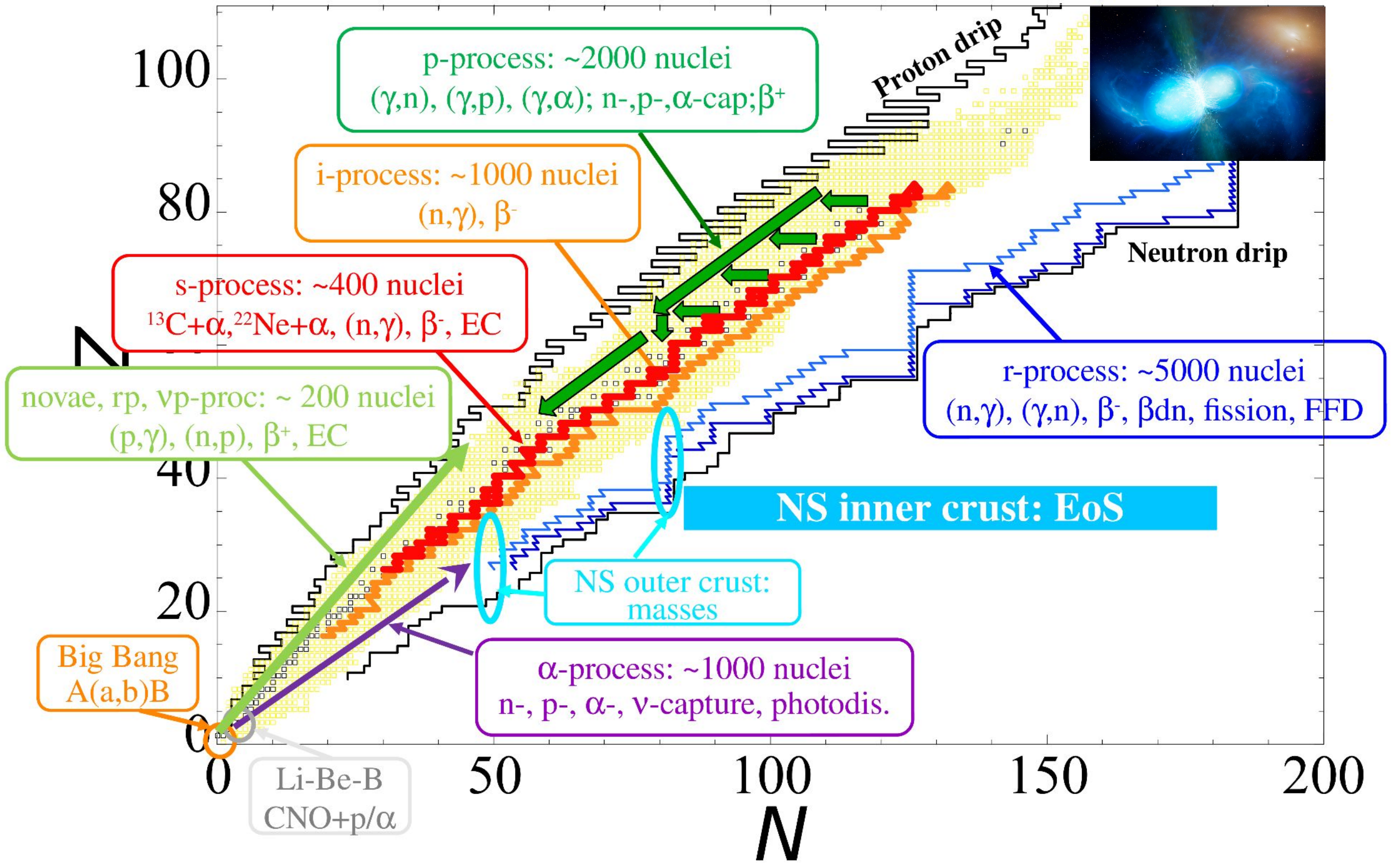

# Nuclear deformation in Brussels Skyrme EDF models

*Pepijn Demol*

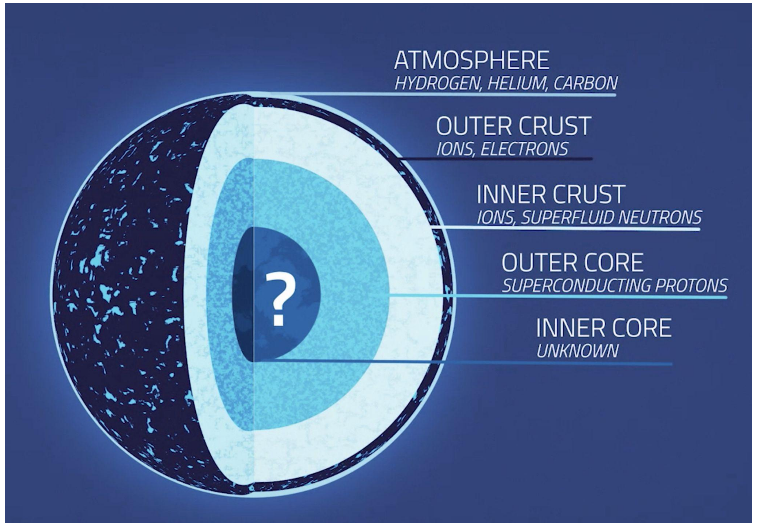
*Hirschegg, Challenges in effective field theory description of nuclei*

*18-24 January 2026*

## Nucleosynthesis

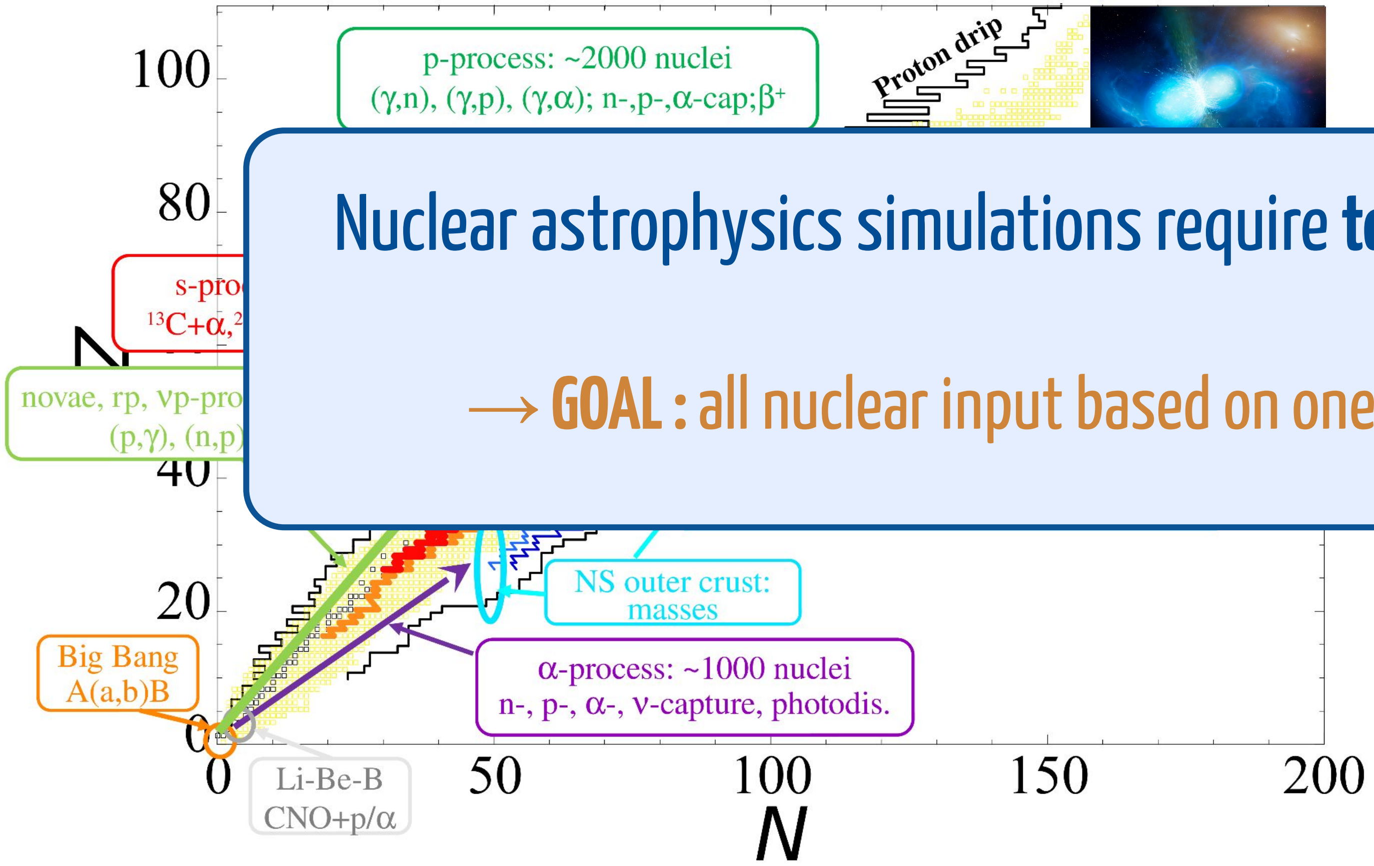


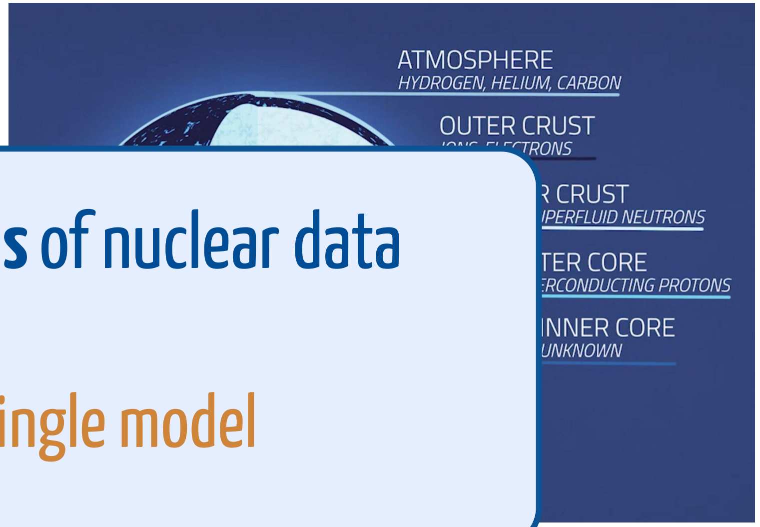

## Neutron stars



## Nucleosynthesis

## Neutron stars




Nuclear astrophysics simulations require **tons** of nuclear data

→ **GOAL :** all nuclear input based on one single model

# Skyrme energy density functional (EDF) theory

Coupling constants to be fitted to data

$$E_{\text{Skyrme}}[\rho] \sim \int d^3\mathbf{r}\, \left[ C^\rho \rho(\mathbf{r})\rho(\mathbf{r}) + C^\tau \tau(\mathbf{r})\rho(\mathbf{r}) + C^\gamma \rho(\mathbf{r})^\gamma \rho(\mathbf{r})\rho(\mathbf{r}) + \cdots \right]$$

Local densities and currents of the wavefunction

$$\min_{\rho} E_{\text{tot}} = E_{\text{Skyrme}} + E_{\text{kin}} + E_{\text{Coul}} + E_{\text{pair}} + E_{\text{cm}}^{(1)} + E_{\text{cm}}^{(2)} + E_{\text{rot}} + E_{\text{W}}$$

Included in mean-field

Corrections treated semi-variationally

Set of trial wavefunctions:
**Mean-field** states = Slater determinant + **symmetry breaking**
$\longrightarrow$ solving the **Hartree-Fock(-Bogoliubov)** problem

# Skyrme energy density functional (EDF) theory

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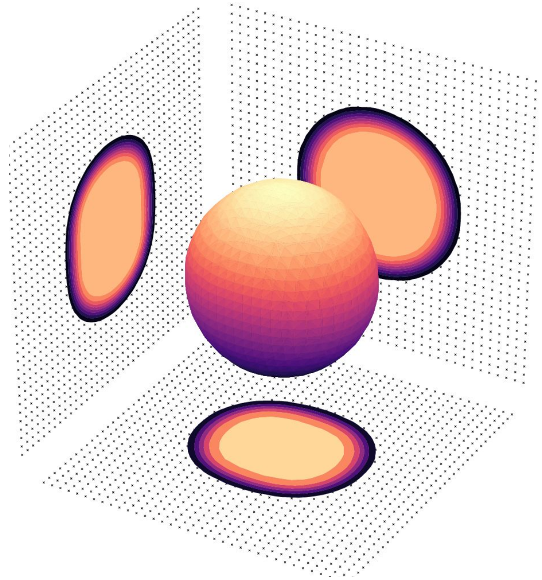
$\longrightarrow$ solving the **Hartree-Fock(-Bogoliubov)** problem

+ Wavefunction with individual nucleons
+ Feasible for 1000s of nuclei (incl. odds)
+ Many observables accessible

− Unclear how to improve functional form
− Lack of systematic uncertainty quantification

# Brussels-Skyrme-on-a-Grid: BSkG



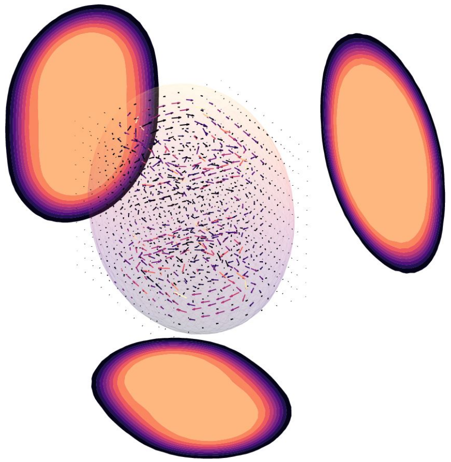
- 3D representation agnostic wrt shape
- shape DOF characterized by multipole moment
- Symmetry breaking enlarges variational space

⟶ captures collective correlations at modest CPU cost
⟶ BUT loss of quantum numbers

# Brussels-Skyrme-on-a-Grid: BSkG

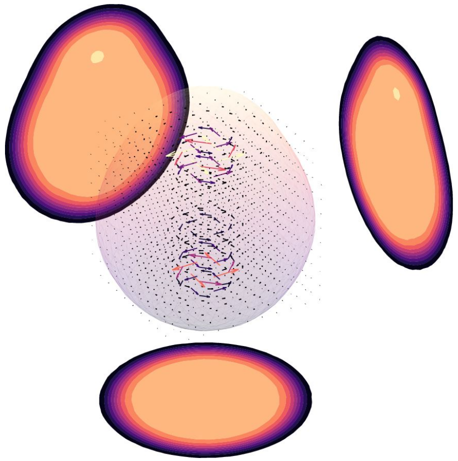
**Triaxial**

$\beta_{20}, \beta_{22}$ or $\beta_2, \gamma$



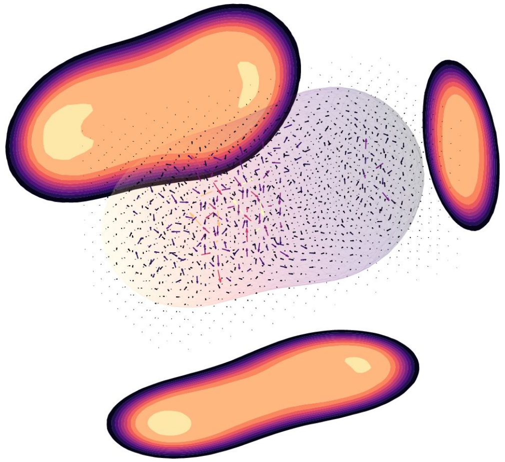
**Octupole**

$\beta_{20}, \beta_{30}$



**Triaxial + octupole**

$\beta_{20}, \beta_{22}$ **and** $\beta_{30}$



$+ \cdots$

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- shape DOF characterized by multipole moment
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BLU-ULB BRUSSELS LABORATORY OF THE UNIVERSE ULB fnrs FREEDOM TO RESEARCH

BSkG1: G. Scamps et al., EPJA **57**, 333 (2021).

# Brussels-Skyrme-on-a-Grid: BSkG

## BSkG1

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

| Rms $\sigma$ | BSkG1 | BSkG2 | BSkG3 | BSkG4 | BSkG5 |
|---|---|---|---|---|---|
| Masses [MeV] | 0.741 | | | | |
| $S_n$ [MeV] | 0.466 | | | | |
| Radii [fm] | 0.024 | | | | |
| Prim. barriers [MeV] | 0.88 | | | | |
| Sec. barriers [MeV] | 0.87 | | | | |
| Fission isomers [MeV] | 1.0 | | | | |
| Max. NS mass [$M_\odot$] | 1.8 | | | | |

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# Brussels-Skyrme-on-a-Grid: BSkG

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## BSkG2

- complete time-reversal breaking
- fit to 45 reference fission barriers
  + 28 fission isomers

| Rms $\sigma$ | BSkG1 | BSkG2 | BSkG3 | BSkG4 | BSkG5 |
|---|---|---|---|---|---|
| Masses [MeV] | 0.741 | 0.678 | | | |
| $S_n$ [MeV] | 0.466 | 0.500 | | | |
| Radii [fm] | 0.024 | 0.027 | | | |
| Prim. barriers [MeV] | 0.88 | 0.44 | | | |
| Sec. barriers [MeV] | 0.87 | 0.47 | | | |
| Fission isomers [MeV] | 1.0 | 0.49 | | | |
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# Brussels-Skyrme-on-a-Grid: BSkG

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|---|---|---|---|---|---|
| Masses [MeV] | 0.741 | 0.678 | 0.631 | | |
| $S_n$ [MeV] | 0.466 | 0.500 | 0.442 | | |
| Radii [fm] | 0.024 | 0.027 | 0.024 | | |
| Prim. barriers [MeV] | 0.88 | 0.44 | 0.33 | | |
| Sec. 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 | | |

## BSkG3

- extended Skyrme EDF form ($t_4$, $t_5$)
- break parity (octupole deformations etc.)

# Brussels-Skyrme-on-a-Grid: BSkG


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|---|---|---|---|---|---|
| Masses [MeV] | 0.741 | 0.678 | 0.631 | 0.633 | |
| $S_n$ [MeV] | 0.466 | 0.500 | 0.442 | 0.402 | |
| Radii [fm] | 0.024 | 0.027 | 0.024 | 0.025 | |
| Prim. barriers [MeV] | 0.88 | 0.44 | 0.33 | 0.36 | |
| Sec. barriers [MeV] | 0.87 | 0.47 | 0.51 | 0.53 | |
| Fission isomers [MeV] | 1.0 | 0.49 | 0.34 | 0.33 | |
| Max. NS mass [$M_\odot$] | 1.8 | 1.8 | 2.3 | 2.3 | |

## BSkG4

- pairing reproduces advanced INM calculations
- ideal for TD simulations in NS crust

## BSkG3

- extended Skyrme EDF form ($t_4$, $t_5$)
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**BSkG1:** G. Scamps et al., EPJA **57**, 333 (2021).
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**BSkG4:** G. Grams et al., EPJA **61,** 35 (2024).
**BSkG5:** G. Grams et al. arXiv:2601:05968 (2026).


## BSkG1

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## BSkG2

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  + 28 fission isomers

## BSkG3

- extended Skyrme EDF form ($t_4$, $t_5$)
- break parity (octupole deformations etc.)

## BSkG4

- pairing reproduces advanced INM calculations
- ideal for TD simulations in NS crust

## BSkG5

- **N2LO** Skyrme functional
- **Fewer** free parameters

DISCLAIMER

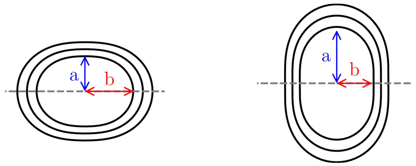
N$k$LO : up to 2$k$ derivatives of density

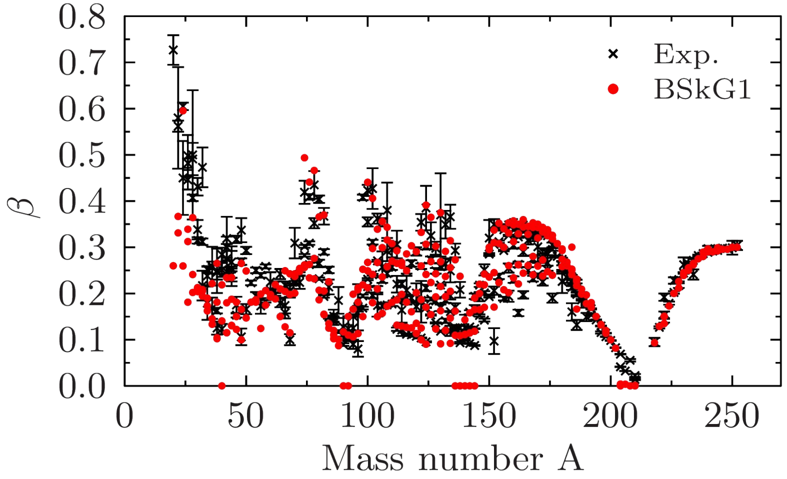
| Rms $\sigma$ | BSkG1 | BSkG2 | BSkG3 | BSkG4 | BSkG5 |
|---|---|---|---|---|---|
| Masses [MeV] | 0.741 | 0.678 | 0.631 | 0.633 | 0.649 |
| $S_n$ [MeV] | 0.466 | 0.500 | 0.442 | 0.402 | 0.409 |
| Radii [fm] | 0.024 | 0.027 | 0.024 | 0.025 | 0.027 |
| Prim. barriers [MeV] | 0.88 | 0.44 | 0.33 | 0.36 | 0.43 |
| Sec. barriers [MeV] | 0.87 | 0.47 | 0.51 | 0.53 | 0.49 |
| Fission isomers [MeV] | 1.0 | 0.49 | 0.34 | 0.33 | 0.59 |
| Max. NS mass [$M_\odot$] | 1.8 | 1.8 | 2.3 | 2.3 | 2.2 |

**BSkG1:** G. Scamps et al., EPJA **57**, 333 (2021).
**BSkG2:** G. Grams et al., EPJA **59**, 270 (2023).

# More on shape and charge distributions

"ordinary" quadrupole deformation



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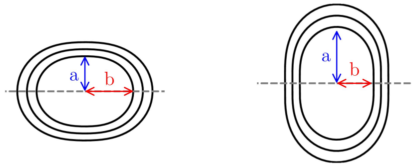
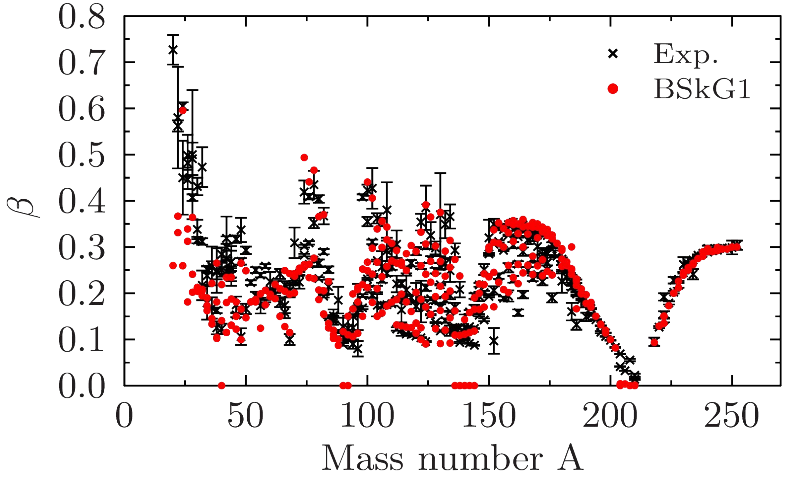
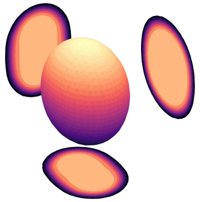
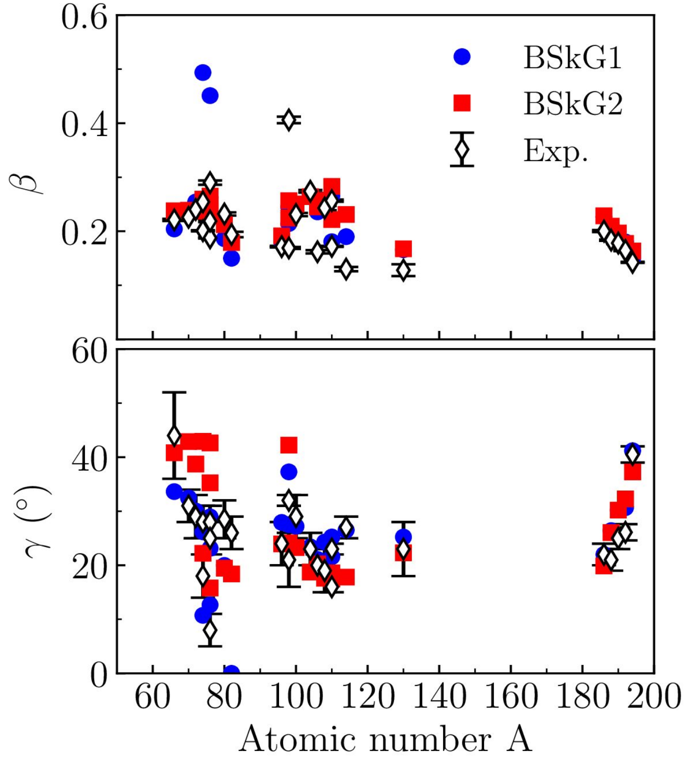



## Triaxial deformation





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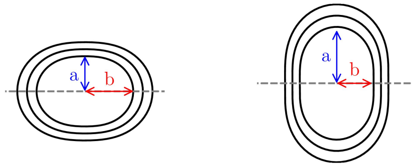


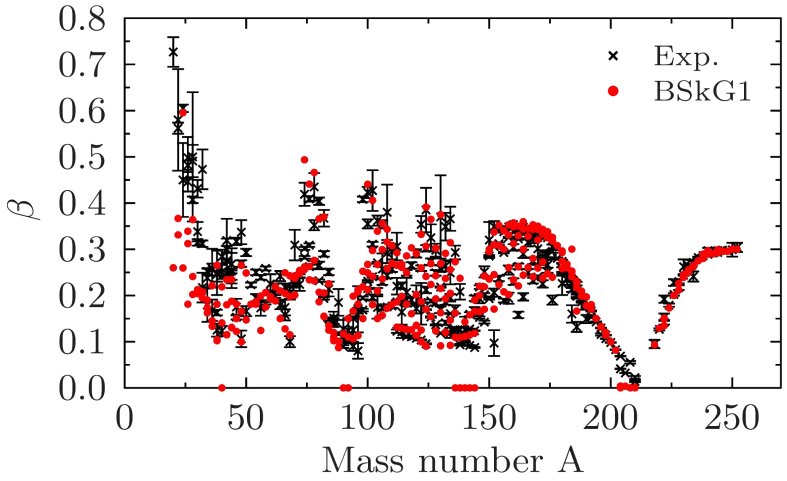


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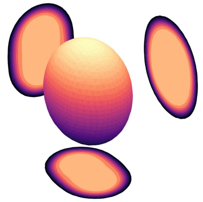
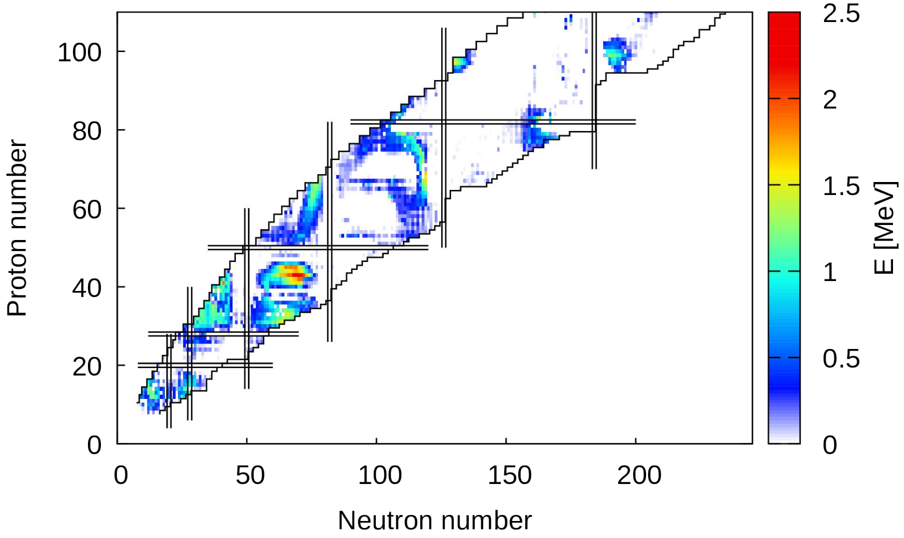
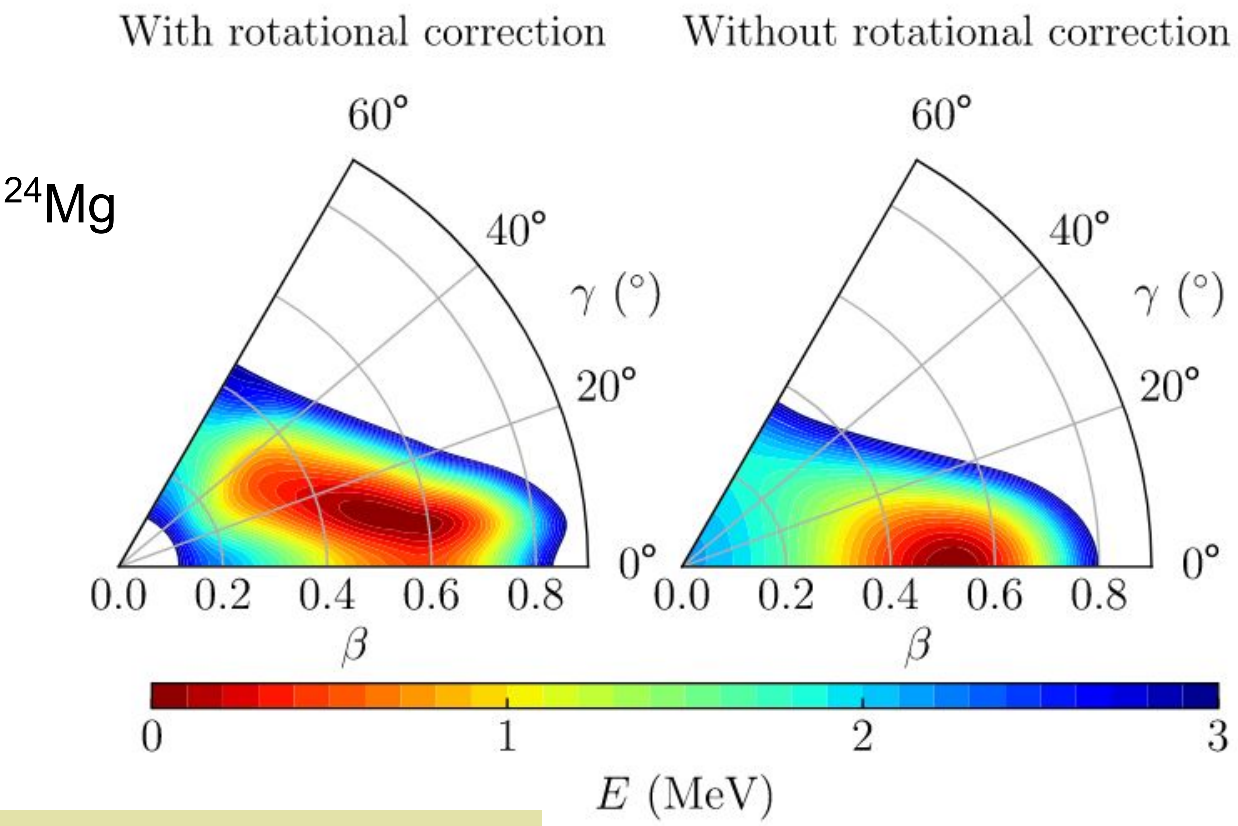




# Rotational correction in $^{24}$Mg with BSkG1




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

Many nuclei triaxially deformed due to semi-variational inclusion of rotational correction

BSkG1: G. Scamps et al., EPJA 57, 333 (2021).
BSkG2: G. Grams et al., EPJA 59, 270 (2023).

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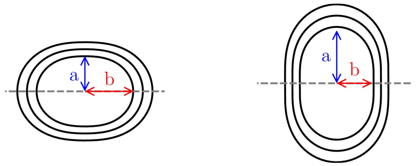
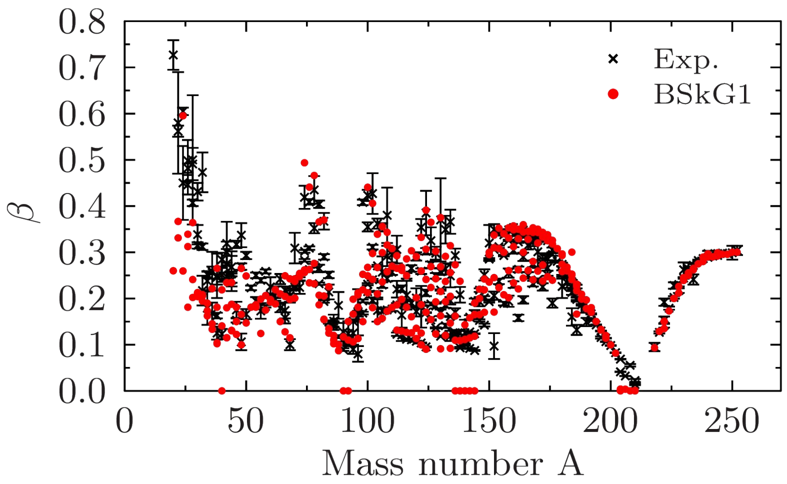
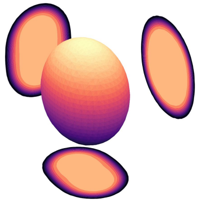
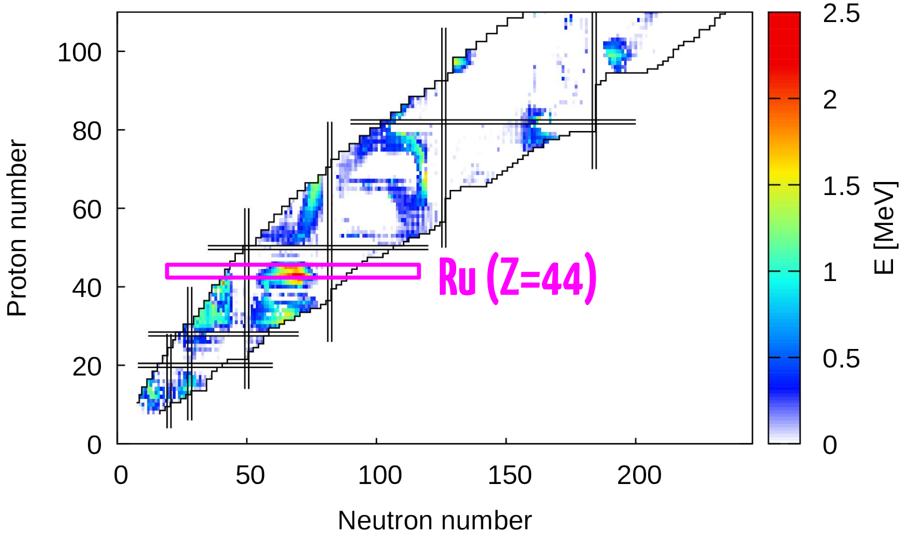


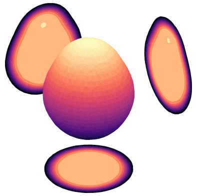


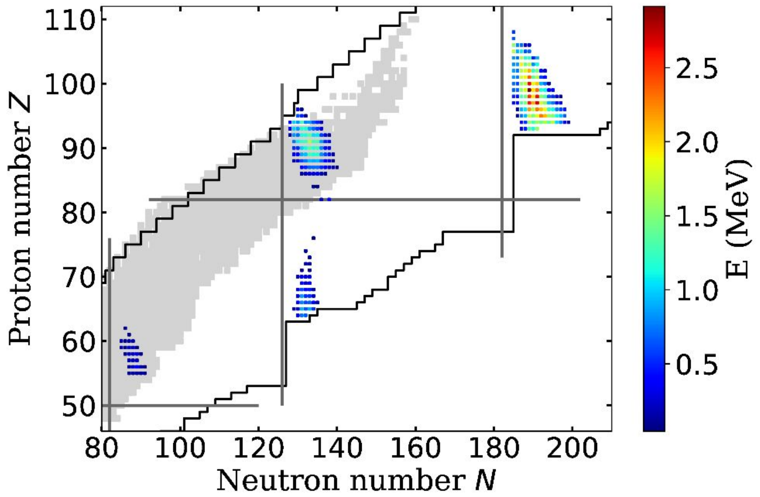

## Triaxial deformation





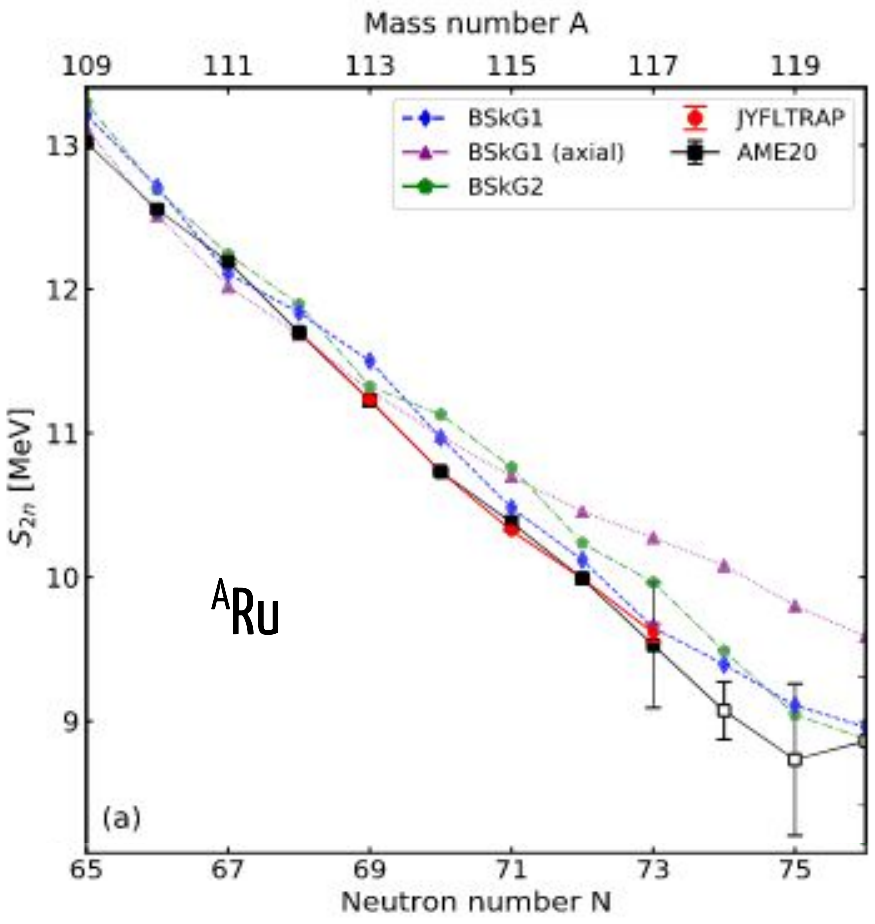

## octupole deformation





M. Hukkanen et al. PRC **108**, 064315 (2023)

# Fingerprints of triaxiality in Ruthenium energies

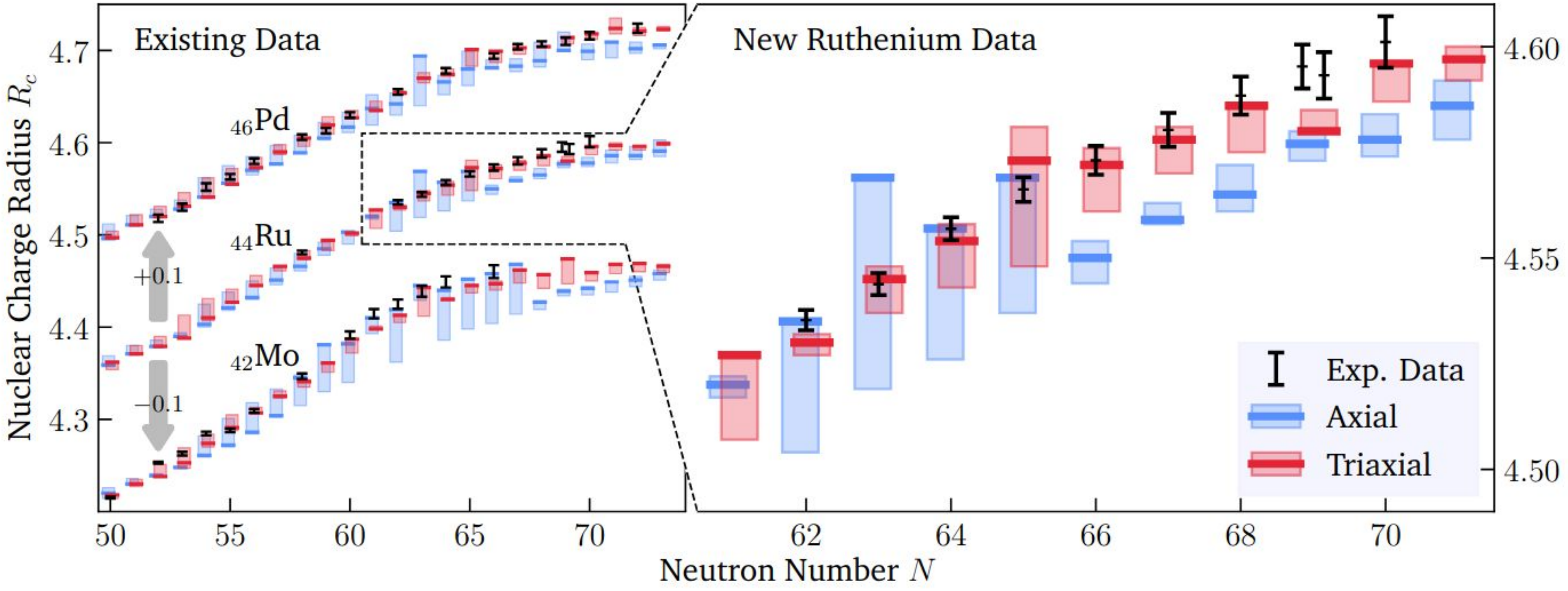


B. Maass, et al. arXiv:2503.07841

# Fingerprints of triaxiality in Ruthenium charge radii

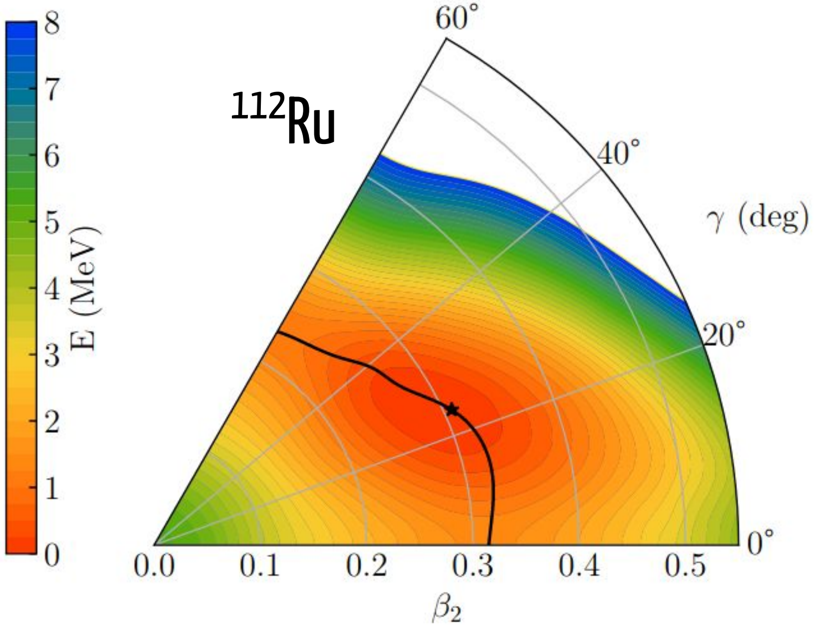
Rigorous uncertainty quantification is impossible within EDF in its current form

⟶ spread between BSkG[1,2,3,4] as proxy for uncertainty

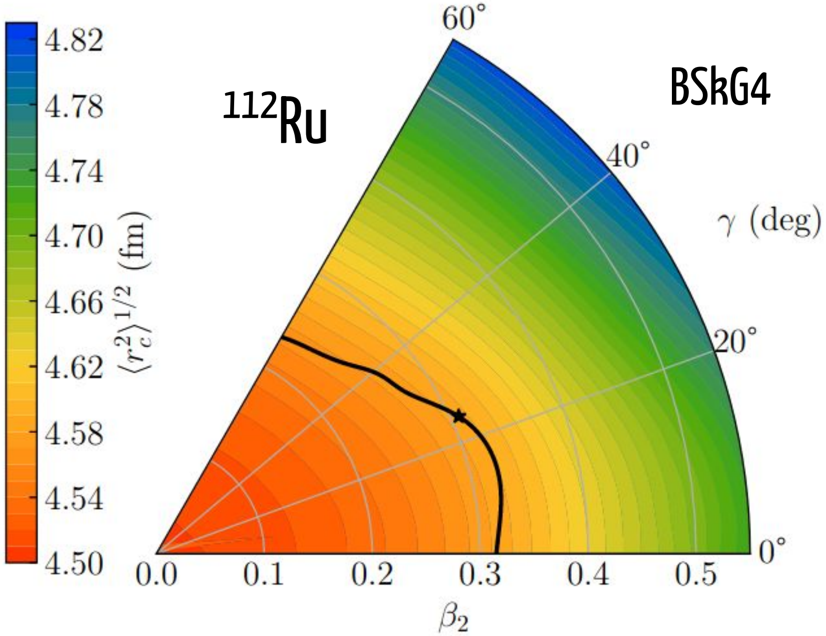


# Fingerprints of triaxiality in Ruthenium charge radii

## Total binding energy

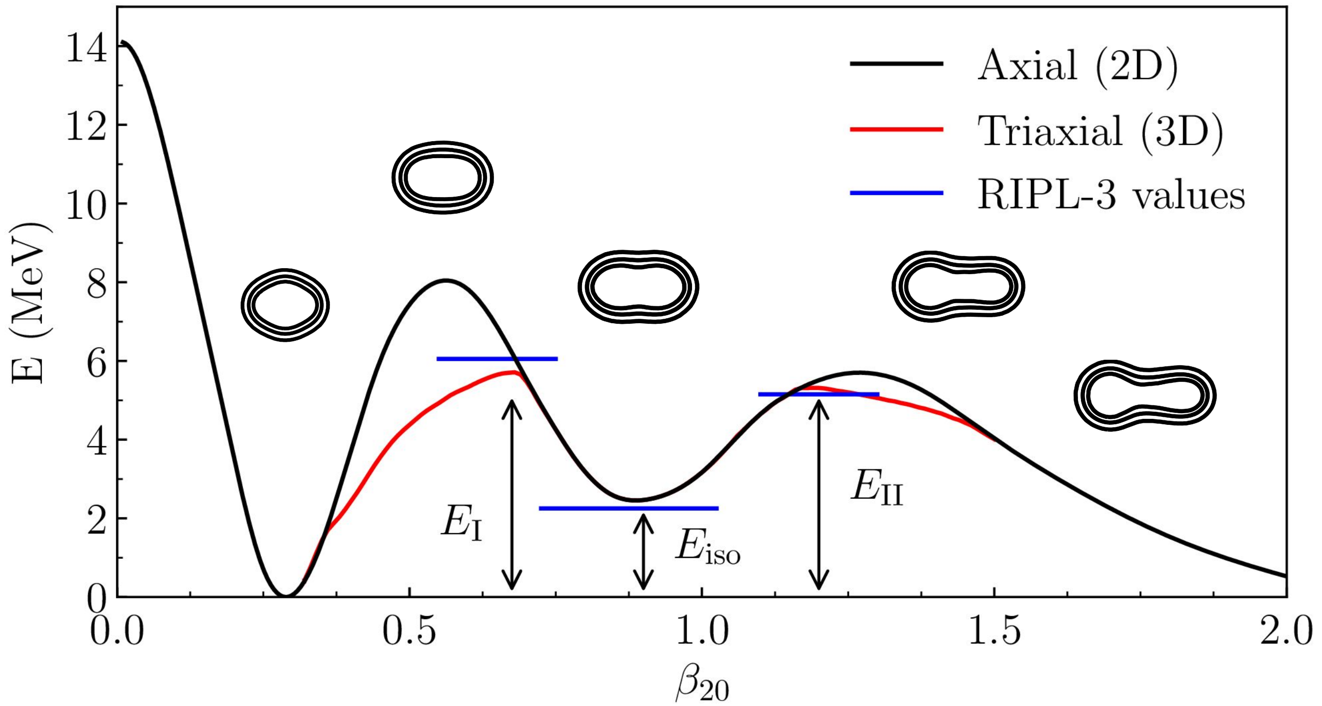



## rms charge radius



W. Ryssens et al., EPJA **59**, 96 (2023).
E. Flynn et al., PRC **105** (2022).
A. Sánchez-Fernández et al., arXiv:2508.16240

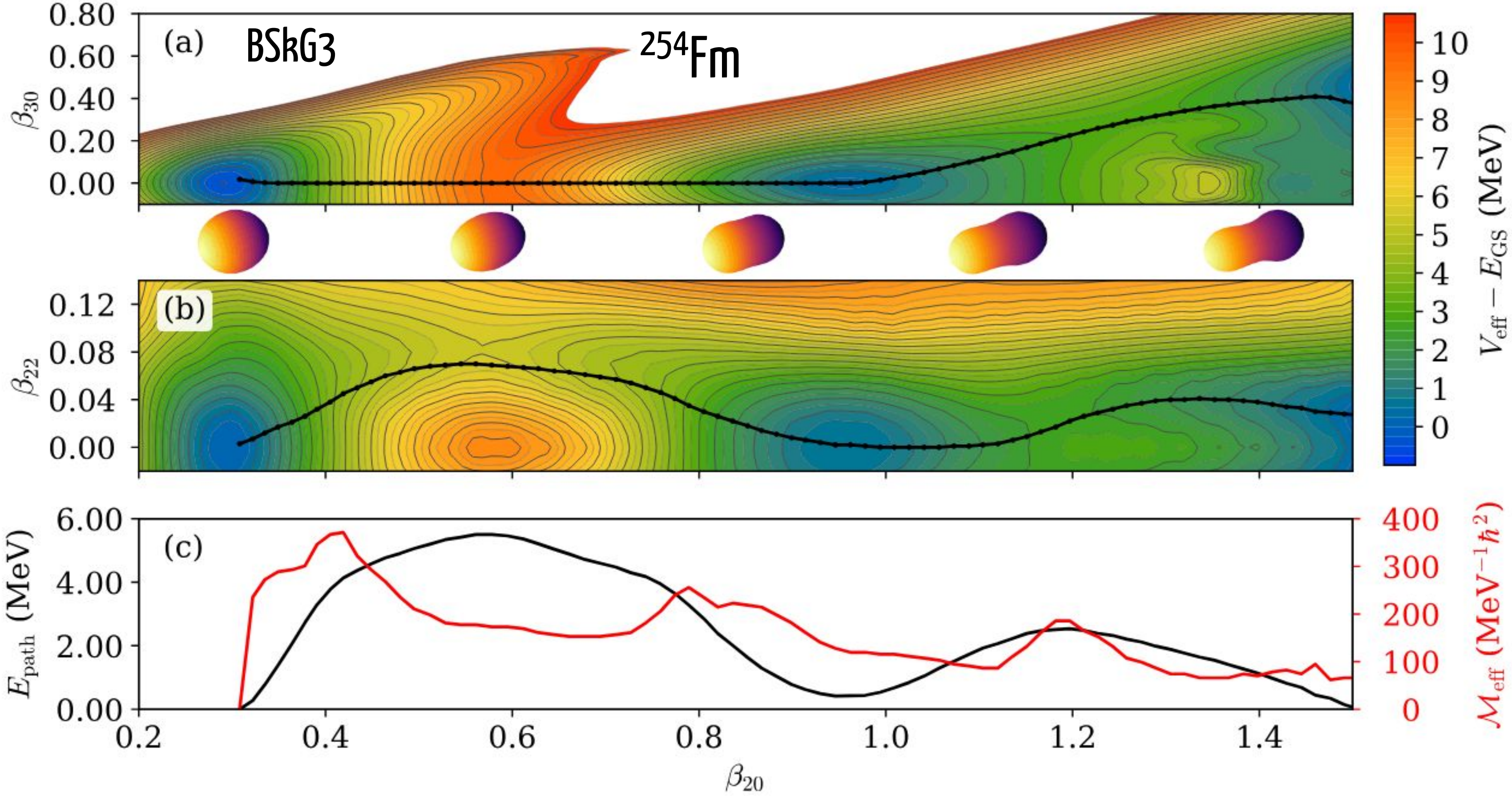
# Fission barriers




- All inner-barriers are triaxial
- All outer-barriers are triaxial + octupole deformed

W. Ryssens et al., EPJA **59**, 96 (2023).
E. Flynn et al., PRC **105** (2022).
A. Sánchez-Fernández et al., arXiv:2508.16240

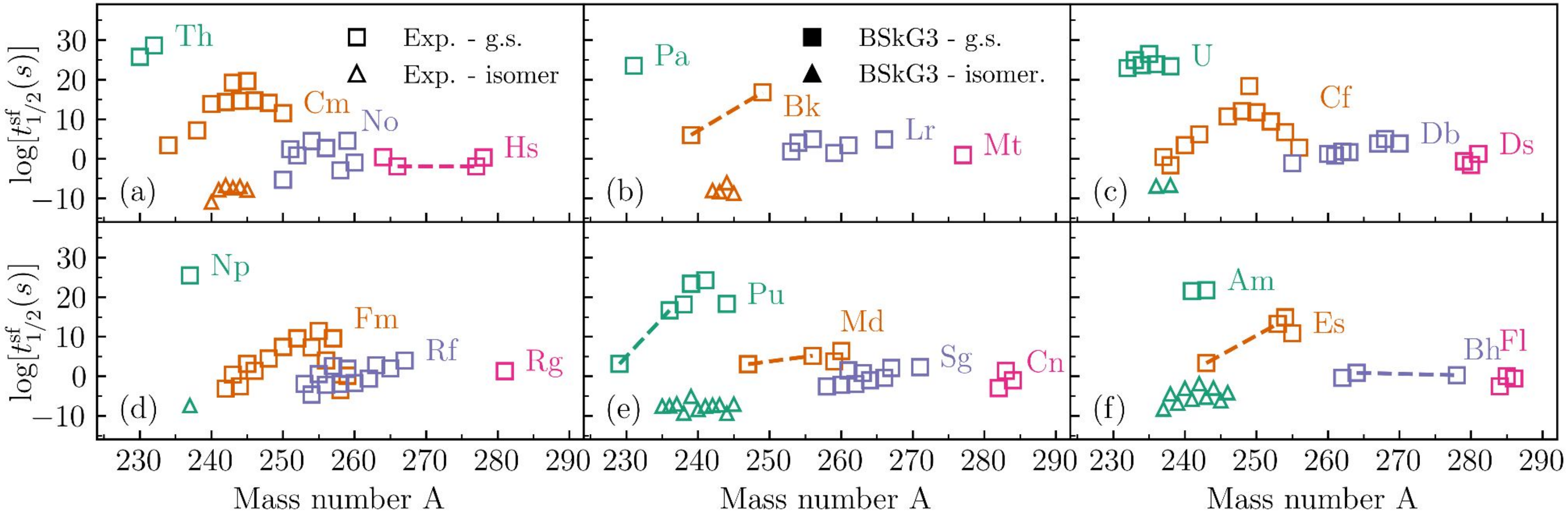
# Fission paths




- Poor-man's 3D collective space : $\beta_{20}$, $\beta_{22}$, $\beta_{30}$
- Least action path (consistent inertias) obtained using PyNEB
- For **3000** fissioning nuclei

W. Ryssens et al., EPJA **59**, 96 (2023).
E. Flynn et al., PRC **105** (2022).
A. Sánchez-Fernández et al., arXiv:2508.16240

# Spontaneous fission half lives




- Exp. data : 124 ground-state + 34 isomer half lives

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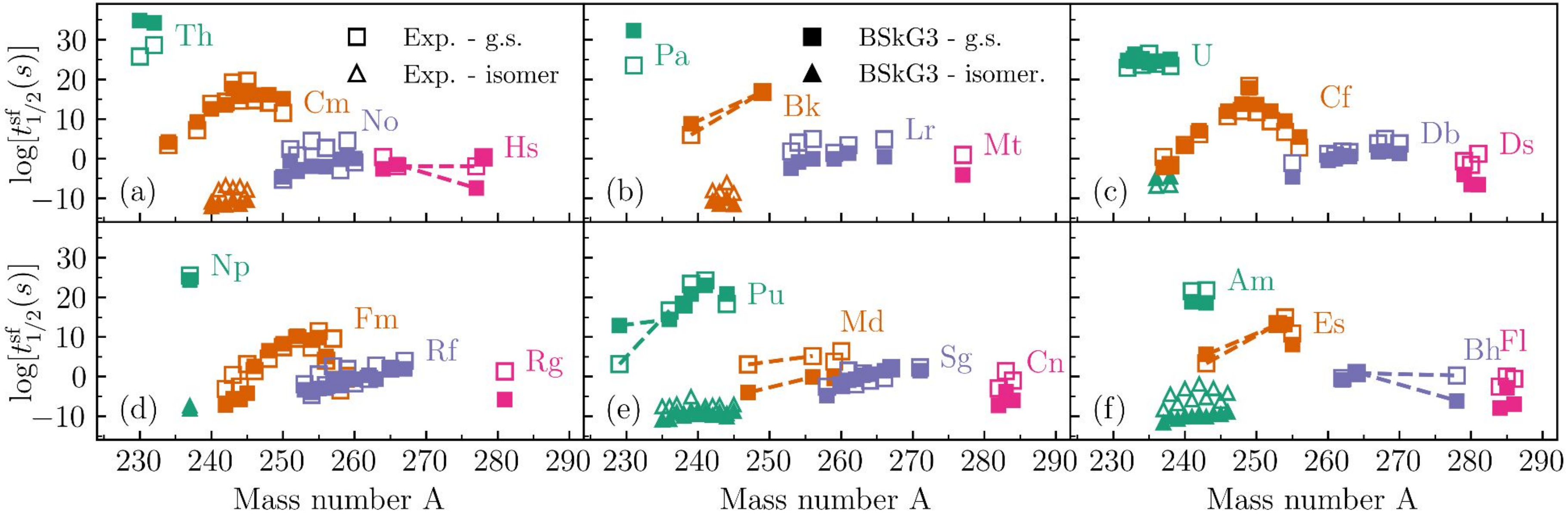
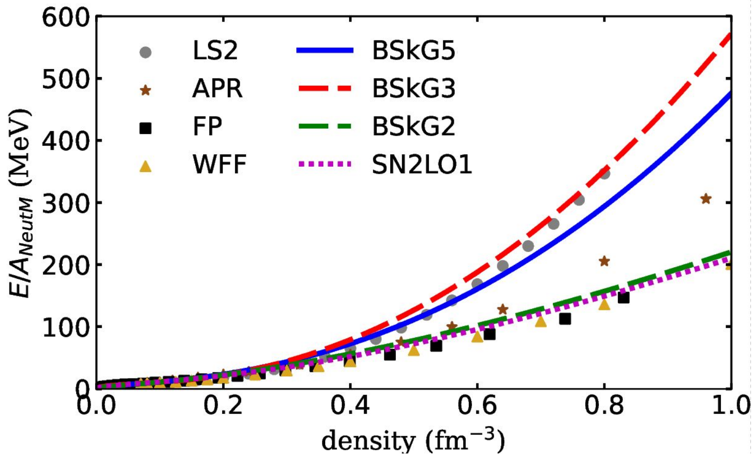



- Exp. data : 124 ground-state + 34 isomer half lives
- BSkG3 comparable to best mic-mac models

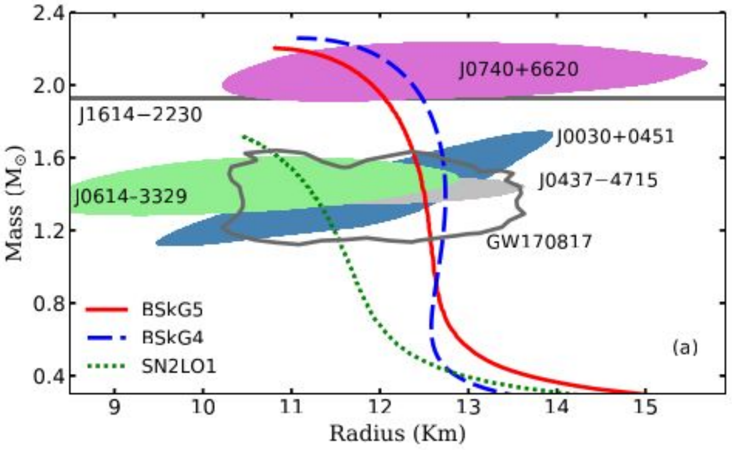
  ⟶ without additional parameter adjustment

# Applications which will not be discussed

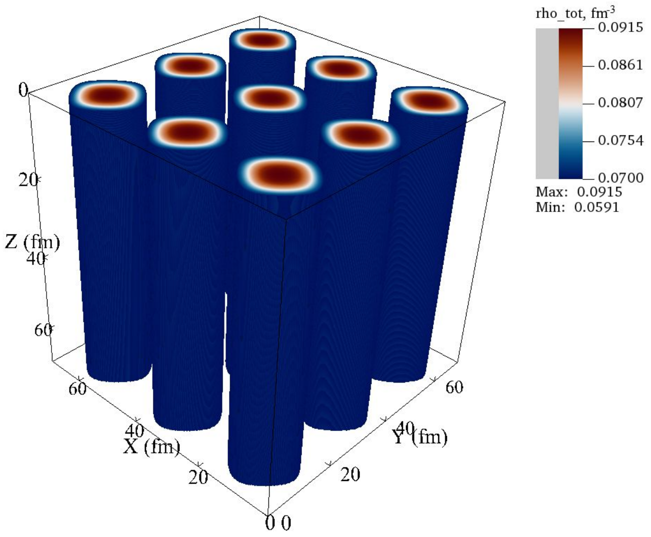
## Neutron star Equation of State (EoS)




G. Grams et al., arXiv2601.05968

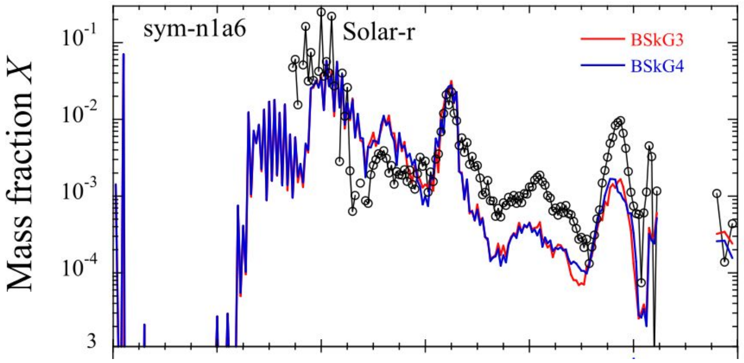



## Nuclear Pasta




N. Shchechilin et al., in preparation

## r-process simulations

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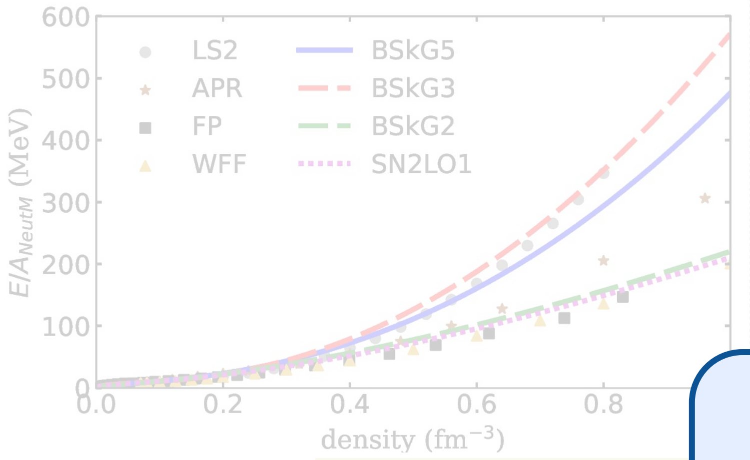
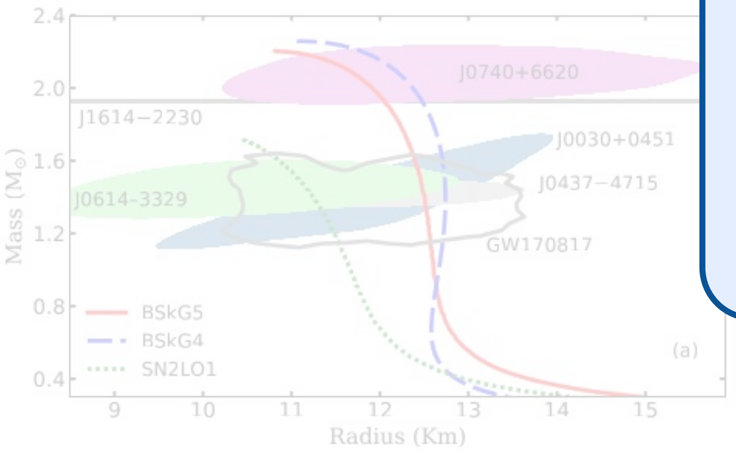


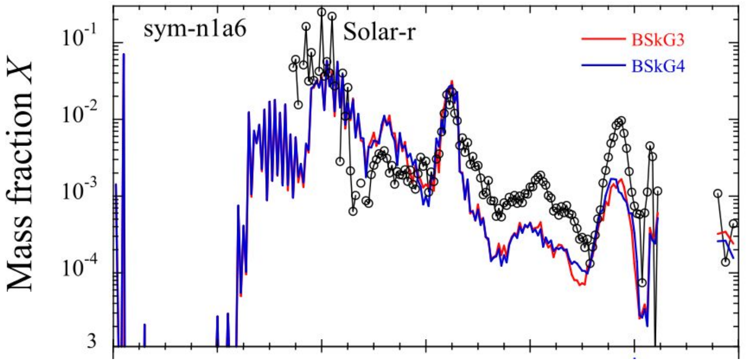

G. Grams et al., arXiv2601.05




## Nuclear Pasta




## r-process simulations




G. Grams et al., arXiv2601.05968

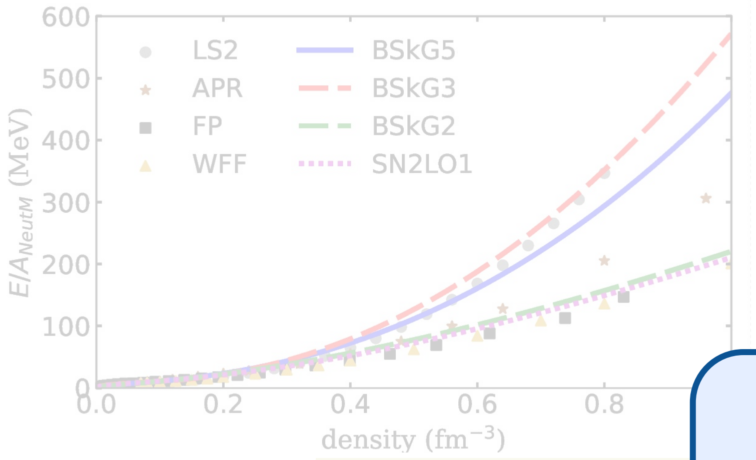
### r-process simulations require **a lot** of data

- Nuclear masses
- Nuclear level densities
- Fission paths and fragment yields
- Electromagnetic and weak strength functions

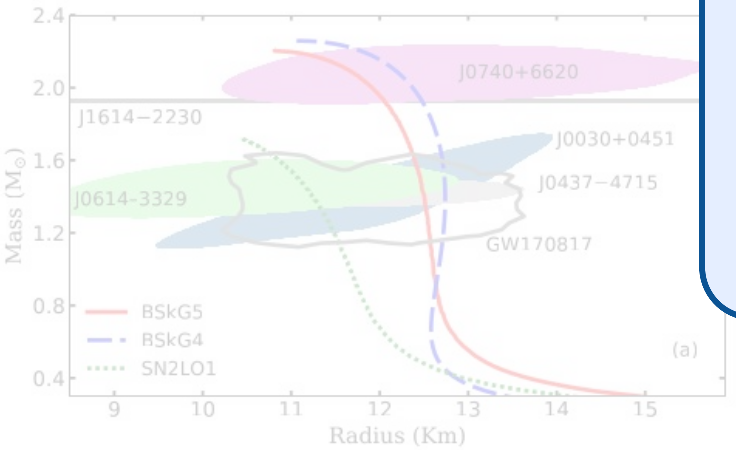
for ALL nuclei

# Applications which will not be discussed

## Neutron star Equation of State (EoS)



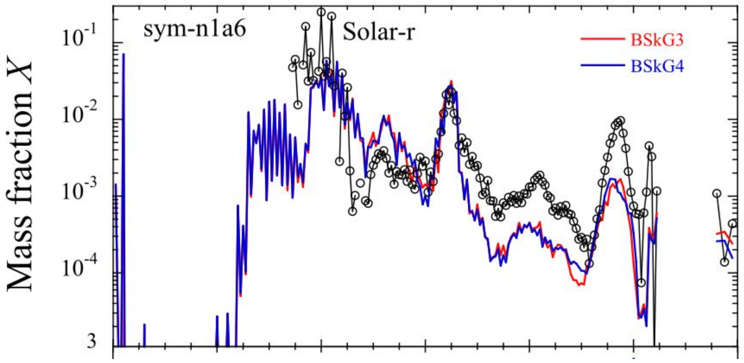

G. Grams et al., arXiv2601.05…




## Nuclear Pasta




## r-process simulations

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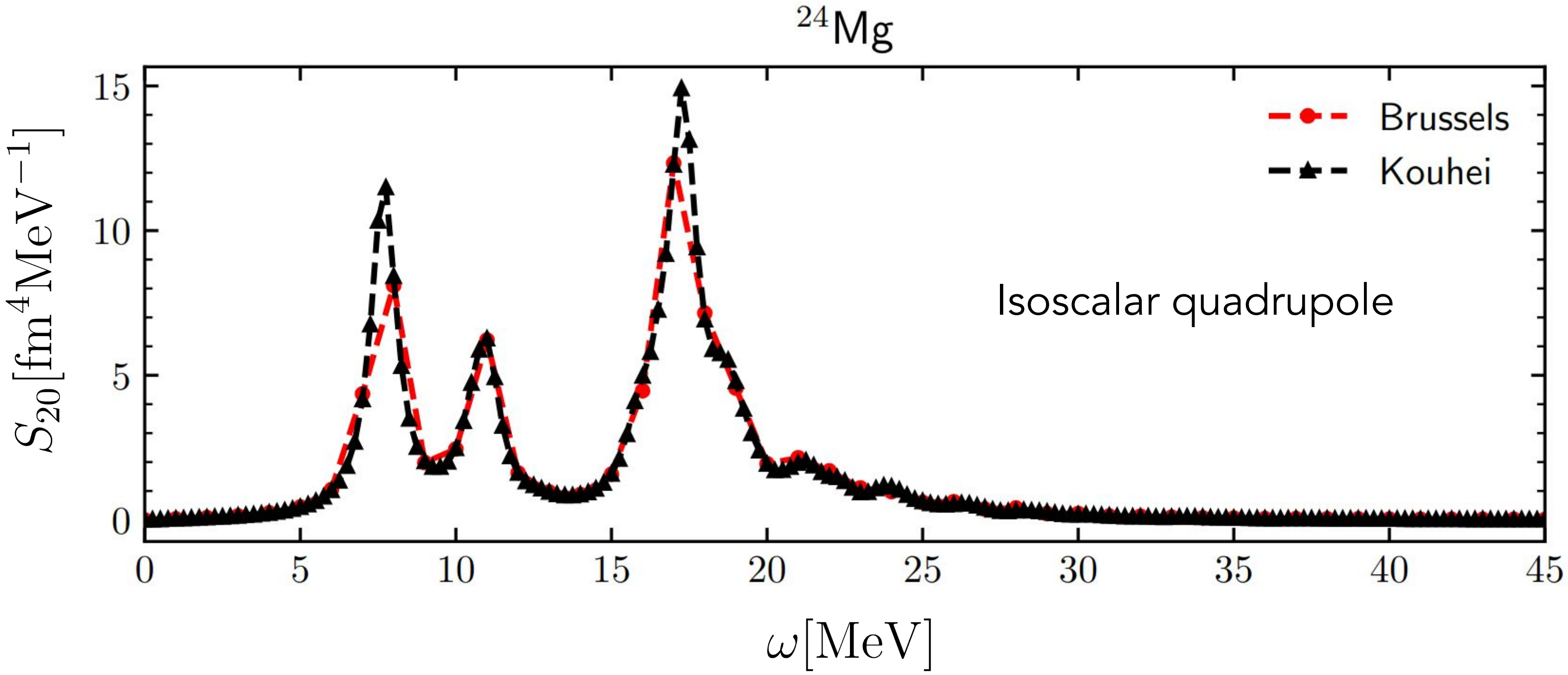
### r-process simulations require **a lot** of data

- ✓ Nuclear masses
- ✓ Nuclear level densities
- ✓ Fission paths and fragment yields
- ✗ Electromagnetic and weak strength functions

for ALL nuclei

# Photon strength functions in BSkG

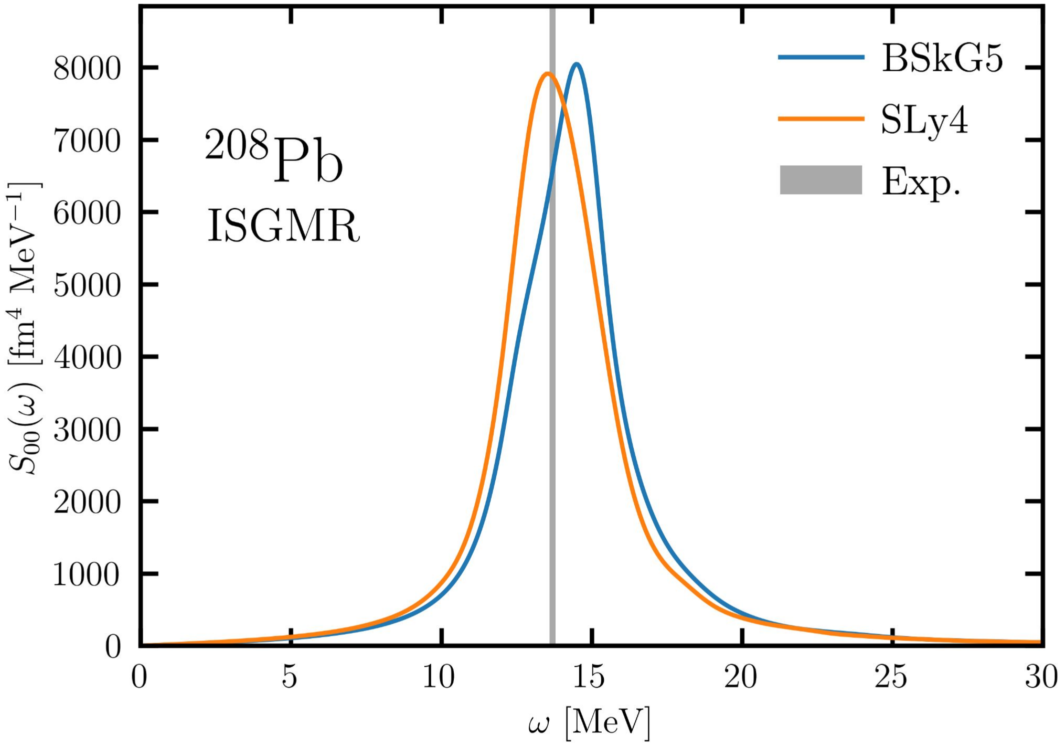
Current effort: implement FAM-QRPA to obtain strength functions




Many thanks to **Kouhei Washiyama** for helping to benchmark the FAM code

# Photon strength functions in BSkG

Current effort: implement FAM-QRPA to obtain strength functions




Very first FAM calculation with an N2LO Skyrme functional

# Emulating FAM via reduced order model

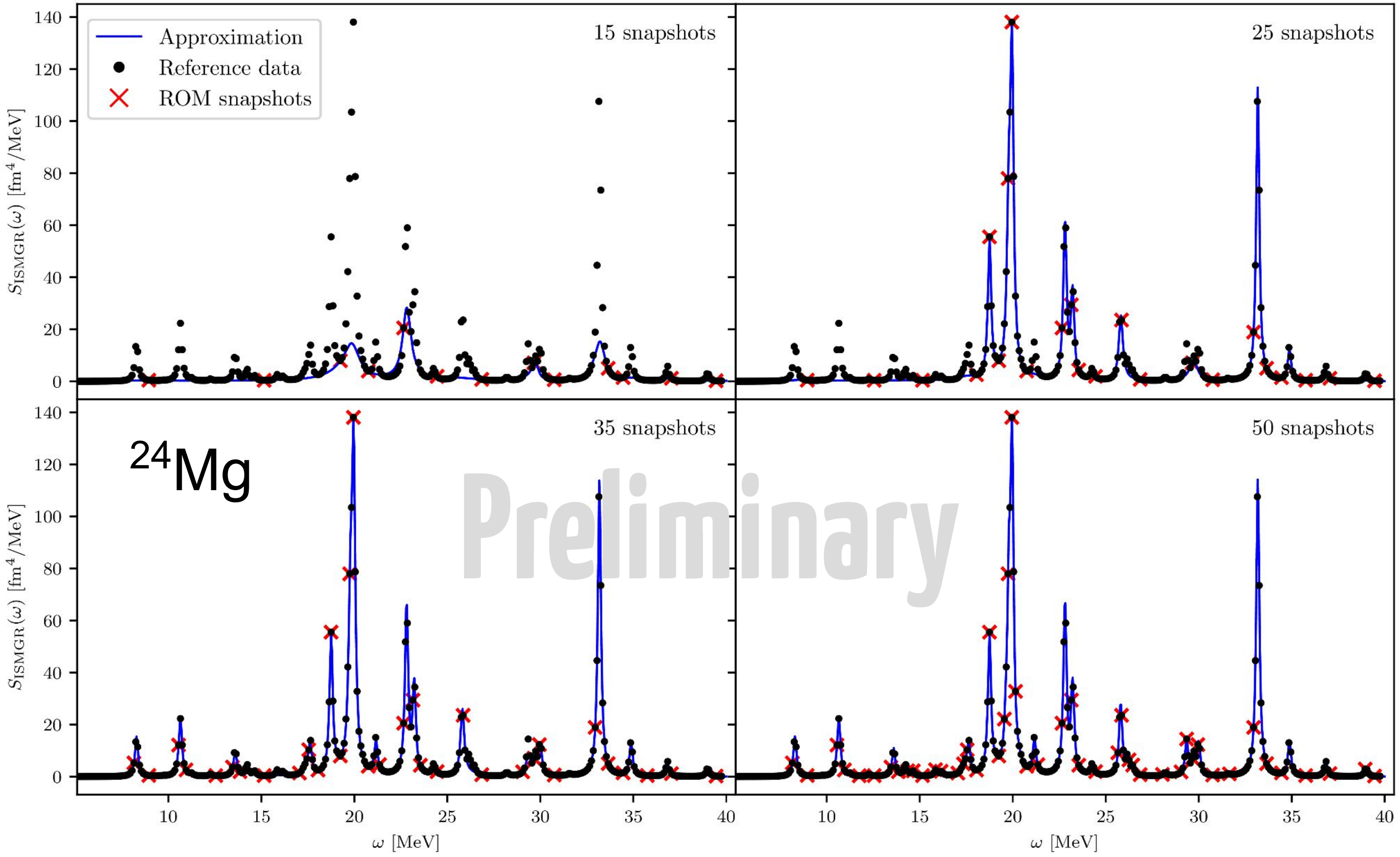
Work of master's student **Emma Vancayseele**

- Solve FAM for few snapshot frequencies $\omega_i$

  $\longrightarrow$ Interpolate X and Y amplitude for any $\omega$

  $\longrightarrow$ Efficient interpolation of strength function

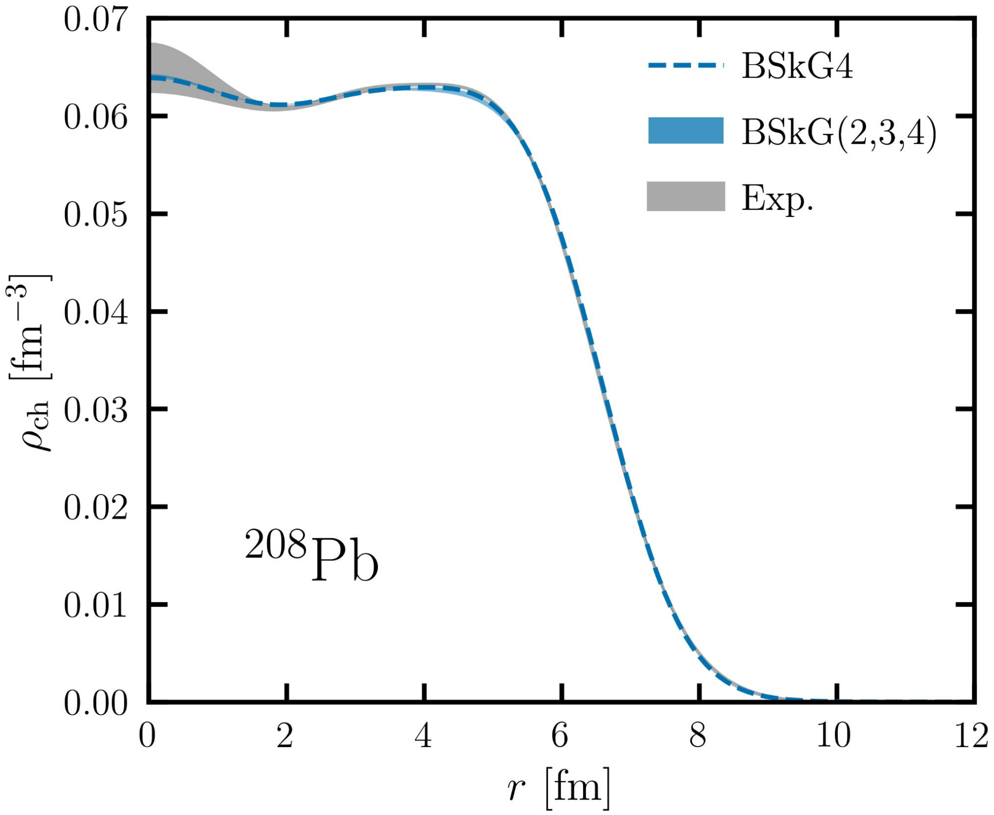
  + Extrapolations in complex frequency plane



**BSkG4:** G. Grams et al., EPJA **61,** 35 (2024).
**Pb208 data:** H. Euteneuer et al., Nuc. Phys A **298,** 3 (1978).

# Quality of charge densities

spread between BSkG[2,3,4] as proxy for uncertainty

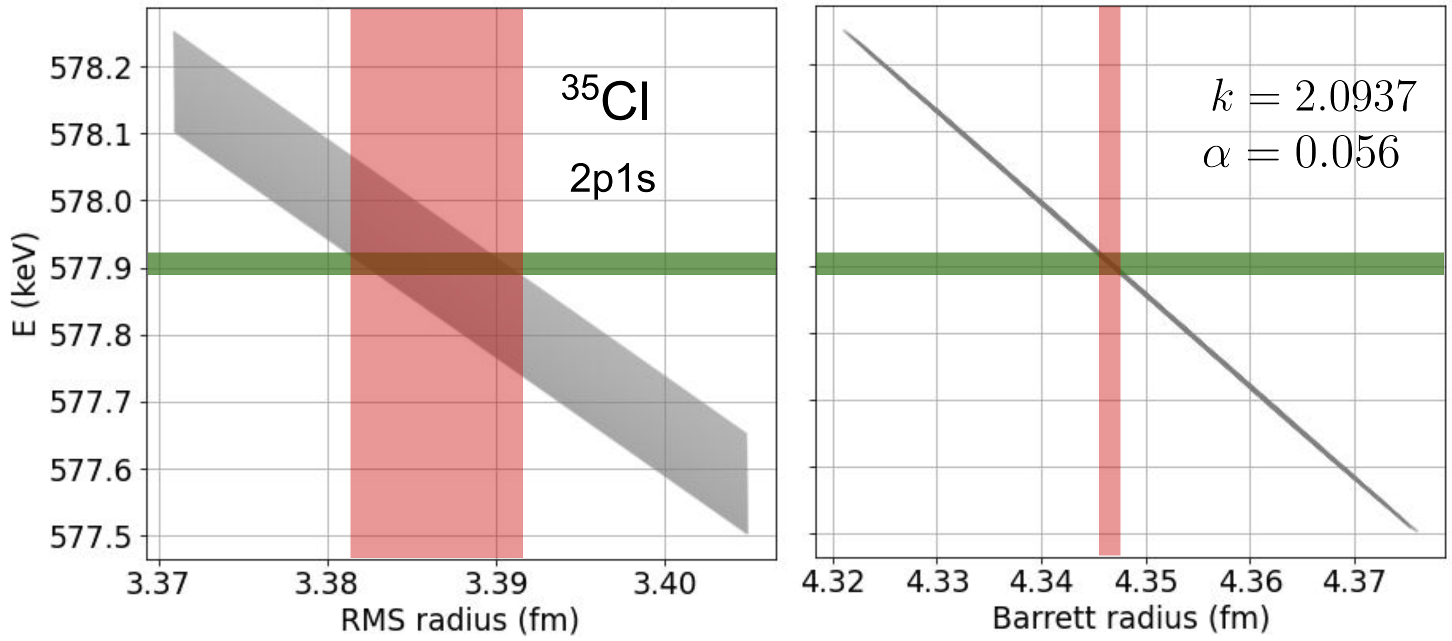


# Measuring charge radii with muonic X-rays

(1) <u>Experiment</u>: Produce muonic atom and measure cascade of X-rays caused by muon falling into the nucleus

(2) <u>QED calculation</u>: link the muonic X-ray energies to the charge radius of the nucleus

$$R_{\text{Bar}} \sim \int r^k e^{-\alpha r} \rho_{ch}(\mathbf{r}) d\mathbf{r} = V_2 \langle r^2 \rangle^{1/2}$$




"Sensitive to shape" "Insensitive to shape"

K. A. Beyer et al., arXiv:2506.08804
Courtesy of Michael Heines

# Measuring charge radii with muonic X-rays

(1) Experiment: Produce muonic atom and measure cascade of X-rays caused by muon falling into the nucleus

(2) QED calculation: link the muonic X-ray energies to the ~~charge~~ Barrett radius of the nucleus

(3) V2 shape correction: determined from $\rho_{ch}(\mathbf{r})$ obtained from electron scattering or through **nuclear theory**

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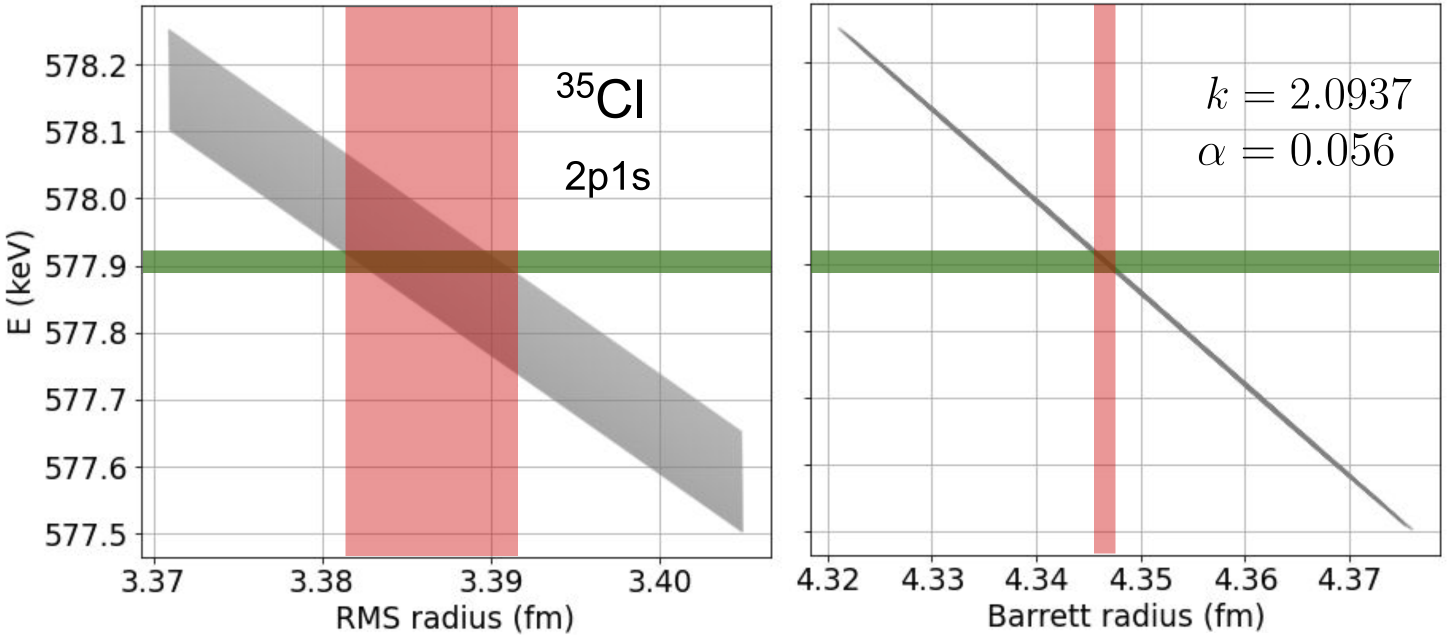


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# Application to muonic X-ray

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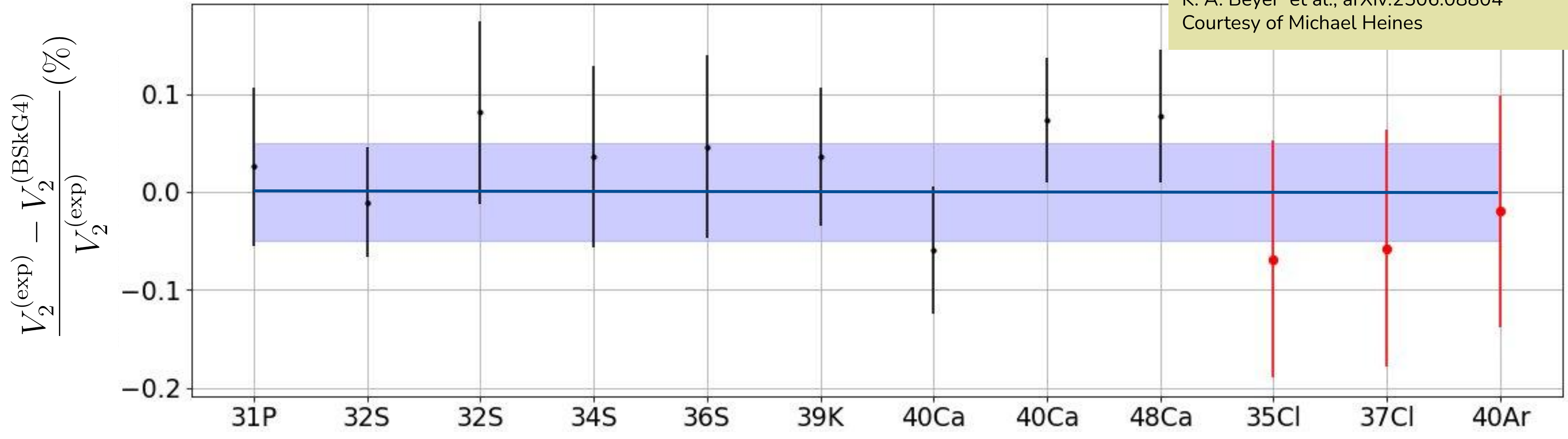


Empirical $V_2$ accuracy : **0.05 %**

Thanks to **Wouter Ryssens** for several slides

# Conclusion

**BSkG** provides **large-scale**, **microscopic** model of nuclear structure

- **Large-scale** : **thousands** of nuclei and **many observable**
- **Microscopic** : simple wave functions yet complex **symmetry breaking** (triaxial, octupole, time-reversal)
- with accurate bulk predictions of **masses, radii, fission properties** and more
- Soon: **strength functions** via **FAM**

## Outlook: synergy with *ab initio*?

Can **BSkG** models be **improved by** constraining on carefully chosen ***ab initio*** **pseudo-data** of exotic nuclei?

# Thanks to all my collaborators

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