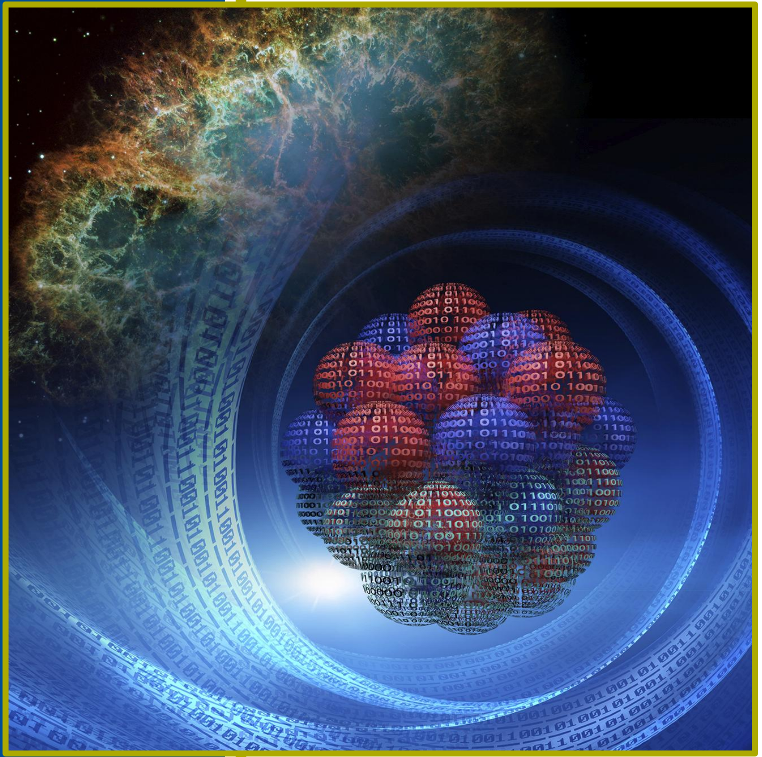
WOUTER RYSSENS



Microscopic models of nuclear structure at scale

W. Ryssens
N. Chamel, S. Bara, G. Grams, N. Shchechilin,
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

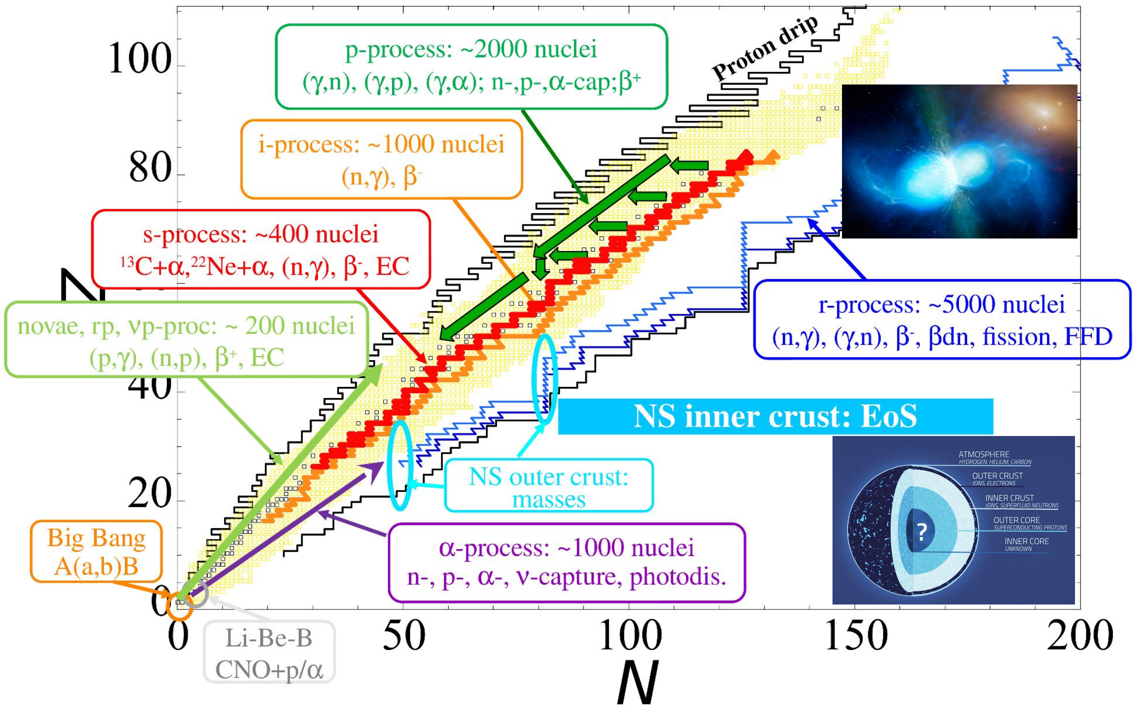
- nucleon number
- energy
- temperature
- density
- ……

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 (**EDF**s)

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

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

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

Local densities and currents of a wavefunction

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

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 (**EDF**s)

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

Energy

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

Local densities and currents of a wavefunction

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

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

Energy

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

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 (**EDF**s)

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

Energy

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

Local densities and currents of a wavefunction

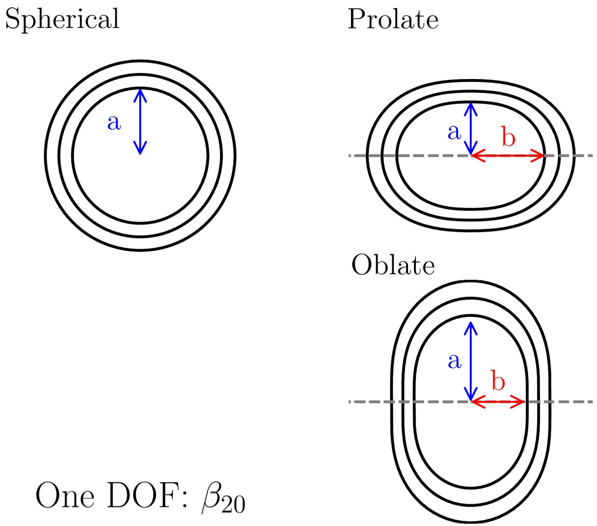
Strong points

- **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

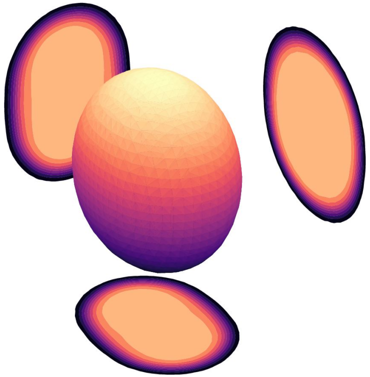


Nuclear deformation

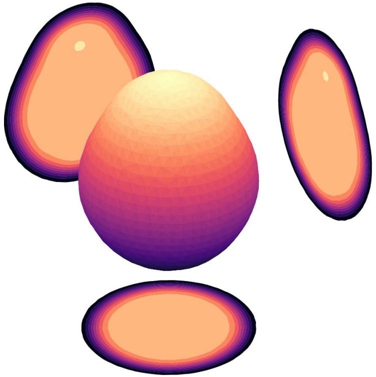
- larger variational space
- shape DOF characterized by multipole moments
- capture correlations at modest CPU cost
- intuitive interpretation

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

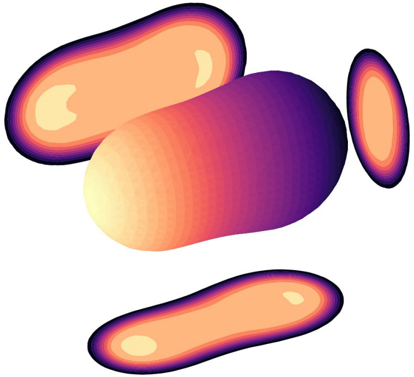
β_{20}, β_{22} or β_2, γ



β_{20}, β_{30}



β_{20}, β_{22} **and** β_{30}



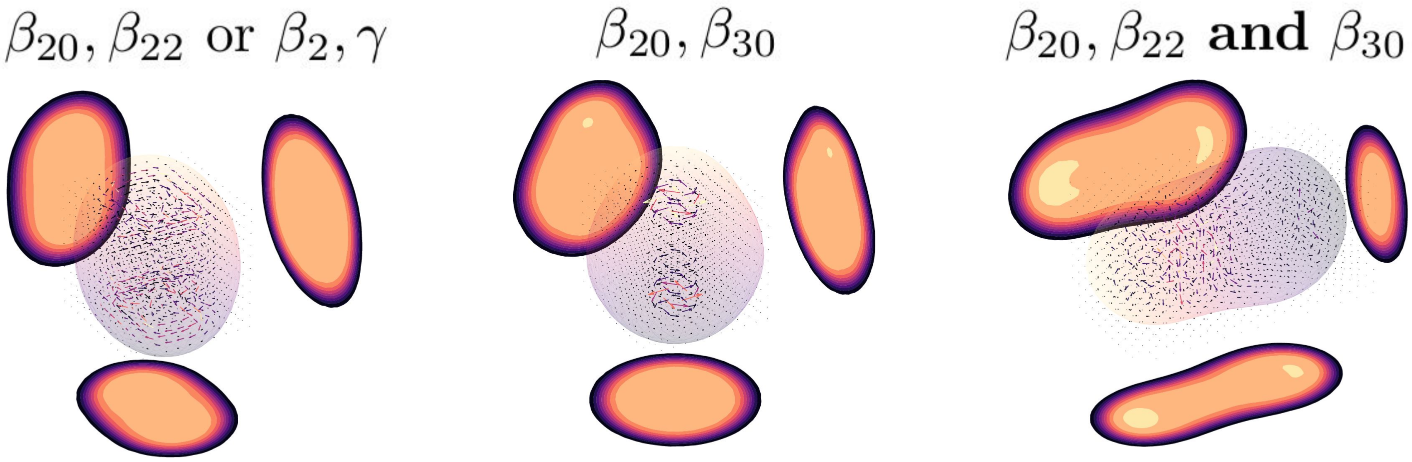
Nuclear deformation

- 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



Nuclear deformation

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

More general configurations

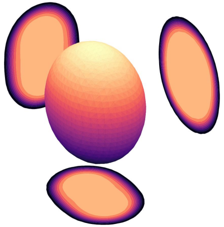
- triaxial shapes
- reflection asymmetry
- elongated shapes
- spin densities and currents

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

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

BSkG1 (2021)

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

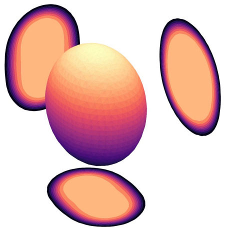


Brussels-**Sk**yrme-on-a-**G**rid: BSkG

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

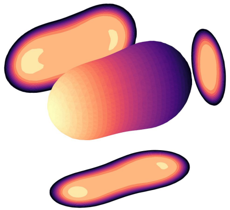
BSkG1 (2021)

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



BSkG2 (2022)

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

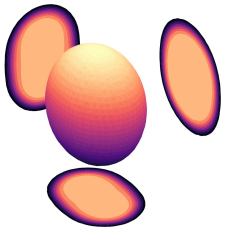


Brussels-**Sk**yrme-on-a-**G**rid: BSkG

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

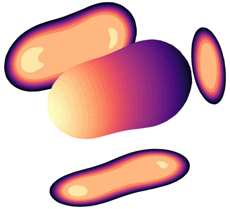
BSkG1 (2021)

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



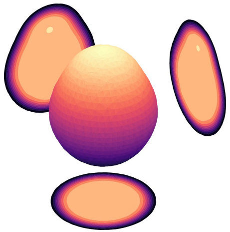
BSkG2 (2022)

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



BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation

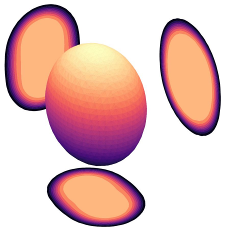


Brussels-**Sk**yrme-on-a-**G**rid: BSkG

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

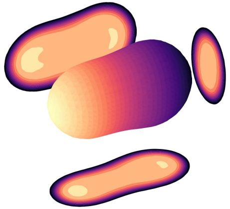
BSkG1 (2021)

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



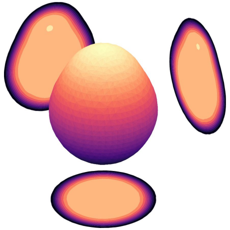
BSkG2 (2022)

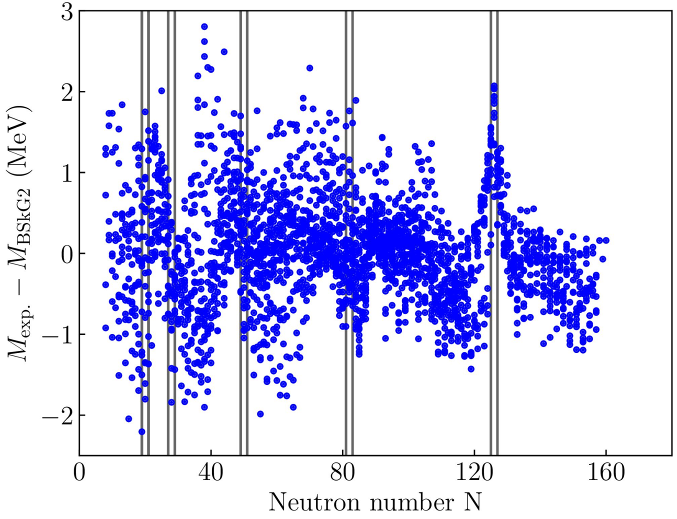
- fitted to 45 fission barriers
- includes spins, currents,...



BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation





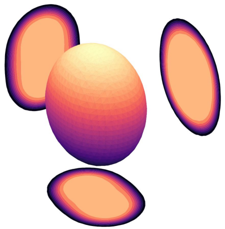
Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]			
Radii [fm]			
Prim. barriers [MeV]			
Secon. barriers [MeV]			
Fission isomers [MeV]			
Max. NS mass [$M_\odot$]			

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

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

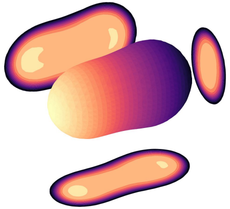
BSkG1 (2021)

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



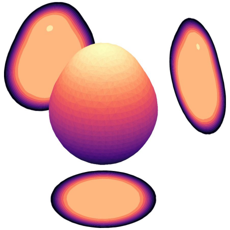
BSkG2 (2022)

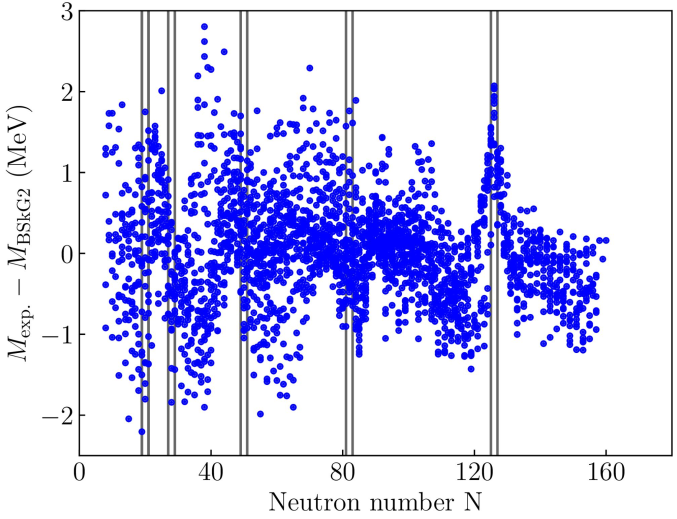
- fitted to 45 fission barriers
- includes spins, currents,...



BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation





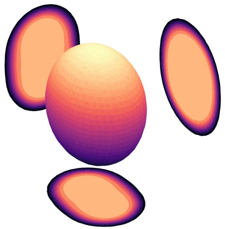
Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
Prim. barriers [MeV]			
Secon. barriers [MeV]			
Fission isomers [MeV]			
Max. NS mass [$M_\odot$]			

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

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

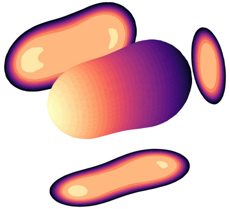
BSkG1 (2021)

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



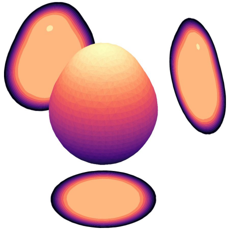
BSkG2 (2022)

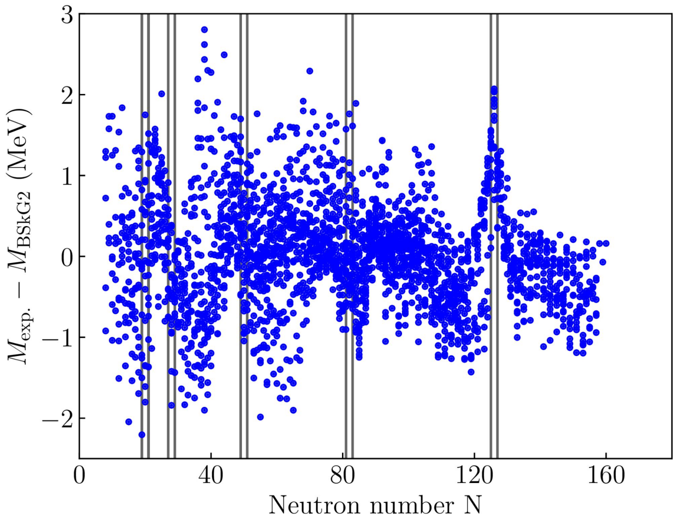
- fitted to 45 fission barriers
- includes spins, currents,...



BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation





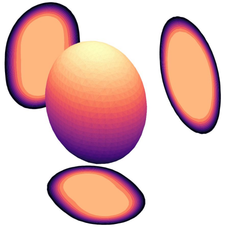
Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
Prim. barriers [MeV]	0.88	0.44	0.33
Secon. barriers [MeV]	0.87	0.47	0.51
Fission isomers [MeV]	1.0	0.49	0.34
Max. NS mass [$M_\odot$]			

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

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

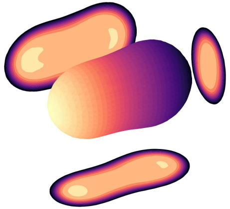
BSkG1 (2021)

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



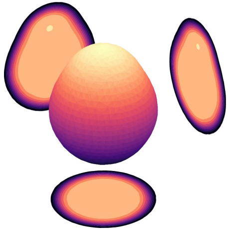
BSkG2 (2022)

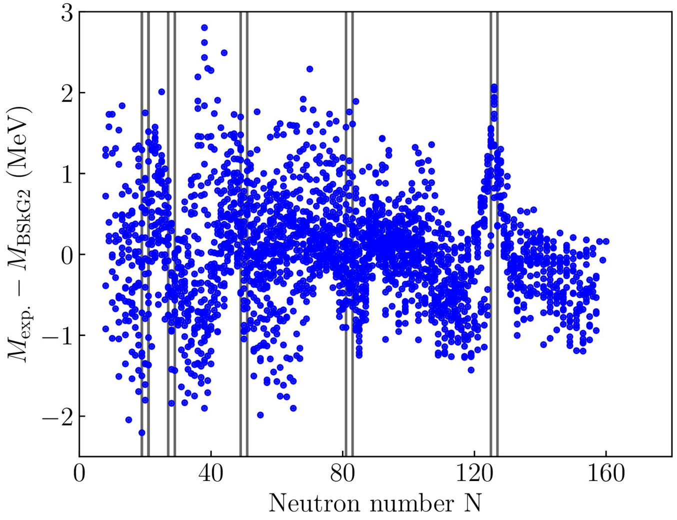
- fitted to 45 fission barriers
- includes spins, currents,...



BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation

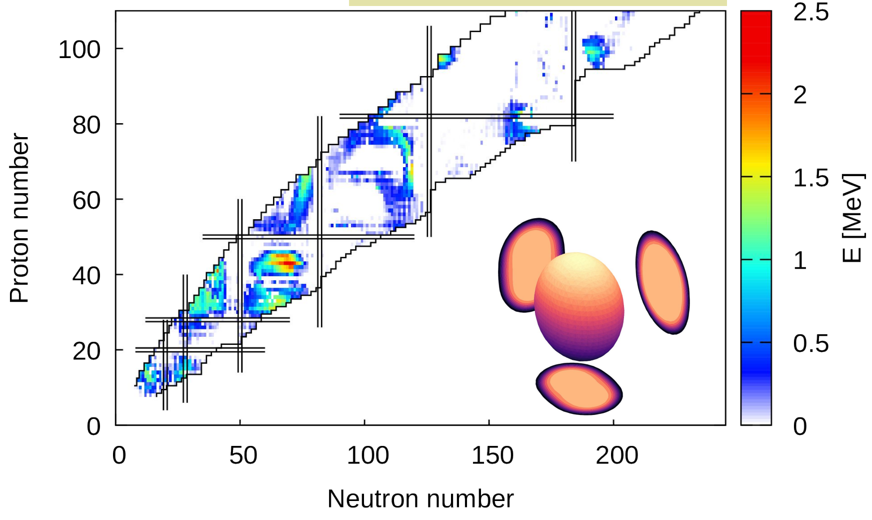




Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
Prim. barriers [MeV]	0.88	0.44	0.33
Secon. barriers [MeV]	0.87	0.47	0.51
Fission isomers [MeV]	1.0	0.49	0.34
Max. NS mass [$M_\odot$]	1.8	1.8	2.3

Masses

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

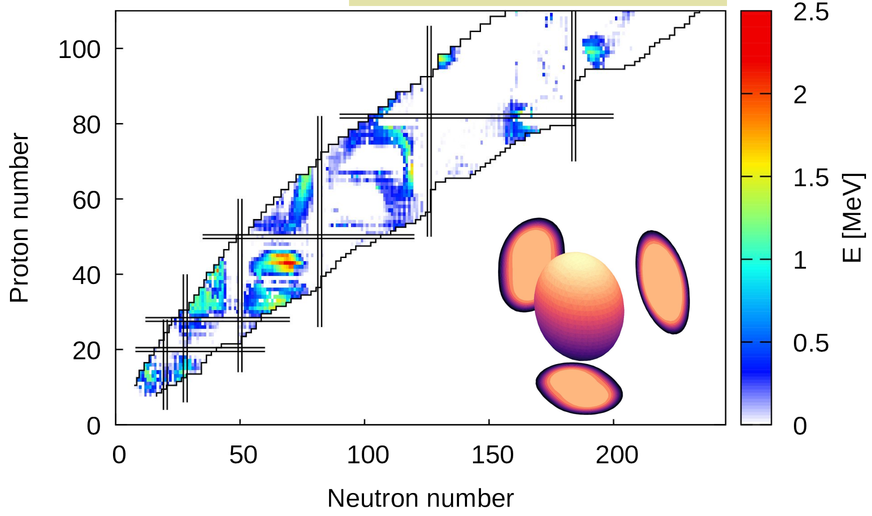


Triaxial deformation

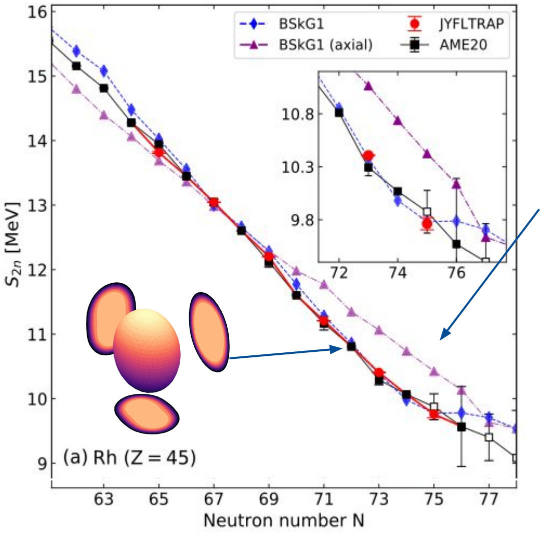
- many nuclei are affected
- effects up to 2.5 MeV near Z~44

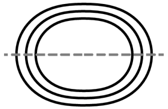
Masses

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



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



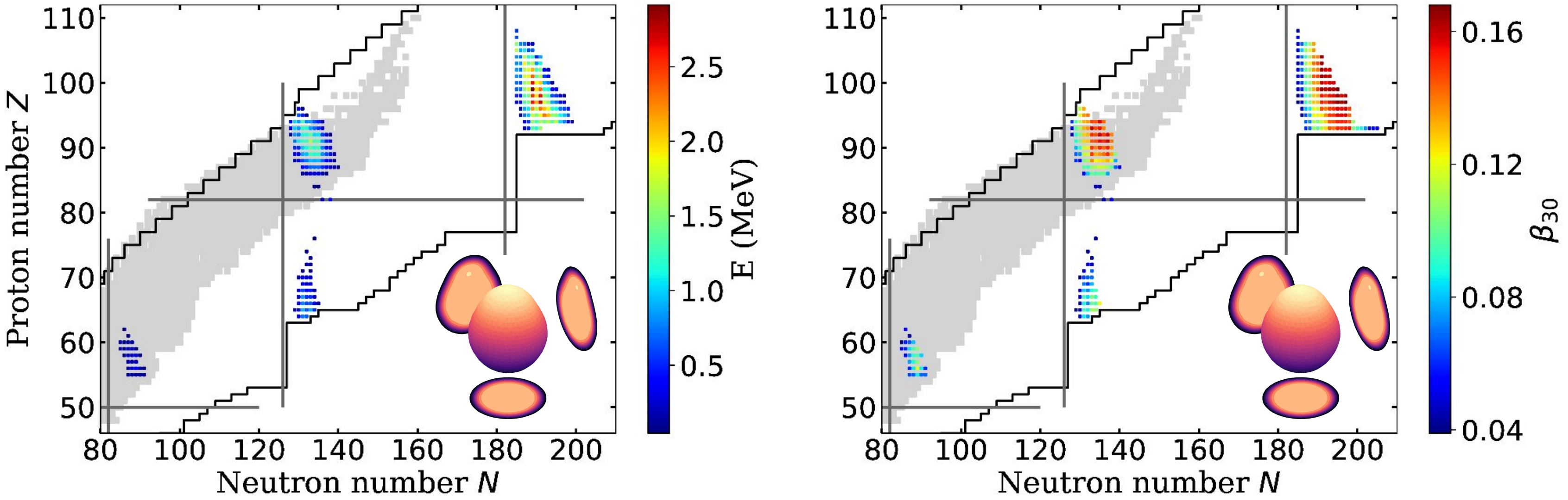


Triaxial deformation

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

Masses

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

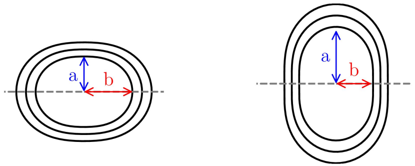


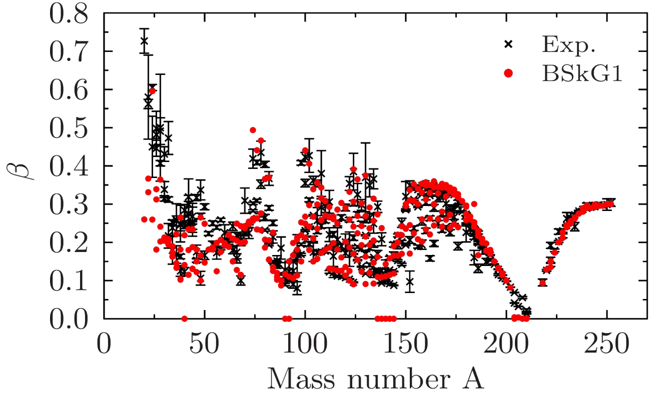
Reflection asymmetry

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

Deformations

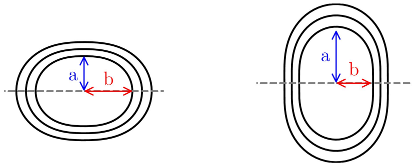
“Ordinary” quadrupole deformation

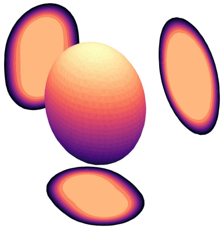


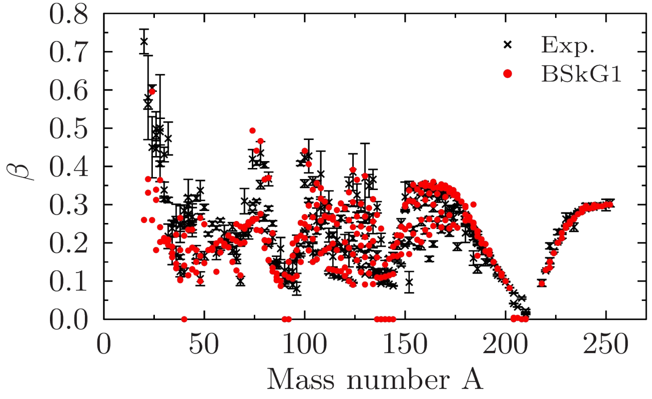


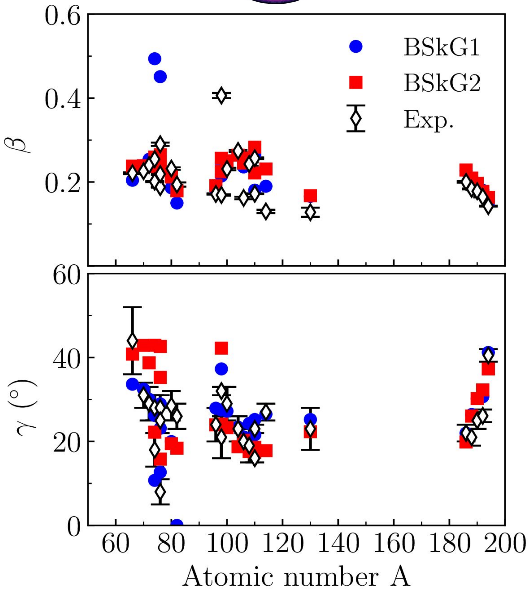
Deformations

“Ordinary” quadrupole deformation … and triaxial deformation …



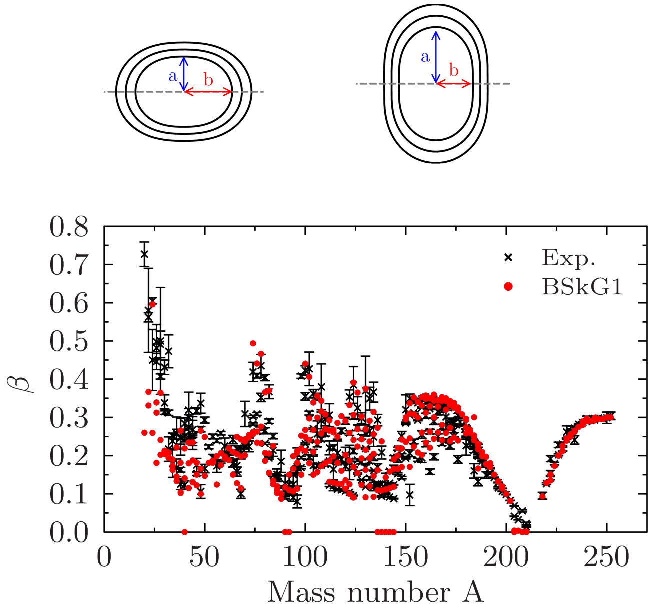




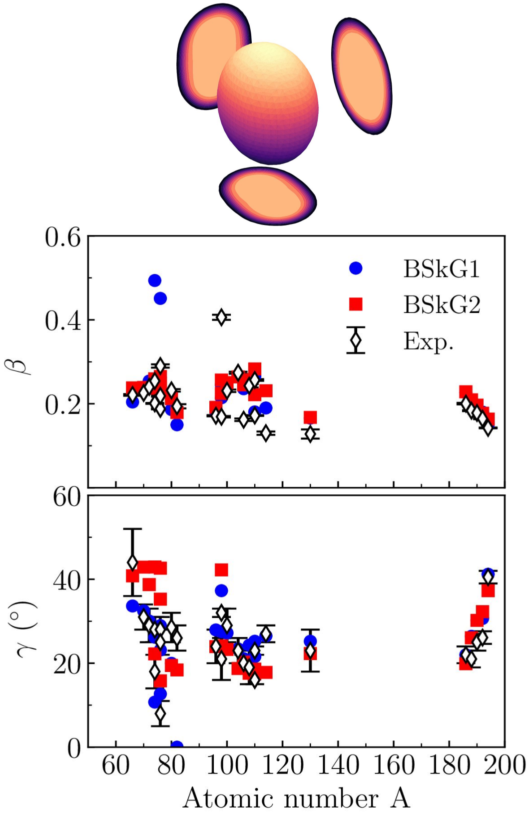


Deformations

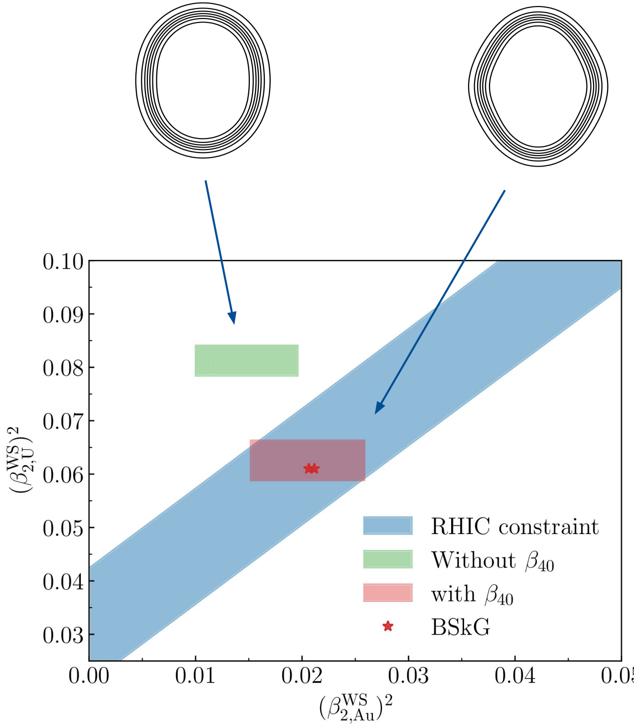
“Ordinary” quadrupole deformation



… and triaxial deformation …

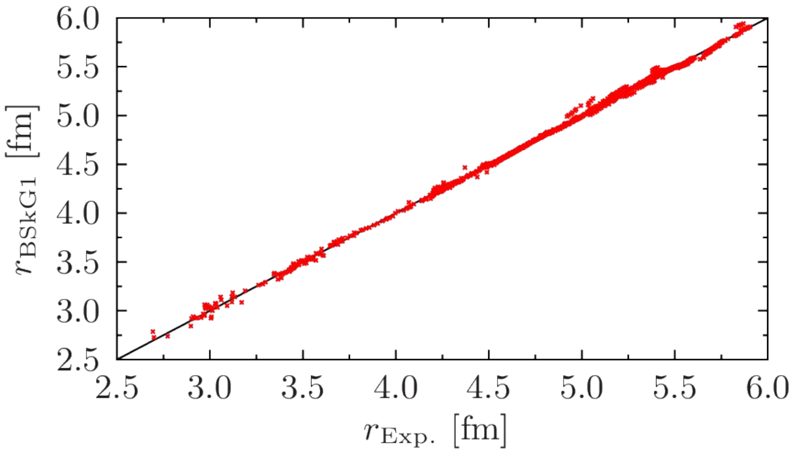


… and even hexadecapole!



W.R. et al., Phys. Rev. Lett. **130**, 212302 (2024)

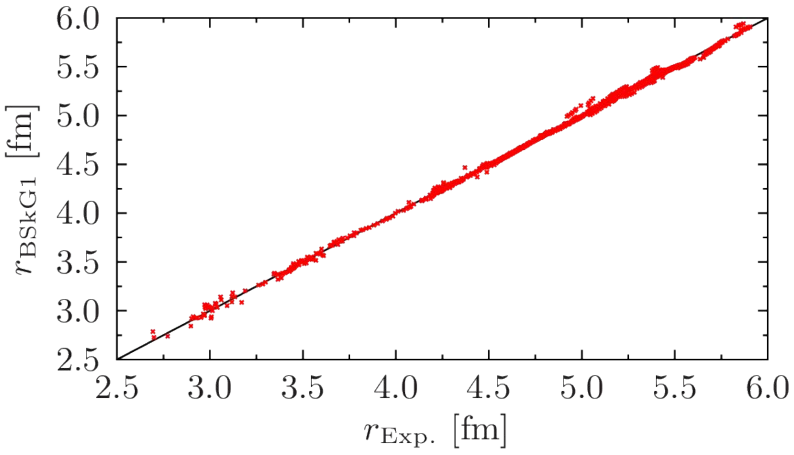
Radii

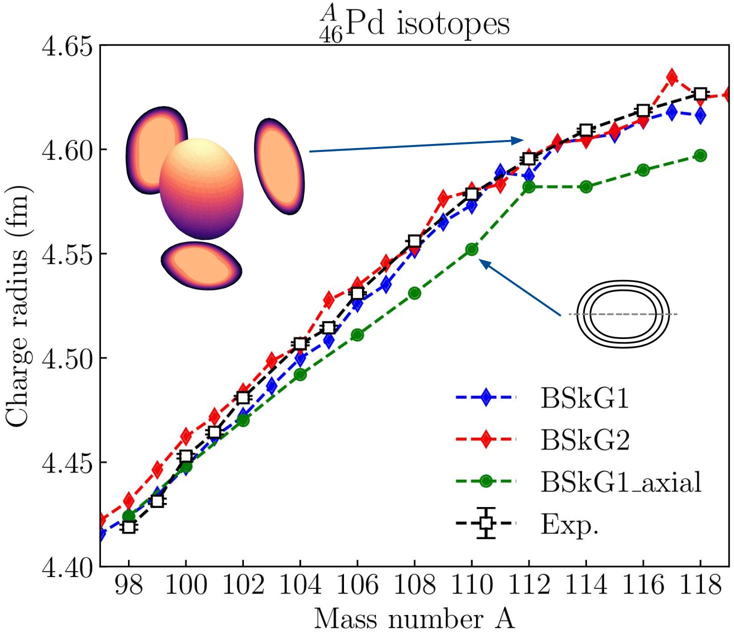


Systematics and details of charge radii

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

Radii





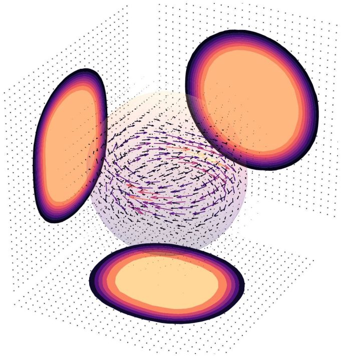
Systematics and details of charge radii

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

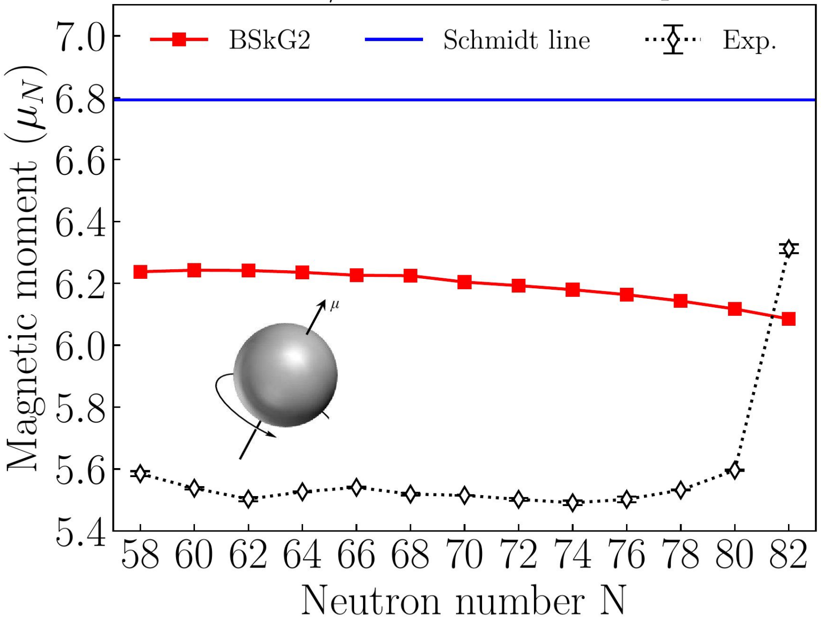
S. Geldhof, PRL **128**, 152501 (2022).
More data on Pd and Ru, coming by the ATLANTIS collaboration!

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).

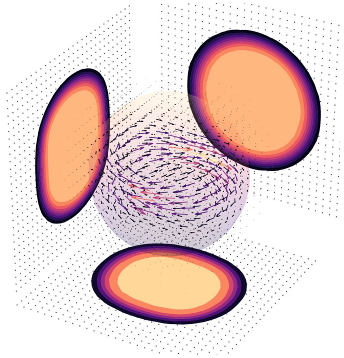


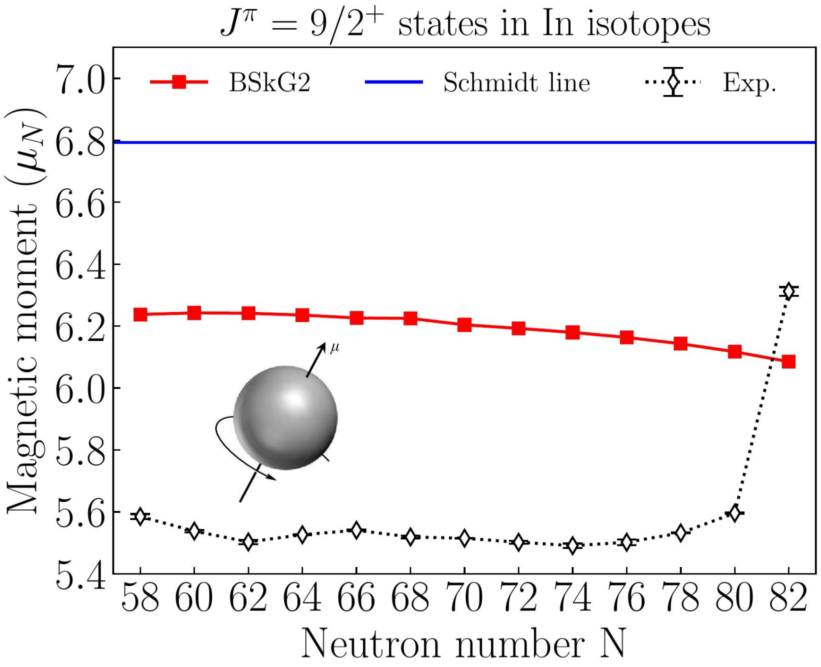
$J^{\pi} = 9/2^{+}$ states in In isotopes

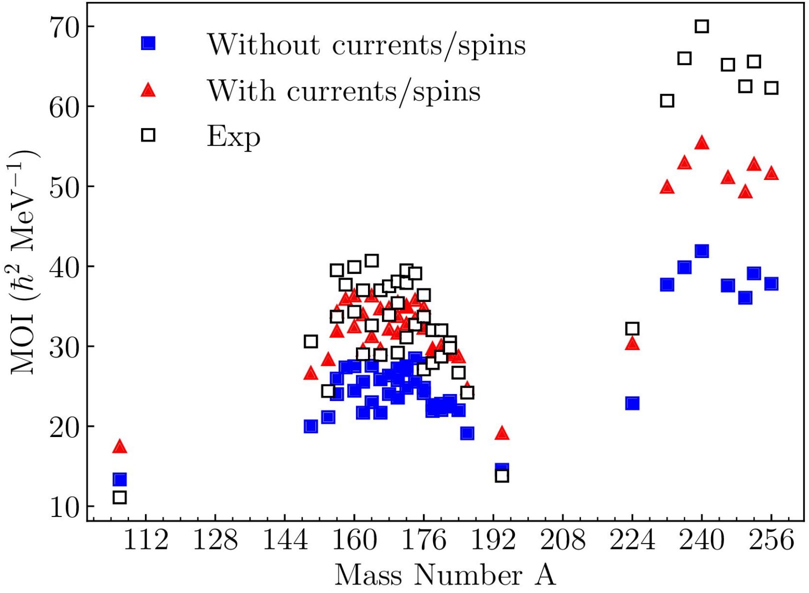


Additional observables

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).

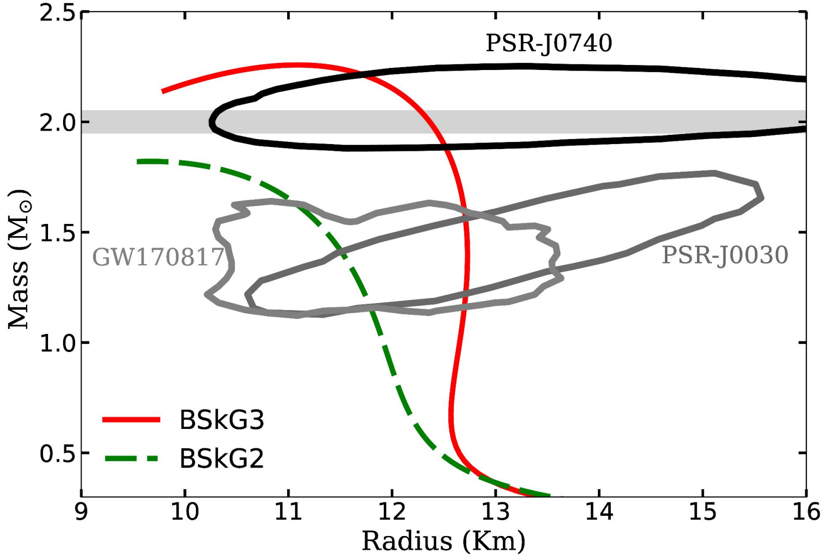






Neutron stars

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

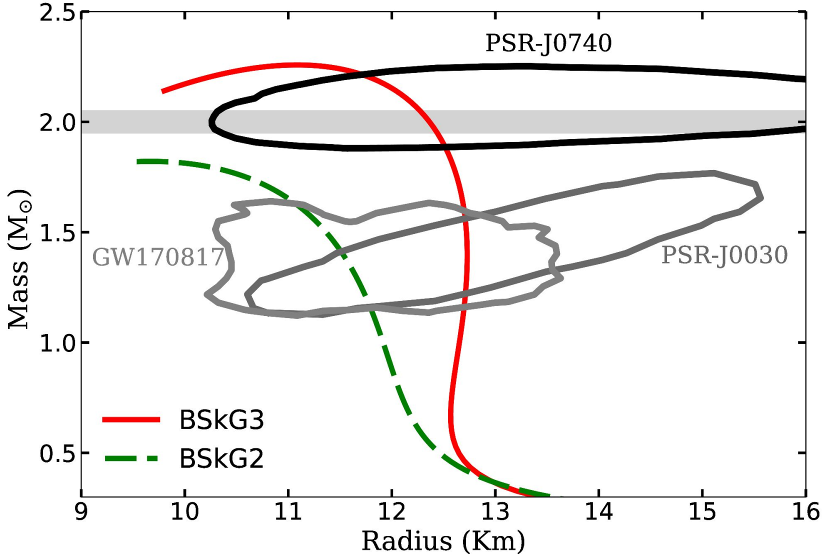


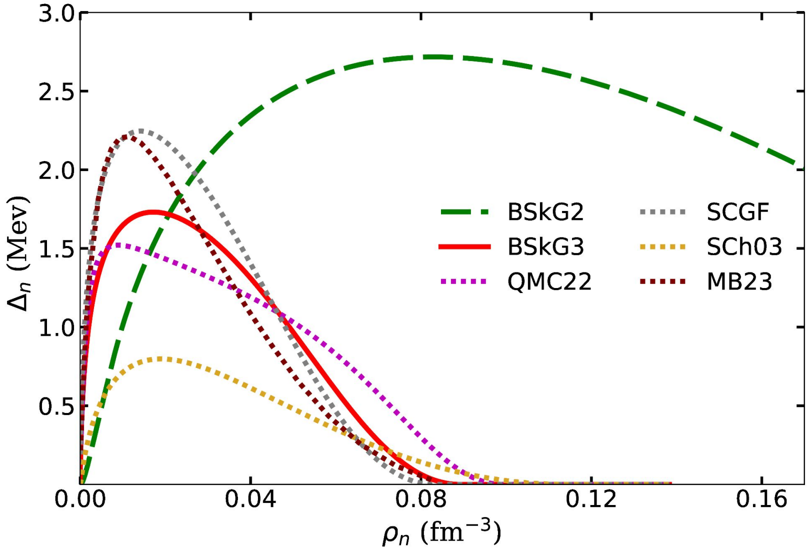
Stiffer EoS

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

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

Neutron stars





Stiffer EoS

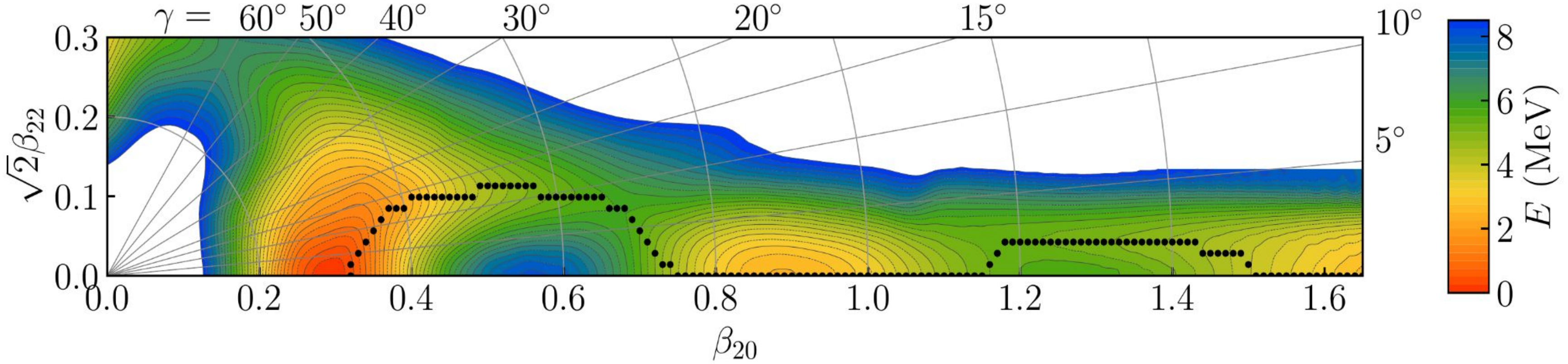
- results in higher maximum mass
- usually incompatible with masses
- we used additional ρ-dependencies

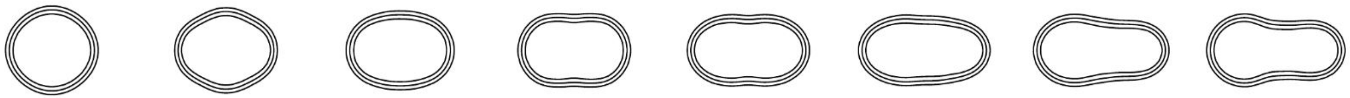
Realistic pairing gaps

- realistic pairing properties in INM
- constrained to advanced calculations

Fission barriers

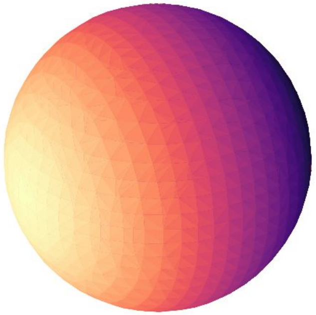
W. R. et al., EPJA **59**, 96 (2023).

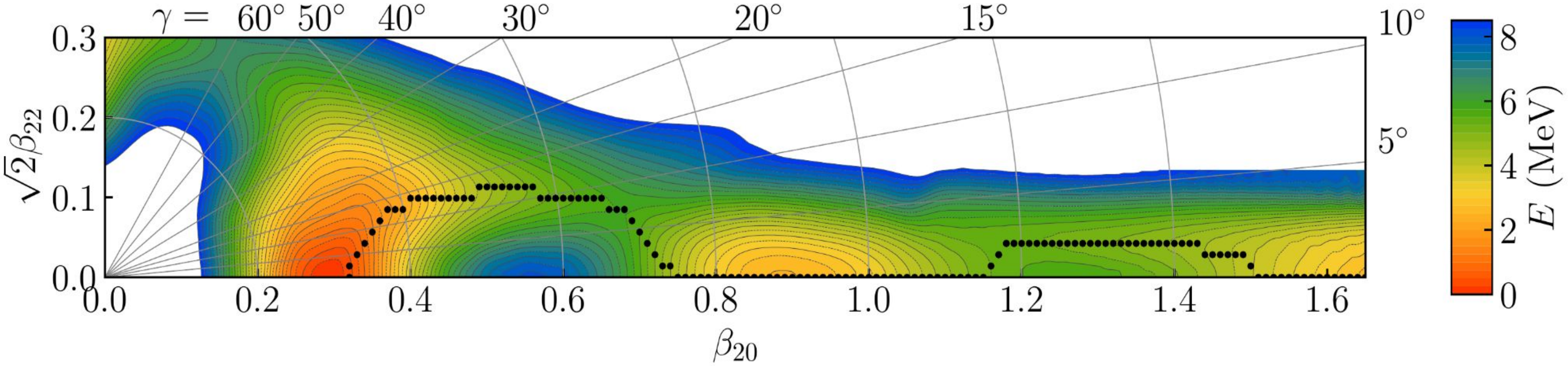


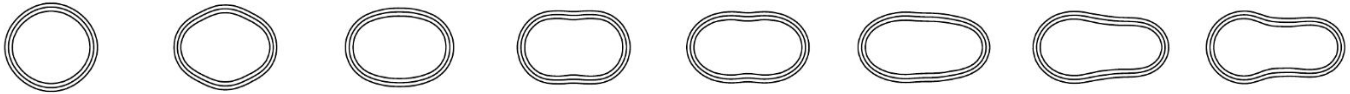


Fission barriers

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

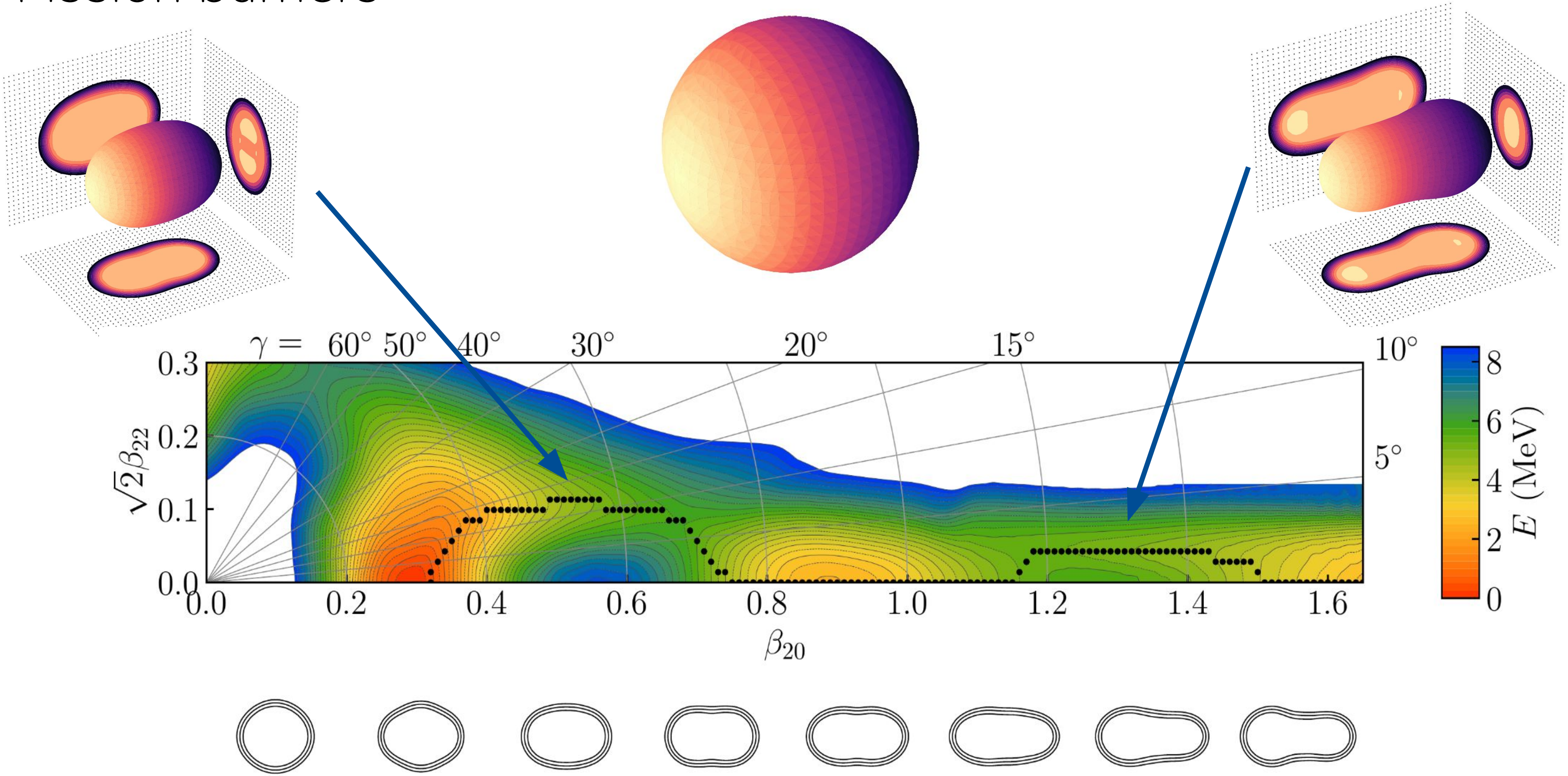






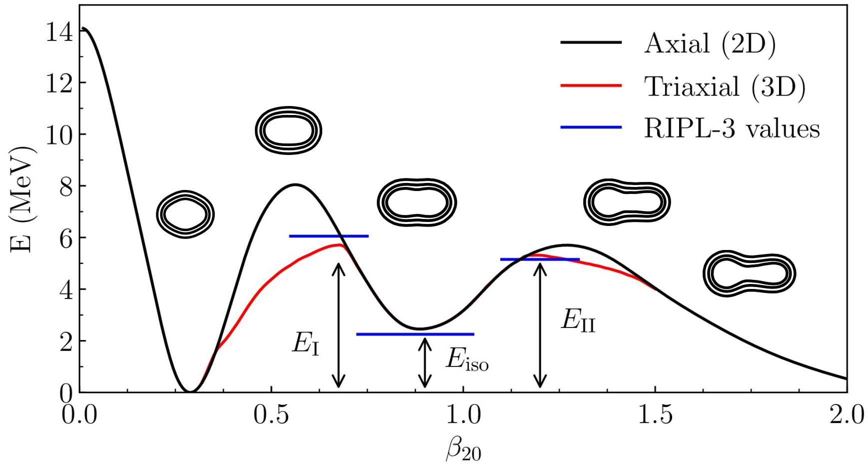
Fission barriers

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



Fission

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

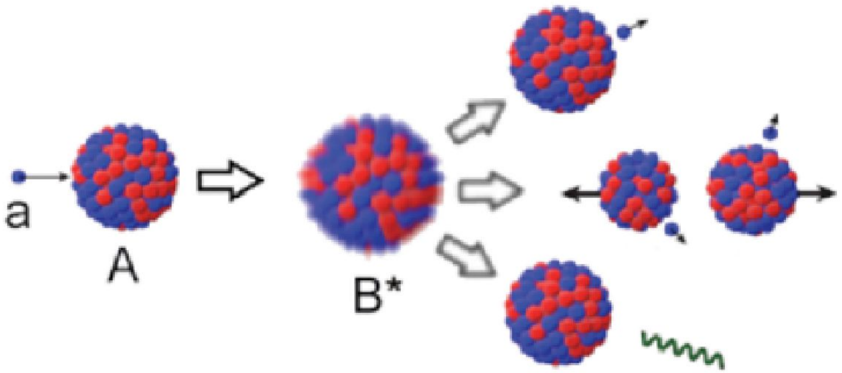


Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
Prim. barriers [MeV]	0.88	0.44	0.33
Secon. barriers [MeV]	0.87	0.47	0.51
Fission isomers [MeV]	1.0	0.49	0.34
Max. NS mass [$M_\odot$]	1.8	1.8	2.3

Fission properties of 45 actinide nuclei

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

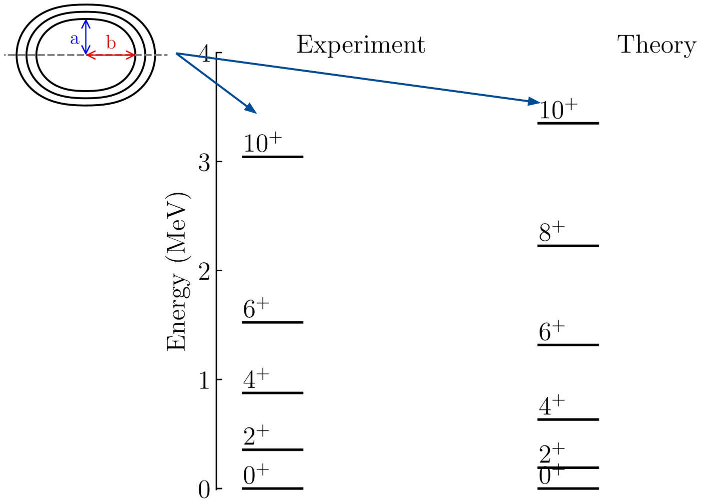
Nuclear level densities



Nuclear level densities

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

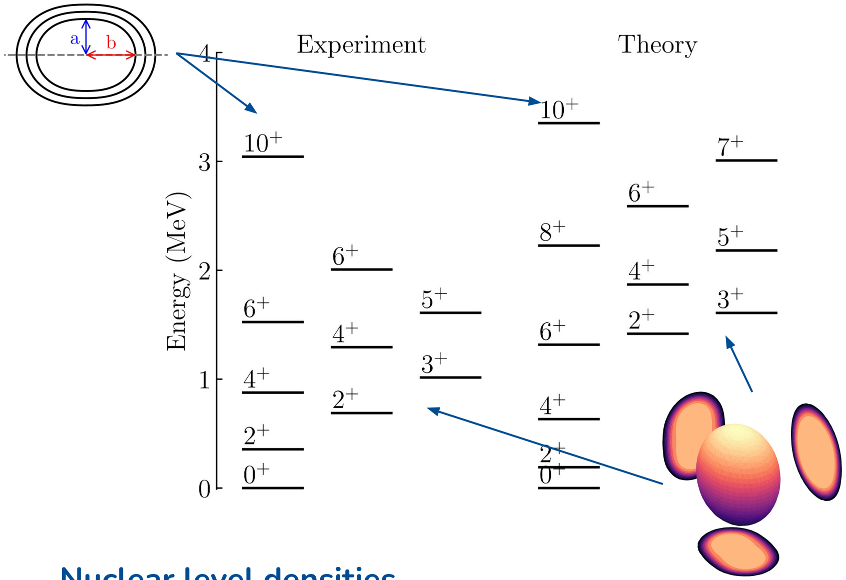
Nuclear level densities: ^{196}Pt



Nuclear level densities

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

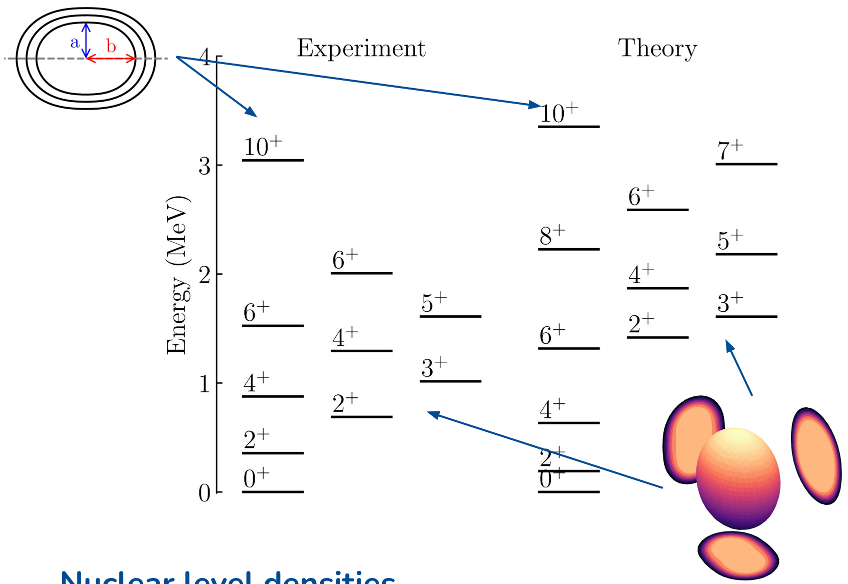
Nuclear level densities: ^{196}Pt

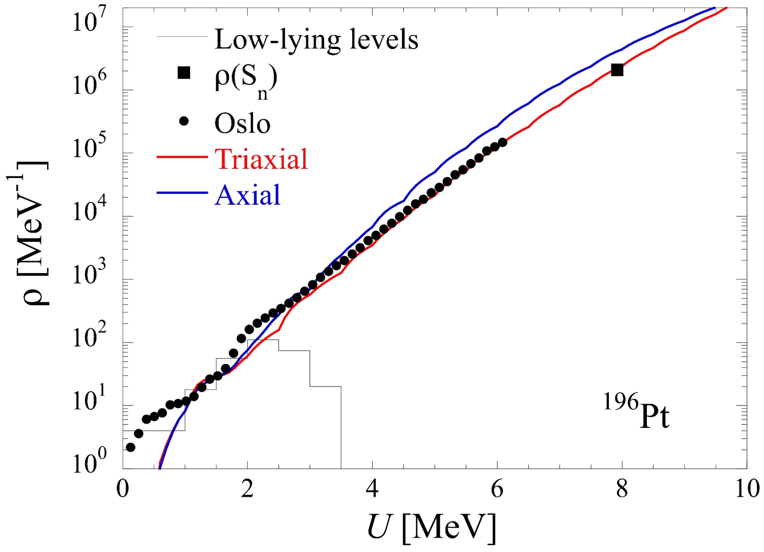


Nuclear level densities

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

Nuclear level densities: ^{196}Pt





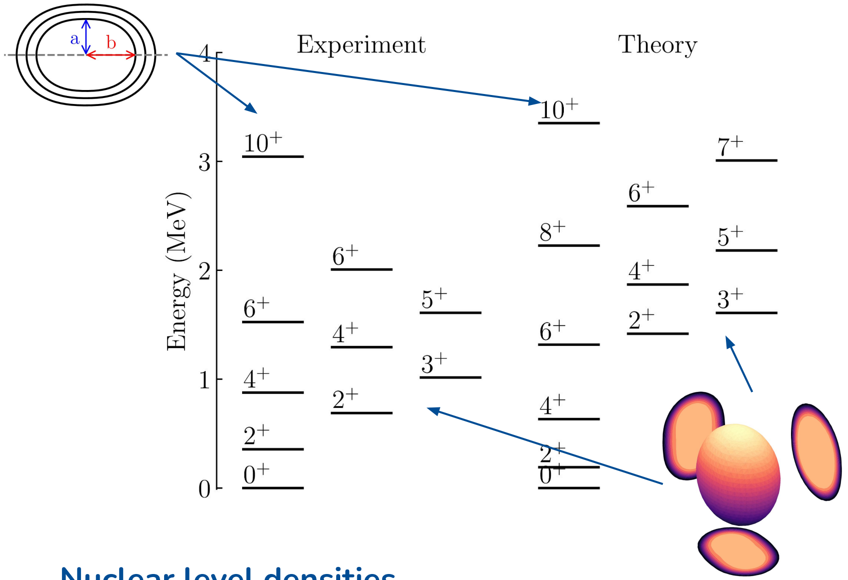
Nuclear level densities

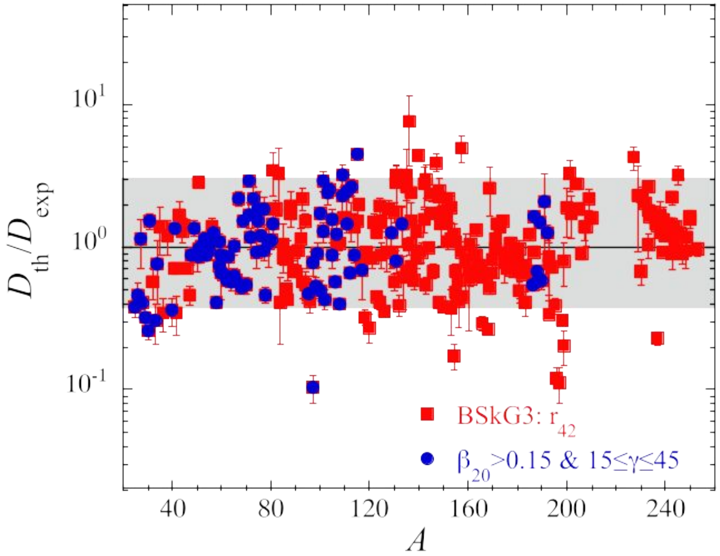
- required for **compound** reactions
- NLDs “count” phase-space
- **little** direct exp. information
- **symmetries** impact level structure

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

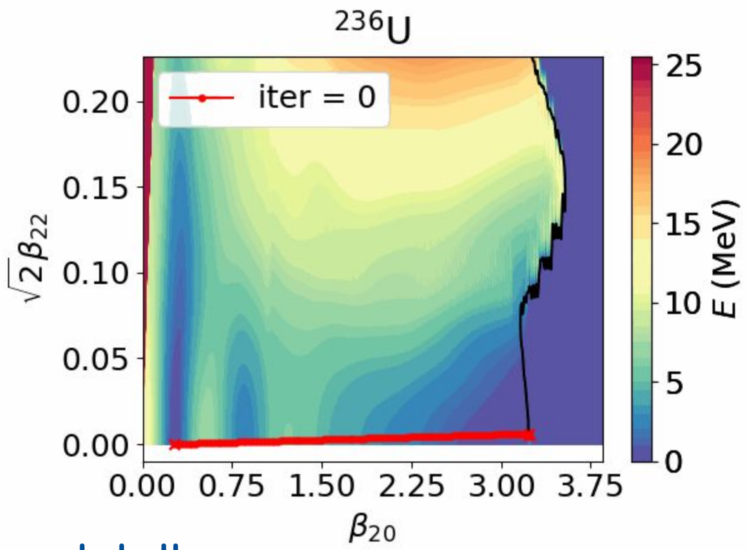
NLDs with BSkG3

- systematic inclusion of triaxiality
- good reproduction of data

W. Ryssens, A. Koning, S. Hilaire and S. Goriely, in preparation.

Large-scale application to fission

Work by Silvia Bara



Several challenges

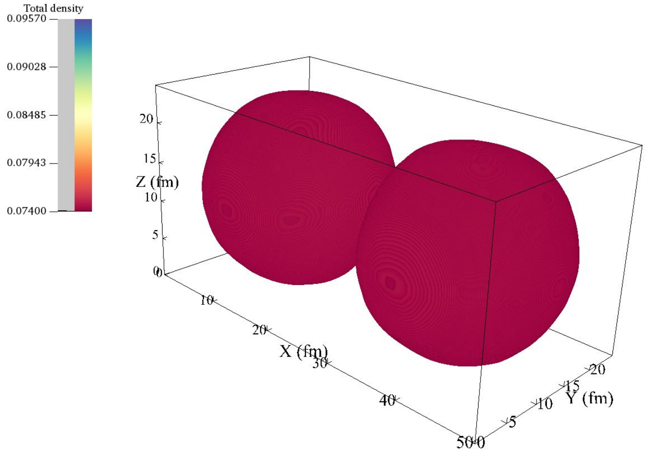
- get multi-D surfaces for 1000s of nuclei
- find the fission path on each surface
- estimate fission rates and yields

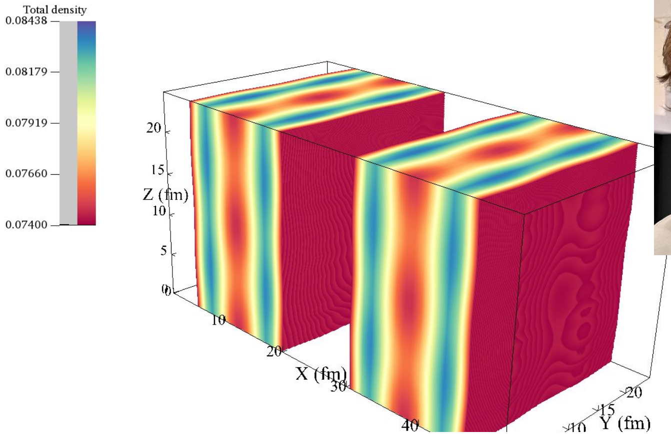
Towards a complete EoS with the BSkGs

Work by Nikolai Shchechilin

Towards a complete EoS with the BSkGs

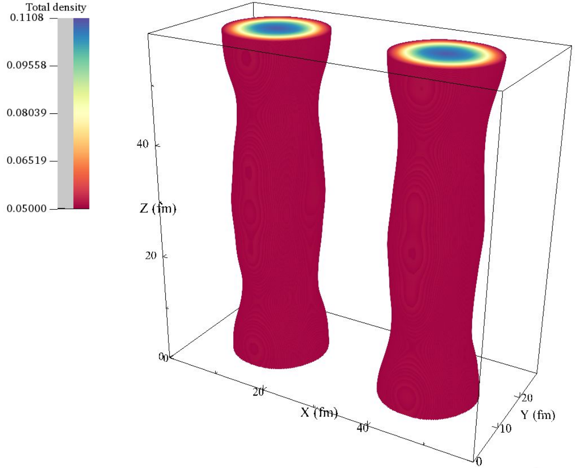
Work by Nikolai Shchechilin





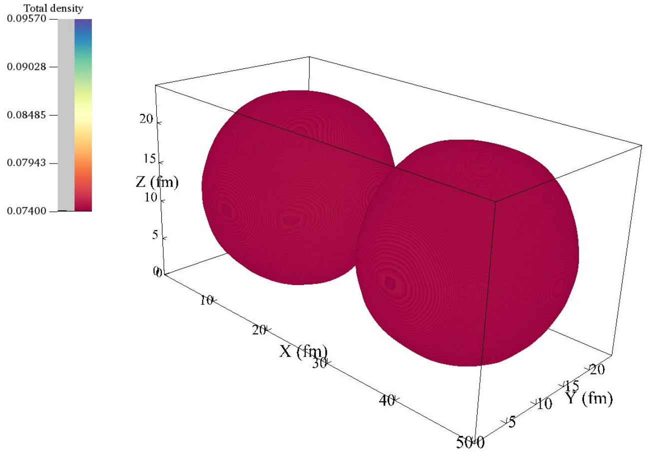
Nuclear pasta

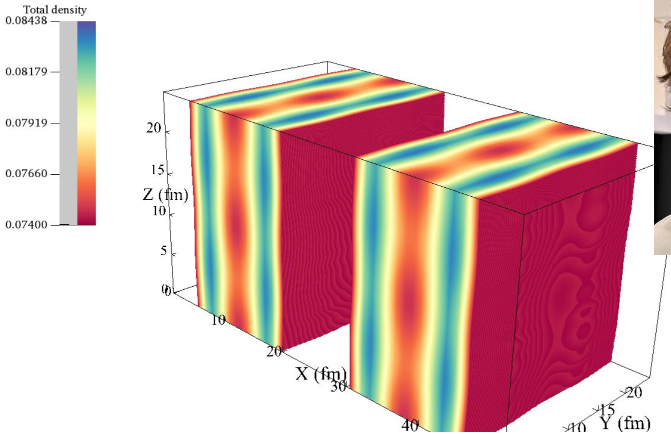
- crystalline structures in NS crust
- impact NS cooling and emitted GW



Towards a complete EoS with the BSkGs

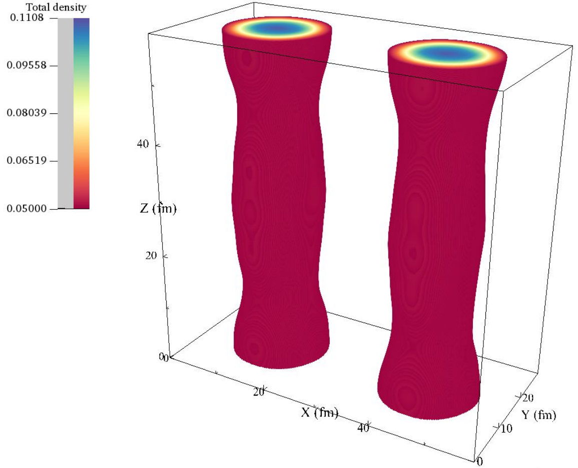
Work by Nikolai Shchechilin





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!



BSkG4

Work by Guilherme Grams

$$
\begin{aligned}
\mathcal{E}^{(0)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(0,1)}_{\mathrm{t,e}}\left(D^{1,1}_t\right)^2 + A^{(0,2)}_{\mathrm{t,e}}\left(D^{1,1}_0\right)^{\alpha}\left(D^{1,1}_t\right)^2\Big],\\
\mathcal{E}^{(2)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(2,1)}_{\mathrm{t,e}}D^{1,1}_t\left(\Delta D^{1,1}_t\right) + A^{(2,2)}_{\mathrm{t,e}}D^{1,1}_t D^{(\nabla,\nabla)}_t + A^{(2,3)}_{\mathrm{t,e}}\sum_{\mu\nu}C^{1,\nabla\sigma}_{t,\mu\nu}C^{1,\nabla\sigma}_{t,\mu\nu} + A^{(2,4)}_{\mathrm{t,e}}D^{1,1}_t\left(\nabla\cdot C^{1,\nabla\times\sigma}_t\right)\Big],\\
\mathcal{E}^{(4)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(4,1)}_{\mathrm{t,e}}\left(\Delta D^{1,1}_t\right)\left(\Delta D^{1,1}_t\right) + A^{(4,2)}_{\mathrm{t,e}}D^{1,1}_t D^{\Delta,\Delta}_t + A^{(4,3)}_{\mathrm{t,e}}D^{(\nabla,\nabla)}_t D^{(\nabla,\nabla)}_t\\
&\quad + A^{(4,4)}_{\mathrm{t,e}}\sum_{\mu\nu}D^{\nabla,\nabla}_{t,\mu\nu}D^{\nabla,\nabla}_{t,\mu\nu} + A^{(4,5)}_{\mathrm{t,e}}\sum_{\mu\nu}D^{\nabla,\nabla}_{t,\mu\nu}\left(\nabla_\mu\nabla_\nu D^{1,1}_t\right)\\
&\quad + A^{(4,6)}_{\mathrm{t,e}}\sum_{\mu\nu}C^{1,\nabla\sigma}_{t,\mu\nu}\left(\Delta C^{1,\nabla\sigma}_{t,\mu\nu}\right) + A^{(4,7)}_{\mathrm{t,e}}\sum_{\mu\nu\kappa}\left(\nabla_\mu C^{1,\nabla\sigma}_{t,\mu\kappa}\right)\left(\nabla_\nu C^{1,\nabla\sigma}_{t,\nu\kappa}\right) + A^{(4,8)}_{\mathrm{t,e}}\sum_{\mu\nu}C^{1,\nabla\sigma}_{t,\mu\nu}C^{\Delta,\nabla\sigma}_{t,\mu\nu}\Big],\\
\mathcal{E}^{(0)}_{\mathrm{Sk,o}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(0,1)}_{\mathrm{t,o}}\vec{D}^{1,\sigma}_t\cdot\vec{D}^{1,\sigma}_t + A^{(0,2)}_{\mathrm{t,o}}(D^{1,1}_0)^{\alpha}\,\vec{D}^{1,\sigma}_t\cdot\vec{D}^{1,\sigma}_t\Big],\\
\mathcal{E}^{(2)}_{\mathrm{Sk,o}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(2,1)}_{\mathrm{t,o}}\vec{D}^{1,\sigma}_t\cdot\left(\Delta\vec{D}^{1,\sigma}_t\right) + A^{(2,2)}_{\mathrm{t,o}}\vec{D}^{1,\sigma}_t\cdot\vec{D}^{(\nabla,\nabla)\sigma}_t + A^{(2,3)}_{\mathrm{t,o}}\vec{C}^{1,\nabla}_t\cdot\vec{C}^{1,\nabla}_t + A^{(2,4)}_{\mathrm{t,o}}\vec{D}^{1,\sigma}_t\cdot\left(\boldsymbol{\nabla}\times\vec{C}^{1,\nabla}_t\right)\Big],\\
\mathcal{E}^{(4)}_{\mathrm{Sk,o}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(4,1)}_{\mathrm{t,o}}\left(\Delta\vec{D}^{1,\sigma}_t\right)\cdot\left(\Delta\vec{D}^{1,\sigma}_t\right) + A^{(4,2)}_{\mathrm{t,o}}\vec{D}^{1,\sigma}_t\cdot\vec{D}^{\Delta,\Delta\sigma}_t + A^{(4,3)}_{\mathrm{t,o}}\vec{D}^{(\nabla,\nabla)\sigma}_t\cdot\vec{D}^{(\nabla,\nabla)\sigma}_t\\
&\quad + A^{(4,4)}_{\mathrm{t,o}}\sum_{\mu\nu\kappa}D^{\nabla,\nabla\sigma}_{\mu\nu\kappa}D^{\nabla,\nabla\sigma}_{\mu\nu\kappa} + A^{(4,5)}_{\mathrm{t,o}}\sum_{\mu\nu\kappa}D^{\nabla,\nabla\sigma}_{\mu\nu\kappa}\left(\nabla_\mu\nabla_\nu D^{1,\sigma}_\kappa\right),\\
&\quad + A^{(4,6)}_{\mathrm{t,o}}\vec{C}^{1,\nabla}_t\cdot\left(\Delta\vec{C}^{1,\nabla}_t\right) + A^{(4,7)}_{\mathrm{t,o}}\left(\boldsymbol{\nabla}\cdot\vec{C}^{1,\nabla}_t\right)\left(\boldsymbol{\nabla}\cdot\vec{C}^{1,\nabla}_t\right) + A^{(4,8)}_{\mathrm{t,o}}\vec{C}^{1,\nabla}_t\cdot\vec{C}^{\Delta,\nabla}_t\Big],
\end{aligned}
$$

N2LO EDF

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

BSkG4

Work by Guilherme Grams

$$
\begin{aligned}
\mathcal{E}^{(0)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(0,1)}_{\mathrm{t,e}}\left(D^{1,1}_t\right)^2 + A^{(0,2)}_{\mathrm{t,e}}\left(D^{1,1}_0\right)^{\alpha}\left(D^{1,1}_t\right)^2\Big], \\
\mathcal{E}^{(2)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(2,1)}_{\mathrm{t,e}}D^{1,1}_t\left(\Delta D^{1,1}_t\right) + A^{(2,2)}_{\mathrm{t,e}}D^{1,1}_t D^{(\nabla,\nabla)}_t + A^{(2,3)}_{\mathrm{t,e}}\sum_{\mu\nu} C^{1,\nabla\sigma}_{t,\mu\nu}C^{1,\nabla\sigma}_{t,\mu\nu} + A^{(2,4)}_{\mathrm{t,e}}D^{1,1}_t\left(\nabla\cdot C^{1,\nabla\times\sigma}_t\right)\Big], \\
\mathcal{E}^{(4)}_{\mathrm{Sk,e}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(4,1)}_{\mathrm{t,e}}\left(\Delta D^{1,1}_t\right)\left(\Delta D^{1,1}_t\right) + A^{(4,2)}_{\mathrm{t,e}}D^{1,1}_t D^{\Delta,\Delta}_t + A^{(4,3)}_{\mathrm{t,e}}D^{(\nabla,\nabla)}_t D^{(\nabla,\nabla)}_t \\
&\quad + A^{(4,4)}_{\mathrm{t,e}}\sum_{\mu\nu} D^{\nabla,\nabla}_{t,\mu\nu}D^{\nabla,\nabla}_{t,\mu\nu} + A^{(4,5)}_{\mathrm{t,e}}\sum_{\mu\nu} D^{\nabla,\nabla}_{t,\mu\nu}\left(\nabla_\mu\nabla_\nu D^{1,1}_t\right) \\
&\quad + A^{(4,6)}_{\mathrm{t,e}}\sum_{\mu\nu} C^{1,\nabla\sigma}_{t,\mu\nu}\left(\Delta C^{1,\nabla\sigma}_{t,\mu\nu}\right) + A^{(4,7)}_{\mathrm{t,e}}\sum_{\mu\nu\kappa}\left(\nabla_\mu C^{1,\nabla\sigma}_{t,\mu\kappa}\right)\left(\nabla_\nu C^{1,\nabla\sigma}_{t,\nu\kappa}\right) + A^{(4,8)}_{\mathrm{t,e}}\sum_{\mu\nu} C^{1,\nabla\sigma}_{t,\mu\nu}C^{\Delta,\nabla\sigma}_{t,\mu\nu}\Big], \\
\mathcal{E}^{(0)}_{\mathrm{Sk,o}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(0,1)}_{\mathrm{t,o}}\vec{D}^{1,\sigma}_t\cdot\vec{D}^{1,\sigma}_t + A^{(0,2)}_{\mathrm{t,o}}(D^{1,1}_0)^{\alpha}\,\vec{D}^{1,\sigma}_t\cdot\vec{D}^{1,\sigma}_t\Big], \\
\mathcal{E}^{(2)}_{\mathrm{Sk,o}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(2,1)}_{\mathrm{t,o}}\vec{D}^{1,\sigma}_t\cdot\left(\Delta\vec{D}^{1,\sigma}_t\right) + A^{(2,2)}_{\mathrm{t,o}}\vec{D}^{1,\sigma}_t\cdot\vec{D}^{(\nabla,\nabla)\sigma}_t + A^{(2,3)}_{\mathrm{t,o}}\vec{C}^{1,\nabla}_t\cdot\vec{C}^{1,\nabla}_t + A^{(2,4)}_{\mathrm{t,o}}\vec{D}^{1,\sigma}_t\cdot\left(\boldsymbol{\nabla}\times\vec{C}^{1,\nabla}_t\right)\Big], \\
\mathcal{E}^{(4)}_{\mathrm{Sk,o}}(\vec{r}) &= \sum_{t=0,1}\Big[A^{(4,1)}_{\mathrm{t,o}}\left(\Delta\vec{D}^{1,\sigma}_t\right)\cdot\left(\Delta\vec{D}^{1,\sigma}_t\right) + A^{(4,2)}_{\mathrm{t,o}}\vec{D}^{1,\sigma}_t\cdot\vec{D}^{\Delta,\Delta\sigma}_t + A^{(4,3)}_{\mathrm{t,o}}\vec{D}^{(\nabla,\nabla)\sigma}_t\cdot\vec{D}^{(\nabla,\nabla)\sigma}_t \\
&\quad + A^{(4,4)}_{\mathrm{t,o}}\sum_{\mu\nu\kappa} D^{\nabla,\nabla\sigma}_{\mu\nu\kappa}D^{\nabla,\nabla\sigma}_{\mu\nu\kappa} + A^{(4,5)}_{\mathrm{t,o}}\sum_{\mu\nu\kappa} D^{\nabla,\nabla\sigma}_{\mu\nu\kappa}\left(\nabla_\mu\nabla_\nu D^{1,\sigma}_\kappa\right), \\
&\quad + A^{(4,6)}_{\mathrm{t,o}}\vec{C}^{1,\nabla}_t\cdot\left(\Delta\vec{C}^{1,\nabla}_t\right) + A^{(4,7)}_{\mathrm{t,o}}\left(\boldsymbol{\nabla}\cdot\vec{C}^{1,\nabla}_t\right)\left(\boldsymbol{\nabla}\cdot\vec{C}^{1,\nabla}_t\right) + A^{(4,8)}_{\mathrm{t,o}}\vec{C}^{1,\nabla}_t\cdot\vec{C}^{\Delta,\nabla}_t\Big],
\end{aligned}
$$

N2LO EDF

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

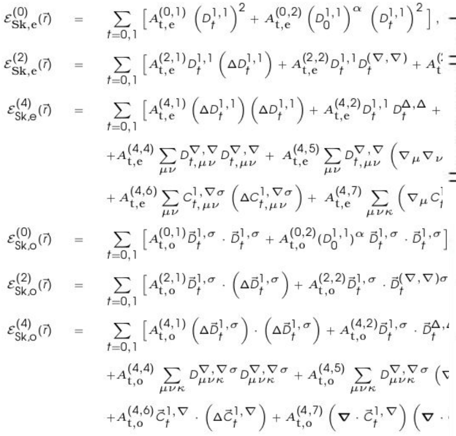
Advantages

- support heavy neutron stars
- less density dependencies
- T-dependent effective mass

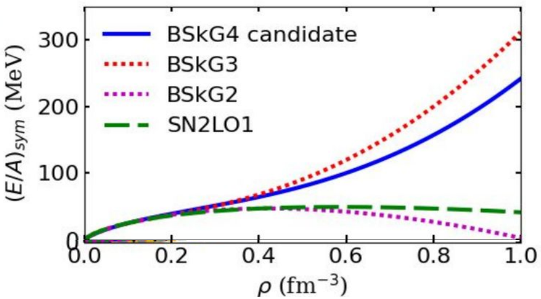
... all with **LESS** parameters!

BSkG4

Work by Guilherme Grams



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

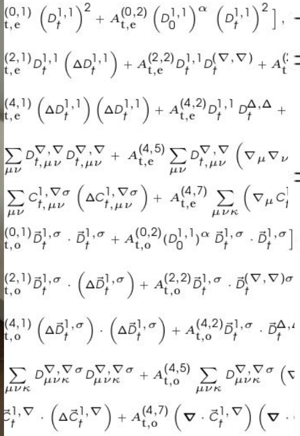
Advantages

- support heavy neutron stars
- less density dependencies
- T-dependent effective mass

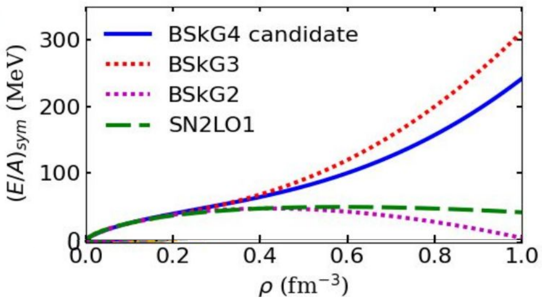
... all with **LESS** parameters!

BSkG4

Work by Guilherme Grams



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

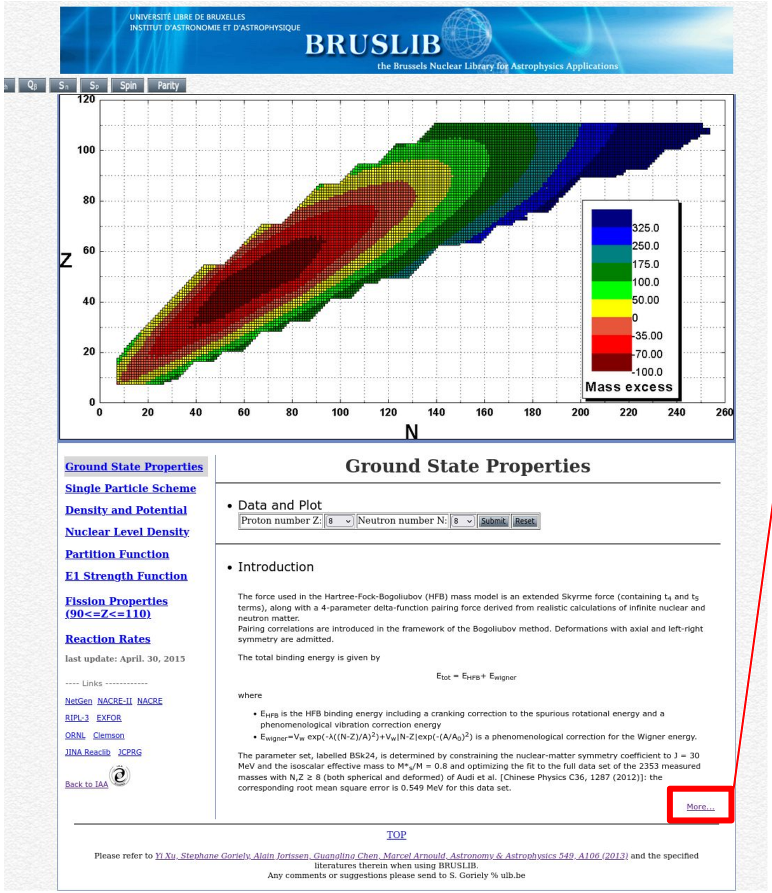
- **systematic** expansion in gradients
- next-to-next-to-leading order
- massively complicates the numerics

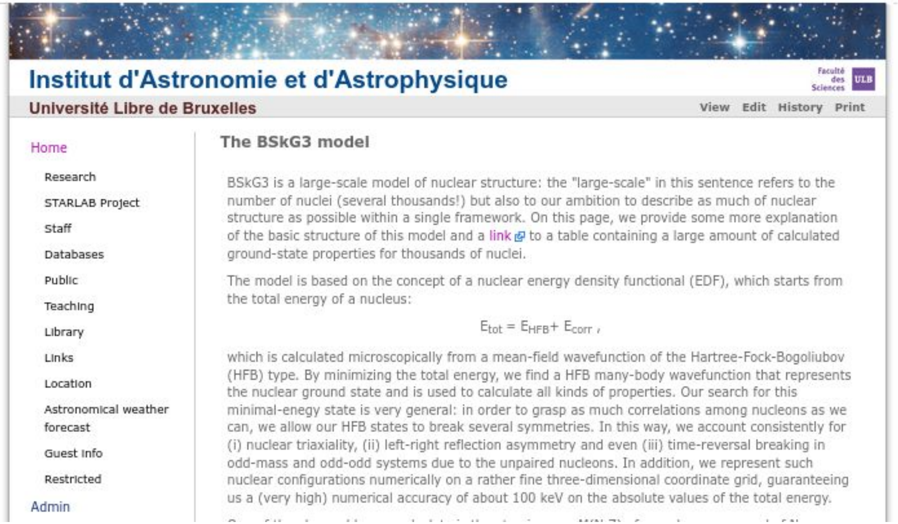
Advantages

- support heavy neutron stars
- less density dependencies
- T-dependent effective mass

... all with **LESS** parameters!

BRUSLIB: http://www.astro.ulb.ac.be/bruslib/





Available right now for BSkG3:

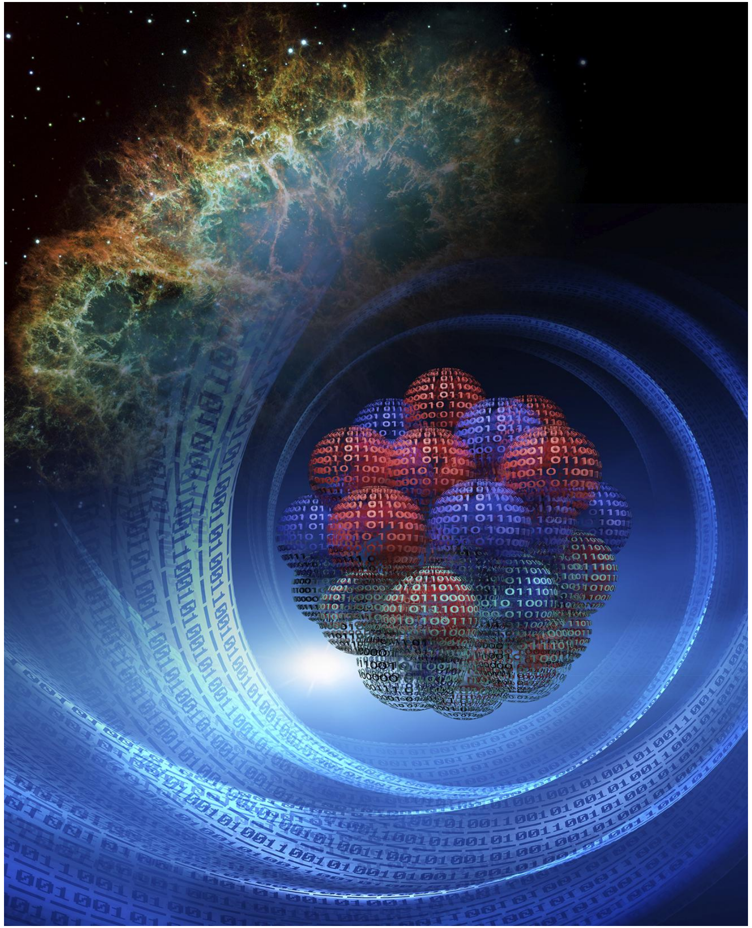
1. ground state properties for 7k nuclei
   a. masses
   b. deformations
   c. charge radii
   d. pairing properties
   e. rotational properties
2. Fission barriers for actinides

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.**



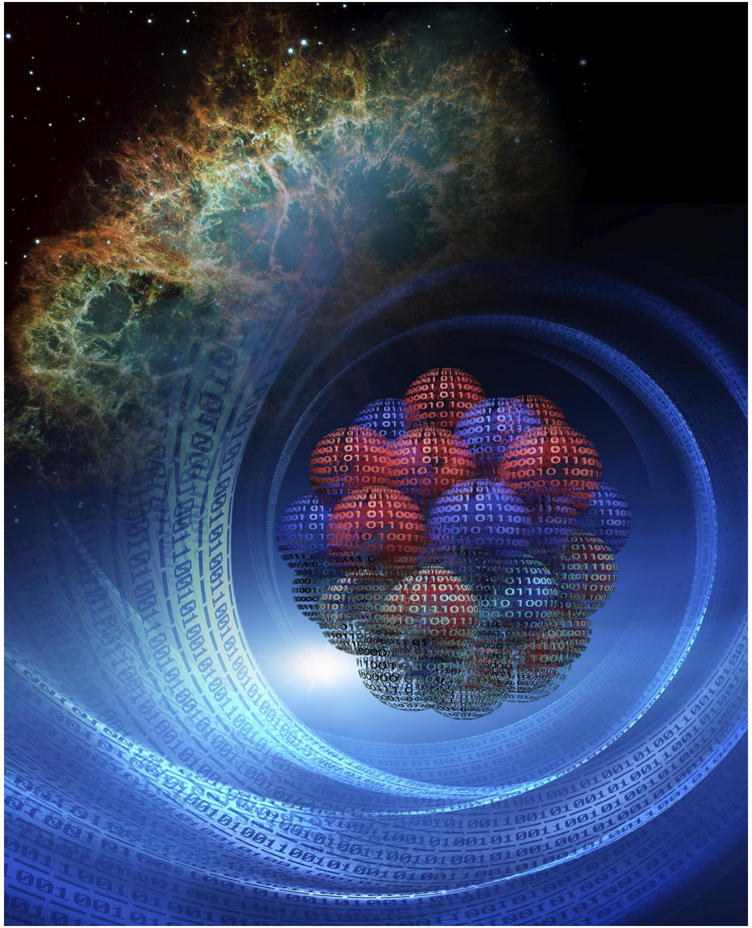
Conclusion

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.

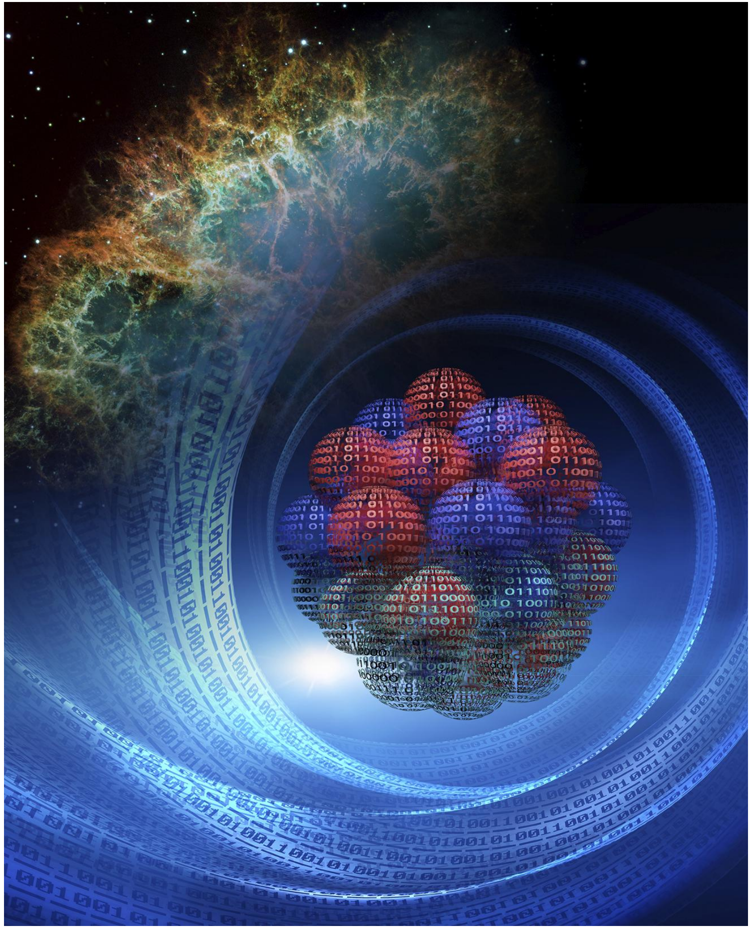
Large-scale = **thousands** of nuclei and **many observables.**
Microscopic = simple wave functions yet complex **symmetry breaking.**

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.**

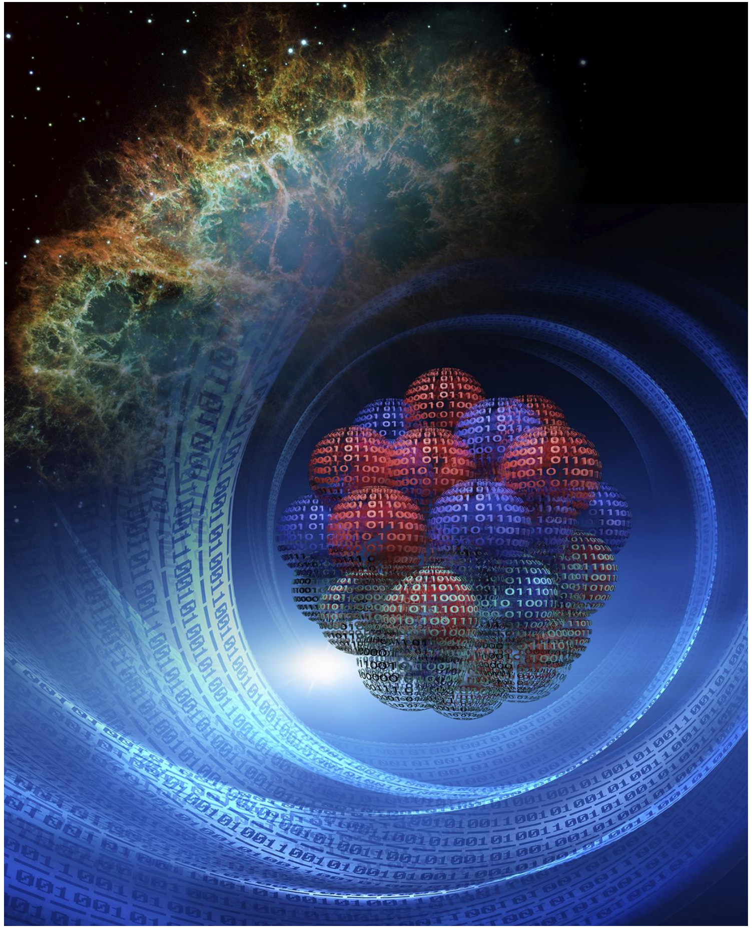
BSkG3

- 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. Shchechilin

S. Hilaire

M. Bender

S. Bara

and several experimental teams!

Thank you for...

...... all the wonderful work!

ULB

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

cea

S. Hilaire

iP2i LES 2 INFINIS LYON

M. Bender

KU LEUVEN

S. Bara

and several experimental teams!

...... the computing time!

CÉCI

EuroHPC Joint Undertaking

Cenaero

Thank you for…

…… all the wonderful work!

ULB

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

cea

S. Hilaire

iP2i LES 2 INFINIS LYON

M. Bender

KU LEUVEN

S. Bara

and several experimental teams!

…… the computing time!

CÉCI

EuroHPC Joint Undertaking

Cenaero

…… the funding!

fnrs LA LIBERTÉ DE CHERCHER

EOS THE EXCELLENCE OF SCIENCE

Thank you for...

...... all the wonderful work!

ULB

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

cea

S. Hilaire

iP2i
LES 2 INFINIS
LYON

M. Bender

KU LEUVEN

S. Bara

and several experimental teams!

...... the computing time!

CÉCI

EuroHPC
Joint Undertaking

Cenaero

...... the funding!

fnrs
LA LIBERTÉ DE CHERCHER

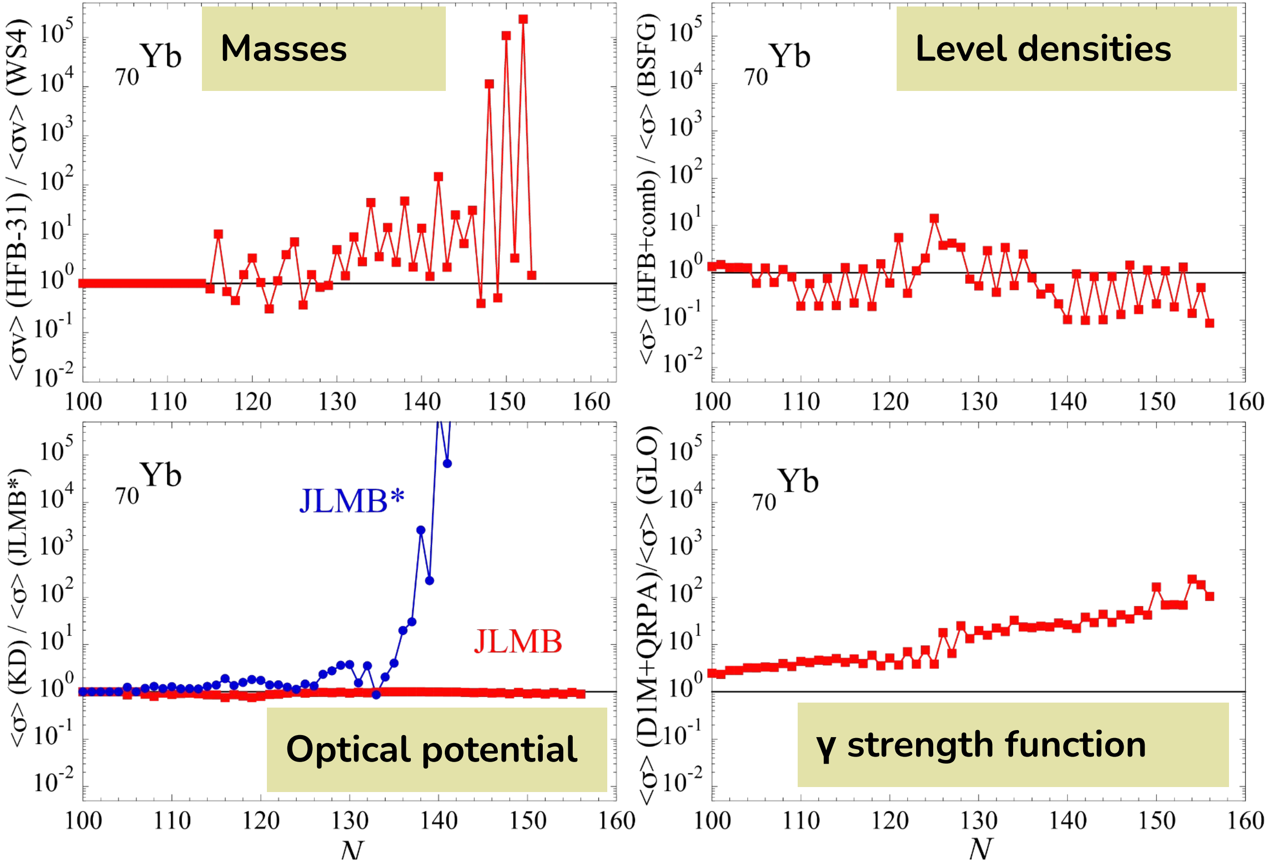
EOS
THE EXCELLENCE
OF SCIENCE

...... your attention!

Bonus!

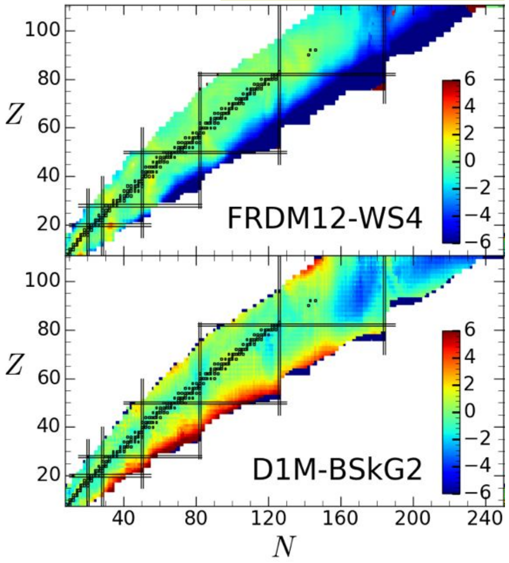
Models can make all the difference…

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

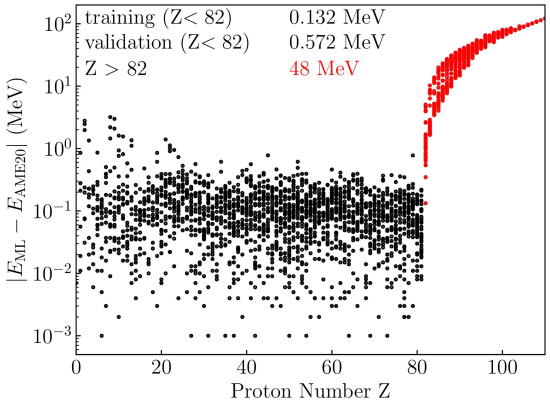


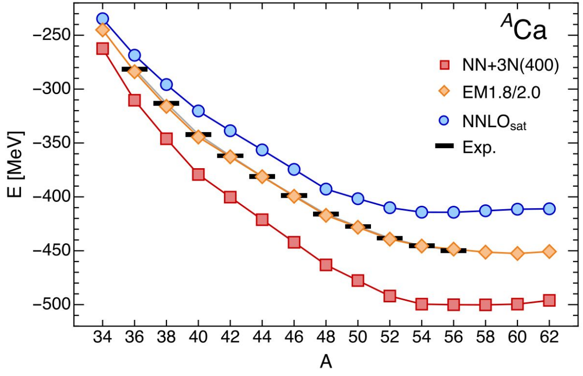
Interlude: why do we do these complex things?

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)