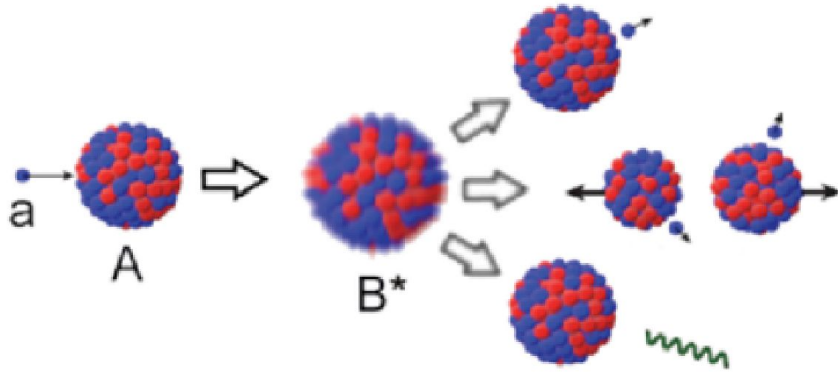


Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
Prim. barriers [MeV]	0.88	0.44	0.33
Secun. barriers [MeV]	0.87	0.47	0.51
Fission isomers [MeV]	1.0	0.49	0.34
Max. NS mass [M_{\odot}]	1.8	1.8	2.3

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

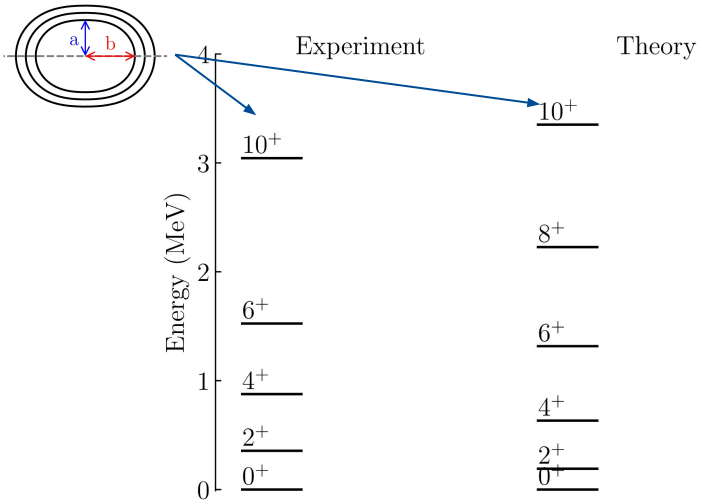
Nuclear level densities



Nuclear level densities

- required for **compound** reactions
- NLDs “count” phase-space
- **little** direct exp. information

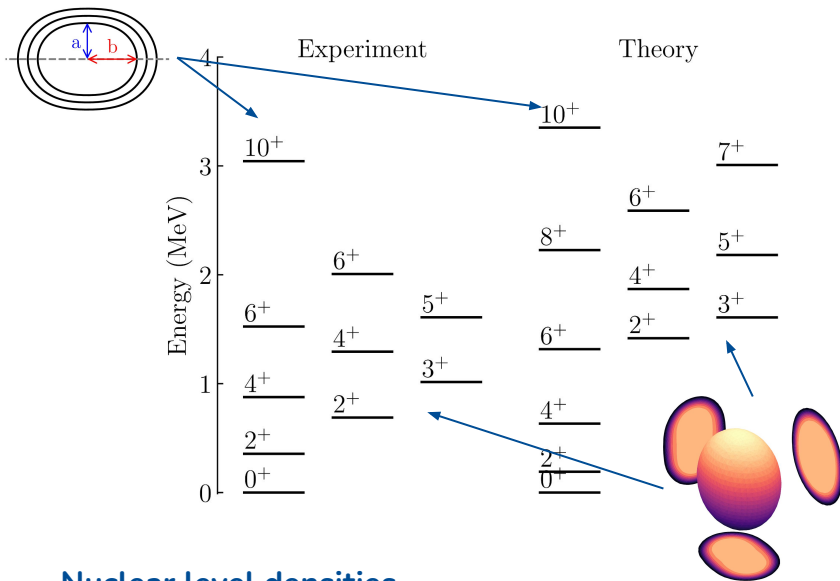
Nuclear level densities: ^{196}Pt



Nuclear level densities

- required for **compound** reactions
- NLDs “count” phase-space
- **little** direct exp. information
- **symmetries** impact level structure

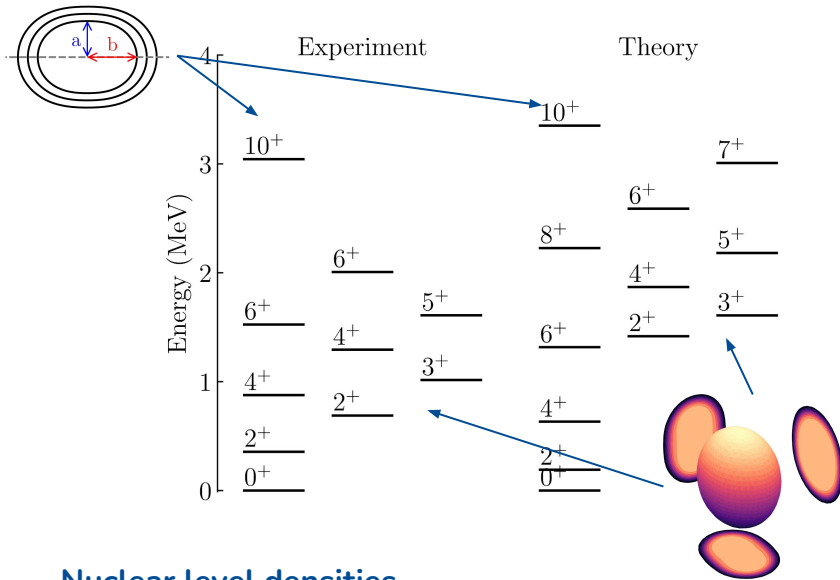
Nuclear level densities: ^{196}Pt



Nuclear level densities

- required for **compound** reactions
- NLDs “count” phase-space
- **little** direct exp. information
- **symmetries** impact level structure

Nuclear level densities: ^{196}Pt



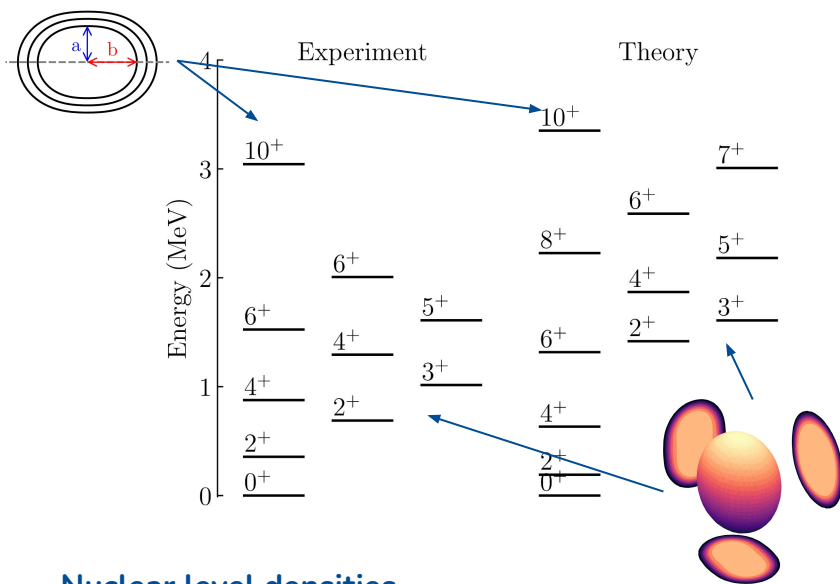
Nuclear level densities

- required for **compound** reactions
- NLDs “count” phase-space
- **little** direct exp. information
- **symmetries** impact level structure

NLDs with BSkG3

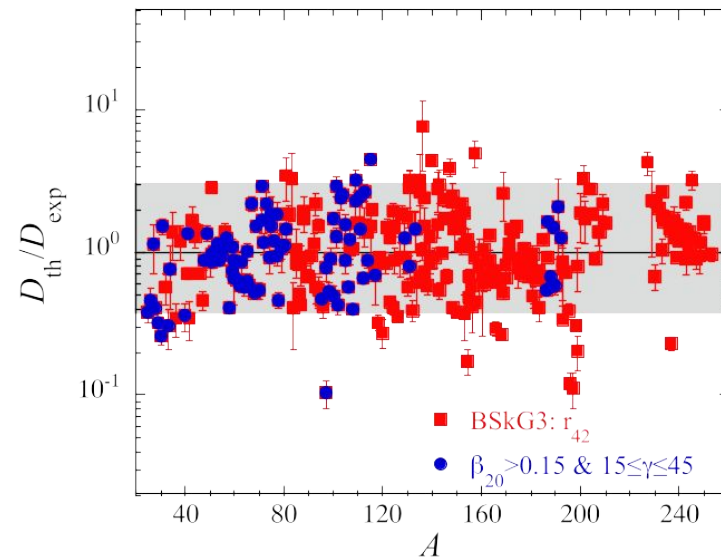
- systematic inclusion of triaxiality
- good reproduction of data

Nuclear level densities: ^{196}Pt



Nuclear level densities

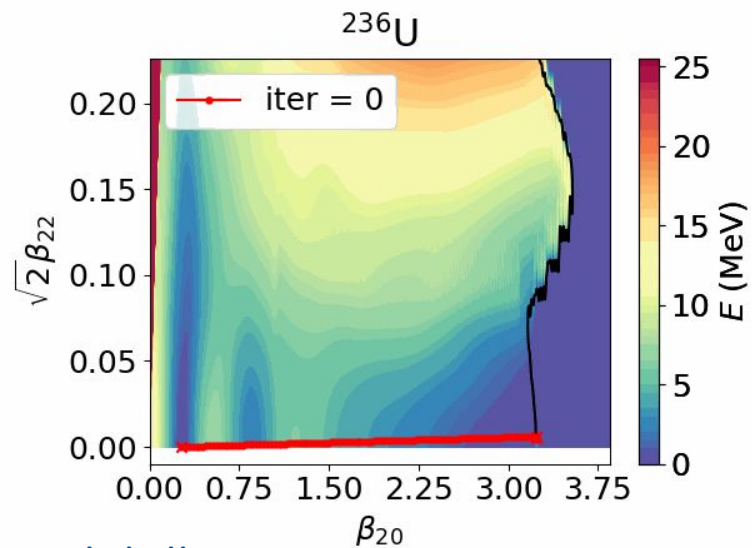
- required for **compound** reactions
- NLDs “count” phase-space
- **little** direct exp. information
- **symmetries** impact level structure



NLDs with BSkG3

- systematic inclusion of triaxiality
- good reproduction of data

Large-scale application to fission



Several challenges

- get multi-D surfaces for 1000s of nuclei
- find the fission path on each surface
- estimate fission rates and yields

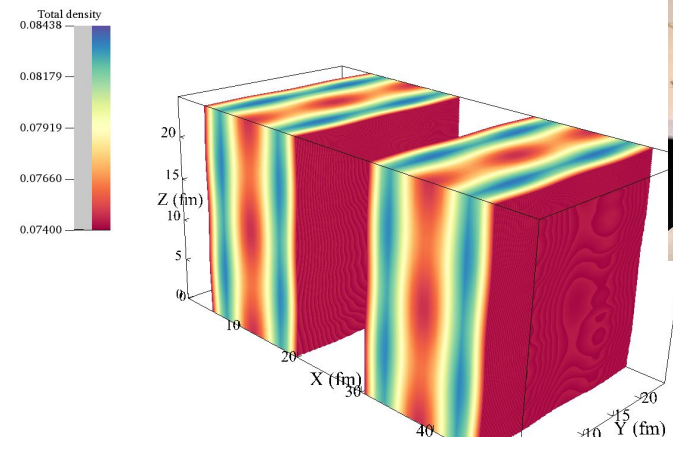
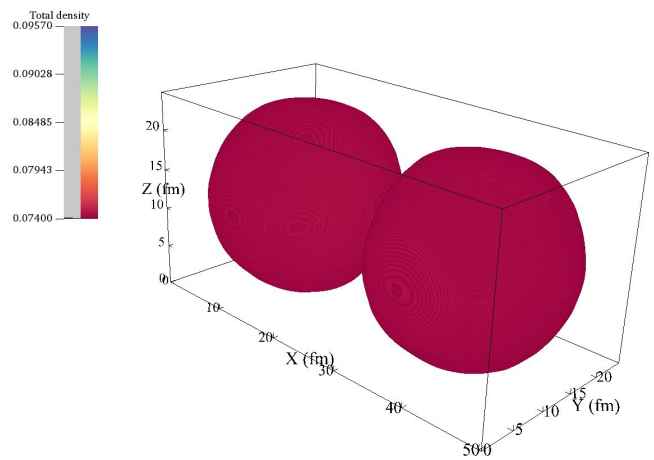
Towards a complete EoS with the BSkGs

Work by Nikolai Shchechilin



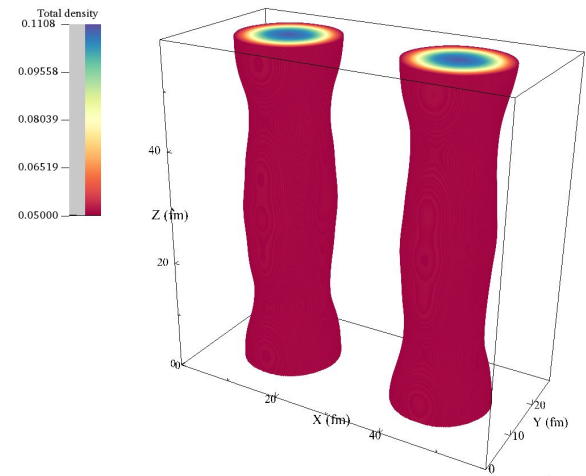
Towards a complete EoS with the BSkGs

Work by Nikolai Shchepochin

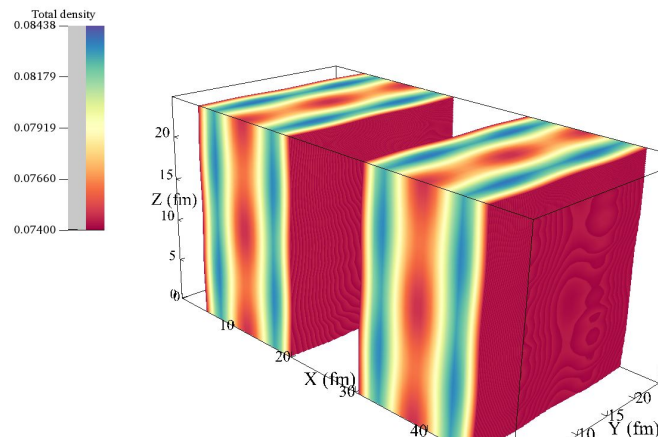
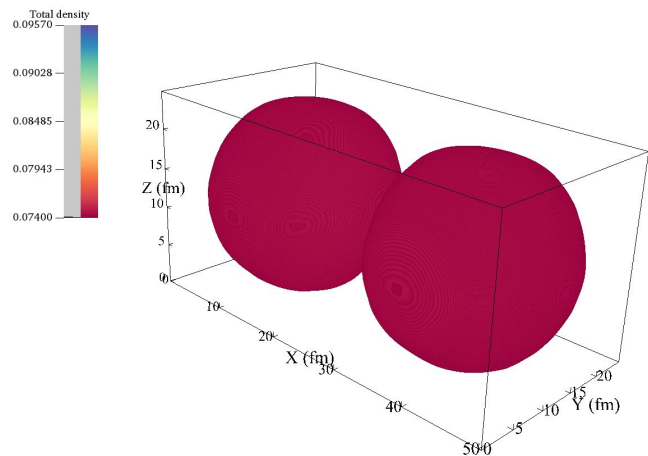


Nuclear pasta

- crystalline structures in NS crust
- impact NS cooling and emitted GW

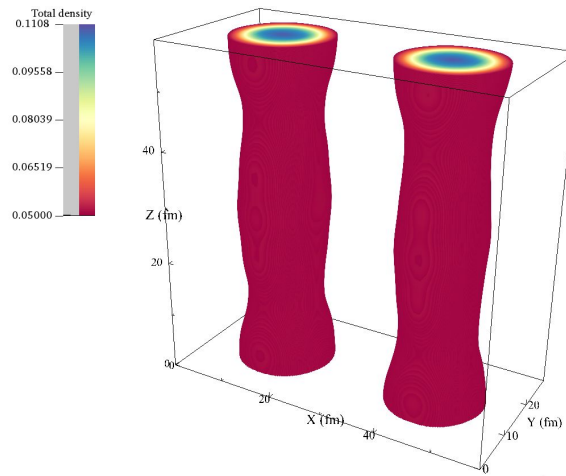


Towards a complete EoS with the BSkGs



Nuclear pasta

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



$$\begin{aligned}
\varepsilon_{\text{Sk},e}^{(0)}(\bar{\eta}) &= \sum_{t=0,1} [A_{t,e}^{(0,1)} (D_t^{1,1})^2 + A_{t,e}^{(0,2)} (D_0^{1,1})^\alpha (D_t^{1,1})^2], \\
\varepsilon_{\text{Sk},e}^{(2)}(\bar{\eta}) &= \sum_{t=0,1} [A_{t,e}^{(2,1)} D_t^{1,1} (\Delta D_t^{1,1}) + A_{t,e}^{(2,2)} D_t^{1,1} D_t^{(\nabla,\nabla)} + A_{t,e}^{(2,3)} \sum_{\mu\nu} C_{t,\mu\nu}^{1,\nabla\sigma} C_{t,\mu\nu}^{1,\nabla\sigma} + A_{t,e}^{(2,4)} D_t^{1,1} (\nabla \cdot C_t^{1,\nabla \times \sigma})], \\
\varepsilon_{\text{Sk},e}^{(4)}(\bar{\eta}) &= \sum_{t=0,1} [A_{t,e}^{(4,1)} (\Delta D_t^{1,1}) (\Delta D_t^{1,1}) + A_{t,e}^{(4,2)} D_t^{1,1} D_t^{\Delta,\Delta} + A_{t,e}^{(4,3)} D_t^{(\nabla,\nabla)} D_t^{(\nabla,\nabla)} \\
&\quad + A_{t,e}^{(4,4)} \sum_{\mu\nu} D_{t,\mu\nu}^{\nabla,\nabla} D_{t,\mu\nu}^{\nabla,\nabla} + A_{t,e}^{(4,5)} \sum_{\mu\nu} D_{t,\mu\nu}^{\nabla,\nabla} (\nabla_\mu \nabla_\nu D_t^{1,1}) \\
&\quad + A_{t,e}^{(4,6)} \sum_{\mu\nu} C_{t,\mu\nu}^{1,\nabla\sigma} (\Delta C_{t,\mu\nu}^{1,\nabla\sigma}) + A_{t,e}^{(4,7)} \sum_{\mu\nu\kappa} (\nabla_\mu C_{t,\mu\kappa}^{1,\nabla\sigma}) (\nabla_\nu C_{t,\nu\kappa}^{1,\nabla\sigma}) + A_{t,e}^{(4,8)} \sum_{\mu\nu} C_{t,\mu\nu}^{1,\nabla\sigma} C_{t,\mu\nu}^{\Delta,\nabla\sigma}], \\
\varepsilon_{\text{Sk},o}^{(0)}(\bar{\eta}) &= \sum_{t=0,1} [A_{t,o}^{(0,1)} \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{1,\sigma} + A_{t,o}^{(0,2)} (D_0^{1,1})^\alpha \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{1,\sigma}], \\
\varepsilon_{\text{Sk},o}^{(2)}(\bar{\eta}) &= \sum_{t=0,1} [A_{t,o}^{(2,1)} \bar{D}_t^{1,\sigma} \cdot (\Delta \bar{D}_t^{1,\sigma}) + A_{t,o}^{(2,2)} \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{(\nabla,\nabla)\sigma} + A_{t,o}^{(2,3)} \bar{C}_t^{1,\nabla} \cdot \bar{C}_t^{1,\nabla} + A_{t,o}^{(2,4)} \bar{D}_t^{1,\sigma} \cdot (\nabla \times \bar{C}_t^{1,\nabla})], \\
\varepsilon_{\text{Sk},o}^{(4)}(\bar{\eta}) &= \sum_{t=0,1} [A_{t,o}^{(4,1)} (\Delta \bar{D}_t^{1,\sigma}) \cdot (\Delta \bar{D}_t^{1,\sigma}) + A_{t,o}^{(4,2)} \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{\Delta,\Delta\sigma} + A_{t,o}^{(4,3)} \bar{D}_t^{(\nabla,\nabla)\sigma} \cdot \bar{D}_t^{(\nabla,\nabla)\sigma} \\
&\quad + A_{t,o}^{(4,4)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} + A_{t,o}^{(4,5)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} (\nabla_\mu \nabla_\nu D_{\kappa}^{1,\sigma}) \\
&\quad + A_{t,o}^{(4,6)} \bar{C}_t^{1,\nabla} \cdot (\Delta \bar{C}_t^{1,\nabla}) + A_{t,o}^{(4,7)} (\nabla \cdot \bar{C}_t^{1,\nabla}) (\nabla \cdot \bar{C}_t^{1,\nabla}) + A_{t,o}^{(4,8)} \bar{C}_t^{1,\nabla} \cdot \bar{C}_t^{\Delta,\nabla}],
\end{aligned}$$

N2LO EDF

- systematic expansion in gradients
- next-to-next-to-leading order
- massively complicates the numerics

$$\begin{aligned}
\varepsilon_{\text{Sk},e}^{(0)}(\bar{n}) &= \sum_{t=0,1} [A_{t,e}^{(0,1)} (D_t^{1,1})^2 + A_{t,e}^{(0,2)} (D_0^{1,1})^\alpha (D_t^{1,1})^2], \\
\varepsilon_{\text{Sk},e}^{(2)}(\bar{n}) &= \sum_{t=0,1} [A_{t,e}^{(2,1)} D_t^{1,1} (\Delta D_t^{1,1}) + A_{t,e}^{(2,2)} D_t^{1,1} D_t^{(\nabla,\nabla)} + A_{t,e}^{(2,3)} \sum_{\mu\nu} c_{t,\mu\nu}^{1,\nabla\sigma} c_{t,\mu\nu}^{1,\nabla\sigma} + A_{t,e}^{(2,4)} D_t^{1,1} (\nabla \cdot c_t^{1,\nabla \times \sigma})], \\
\varepsilon_{\text{Sk},e}^{(4)}(\bar{n}) &= \sum_{t=0,1} [A_{t,e}^{(4,1)} (\Delta D_t^{1,1}) (\Delta D_t^{1,1}) + A_{t,e}^{(4,2)} D_t^{1,1} D_t^{\Delta,\Delta} + A_{t,e}^{(4,3)} D_t^{(\nabla,\nabla)} D_t^{(\nabla,\nabla)} \\
&\quad + A_{t,e}^{(4,4)} \sum_{\mu\nu} D_{t,\mu\nu}^{\nabla,\nabla} D_{t,\mu\nu}^{\nabla,\nabla} + A_{t,e}^{(4,5)} \sum_{\mu\nu} D_{t,\mu\nu}^{\nabla,\nabla} (\nabla_\mu \nabla_\nu D_t^{1,1}) \\
&\quad + A_{t,e}^{(4,6)} \sum_{\mu\nu} c_{t,\mu\nu}^{1,\nabla\sigma} (\Delta c_{t,\mu\nu}^{1,\nabla\sigma}) + A_{t,e}^{(4,7)} \sum_{\mu\nu\kappa} (\nabla_\mu c_{t,\mu\kappa}^{1,\nabla\sigma}) (\nabla_\nu c_{t,\nu\kappa}^{1,\nabla\sigma}) + A_{t,e}^{(4,8)} \sum_{\mu\nu} c_{t,\mu\nu}^{1,\nabla\sigma} c_{t,\mu\nu}^{\Delta,\nabla\sigma}], \\
\varepsilon_{\text{Sk},o}^{(0)}(\bar{n}) &= \sum_{t=0,1} [A_{t,o}^{(0,1)} \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{1,\sigma} + A_{t,o}^{(0,2)} (D_0^{1,1})^\alpha \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{1,\sigma}], \\
\varepsilon_{\text{Sk},o}^{(2)}(\bar{n}) &= \sum_{t=0,1} [A_{t,o}^{(2,1)} \bar{D}_t^{1,\sigma} \cdot (\Delta \bar{D}_t^{1,\sigma}) + A_{t,o}^{(2,2)} \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{(\nabla,\nabla)\sigma} + A_{t,o}^{(2,3)} \bar{c}_t^{1,\nabla} \cdot \bar{c}_t^{1,\nabla} + A_{t,o}^{(2,4)} \bar{D}_t^{1,\sigma} \cdot (\nabla \times \bar{c}_t^{1,\nabla})], \\
\varepsilon_{\text{Sk},o}^{(4)}(\bar{n}) &= \sum_{t=0,1} [A_{t,o}^{(4,1)} (\Delta \bar{D}_t^{1,\sigma}) \cdot (\Delta \bar{D}_t^{1,\sigma}) + A_{t,o}^{(4,2)} \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{\Delta,\Delta\sigma} + A_{t,o}^{(4,3)} \bar{D}_t^{(\nabla,\nabla)\sigma} \cdot \bar{D}_t^{(\nabla,\nabla)\sigma} \\
&\quad + A_{t,o}^{(4,4)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} + A_{t,o}^{(4,5)} \sum_{\mu\nu\kappa} D_{\mu\nu\kappa}^{\nabla,\nabla\sigma} (\nabla_\mu \nabla_\nu D_{\kappa}^{1,\sigma}) \\
&\quad + A_{t,o}^{(4,6)} \bar{c}_t^{1,\nabla} \cdot (\Delta \bar{c}_t^{1,\nabla}) + A_{t,o}^{(4,7)} (\nabla \cdot \bar{c}_t^{1,\nabla}) (\nabla \cdot \bar{c}_t^{1,\nabla}) + A_{t,o}^{(4,8)} \bar{c}_t^{1,\nabla} \cdot \bar{c}_t^{\Delta,\nabla}],
\end{aligned}$$

N2LO EDF

- systematic expansion in gradients
- next-to-next-to-leading order
- massively complicates the numerics

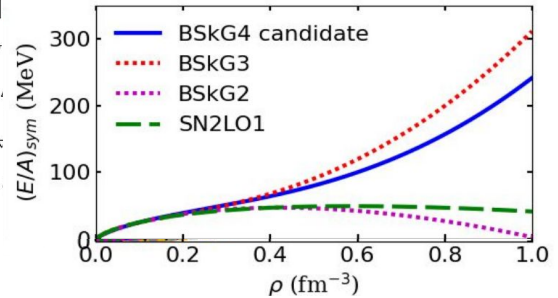
Advantages

- support heavy neutron stars
 - less density dependencies
 - T-dependent effective mass
- ... all with **LESS** parameters!

BSkG4

$$\begin{aligned} \varepsilon_{\text{Sk},e}^{(0)}(\bar{n}) &= \sum_{t=0,1} [A_{t,e}^{(0,1)} (D_t^{1,1})^2 + A_{t,e}^{(0,2)} (D_0^{1,1})^\alpha (D_t^{1,1})^2], \\ \varepsilon_{\text{Sk},e}^{(2)}(\bar{n}) &= \sum_{t=0,1} [A_{t,e}^{(2,1)} D_t^{1,1} (\Delta D_t^{1,1}) + A_{t,e}^{(2,2)} D_t^{1,1} D_t^{(\nabla,\nabla)} + A_{t,e}^{(2,3)} D_t^{1,1} D_t^{\Delta,\Delta}], \\ \varepsilon_{\text{Sk},e}^{(4)}(\bar{n}) &= \sum_{t=0,1} [A_{t,e}^{(4,1)} (\Delta D_t^{1,1}) (\Delta D_t^{1,1}) + A_{t,e}^{(4,2)} D_t^{1,1} D_t^{\Delta,\Delta} + \\ &\quad + A_{t,e}^{(4,4)} \sum_{\mu\nu} D_{t,\mu\nu}^{\nabla,\nabla} D_{t,\mu\nu}^{\nabla,\nabla} + A_{t,e}^{(4,5)} \sum_{\mu\nu} D_{t,\mu\nu}^{\nabla,\nabla} (\nabla_\mu \nabla_\nu \\ &\quad + A_{t,e}^{(4,6)} \sum_{\mu\nu} C_{t,\mu\nu}^{1,\nabla\sigma} (\Delta C_{t,\mu\nu}^{1,\nabla\sigma}) + A_{t,e}^{(4,7)} \sum_{\mu\nu\kappa} (\nabla_\mu C_{t,\nu\kappa}^1 \\ \varepsilon_{\text{Sk},o}^{(0)}(\bar{n}) &= \sum_{t=0,1} [A_{t,o}^{(0,1)} \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{1,\sigma} + A_{t,o}^{(0,2)} (D_0^{1,1})^\alpha \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{1,\sigma}] \\ \varepsilon_{\text{Sk},o}^{(2)}(\bar{n}) &= \sum_{t=0,1} [A_{t,o}^{(2,1)} \bar{D}_t^{1,\sigma} \cdot (\Delta \bar{D}_t^{1,\sigma}) + A_{t,o}^{(2,2)} \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{(\nabla,\nabla)\sigma} \\ \varepsilon_{\text{Sk},o}^{(4)}(\bar{n}) &= \sum_{t=0,1} [A_{t,o}^{(4,1)} (\Delta \bar{D}_t^{1,\sigma}) \cdot (\Delta \bar{D}_t^{1,\sigma}) + A_{t,o}^{(4,2)} \bar{D}_t^{1,\sigma} \cdot \bar{D}_t^{\Delta,\mu} \\ &\quad + A_{t,o}^{(4,4)} \sum_{\mu\nu\kappa} D_{t,\mu\nu\kappa}^{\nabla,\nabla\sigma} D_{t,\mu\nu\kappa}^{\nabla,\nabla\sigma} + A_{t,o}^{(4,5)} \sum_{\mu\nu\kappa} D_{t,\mu\nu\kappa}^{\nabla,\nabla\sigma} (\nabla_\mu \nabla_\nu \nabla_\kappa \\ &\quad + A_{t,o}^{(4,6)} \bar{C}_t^{1,\nabla} \cdot (\Delta \bar{C}_t^{1,\nabla}) + A_{t,o}^{(4,7)} (\nabla \cdot \bar{C}_t^{1,\nabla}) (\nabla \cdot \bar{C}_t^{1,\nabla}) \end{aligned}$$

Model	BSkG3	BSkG4?
Masses [MeV]	0.631	0.680
Radii [fm]	0.024	0.024
Max. NS mass [M_\odot]	2.3	2.3



N2LO EDF

- systematic expansion in gradients
- next-to-next-to-leading order
- massively complicates the numerics

Advantages

- support heavy neutron stars
- less density dependencies
- T-dependent effective mass
- ... all with **LESS** parameters!

BRUSLIB
the Brussels Nuclear Library for Astrophysics Applications

UNIVERSITÉ LIBRE DE BRUXELLES
INSTITUT D'ASTRONOMIE ET D'ASTROPHYSIQUE

Q. S. Spin Parity

Ground State Properties

Single Particle Scheme
Density and Potential
Nuclear Level Density
Partition Function
E1 Strength Function
Fission Properties (90<=Z<=110)
Reaction Rates

Last update: April, 30, 2015

Links

MeGen NACRE-II NACRE
SIP-3 EXFOR
ORNL CERNLIB
JINA ReacLib ICFRG

Back to JAA

Ground State Properties

• Data and Plot
Proton number Z: [8] Neutron number N: [8]

• Introduction

The force used in the Hartree-Fock-Bogoliubov (HFB) mass model is an extended Skyrme force (containing t_4 and t_5 terms), along with a 4-parameter delta-function pairing force derived from realistic calculations of infinite nuclear and neutron matter. Pairing correlations are introduced in the framework of the Bogoliubov method. Deformations with axial and left-right symmetry are admitted.

The total binding energy is given by

$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{Wigner}}$$

where

- E_{HFB} is the HFB binding energy including a cranking correction to the spurious rotational energy and a phenomenological vibration correction energy
- $E_{\text{Wigner}} = V_p \exp(-N(N-2)/A^2) + N_n(N_n-2)\exp(-A/A_0)^2$ is a phenomenological correction for the Wigner energy.

The parameter set, labelled BSk24, is determined by constraining the nuclear-matter symmetry coefficient to $\beta = 30$ MeV and the isoscalar effective mass to $M^*/M = 0.8$ and optimizing the fit to the full data set of the 2353 measured masses with $N, Z \geq 8$ (both spherical and deformed) of Audi et al. [Chinese Physics C36, 1287 (2012)]: the corresponding root mean square error is 0.549 MeV for this data set.

TOP

Please refer to Yi Xu, Steinhilber Corley, Alain Fortson, Guangming Chen, Marcel Aronoff, *Astronomy & Astrophysics* 549, A166 (2013) and the specified literature therein when using BRUSLIB.

Any comments or suggestions please send to S. Corley % ulb.be

Institut d'Astronomie et d'Astrophysique
Université Libre de Bruxelles

Faculté des Sciences U.L.B.

View Edit History Print

Home

Research
STARLAB Project
Staff
Databases
Public
Teaching
Library
Links
Location
Astronomical weather forecast
Guest Info
Restricted
Admin

The BSkG3 model

BSkG3 is a large-scale model of nuclear structure: the "large-scale" in this sentence refers to the number of nuclei (several thousands!) but also to our ambition to describe as much of nuclear structure as possible within a single framework. On this page, we provide some more explanation of the basic structure of this model and a [link](#) to a table containing a large amount of calculated ground-state properties for thousands of nuclei.

The model is based on the concept of a nuclear energy density functional (EDF), which starts from the total energy of a nucleus:

$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{corr}}$$

which is calculated microscopically from a mean-field wavefunction of the Hartree-Fock-Bogoliubov (HFB) type. By minimizing the total energy, we find a HFB many-body wavefunction that represents the nuclear ground state and is used to calculate all kinds of properties. Our search for this minimal-energy state is very general: in order to grasp as much correlations among nucleons as we can, we allow our HFB states to break several symmetries. In this way, we account consistently for (i) nuclear triaxiality, (ii) left-right reflection asymmetry and even (iii) time-reversal breaking in odd-mass and odd-odd systems due to the unpaired nucleons. In addition, we represent such nuclear configurations numerically on a rather fine three-dimensional coordinate grid, guaranteeing us a (very high) numerical accuracy of about 100 keV on the absolute values of the total energy.

Available right now for BSkG3:

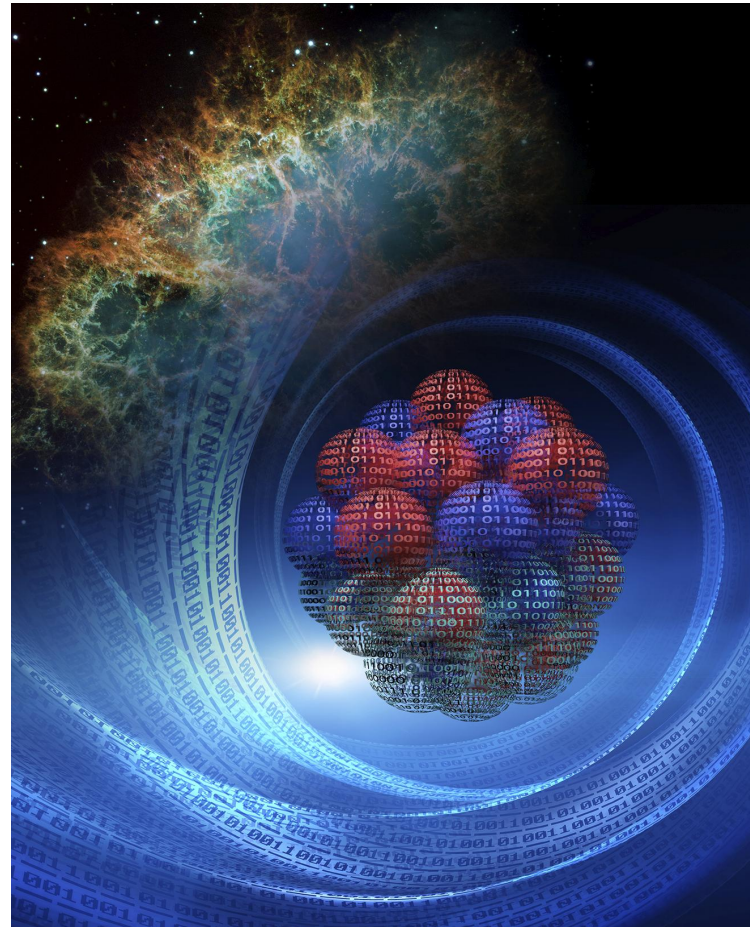
- ground state properties for 7k nuclei
 - masses
 - deformations
 - charge radii
 - pairing properties
 - rotational properties
 - Fission barriers for actinides
- Expansion/modernisation (slowly) ongoing.

Conclusion

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

Large-scale = thousands of nuclei and many observables.

Microscopic = simple wave functions yet complex **symmetry breaking**.



Conclusion

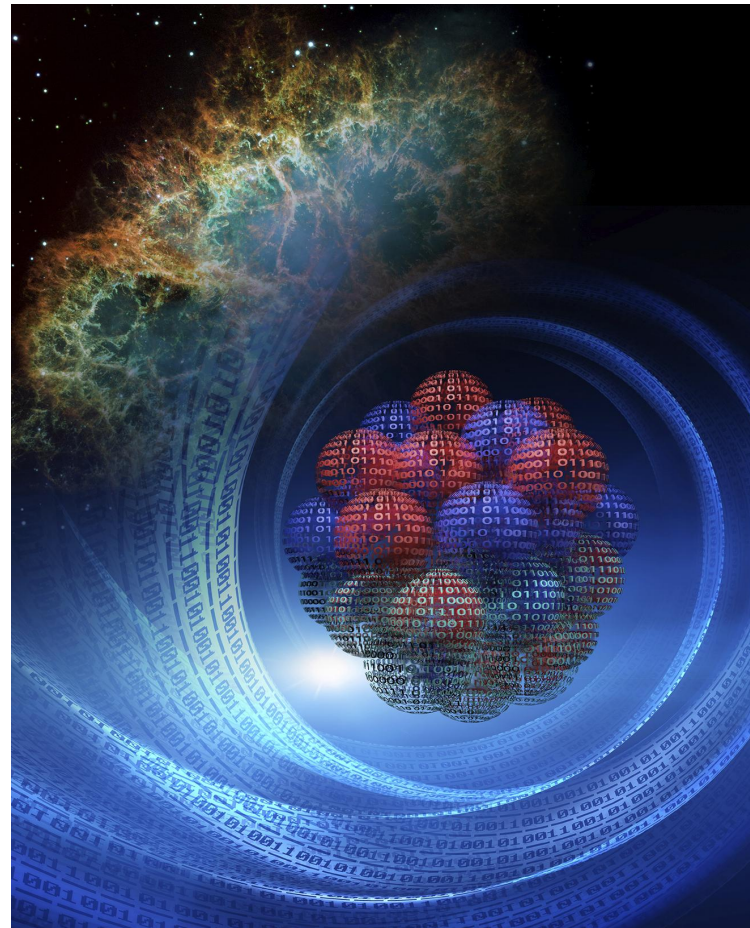
We build large-scale, microscopic models for (astro) applications.

Large-scale = thousands of nuclei and many observables.

Microscopic = simple wave functions yet complex **symmetry breaking**.

BSkG3

- triaxial, octupole and time-reversal deformation
- competitive for masses and charge radii
- unmatched for fission properties
- consistent with NS observations
- masses and densities in TALYS!



Conclusion

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

Large-scale = thousands of nuclei and many observables.

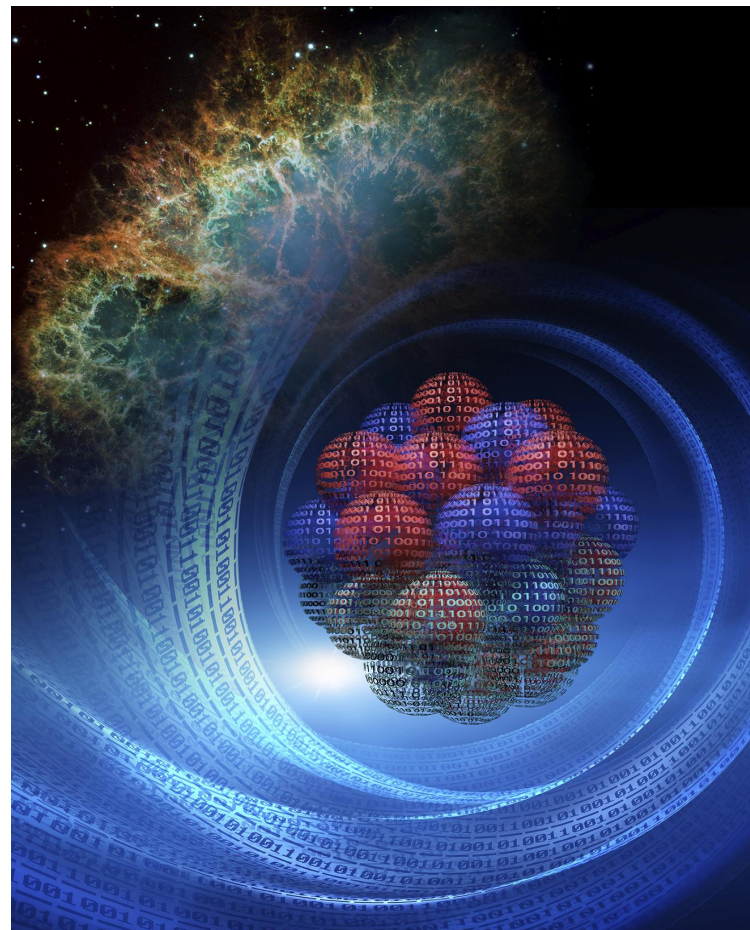
Microscopic = simple wave functions yet complex **symmetry breaking**.

BSkG3

- triaxial, octupole and time-reversal deformation
- competitive for masses and charge radii
- unmatched for fission properties
- consistent with NS observations
- masses and densities in TALYS!

The immediate future:

- complete NLDs for BSkG1/2/3
- fission calculations at an extreme scale
- unified EoS for neutron star applications
- more with less: BSkG4



Conclusion

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

Large-scale = thousands of nuclei and many observables.

Microscopic = simple wave functions yet complex **symmetry breaking**.

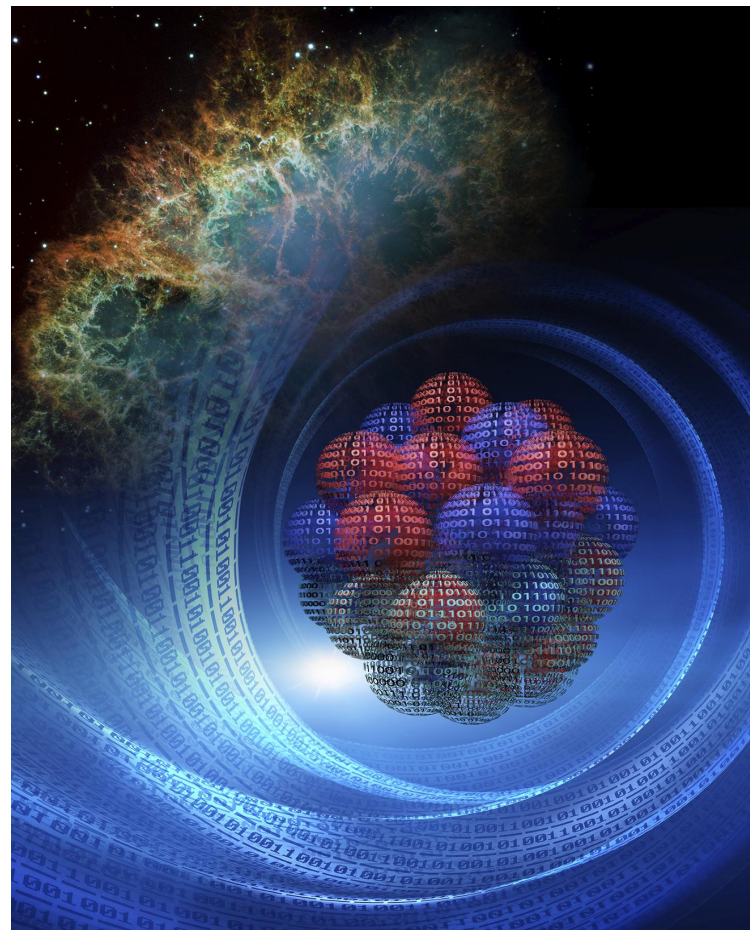
BSkG3

- triaxial, octupole and time-reversal deformation
- competitive for masses and charge radii
- unmatched for fission properties
- consistent with NS observations
- masses and densities in TALYS!

The immediate future:

- complete NLDs for BSkG1/2/3
- fission calculations at an extreme scale
- unified EoS for neutron star applications
- more with less: BSkG4

.... and much more to come!



Conclusion

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

Large-scale = thousands of nuclei and many observables.

Microscopic = simple wave functions yet complex **symmetry breaking**.

BSkG3

- triaxial, octupole and time-reversal deformation
- competitive for masses and charge radii
- unmatched for fission properties
- consistent with NS observations
- masses and densities in TALYS!

The immediate future:

- complete NLDs for BSkG1/2/3
- fission calculations at an extreme scale
- unified EoS for neutron star applications
- more with less: BSkG4

.... and much more to come!



Thank you for...

..... all the wonderful work!



S. Goriely
G. Grams
N. Chamel
N. Shchечilin



S. Hilaire



M. Bender



S. Bara

and several experimental teams!

Thank you for...

..... all the wonderful work!



S. Goriely
G. Grams
N. Chamel
N. Shchepochin



S. Hilaire



M. Bender



S. Bara

and several experimental teams!

..... the computing time!



EuroHPC
Joint Undertaking



Thank you for...

..... all the wonderful work!



S. Goriely
G. Grams
N. Chamel
N. Shchечilin



S. Hilaire



M. Bender



S. Bara

and several experimental teams!

..... the computing time!



EuroHPC
Joint Undertaking



..... the funding!



Thank you for...

..... all the wonderful work!



S. Goriely
G. Grams
N. Chamel
N. Shchечilin



S. Hilaire



M. Bender



S. Bara

and several experimental teams!

..... the computing time!



EuroHPC
Joint Undertaking



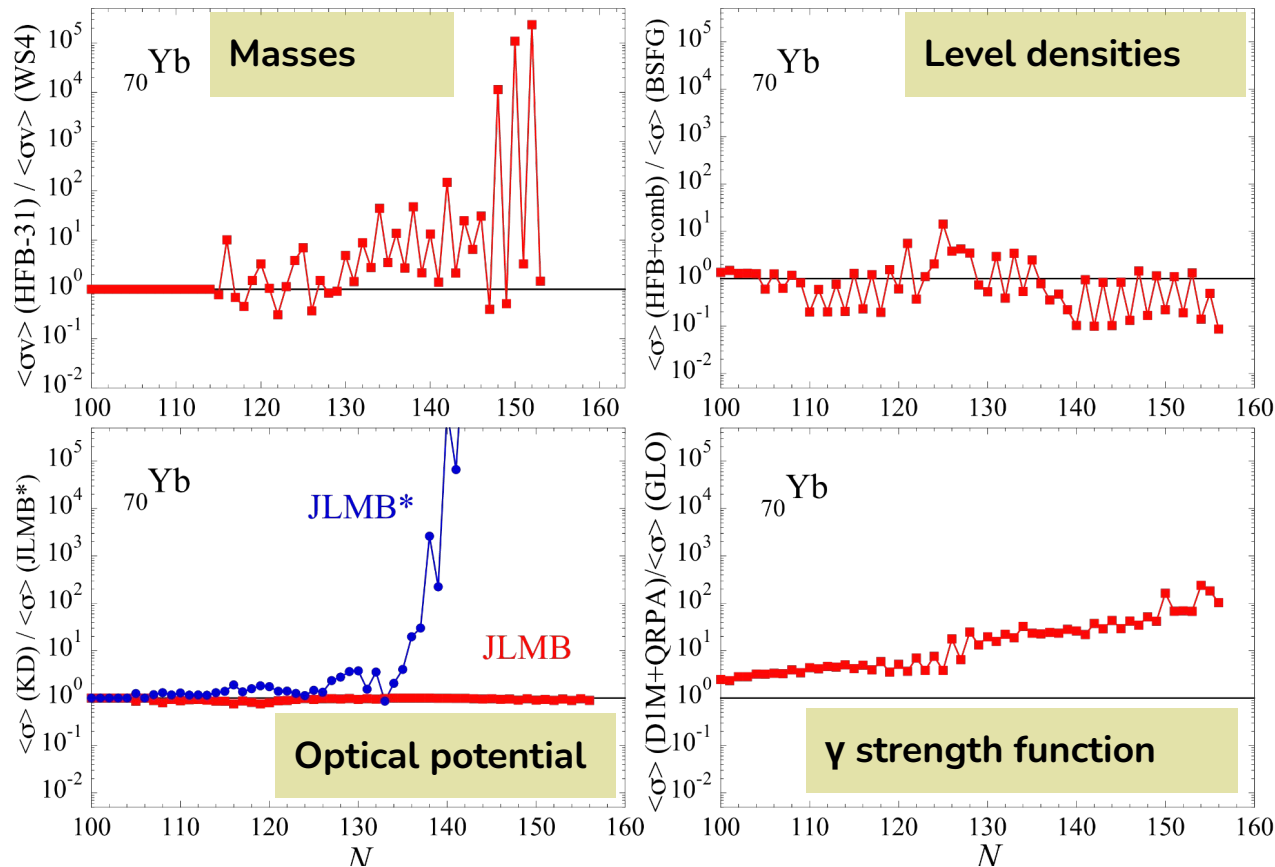
..... the funding!



..... your attention!

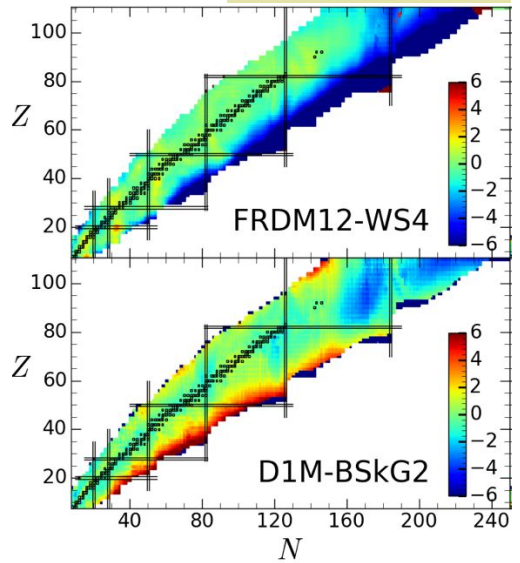
Bonus!

Models can make all the difference...

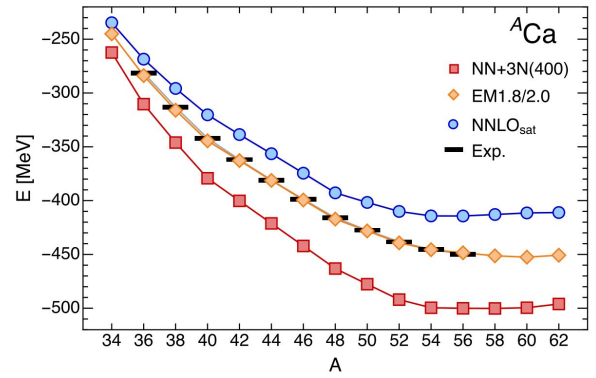
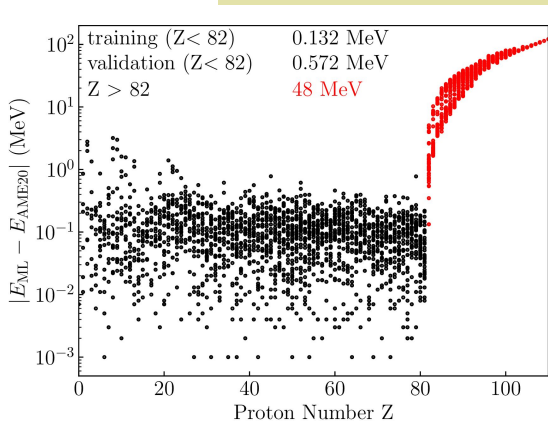


Interlude: why do we do these complex things?

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)