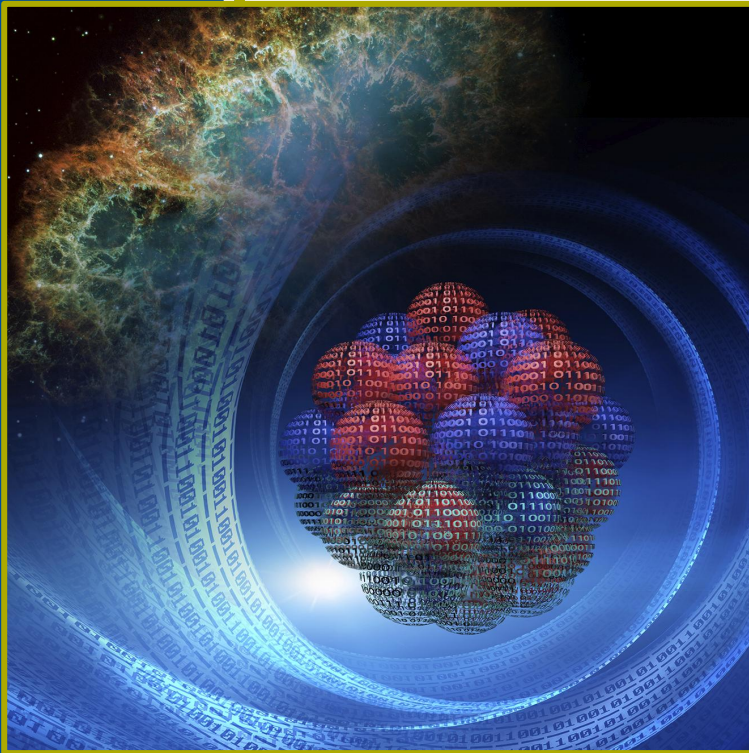


WOUTER RYSENS



Andy Sproles, ORNL



wryssens.com

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Towards a truly global description of nuclei

W. Ryssens

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

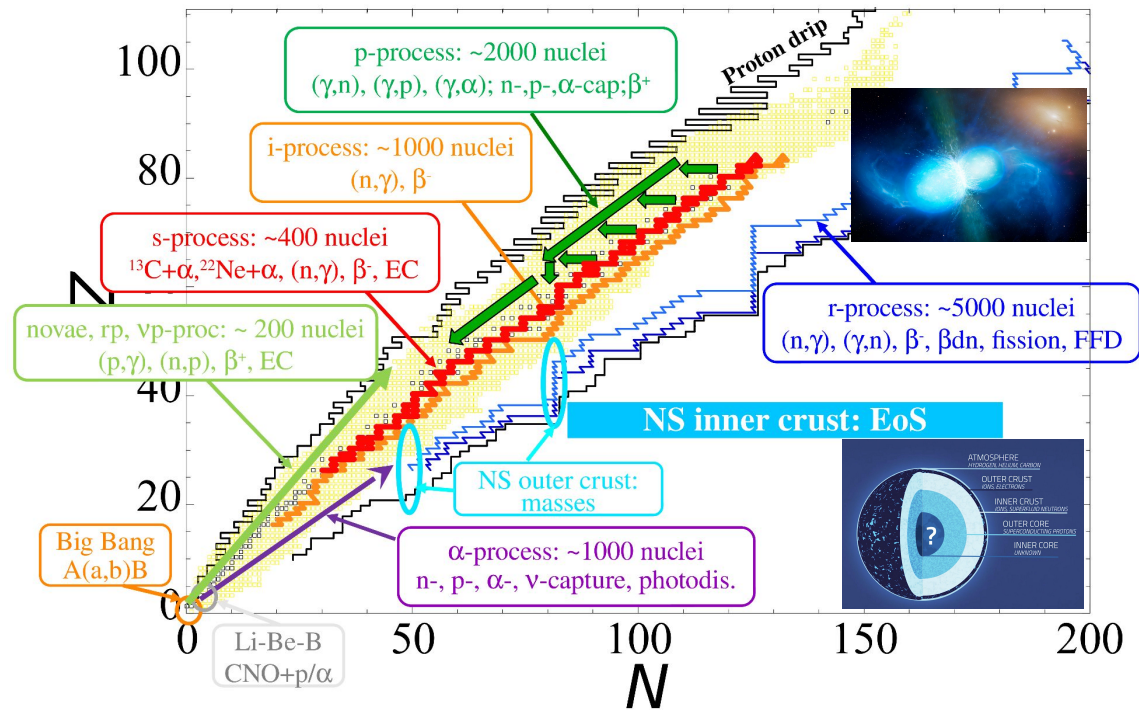
7th of June 2024



The nuclear chart and the processes traversing it

Extrapolations in

- nucleon number
- energy
- temperature
- density
-



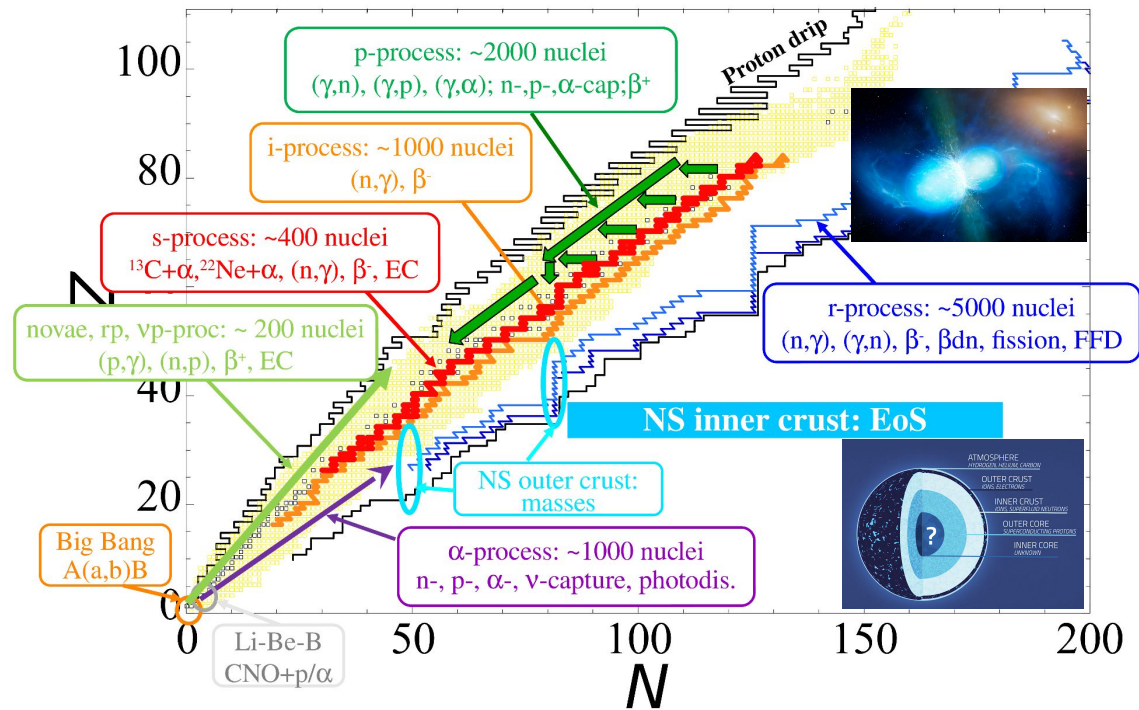
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and all of that for

- ~7000 nuclei
- many reactions



The nuclear chart and the processes traversing it

Extrapolations in

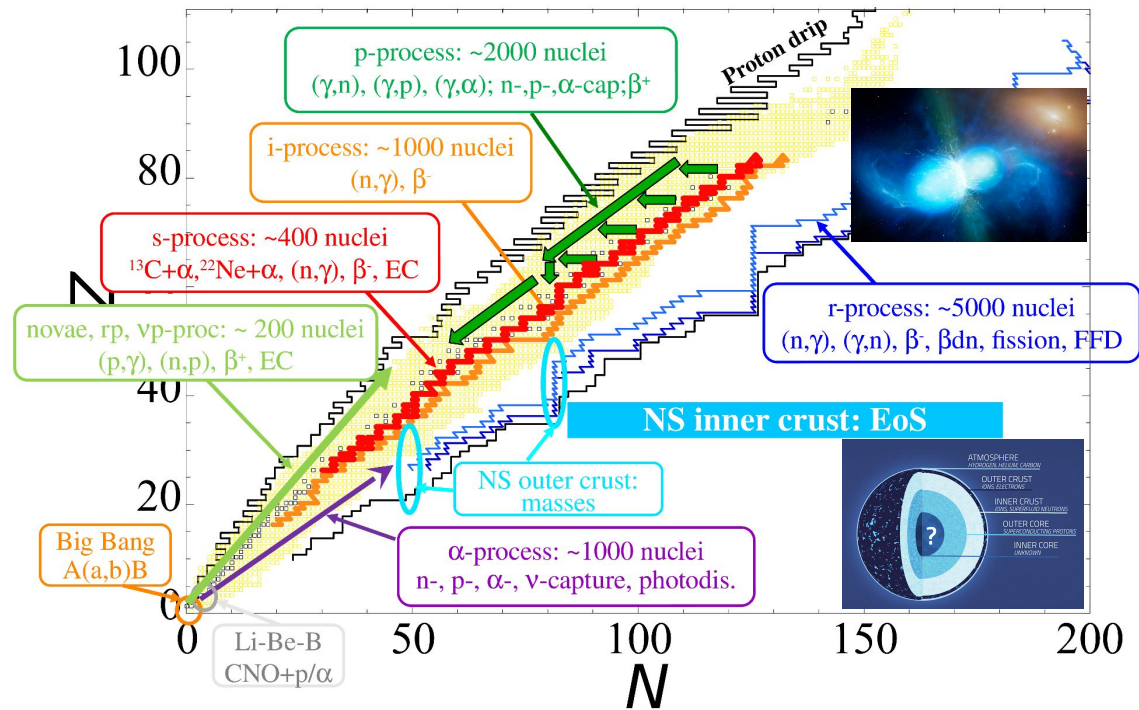
- nucleon number
- energy
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and all of that for

- ~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**)

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



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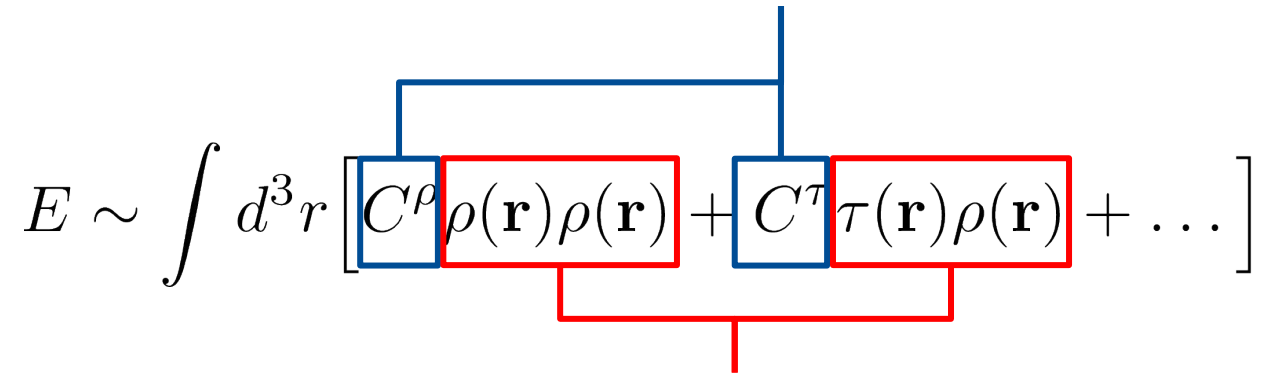
$$E \sim \int d^3r \left[C^\rho \boxed{\rho(\mathbf{r})\rho(\mathbf{r})} + C^\tau \boxed{\tau(\mathbf{r})\rho(\mathbf{r})} + \dots \right]$$


Local densities and currents of a wavefunction



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Local densities and currents of a wavefunction

Strong points

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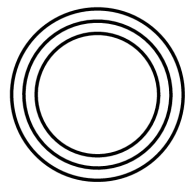
- **simple** wavefunctions but **individual** nucleons
- based on “in-medium” N-N interaction
- many observables accessible
- Feasible for ~**7000** nuclei

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 dimensions

Spherical

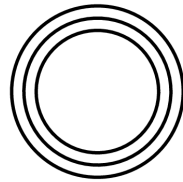


$$\beta_{20} = 0$$



Large-scale models in 1-2 dimensions

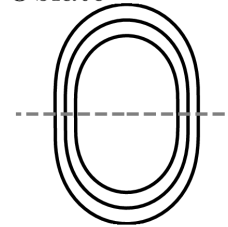
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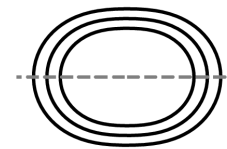


Oblate



$$\beta_{20} < 0$$

Prolate



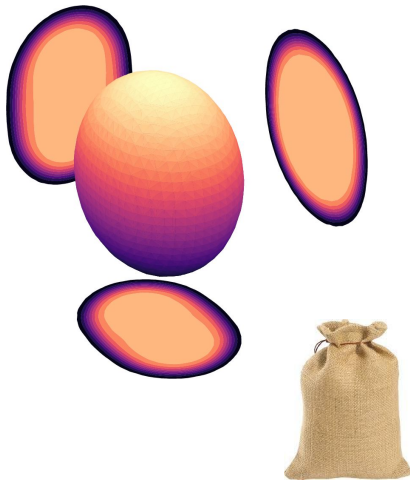
$$\beta_{20} > 0$$

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



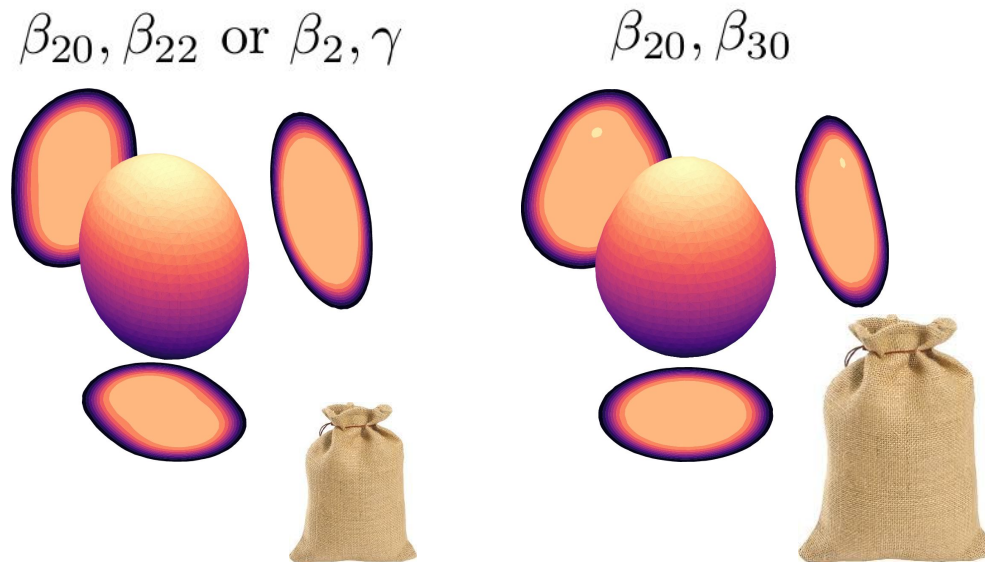
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More general configurations

- triaxial shapes
- reflection asymmetry
- elongated shapes

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



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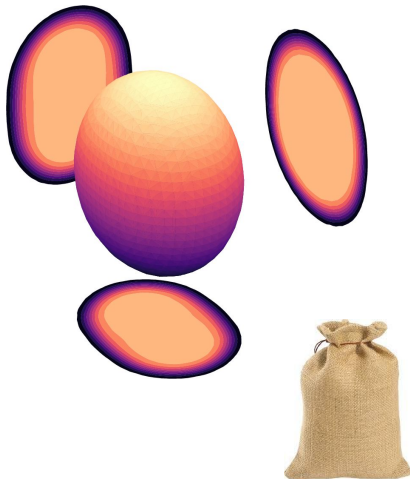
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β_{20}, β_{22} **and** β_{30}



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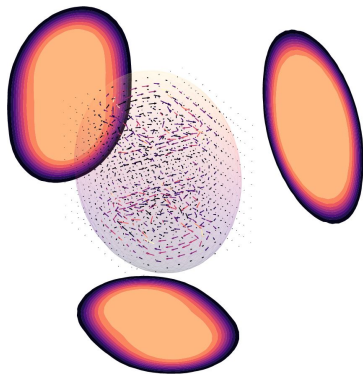
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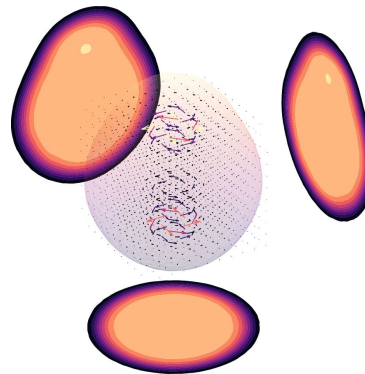
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Large-scale models in 1-2-**3** dimensions

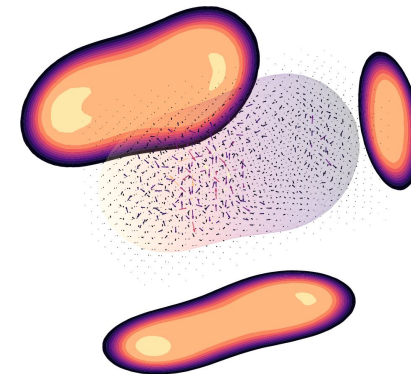
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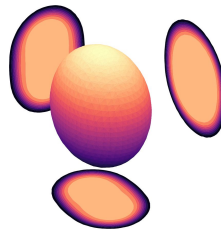
More general configurations

- 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

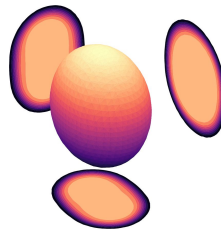


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Brussels-Skyrme-on-a-Grid: BSkg

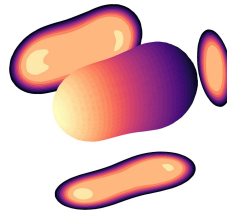
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BSkg2 (2022)

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

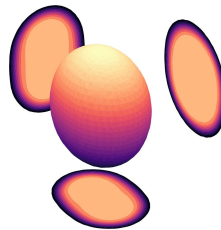


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Brussels-Skyrme-on-a-Grid: BSkG

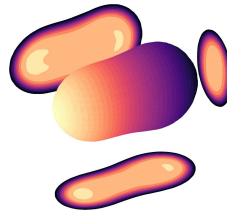
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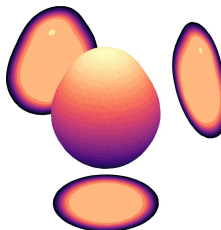
BSkG2 (2022)

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BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation

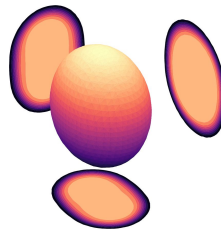


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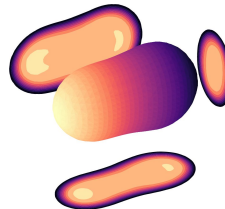
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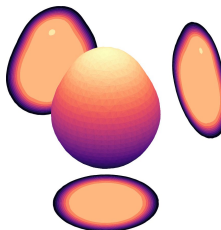
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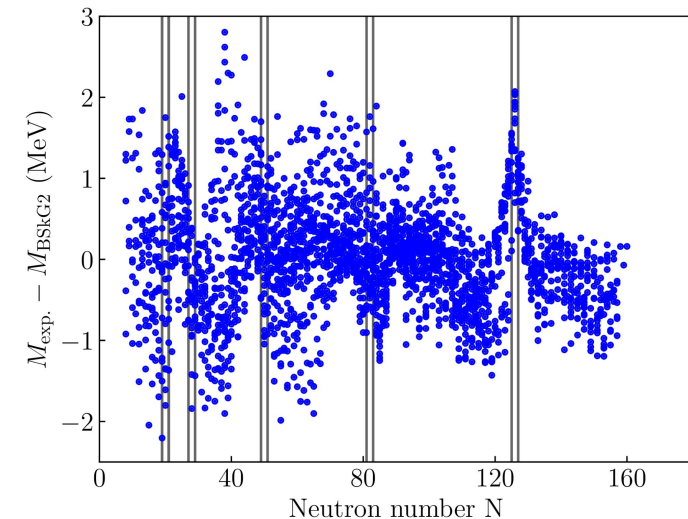


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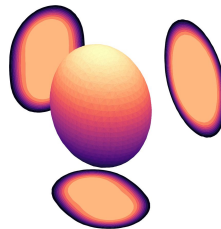


Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]			
Radii [fm]			
Prim. barriers [MeV]			
Secon. barriers [MeV]			
Fission isomers [MeV]			
Max. NS mass [$M_{\odot}$]			

Brussels-Skyrme-on-a-Grid: BSkG

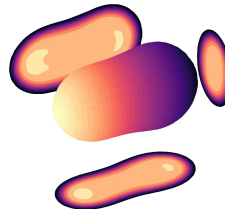
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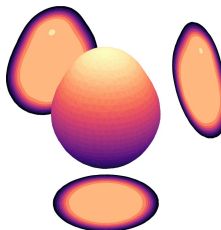
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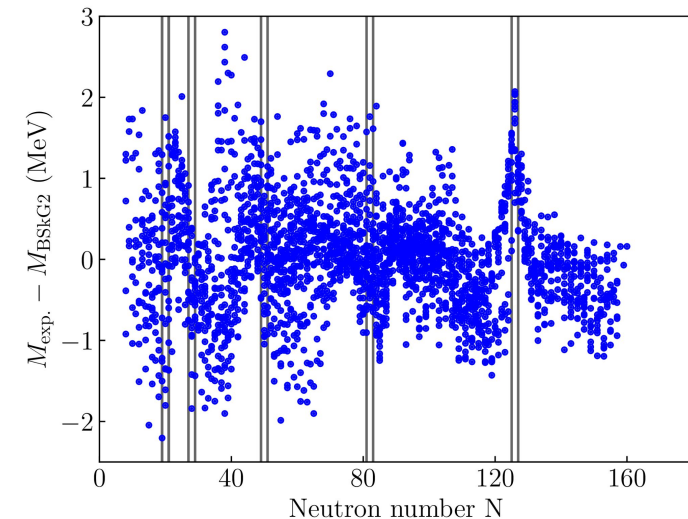


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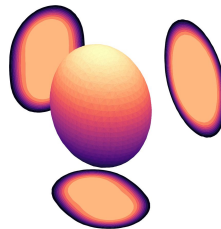


Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
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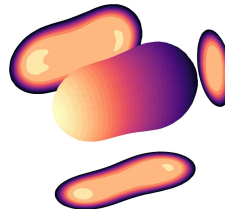
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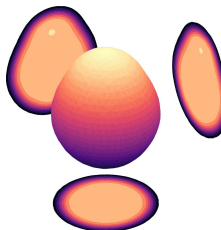
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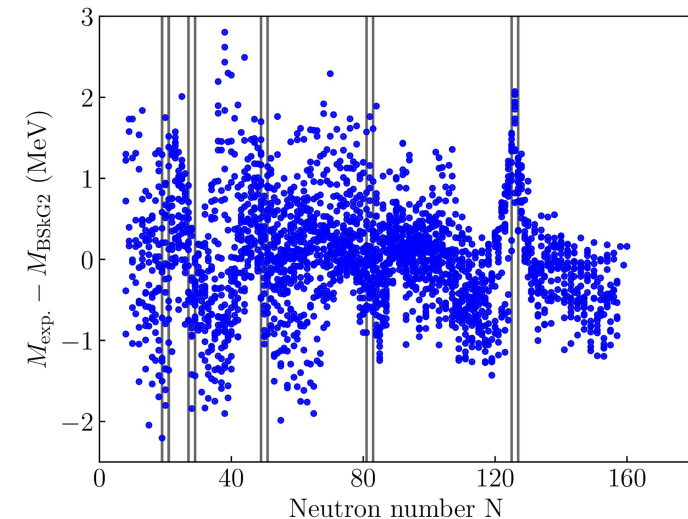


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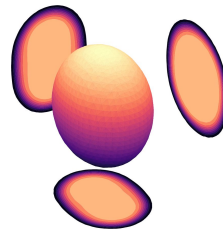


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Brussels-Skyrme-on-a-Grid: BSkG

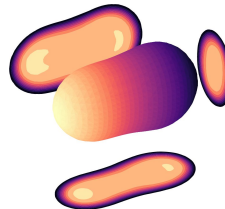
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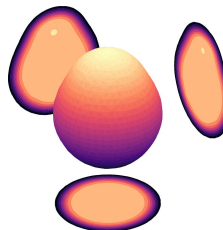
BSkG2 (2022)

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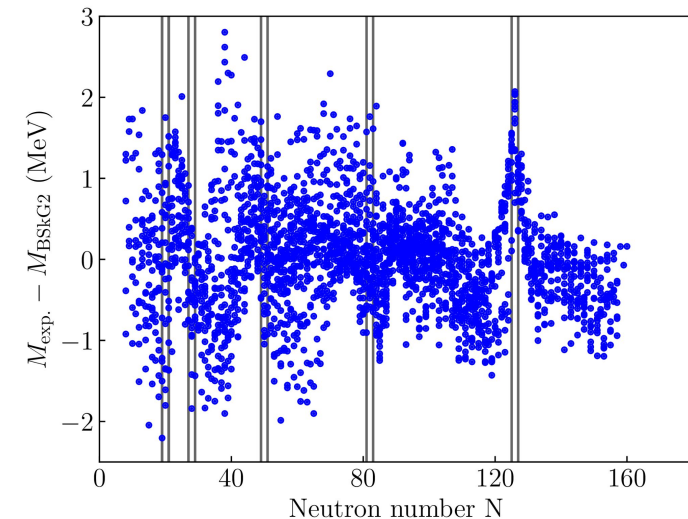


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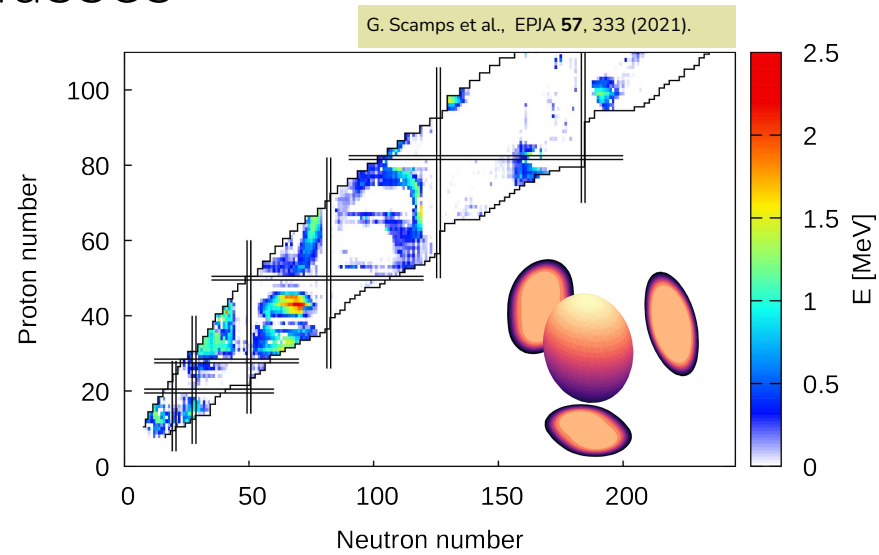


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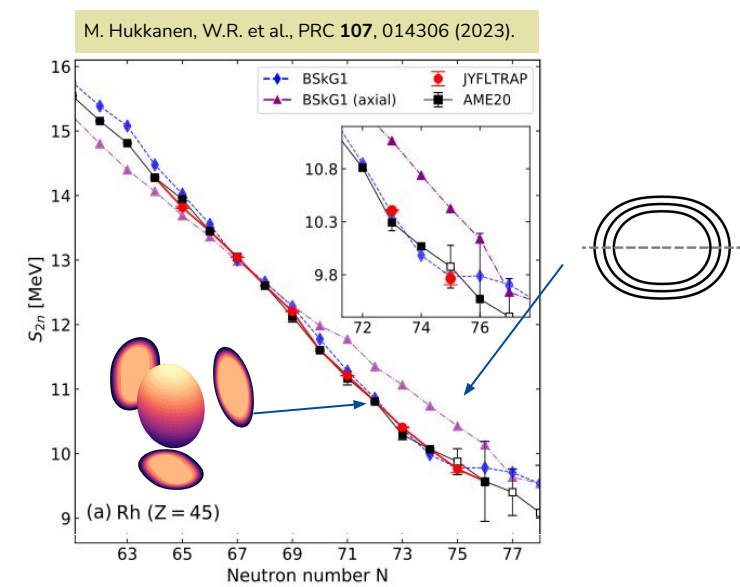
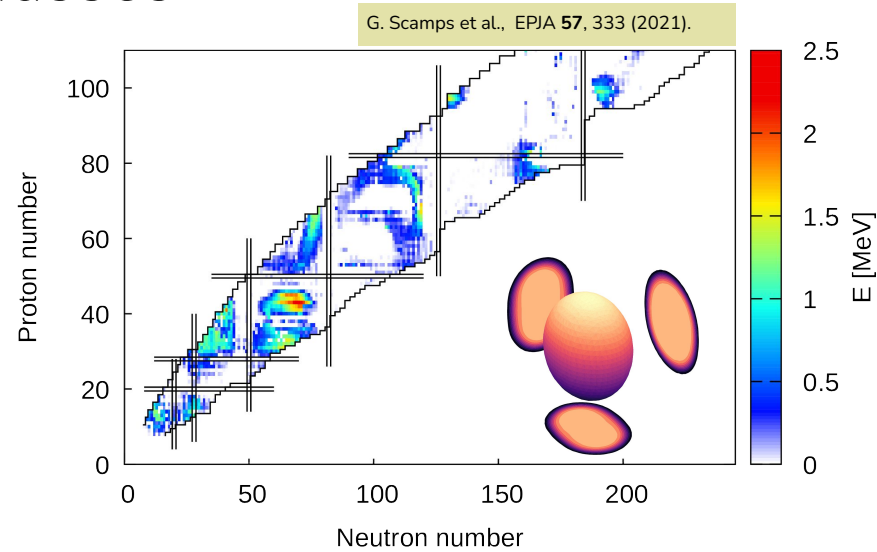
Masses



Triaxial deformation

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

Masses

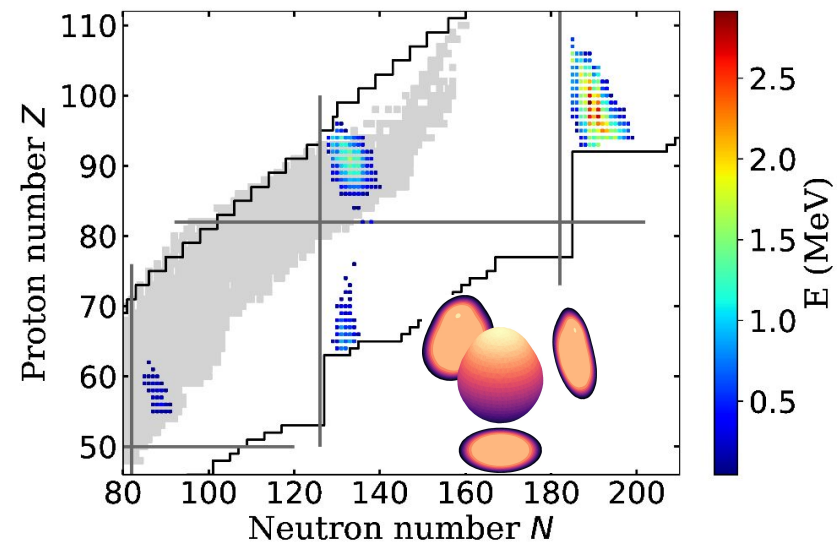


Triaxial deformation

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

Masses

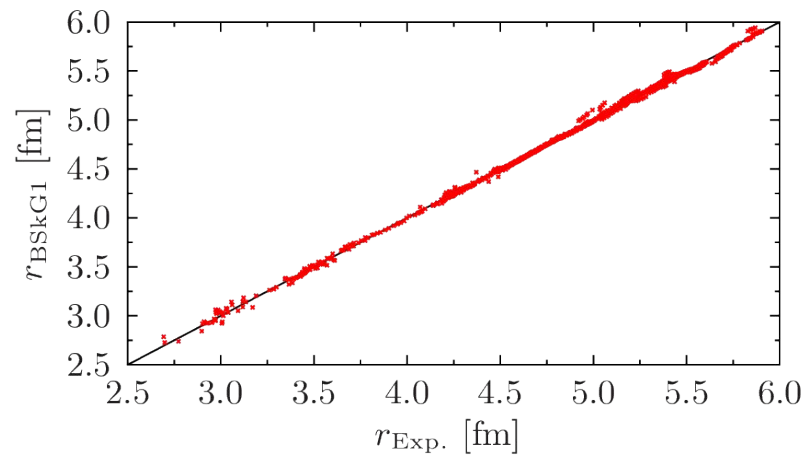
G. Grams et al., EPJA **59**, 270 (2023).



Reflection asymmetry

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

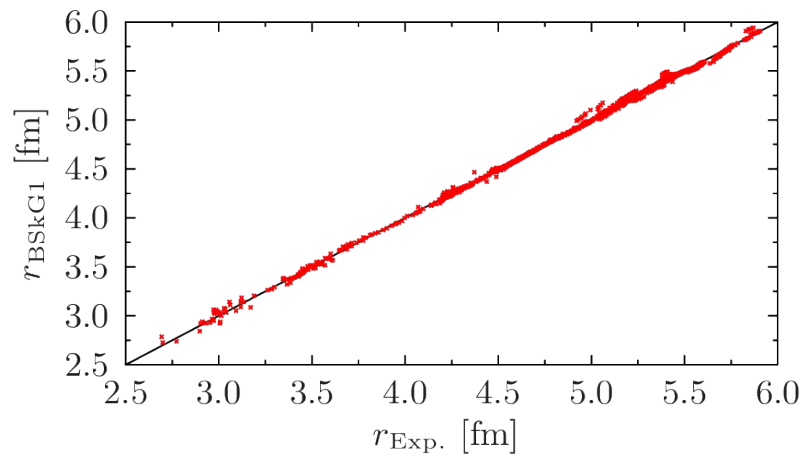
Radii



Systematics and details of charge radii

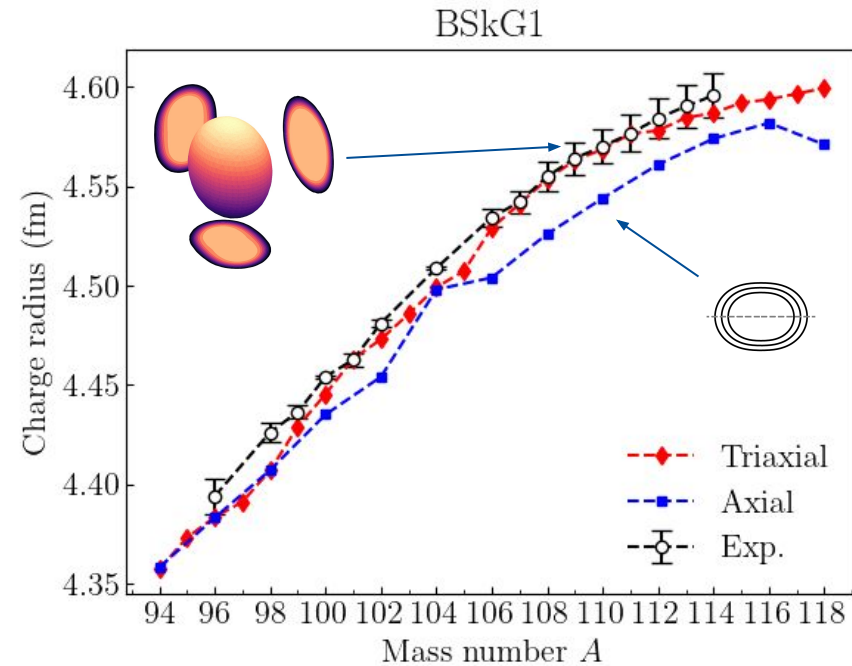
- rms (charge radii) ~ 0.027 fm
- complete charge densities
- ALL deformation affects radii!

Radii



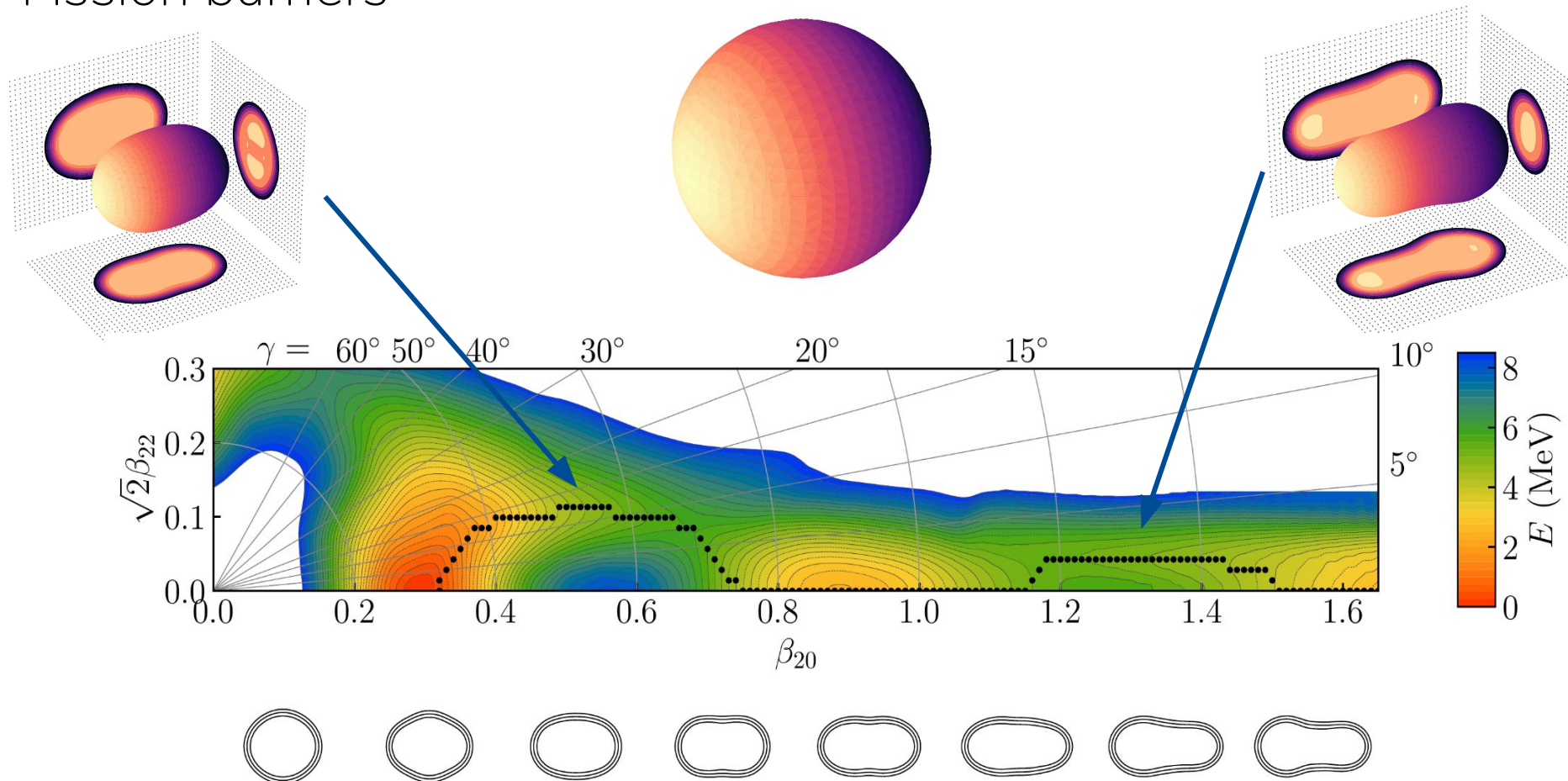
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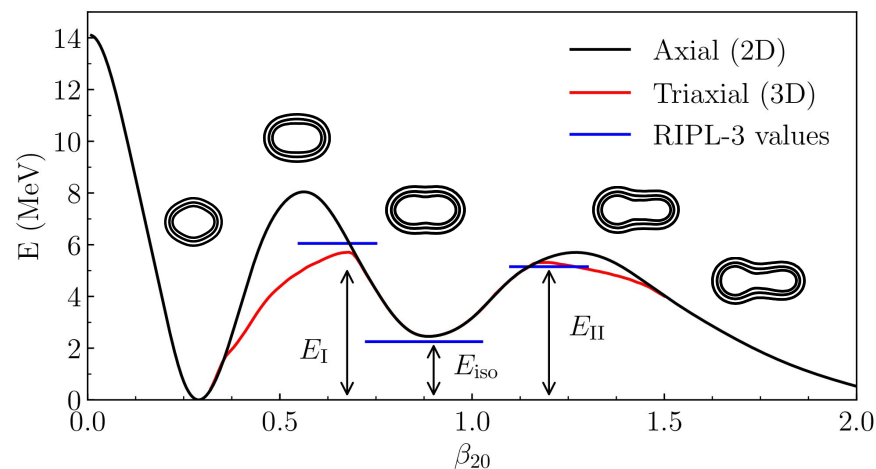


See talk by B. Maaß on Tuesday.

Fission barriers



Fission

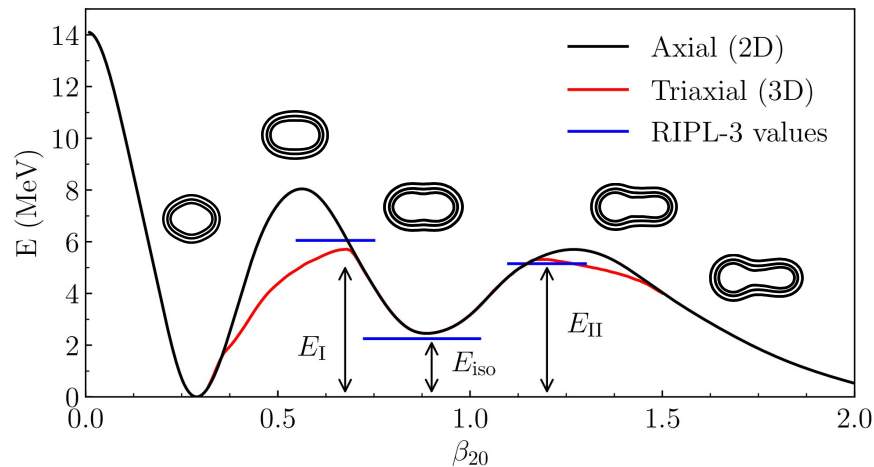


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Fission properties of 45 actinide nuclei

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

Fission



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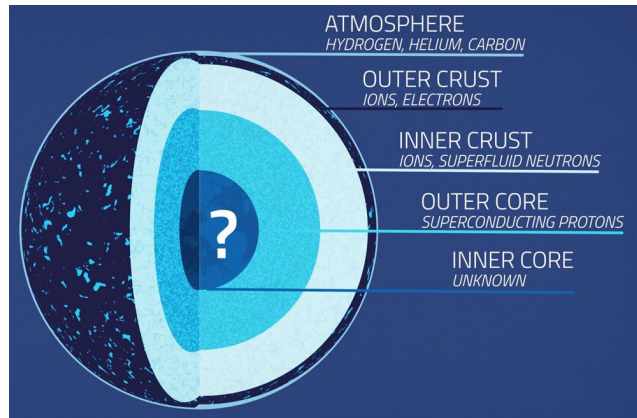
Fission properties of 45 actinide nuclei

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- all outer barriers exploit
 - octupole deformation
 - triaxial deformation

.... to those of **thousands** of nuclei!

- calculations started: G. Grams
- pathfinding: S. Bara
- big effort in code optimisation

Neutron stars

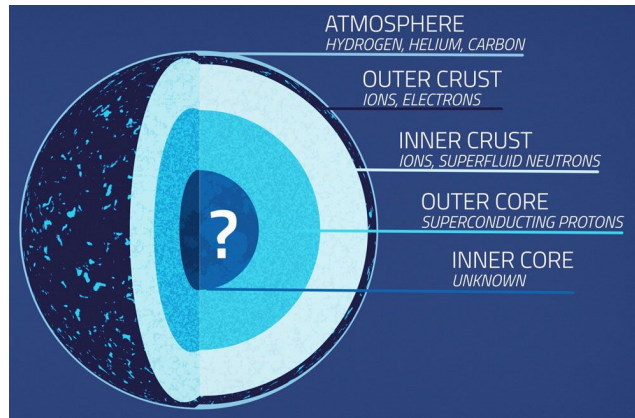


Simulations of crust composition

- does nuclear pasta exist?

Work by N. Shchechilin

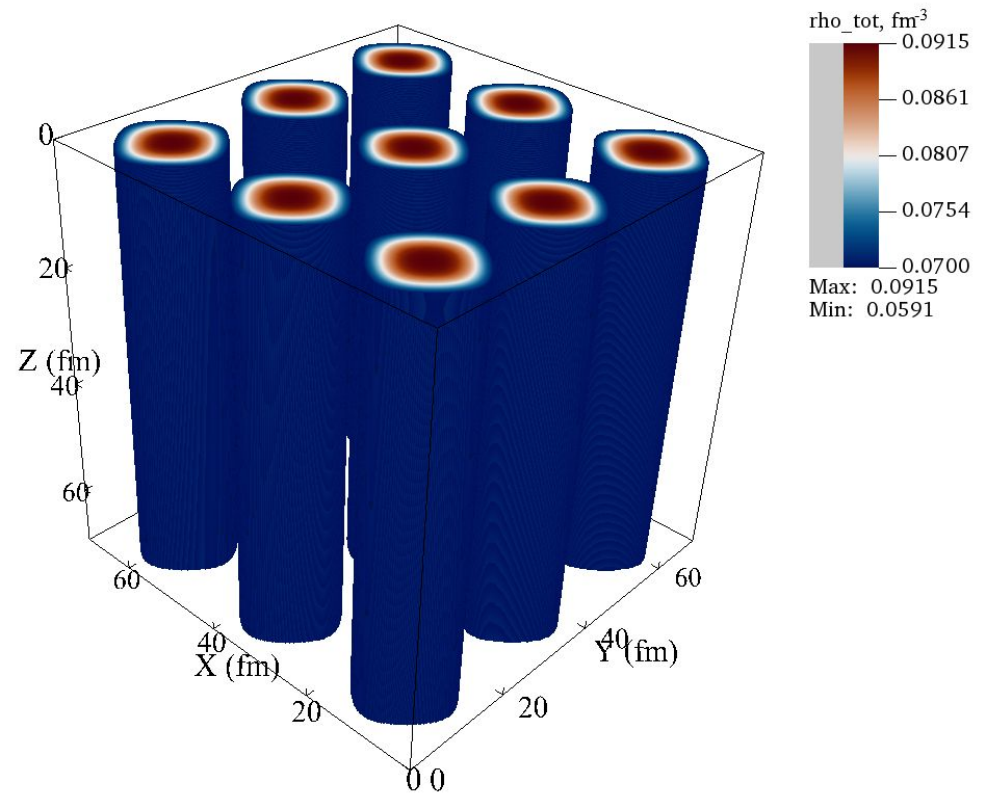
Neutron stars



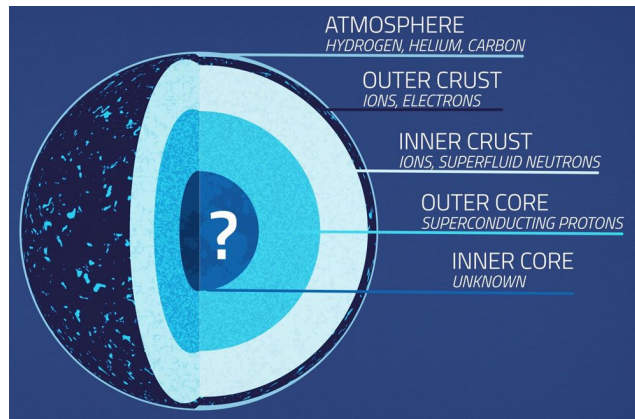
Simulations of crust composition

- does nuclear pasta exist?
- from ~200 to 25000 particles

Work by N. Shchechilin



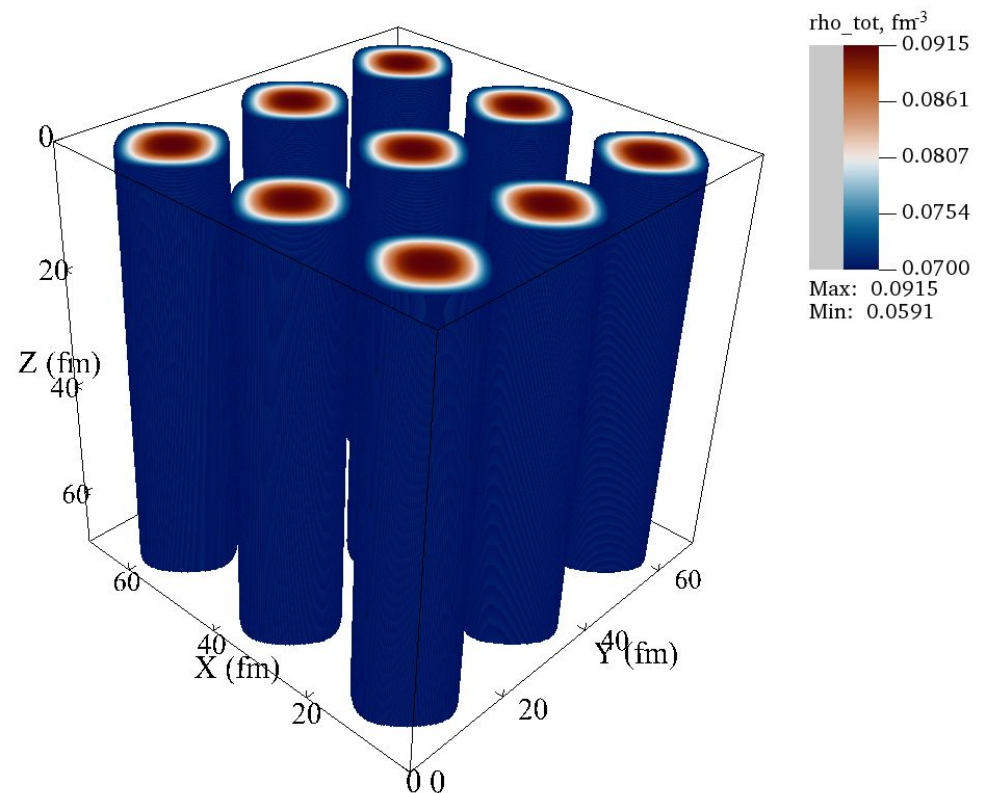
Neutron stars



Simulations of crust composition

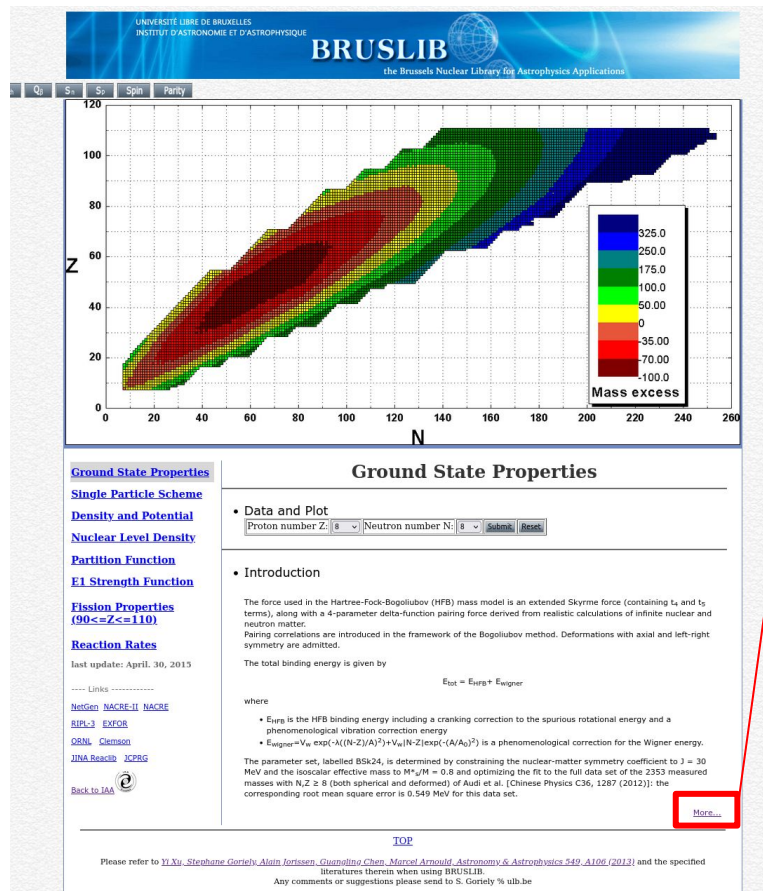
- does nuclear pasta exist?
- from ~200 to 25000 particles
- ... up to 100.000 will be possible!

Work by N. Shchechilin



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

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



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

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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

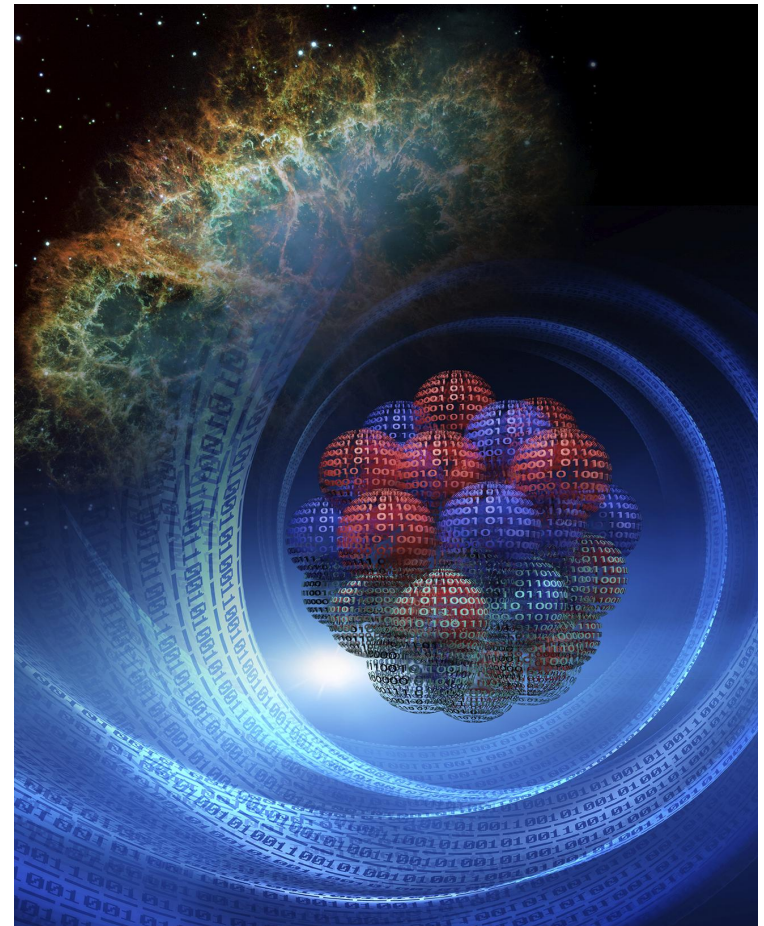
... or check the supplementary material!

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

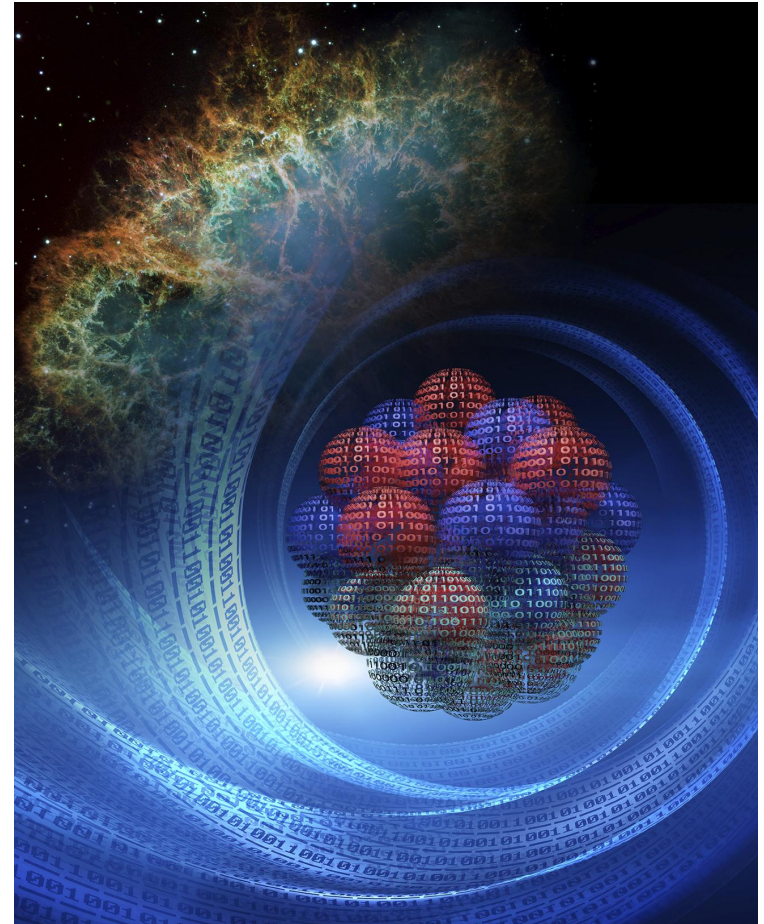
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BSkG3

- 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!



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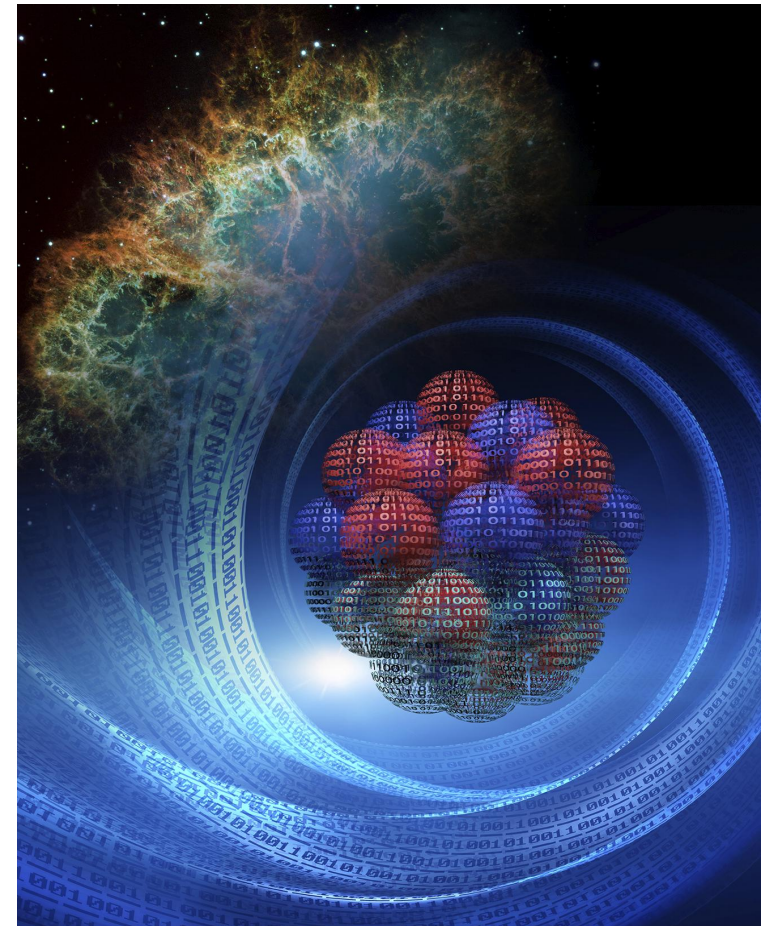
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The immediate future:

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



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Thank you for...

..... all the wonderful work!



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



M. Bender



E. Tijskens



S. Hilaire



S. Bara

+ several experimental teams!

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EuroHPC
Joint Undertaking



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