

Andy Sproles, ORNL

BSkG models versus experiments

Wouter Ryssens

4th of December 2023

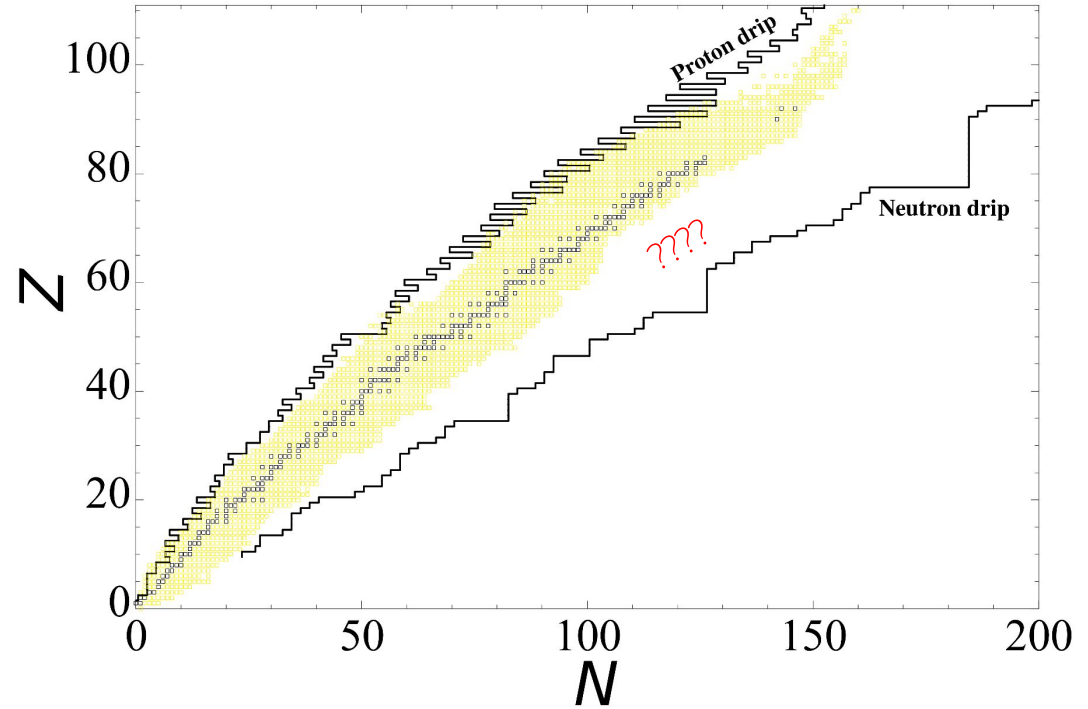


wryssens.com

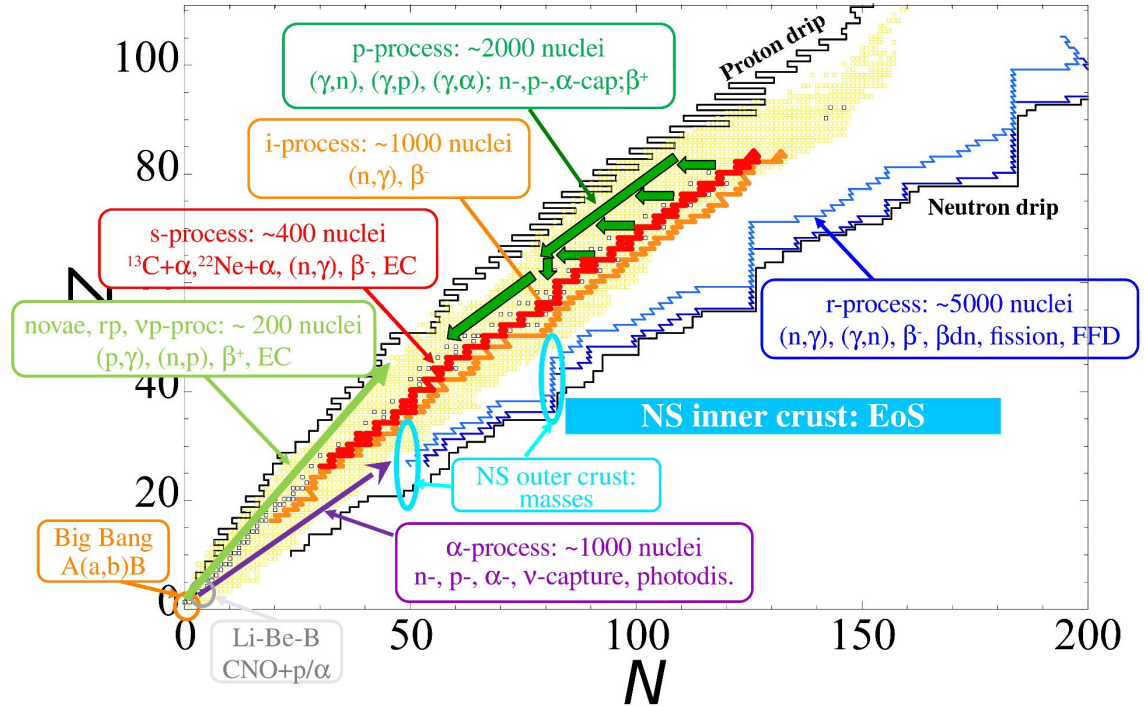
wryssens@ulb.be



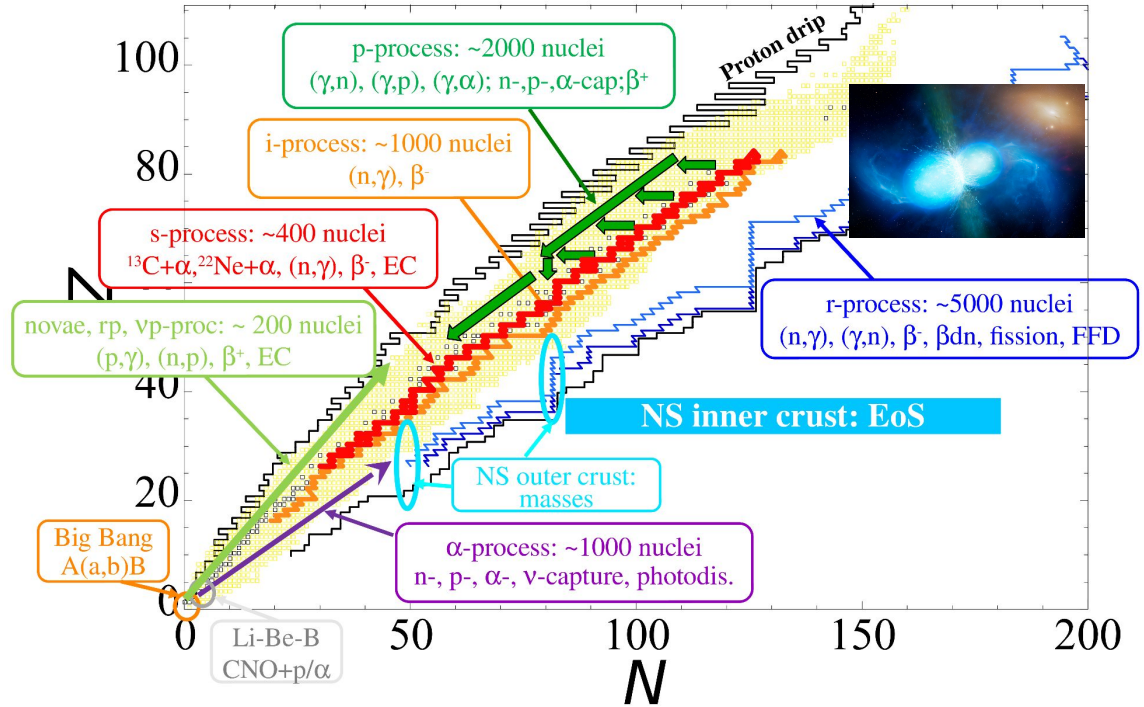
The nuclear chart...



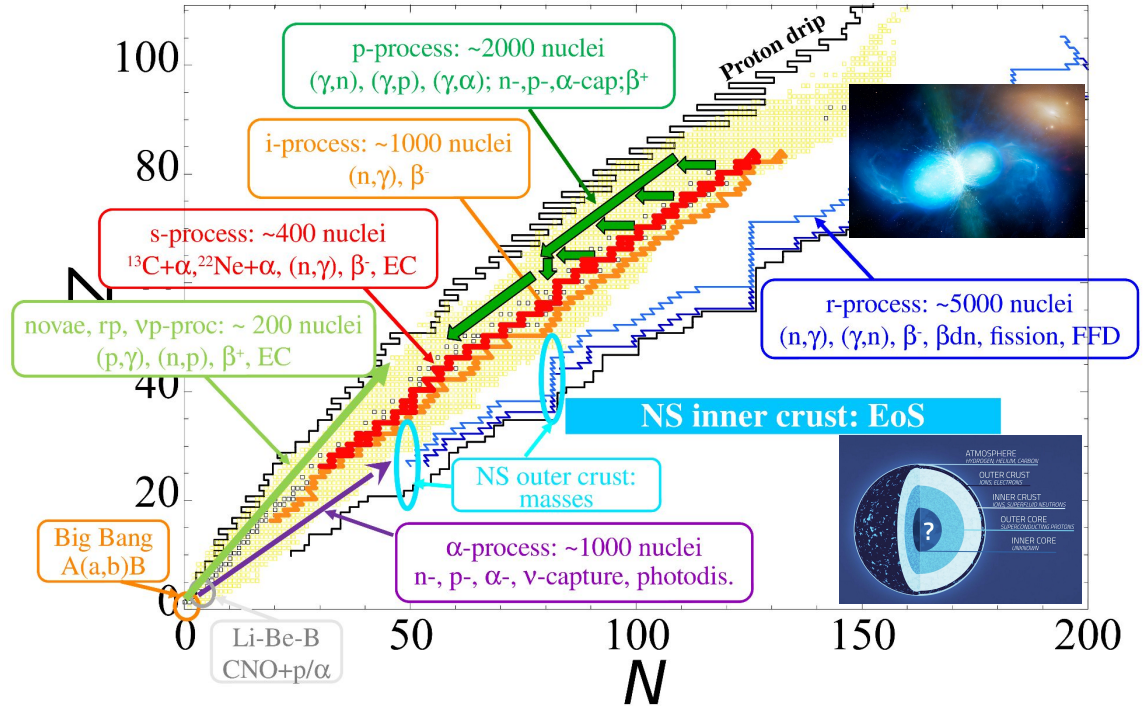
The nuclear chart and the processes traversing it



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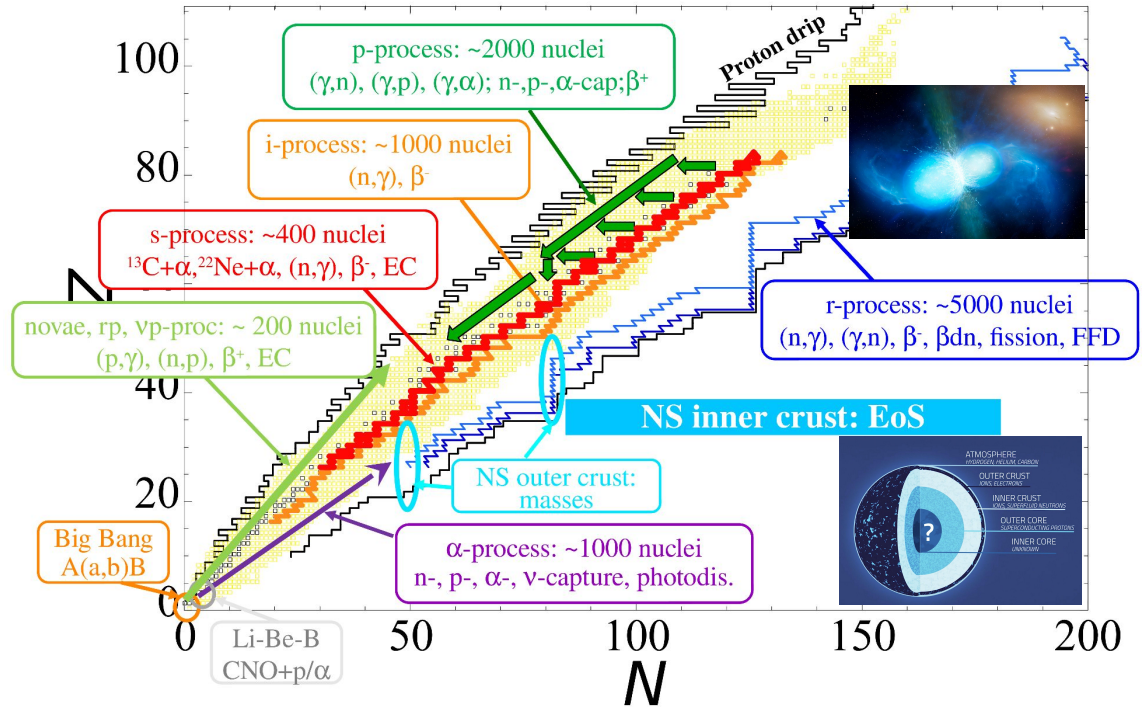


The nuclear chart and the processes traversing it

Extrapolations in N, Z, E, T, ρ, \dots
for ~ 7000 nuclei and **many** reactions!

We need models that should be

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



The nuclear chart and the processes traversing it

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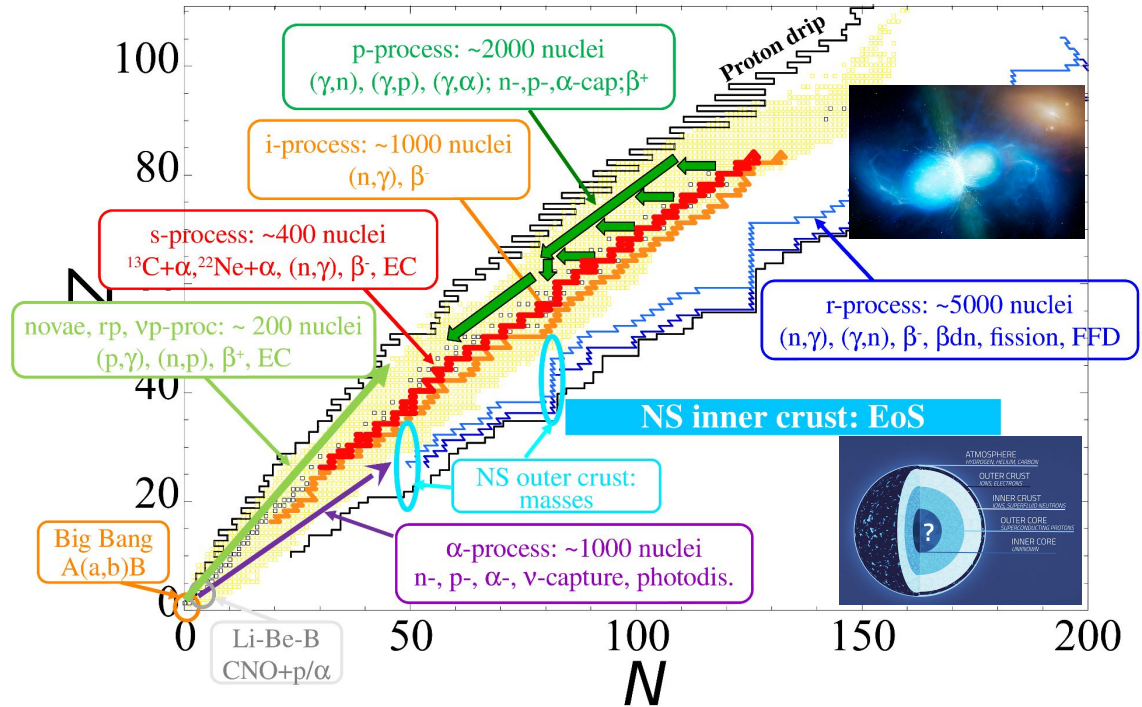
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Energy Density Functional models

- ≈ 25 parameters fitted to data

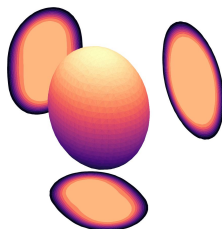
- ✓ based on “in-medium” interaction
- ✓ wavefunctions with nucleons
- ✓ many observables accessible
- ✓ feasible for ~ 7000 nuclei
- ✓ symmetry-breaking \Rightarrow 3D shapes



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).

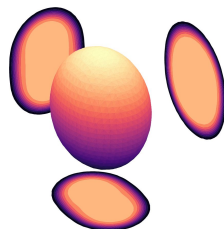
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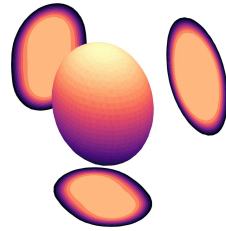
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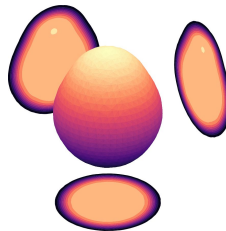
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- larger max. neutron star mass
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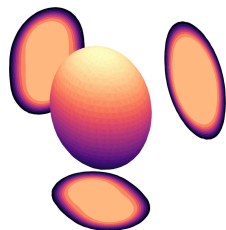
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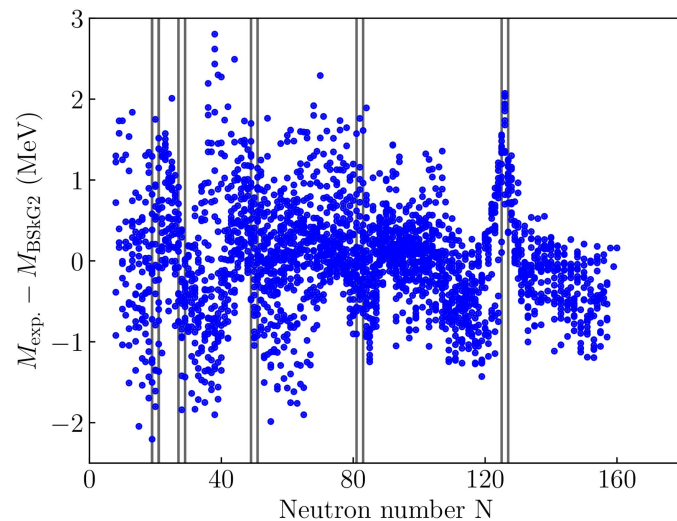
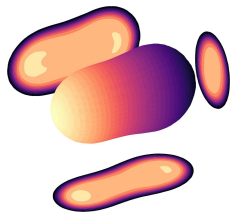
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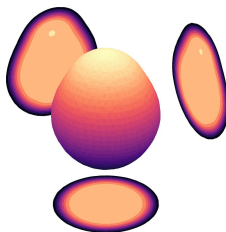
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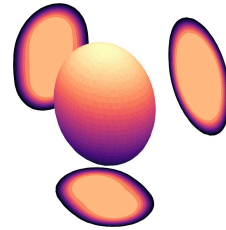
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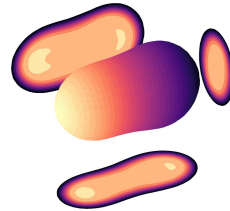
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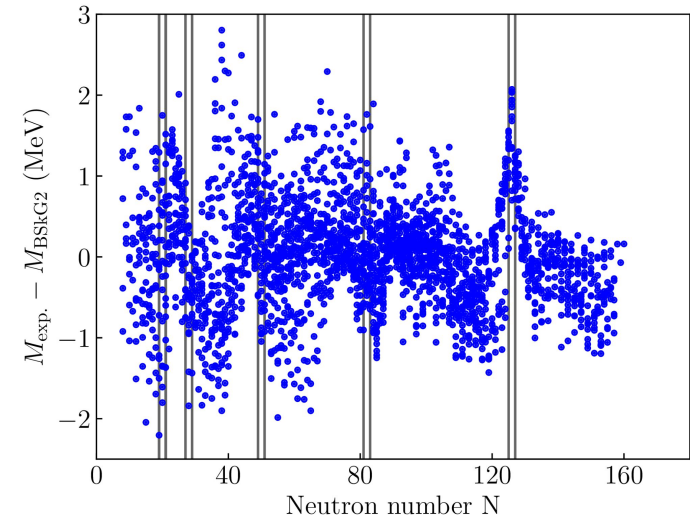
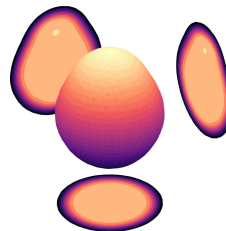
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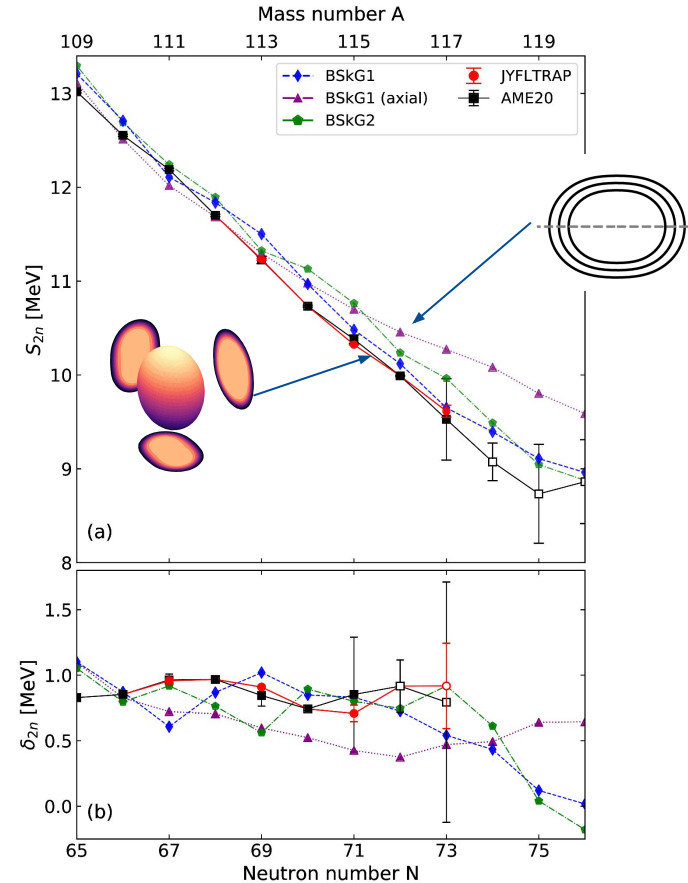


| Rms σ | BSkG1 | BSkG2 | BSkG3 |
|------------------------------|-------|-------|-------|
| Masses [MeV] | 0.741 | 0.678 | 0.631 |
| Radii [fm] | 0.024 | 0.027 | 0.024 |
| Prim. barriers [MeV] | 0.88 | 0.44 | 0.33 |
| Secun. barriers [MeV] | 0.87 | 0.47 | 0.51 |
| Fission isomers [MeV] | 1.0 | 0.49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

Masses

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

M. Hukkanen, W.R. et al., arXiv:2306.04517 [nucl-ex] (2023).



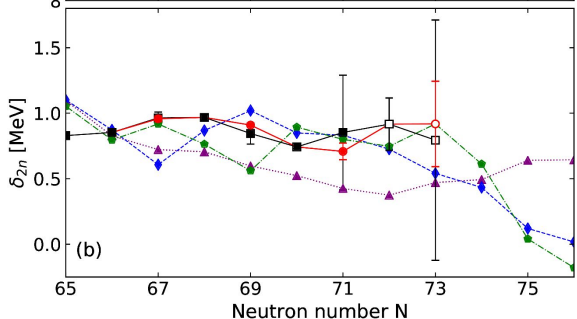
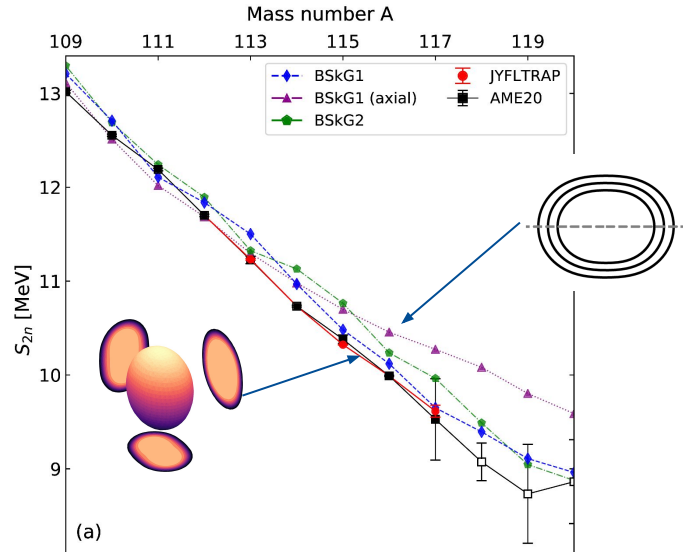
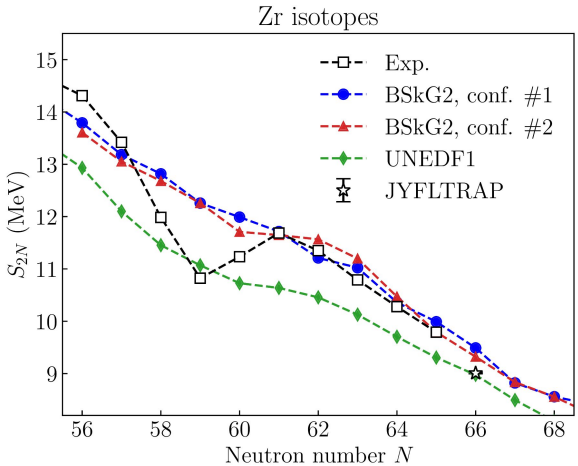
JYFLTRAP mass measurements

- neutron-rich Rh & neutron-rich Ru
 - triaxiality from spectroscopy
 - ... and (indirectly) from masses

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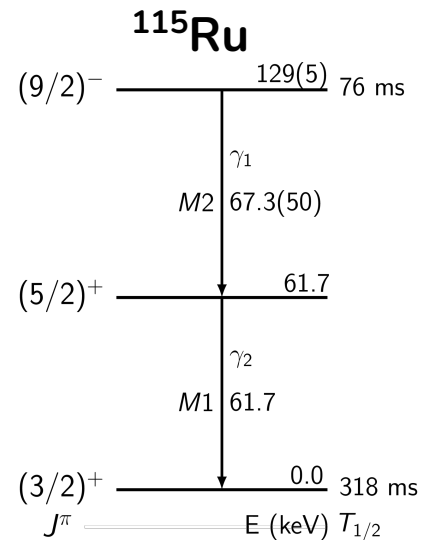
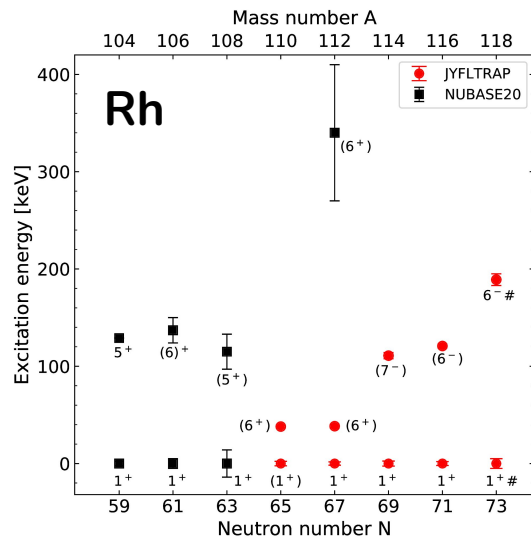
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JYFLTRAP mass measurements

- neutron-rich Rh & neutron-rich Ru
 - triaxiality from spectroscopy
 - ... and (indirectly) from masses
- neutron-rich Y,Zr, Nb, Mo
 - shape coexistence
 - failure to get details right

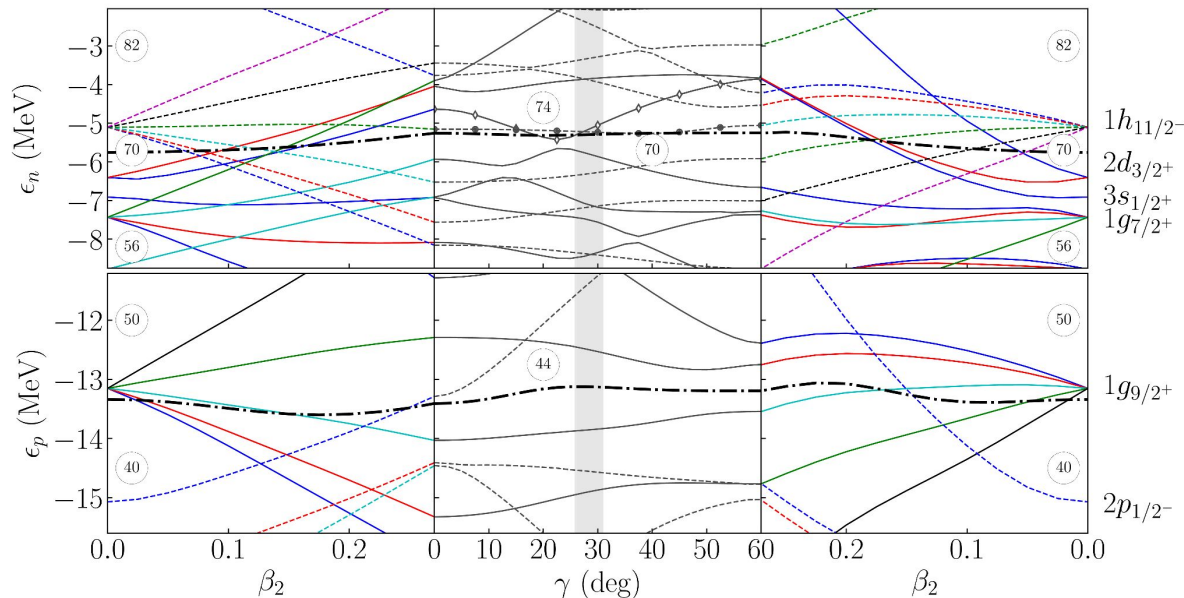
Isomers



..... with Phase-Imaging-ICR!

- massive resolving power for isomers
- set of low-lying isomers in Rh
- new low-lying isomer in Ru

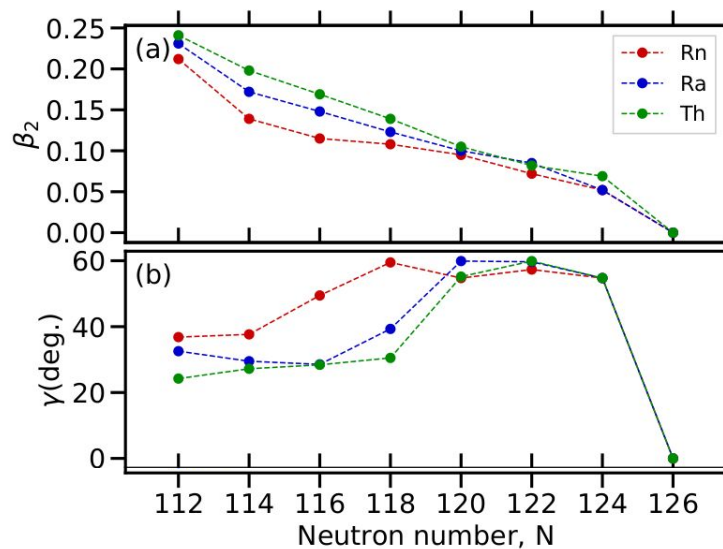
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- qualitatively interpreted with BSkG's!

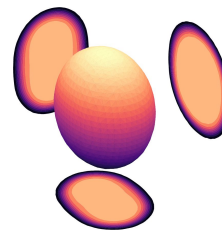
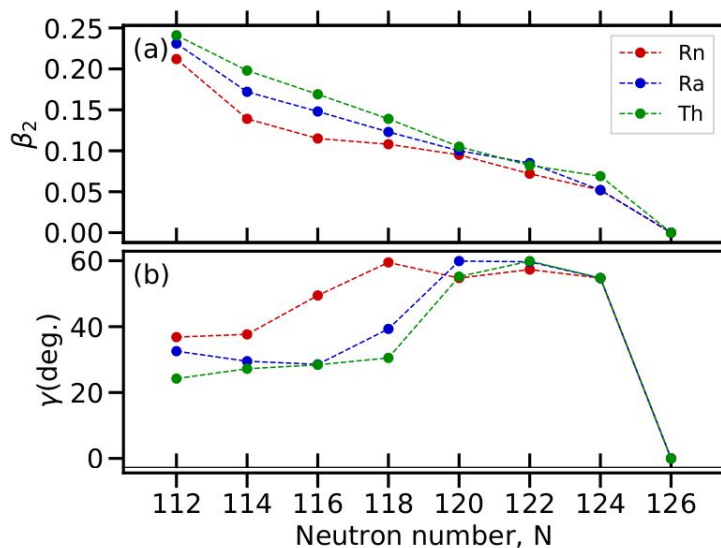
Spectroscopy



Neutron-deficient Radium isotopes

- in-beam γ -ray spectroscopy @ JYFL
- looking for highly-deformed states

Spectroscopy

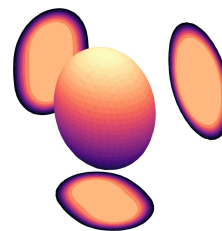
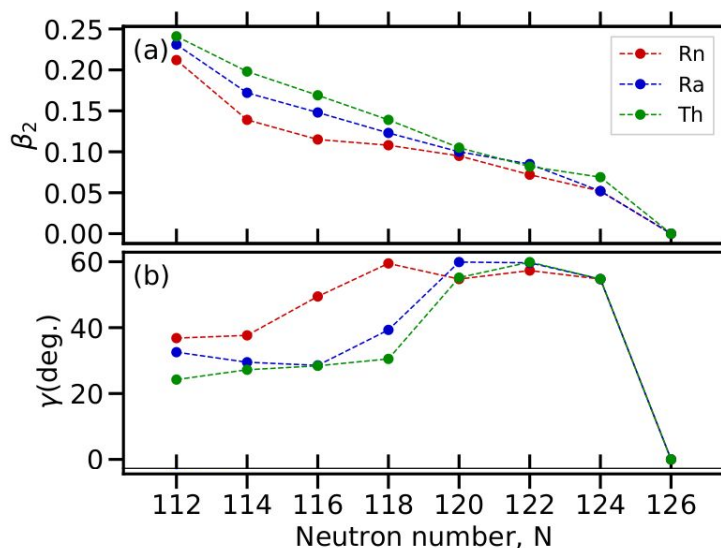


$$+ \hat{H}_{\text{rot}} = \sum_{\mu=x,y,z} \frac{\hat{j}_{\mu}^2}{2\mathcal{I}_{\mu}}$$

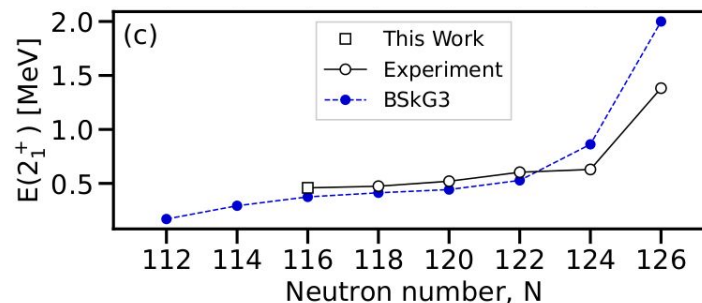
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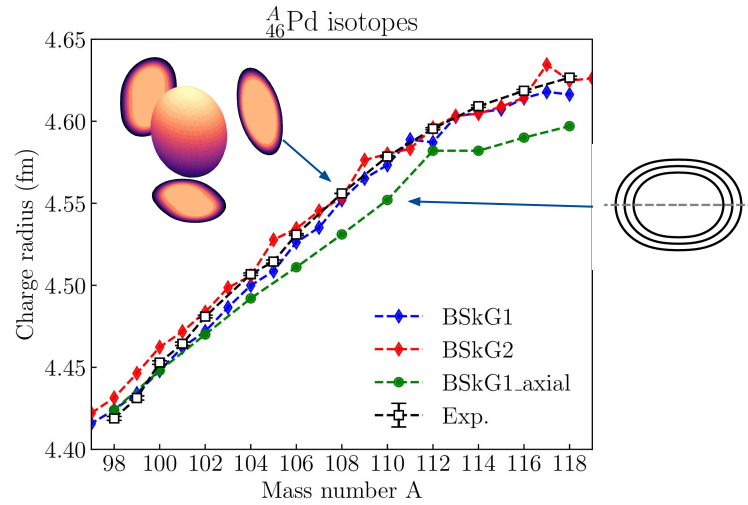
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Neutron-deficient Radium isotopes

- in-beam γ -ray spectroscopy @ JYFL
- looking for highly-deformed states
- no immediate evidence for that
(as predicted by BSkG3!)

Radii

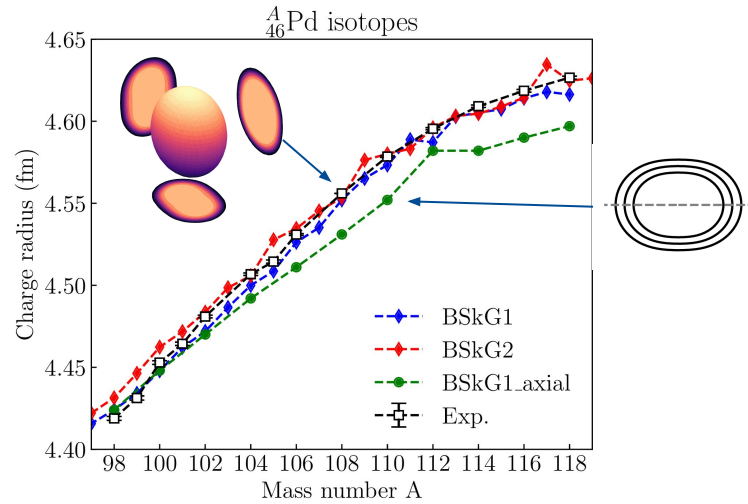


Radii of triaxial nuclei

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

- all deformation impact radii
- not just β_{20} , but also β_{22} , β_{30} , β_{40} , ...!

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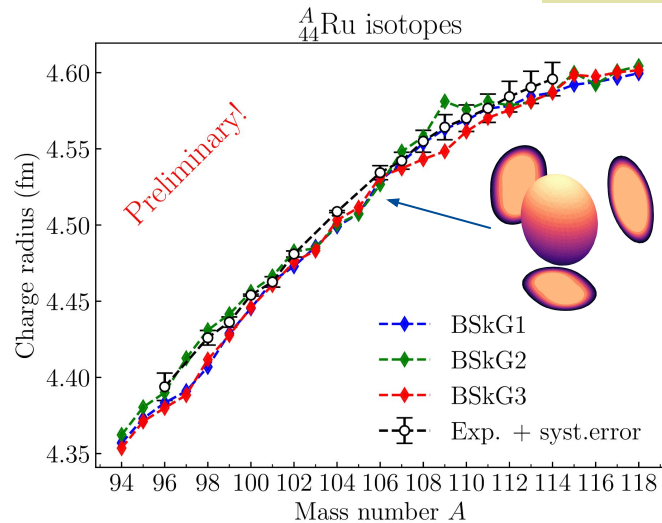
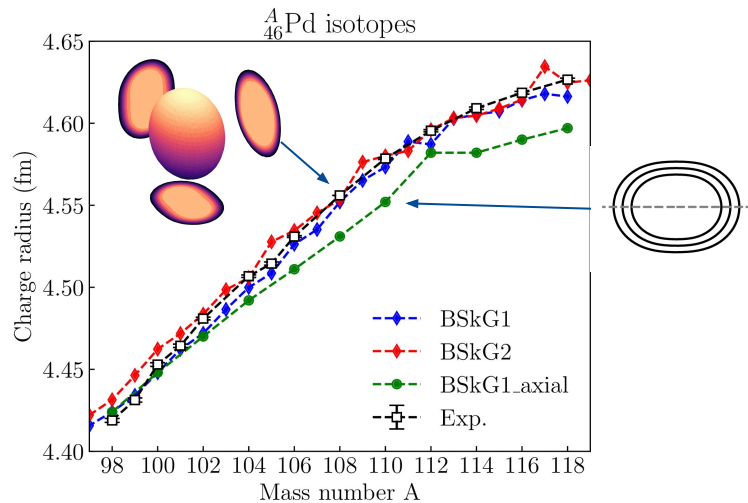


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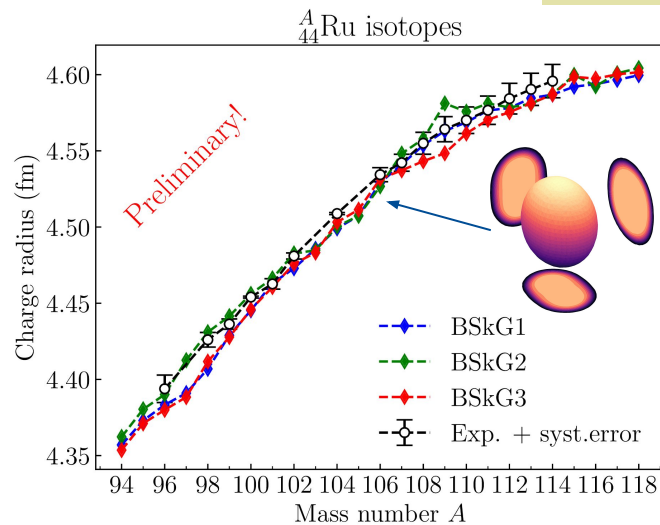
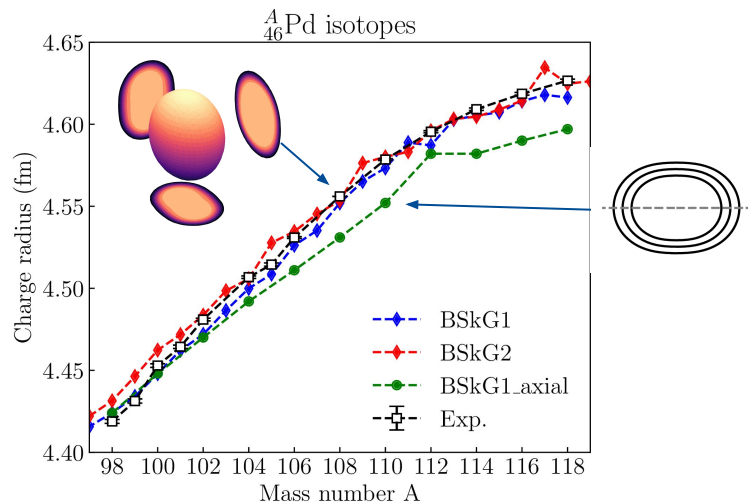


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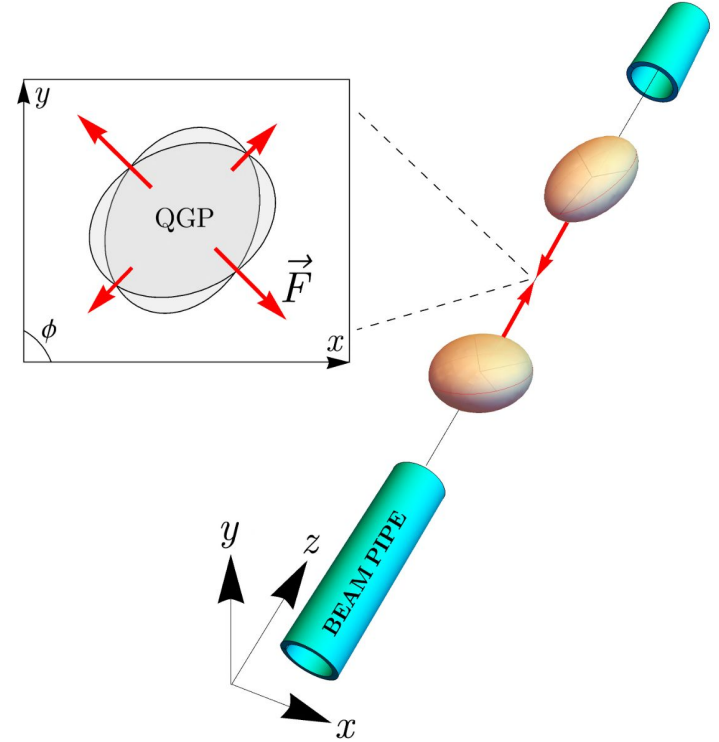
Other projects ongoing

- onset of deformation in Y & Nb chains
- radii of superheavies: Fm

Deformation

Relativistic collisions probe structure

- ^{238}U , ^{197}Au @BNL => deformation
- ^{208}Pb @ CERN => neutron skin



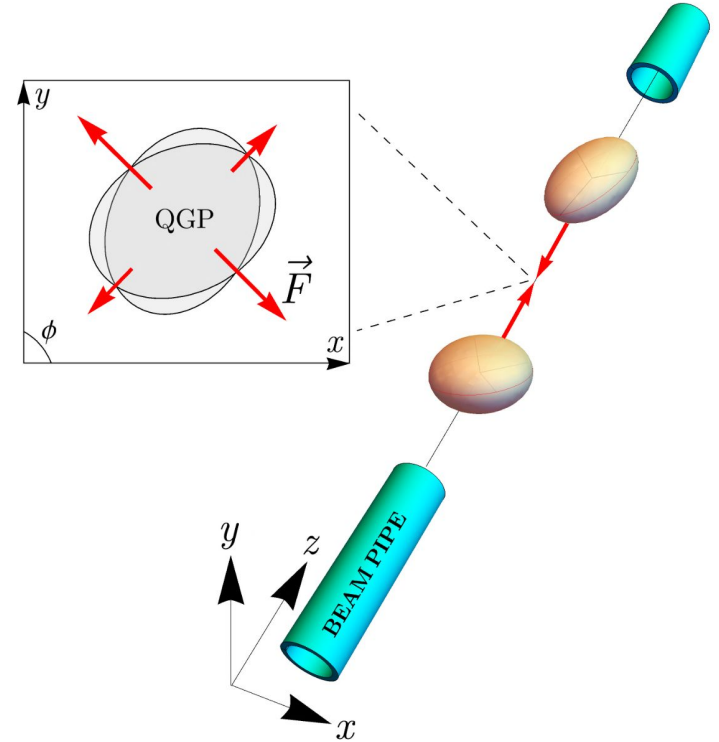
Deformation

$$\rho^{\text{WS}}(\mathbf{r}) = \frac{\rho_0}{1 + \exp([r - R(\theta, \phi)]/a)},$$

$$R(\theta, \phi) = R_d \left[1 + \sum_{\ell=2}^{\ell_{\text{max}}} \sum_{m=-\ell}^{\ell} \beta_{\ell m}^{\text{WS}} Y_{\ell m}(\theta, \phi) \right],$$

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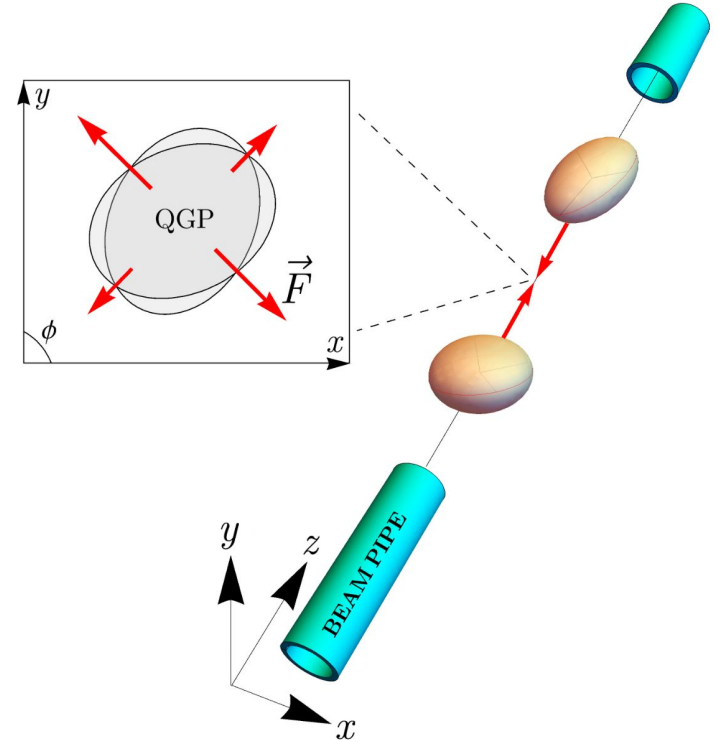
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 - Wood-Saxon parameterisation
 - with naive input from B(E2) rates



Deformation

Volume deformation

$$\beta_{20} = \frac{R_d^2}{R_0^2} \left[\beta_{20}^{\text{WS}} + \frac{2}{7} \sqrt{\frac{5}{\pi}} (\beta_{20}^{\text{WS}})^2 + \frac{12}{7\sqrt{\pi}} \beta_{20}^{\text{WS}} \beta_{40}^{\text{WS}} \right],$$

Surface deformation

... but this misses low-energy physics!

- low-energy experiments measure **volume deformation!**

Deformation

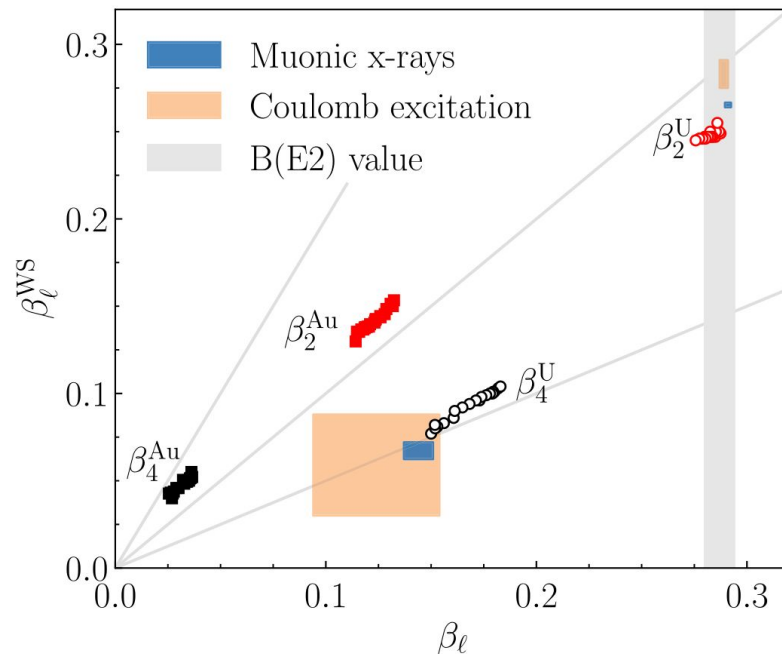
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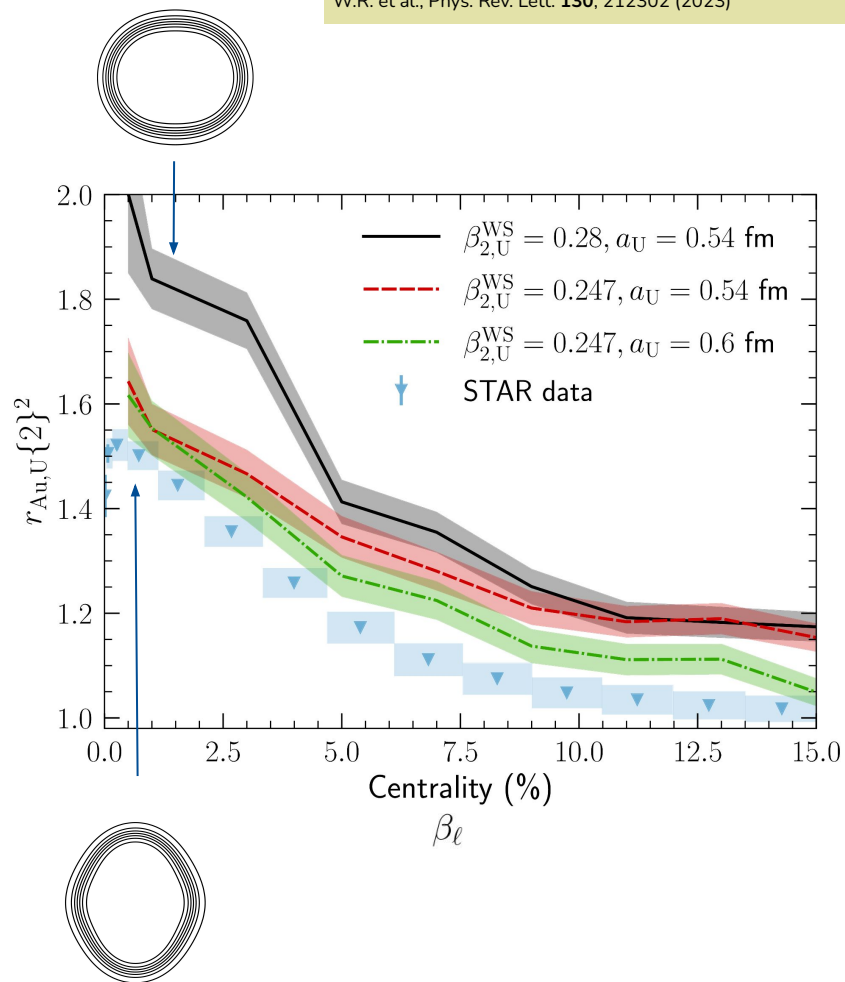
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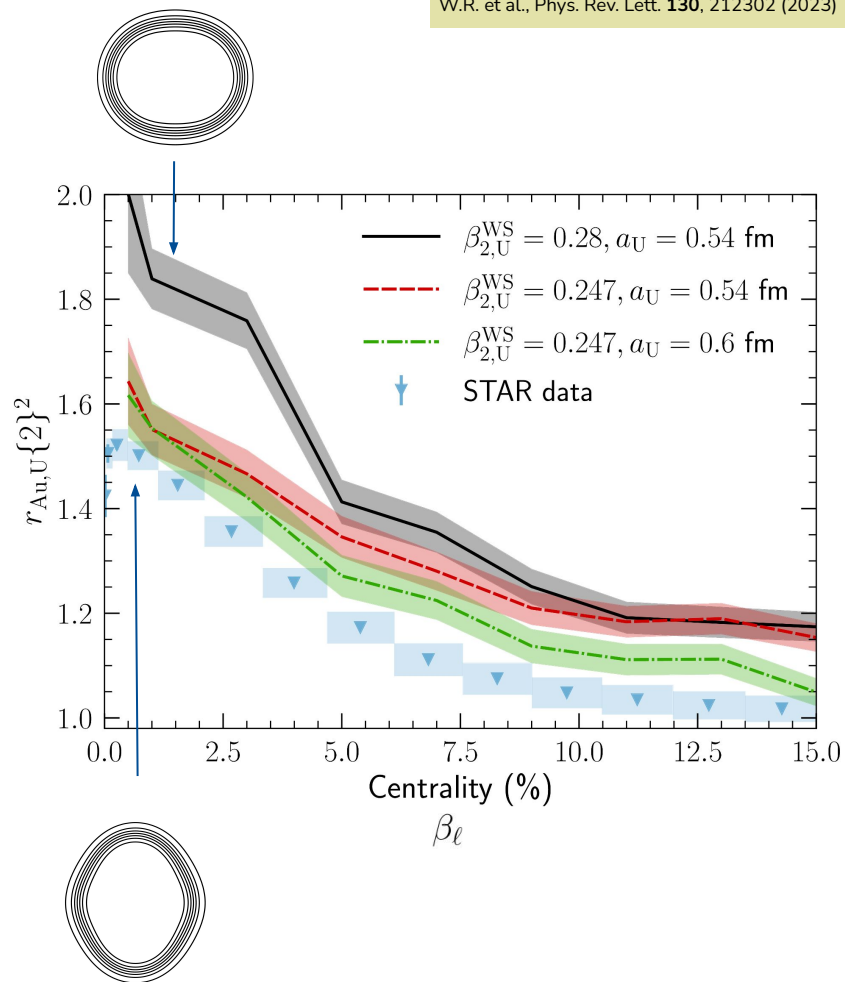
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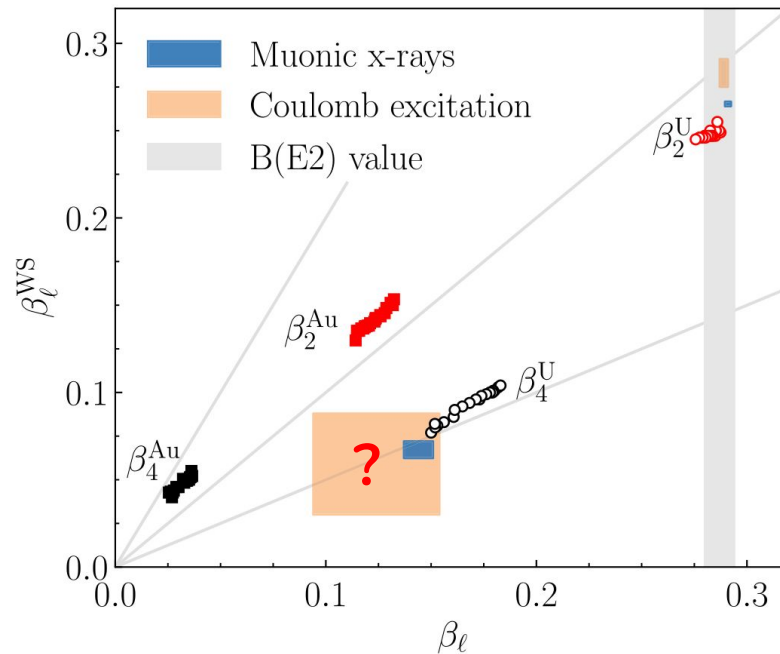
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Surface deformation

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- First evidence of β_{40} deformation
- What will the future bring?

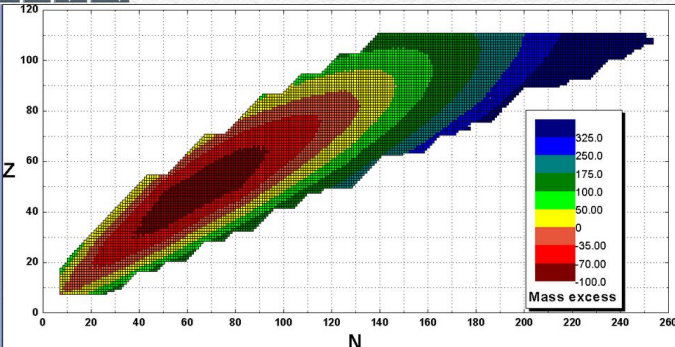


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[Single Particle Scheme](#)

[Density and Potential](#)

[Nuclear Level Density](#)

[Partition Function](#)

[F1 Strength Function](#)

[Fission Properties \(90<=Z<=110\)](#)

[Reaction Rates](#)

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Ground State Properties

• **Data and Plot**

• **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
- $E_{\text{Wigner}} = V_p \exp(-\lambda|(N-Z)/A|^\lambda) + N_p(N-Z) \exp(-\lambda(A_p)^2)$ is a phenomenological correction for the Wigner energy.

The parameter set, labelled BSs24, is determined by constraining the nuclear-matter symmetry coefficient to $J = 30$ 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.

More...

[TOP](#)

Please refer to [Yi Xu, Steenhart Goriely, Alain Fortson, Chuanqiang Chen, Marcel Arnould, Astronomy & Astrophysics 549, A106 \(2012\)](#) and the specified literatures therein when using BRUSLIB.

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

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Q. S. Spin Parity

Ground State Properties

Single Particle Scheme
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E1 Strength Function
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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
- $E_{\text{Wigner}} = V_p \exp(-N(Z/A)^2) + N_n(N-Z) \exp(-N(A_n)^2)$ is a phenomenological correction for the Wigner energy.

The parameter set, labelled BSk24, is determined by constraining the nuclear-matter symmetry coefficient to $J = 30$ 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, Guangling Chen, Marcel Arnould, *Astronomy & Astrophysics* 549, A166 (2012) and the specified literature therein when using BRUSLIB.

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

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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.

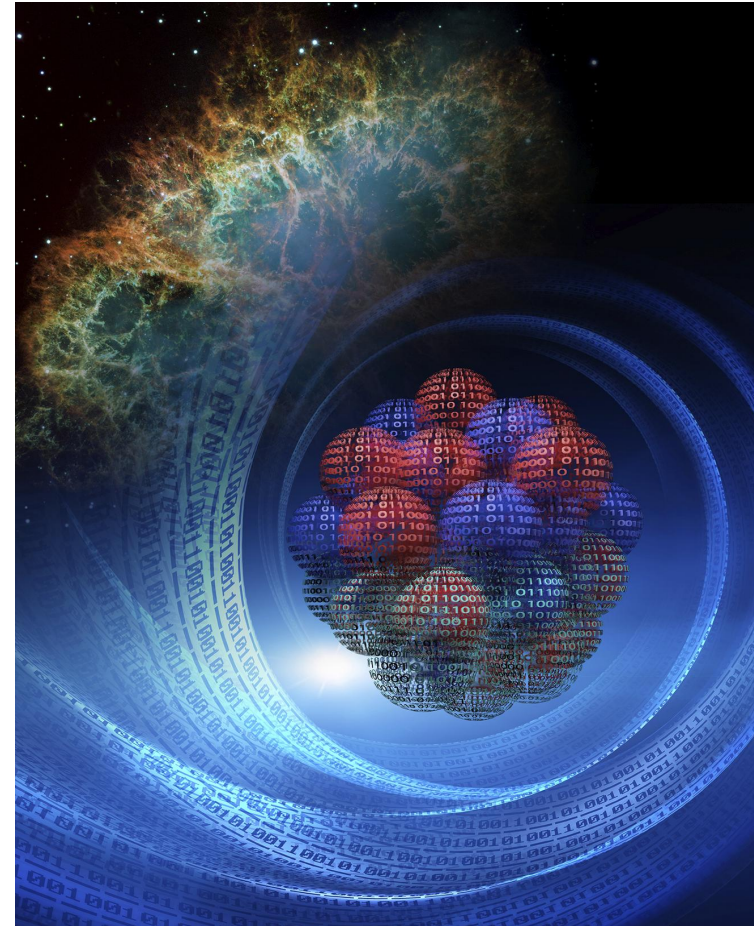
Available right now for BSkG3:

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

Conclusion

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

The interplay theory \leftrightarrow experiment is crucial,
... and this is something we invest in!

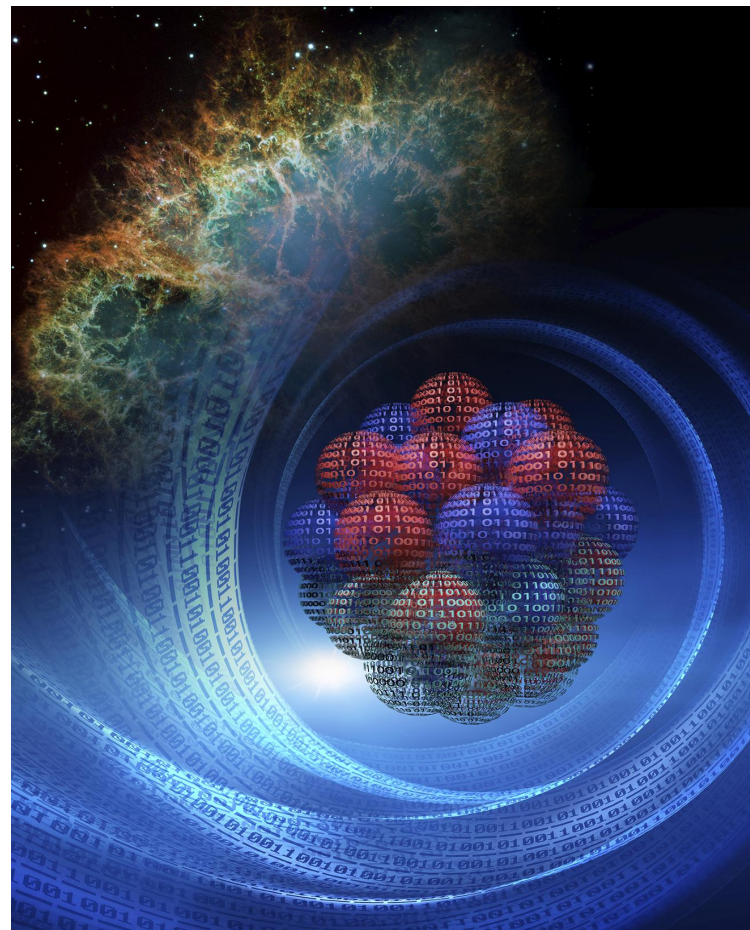


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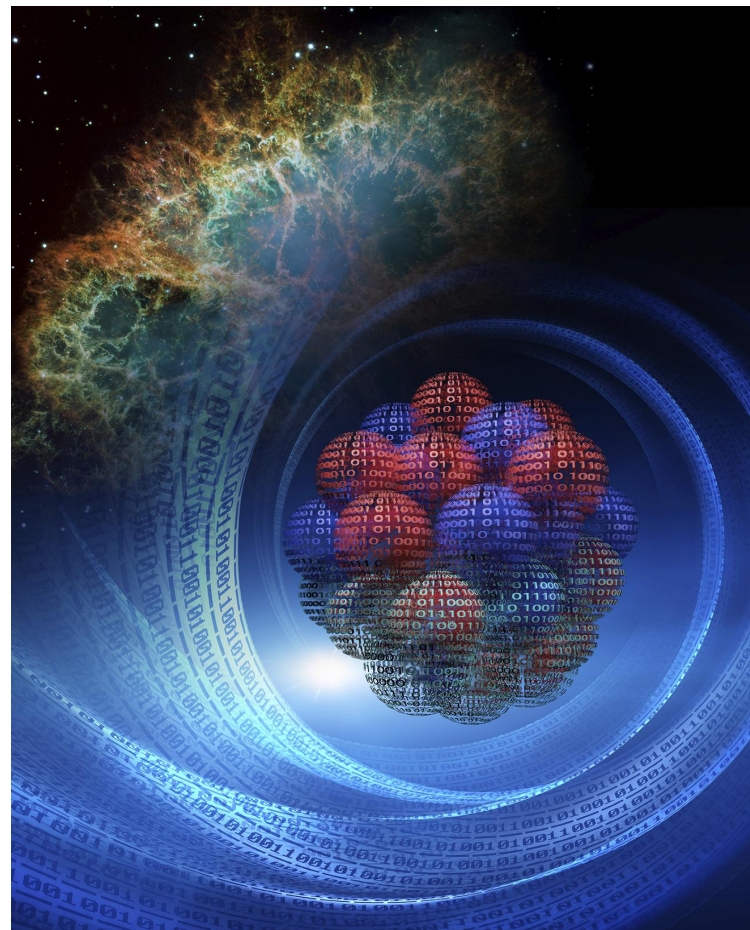
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Coming up soon for comparison:

1. level densities
2. repository of nuclear level densities
3. fission properties \Rightarrow S. Bara



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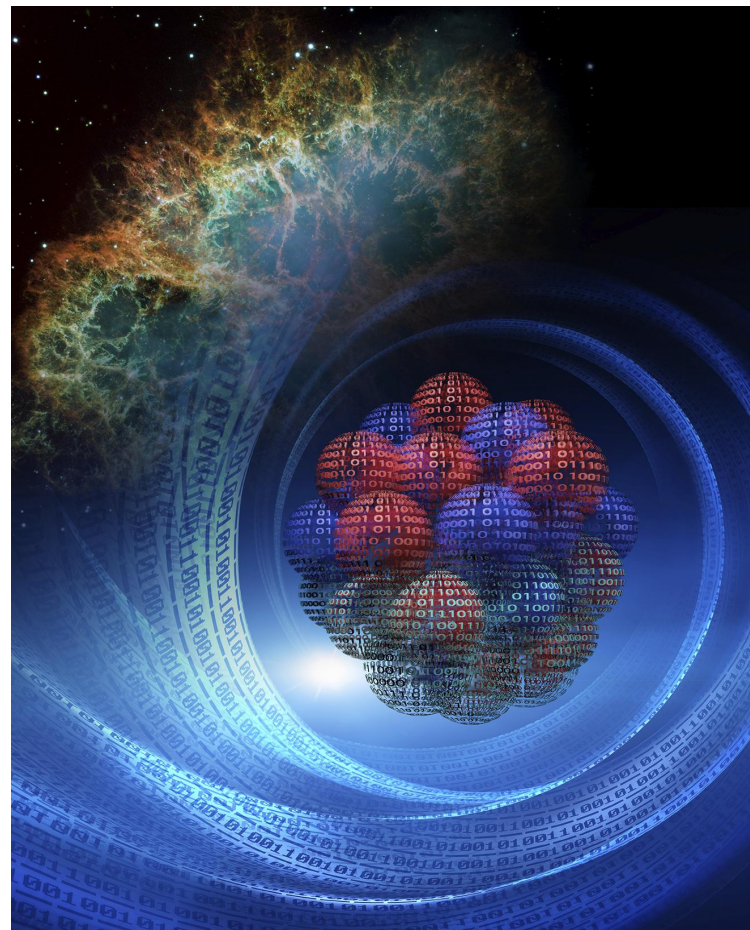
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Other exciting things:

1. BSkG4 \Rightarrow G. Grams
2. Neutron stars \Rightarrow N. Shchechilin, C. Mondal



Thank you for...

..... all the wonderful work!



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



M. Bender



G. Scamps



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..... the computing time!



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