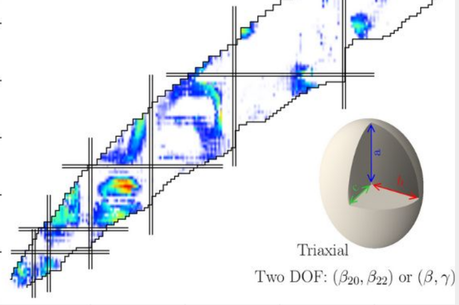
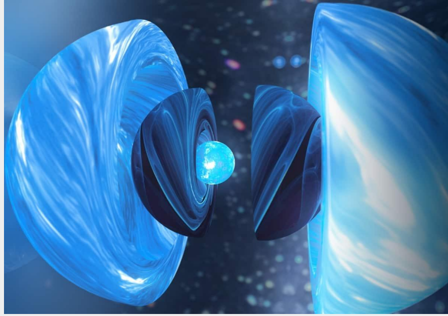




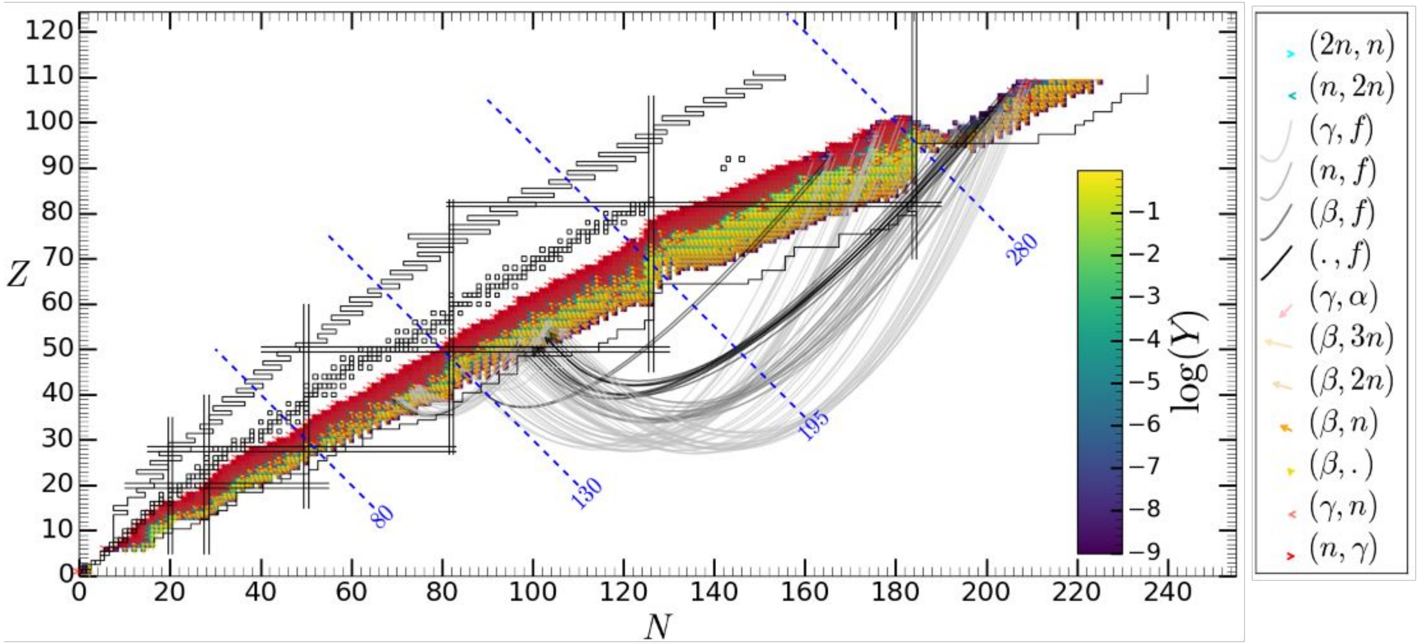
Nuclear models based on energy density functional for astrophysics applications

Guilherme Grams,
W. Ryssens, N. Shchechilin, G. Scamps,
S. Goriely and N. Chamel
Astronomy and Astrophysics Institute (IAA) - ULB

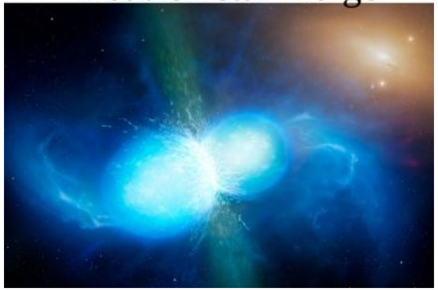
**The 11th International Symposium
on Nuclear Symmetry Energy,
Darmstadt - 20/09/23**

Motivation

r-process nucleosynthesis



Neutron star merger

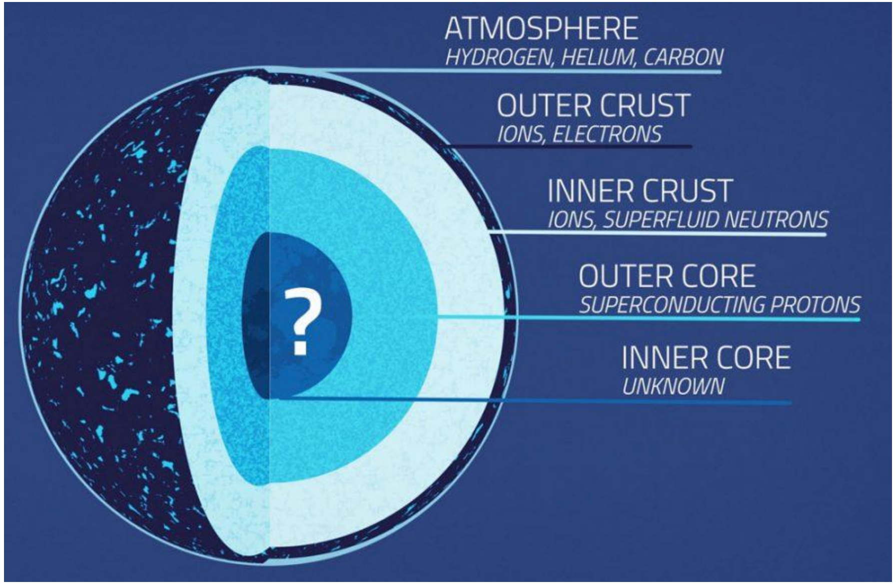


Supernova explosion

Description of **nuclear masses** and **fission** paths in *experimentally unknown* regions.

Motivation

Neutron star physics



Credit image: NASA's Conceptual Image Lab

Nuclear physics inputs:

- **nuclear masses** for the neutron star (NS) crust;
- **infinite nuclear matter (INM) properties** for the NS core and neutron fluid in the inner crust.

Skyrme Energy Density Functional (EDF)

Energy

Coupling constants

Local densities ρ and kinetic density τ of a HFB state

$$E = \boxed{C_1(\rho)}\rho^2 + \boxed{C_2}\rho\tau + \boxed{C_3}\nabla\rho\nabla\rho + \ldots$$

Skyrme Energy Density Functional (EDF)

Energy

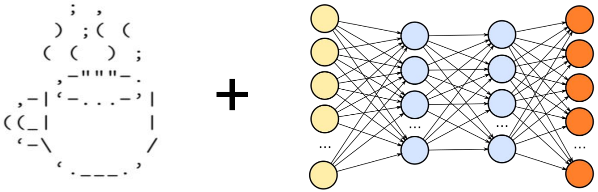
Coupling constants

Local densities ρ and kinetic density τ of a HFB state

$$E = \boxed{C_1(\rho)}\rho^2 + \boxed{C_2}\rho\tau + \boxed{C_3}\nabla\rho\nabla\rho + \dots$$

Brussels-Skyrme-on-a-grid (BSkG)

- Solve HFB equations with MOCCa code;
- fitted to essentially all experimental masses;
- constraints on infinite nuclear matter properties;
- machine learning to accelerate the fit.

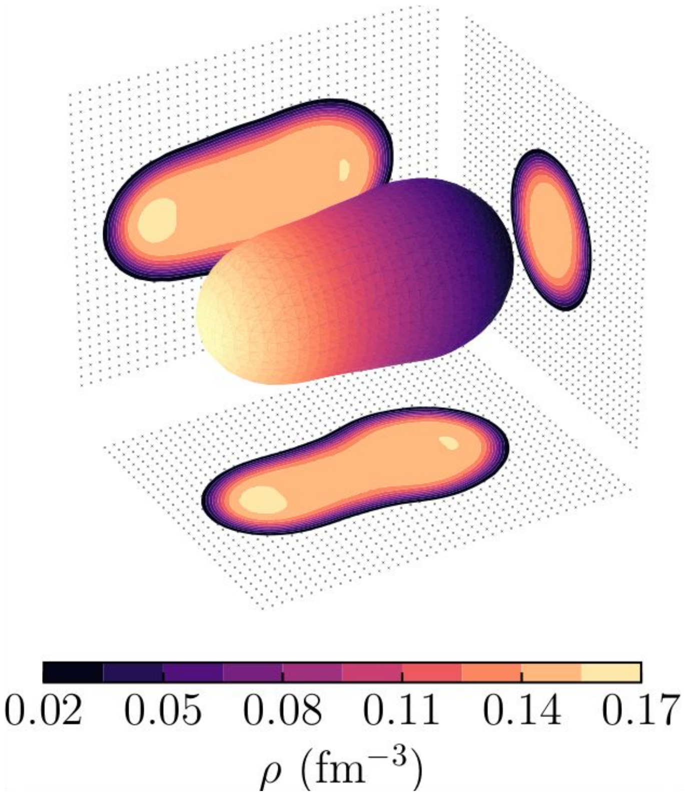


The BSk**G** functionals

- HFB code based coordinate space in 3D mesh -> MOCCa code;
- better control of numerical accuracy;
- improve the description of **deformed nuclei** .

EPJA **57**, 333 (2021)

EPJA **58**, 246 (2022)



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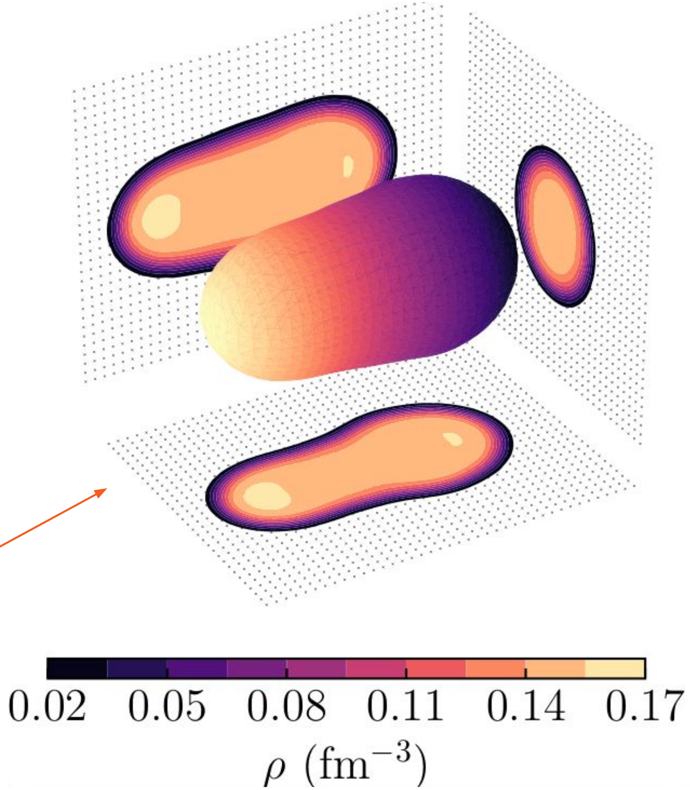
EPJA **57**, 333 (2021)

EPJA **58**, 246 (2022)

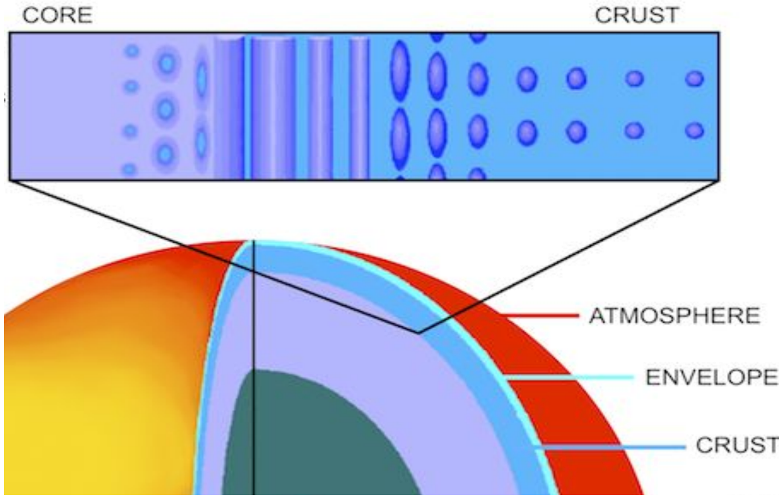


Elongated shape of ^{240}Pu encountered along the **fission** path.

EPJA **59**, 96 (2023)

Pasta phases: see poster of **Nikolai Shchechilin**.

Pasta sequence for different BSks (with various **symmetry energies**)



The BSkG3 functional

Connects the best features of Brussels functionals.

From BSk series

- Skyrme EDF + HFB method;
- fitted to essentially all experimental masses;
- constraints on infinite nuclear matter properties;
- stiff neutron matter equation of state;
- realistic pairing with self-energy corrections.

From BSkG series

- 3D coordinate-space on Lagrangian mesh (high numerical accuracy);
- triaxial and octupole deformation;
- breaks time-reversal symmetry (time-odd terms);
- fission properties included in the fit.

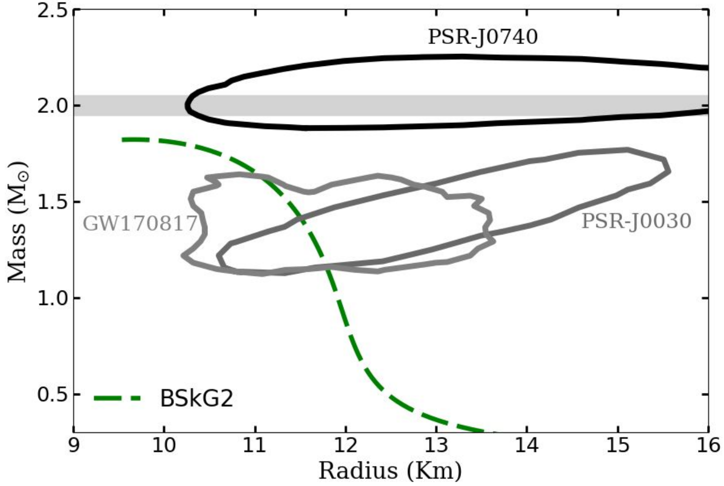
The BSkG3 functional

Connects the best features of Brussels functionals.

From BSk series

- Skyrme EDF + HFB method;
- fitted to essentially all experimental masses;
- constraints on infinite nuclear matter
- stiff neutron matter equation of state;
- realistic pairing with self-energy corrections.

Not present in previous BSkG models.



- Necessary to describe **heavy pulsars**.
- Important for the description of **superfluids in neutron stars**.

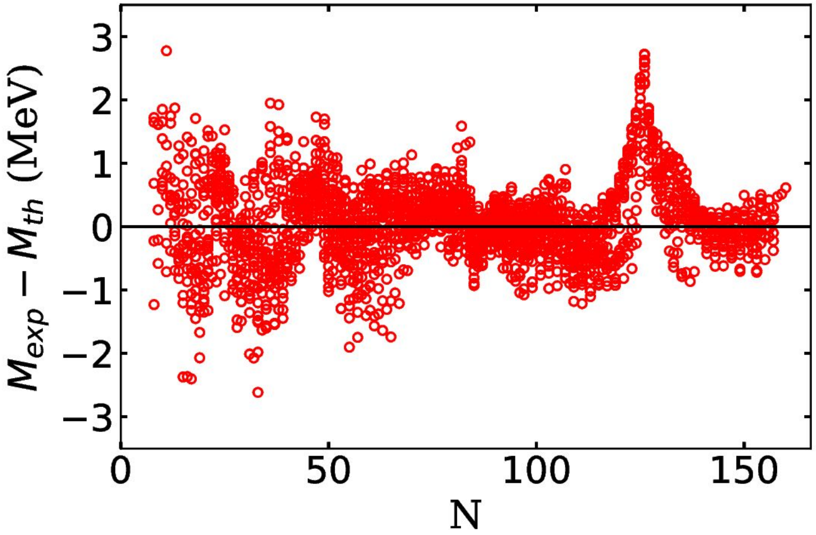
The BSkG3 mass model

Reproduction of known nuclear masses.

σ (M) = 0.631 MeV

σ (R_C) = 0.0237 fm

All 2457 nuclei in the AME2020.



The BSkG3 mass model

Reproduction of known nuclear masses.

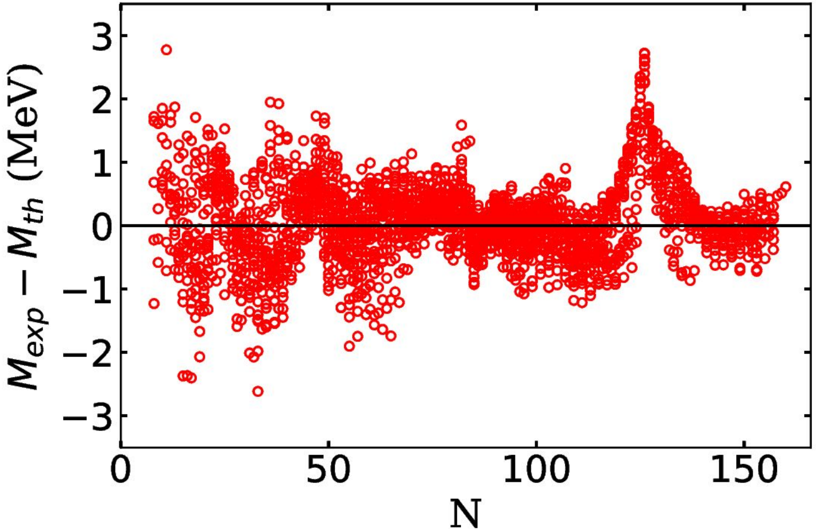
σ (M) = 0.631 MeV

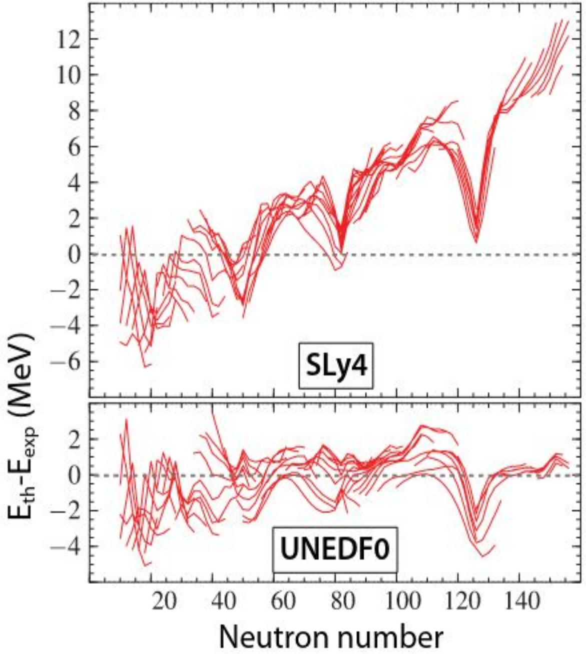
σ (R_C) = 0.0237 fm

All 2457 nuclei in the AME2020.

Comparison:

BSkG2 σ (M) = 0.678 MeV **BSkG1** σ (M) = 0.741 MeV	**SLy4** σ (M) = 4.80 MeV **UNEDF0** σ (M) = 1.45 MeV

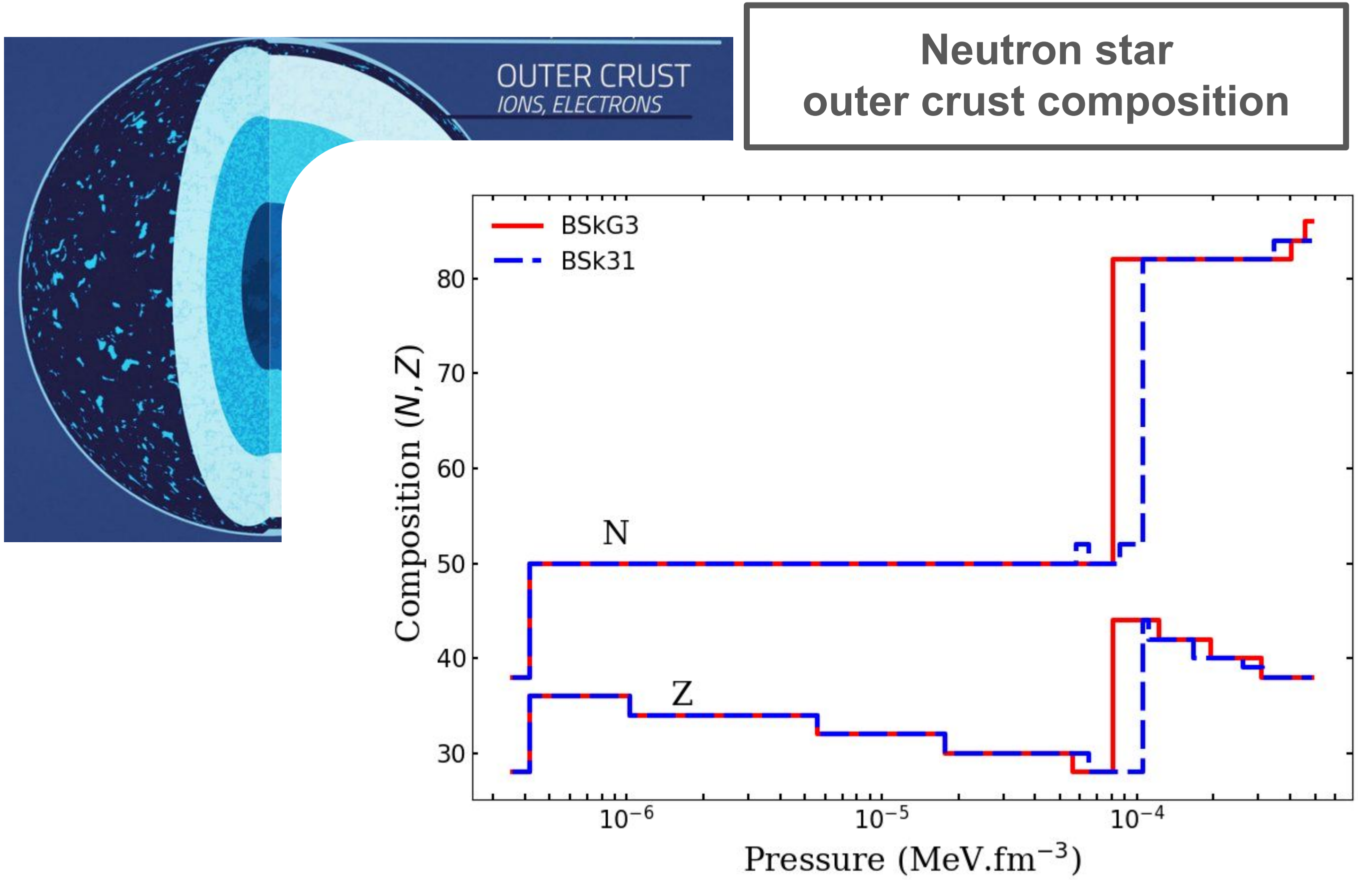




SLy4: E. Chabanat, et al., Phys. Scr. T 56, 231 (1995).
UNEDF0: M. Kortelainen, et al., Phys. Rev. C 82, 024313 (2010).

The BSkG3 mass model

**Neutron star
outer crust composition**

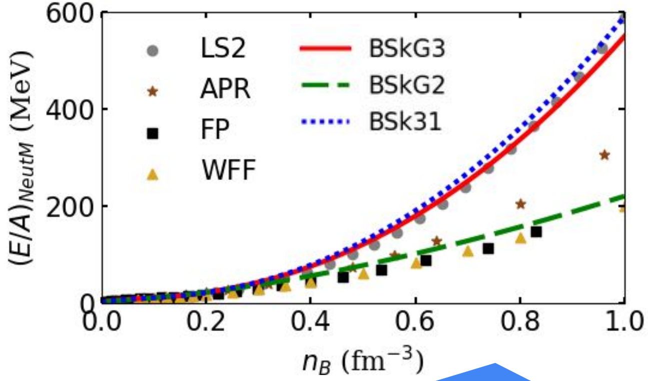


The BSkG3 parameterization

Neutron matter (NeutM) energy

Constraint in *high density* neutron matter energy included in the fit protocol

Neutron matter energy



important for describing massive neutron star

The BSkG3 parameterization

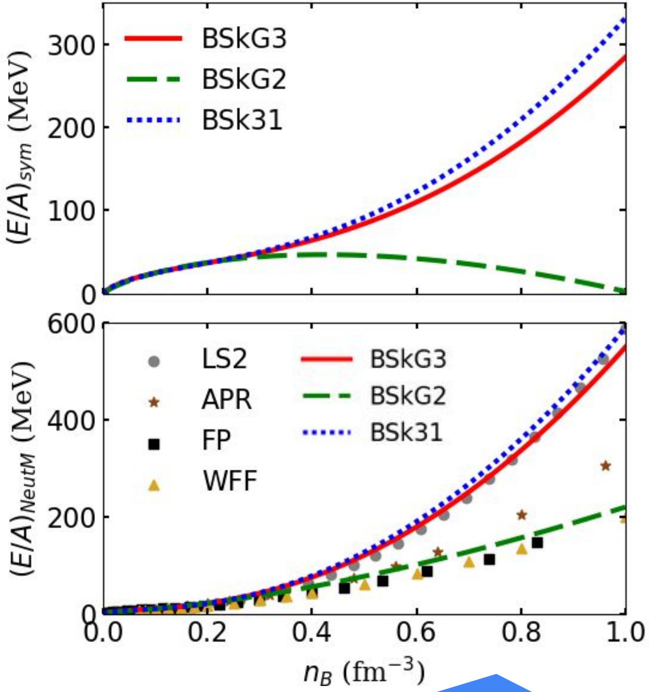
Neutron matter (NeutM) & symmetry energy

Symmetry energy = $e_{\mathrm{NeutM}} - e_{\mathrm{SM}}$

Symmetry energy properties at saturation:

J = 31 MeV
L = 55 MeV
K_{sym} = -21 MeV

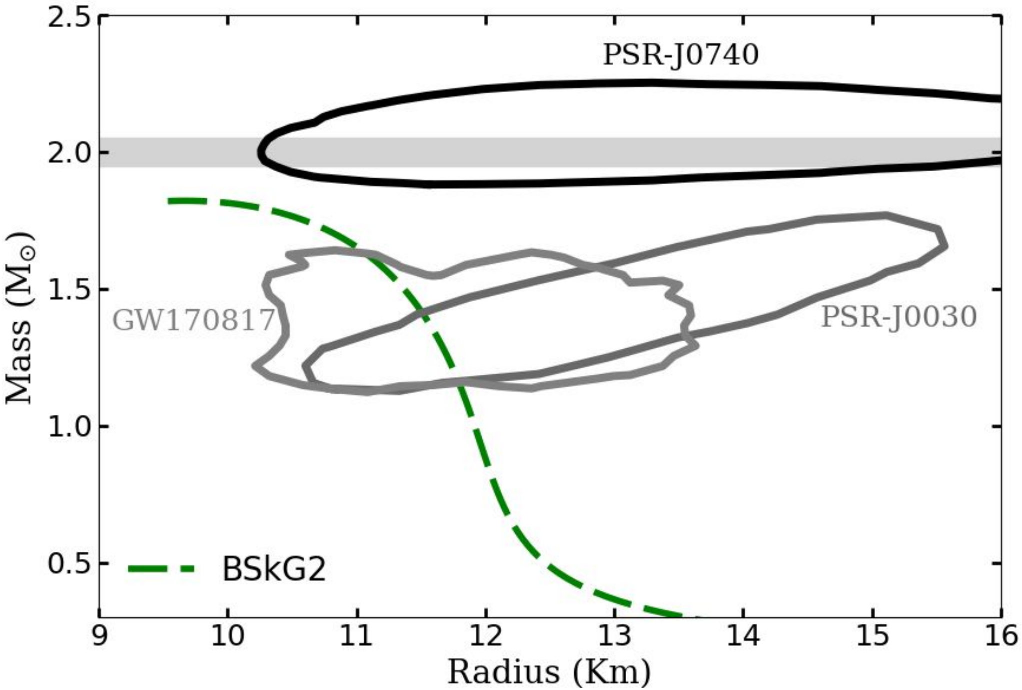
Neutron matter energy



important for describing massive neutron star

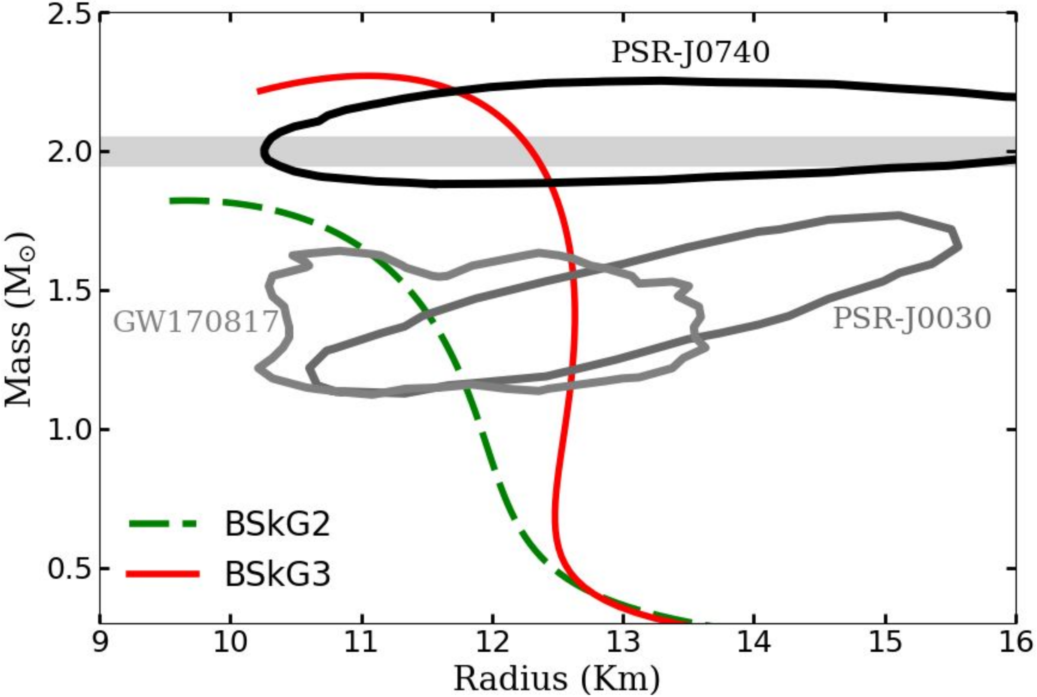
The BSkG3 parameterization

Neutron star properties



The BSkG3 parameterization

Neutron star properties



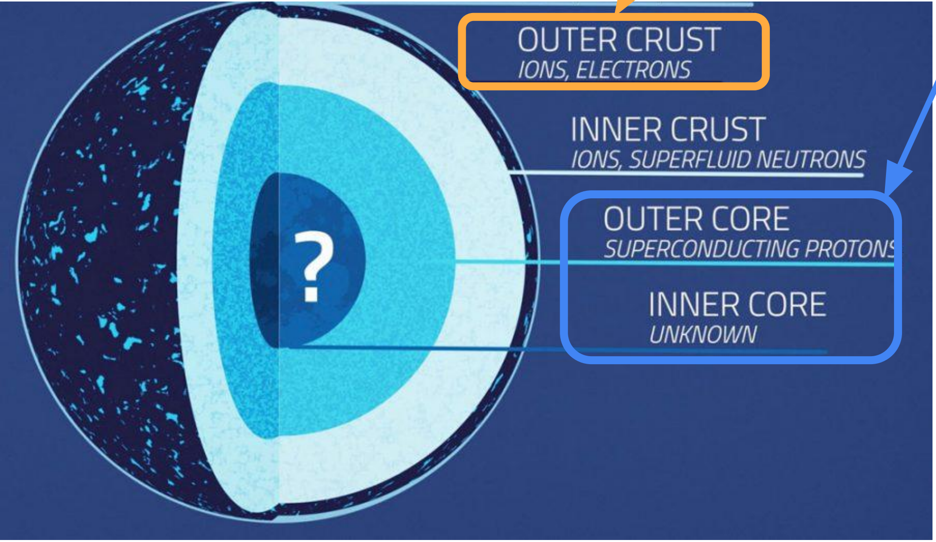
$R_{1.4}$ = 12.6 km

M_{max} = 2.3 Msun

R_{Mmax} = 11.1 km

Summary

Root-mean-square on experimental masses:
σ (M) < 650 KeV



- **stiff neutron matter EoS at high densities**, which allows the description of **heavy pulsars**;

The road ahead:

- systematic exploration of symmetry energy;
- finite temperature EoS;
- explore extensions of the Skyrme EDF;
- investigation of pasta phase within HFB calculation in 3D coordinate space.

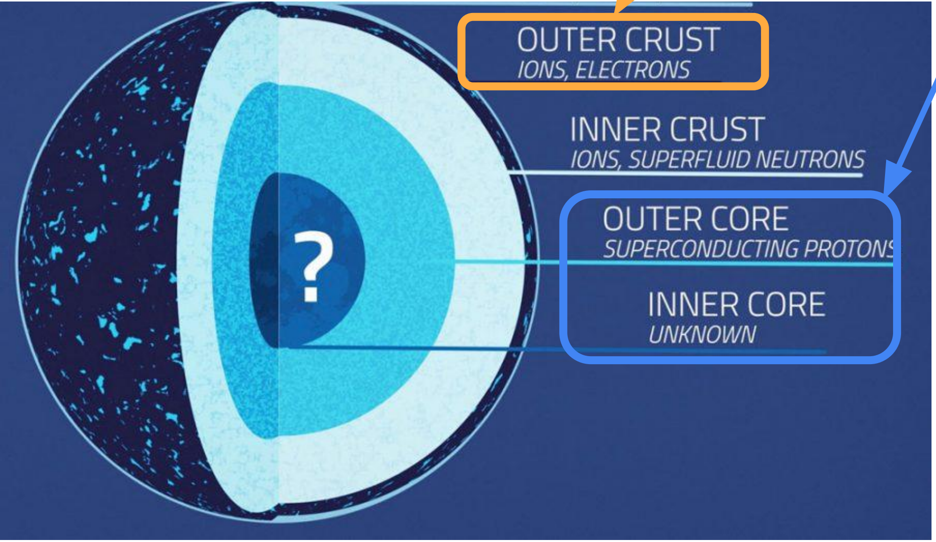
For the complete BSkG3 work!

arXiv: 2307.14276

Summary

What are the most important **physics aspects of dense matter** not yet captured by EDF models?
How can we include them?

Root-mean-square on experimental masses:
σ (M) < 650 KeV



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- systematic exploration of symmetry energy;
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For the complete BSkG3 work!

arXiv: 2307.14276

Acknowledgements

I thank:

- My collaborators: Wouter Ryssens, Nikolai Shchechilin, Guillaume Scamps, Stéphane Goriely, and Nicolas Chamel.
- The *Consortium des Équipements de Calcul Intensif* (CECI) for providing computational resources.
- The agencies FNRS and FWO for funding EVEREST and MANASLU EOS projects.

- **Thank you for your attention!**

ULB UNIVERSITÉ LIBRE DE BRUXELLES

IAA bruxelles

EOS THE EXCELLENCE OF SCIENCE

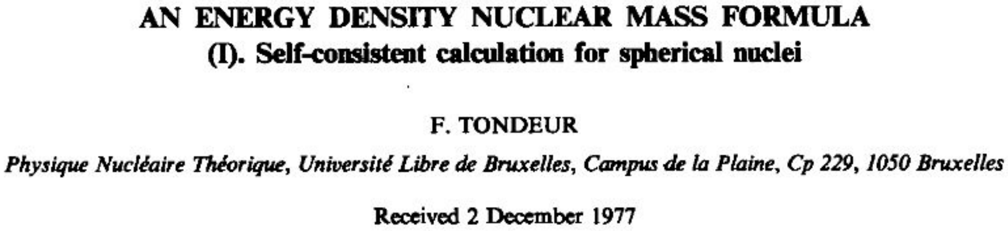
fnrs FREEDOM TO RESEARCH

fwo

extra slides

The road to here

Brussels
mass models



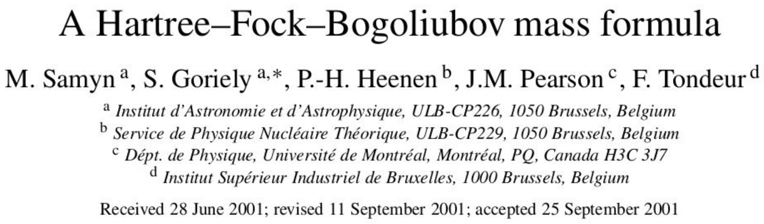
AN ENERGY DENSITY NUCLEAR MASS FORMULA
(I). Self-consistent calculation for spherical nuclei

F. TONDEUR

Physique Nucléaire Théorique, Université Libre de Bruxelles, Campus de la Plaine, Cp 229, 1050 Bruxelles

Received 2 December 1977

HFB-1 mass model
BSk-1 Skyrme interaction



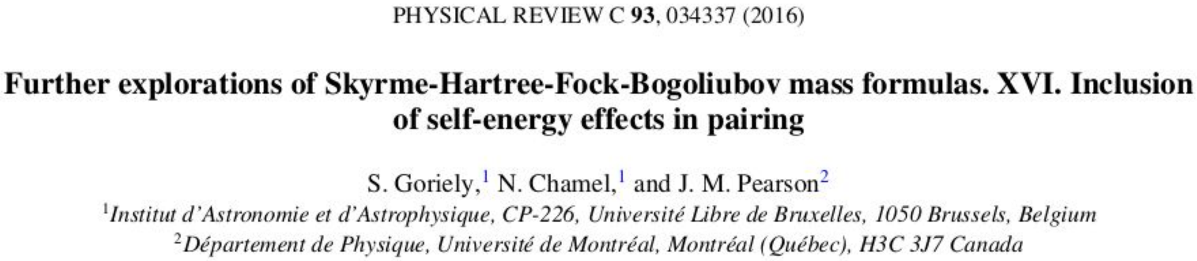
A Hartree–Fock–Bogoliubov mass formula

M. Samyn [a], S. Goriely [a,*], P.-H. Heenen [b], J.M. Pearson [c], F. Tondeur [d]

[a] *Institut d'Astronomie et d'Astrophysique, ULB-CP226, 1050 Brussels, Belgium*
[b] *Service de Physique Nucléaire Théorique, ULB-CP229, 1050 Brussels, Belgium*
[c] *Dépt. de Physique, Université de Montréal, Montréal, PQ, Canada H3C 3J7*
[d] *Institut Supérieur Industriel de Bruxelles, 1000 Brussels, Belgium*

Received 28 June 2001; revised 11 September 2001; accepted 25 September 2001

HFB-32 mass model
BSk-32 Skyrme interaction



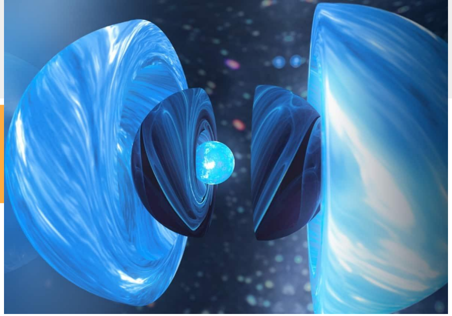
PHYSICAL REVIEW C **93**, 034337 (2016)

Further explorations of Skyrme-Hartree-Fock-Bogoliubov mass formulas. XVI. Inclusion of self-energy effects in pairing

S. Goriely,[1] N. Chamel,[1] and J. M. Pearson[2]

[1] *Institut d'Astronomie et d'Astrophysique, CP-226, Université Libre de Bruxelles, 1050 Brussels, Belgium*
[2] *Département de Physique, Université de Montréal, Montréal (Québec), H3C 3J7 Canada*

The BSks functionals



Astrophysics interest.

From BSk/HFB series

- Skyrme EDF + HFB method;
- fitted to essentially all experimental masses;
- constraints on infinite nuclear matter properties;
- extended Skyrme functional to obtain stiff neutron matter equation of state;
- realistic pairing with self-energy corrections.

- Description of **masses** of nuclei in NS **outer-crust**.
- INM, *e.g.*, the symmetry energy coefficient J, and its slope L, are crucial for many NS properties, such as **crust-core transition and NS radius**.
- Necessary to describe **heavy pulsars**.
- Important for the description of **superfluids in NS**.

The BSk**G** functionals

BSkG1

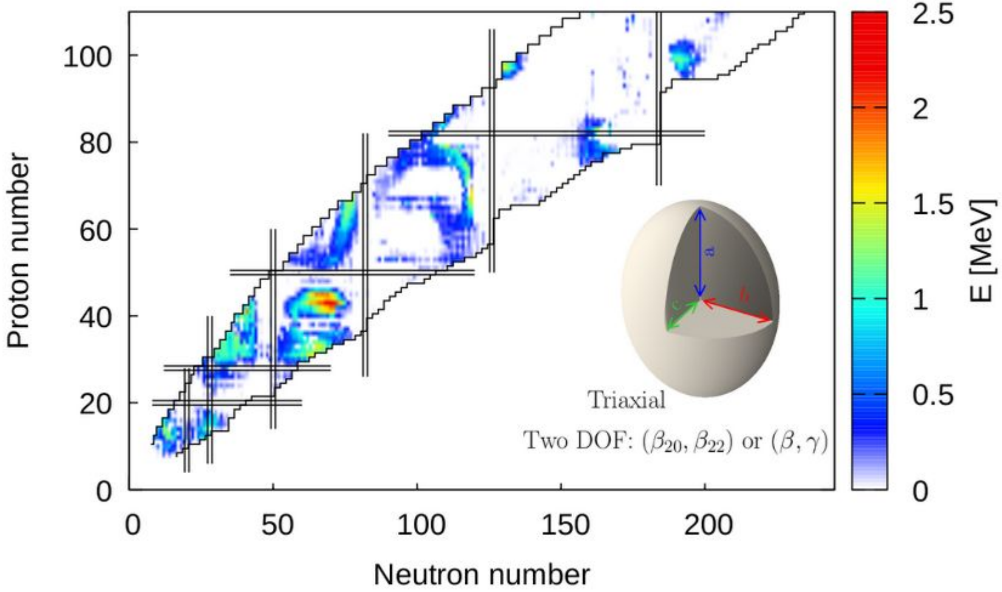
EPJA **57**, 333 (2021)

Skyrme-Hartree-Fock-Bogoliubov mass models on a 3D mesh: effect of triaxial shape

Guillaume Scamps[1,a], **Stephane Goriely**[1], **Erik Olsen**[1], **Michael Bender**[2], **Wouter Ryssens**[1,3]

[1] Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles, Campus de la Plaine CP 226, 1050 Brussels, Belgium
[2] Université de Lyon, Université Claude Bernard Lyon 1, CNRS, IP2I Lyon / IN2P3, UMR 5822, 69622 Villeurbanne, France
[3] Center for Theoretical Physics, Sloane Physics Laboratory, Yale University, New Haven, CT 06520, USA

- Brussels-Skyrme-on-the-**grid** (BSkG);
- HFB code based coordinate space in 3D mesh -> MOCCa code (Ryssens et. al., EPJA 55, 93 (2019));
- better control of numerical accuracy;
- allow **triaxial deformation**.



The BSk**G** functionals

BSk**G**1

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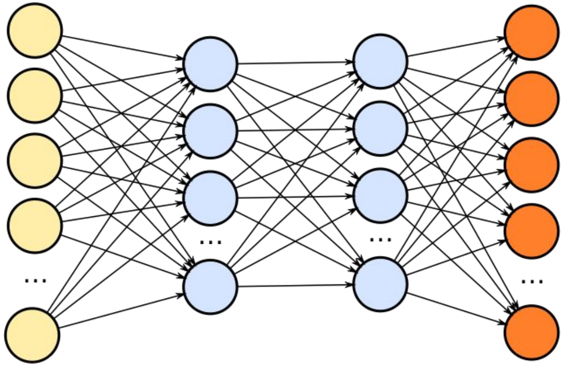
- better control of numerical accuracy;
- allow **triaxial deformation**.
- *machine learning* to accelerate the fit.

machine learning as emulator of MOCCa.
MOCCa predictions for one nucleus ~ 20 minutes.
Machine learning prediction for one nucleus ~ a few seconds.



The BSkG3 mass model

Reproduction of known nuclear masses.

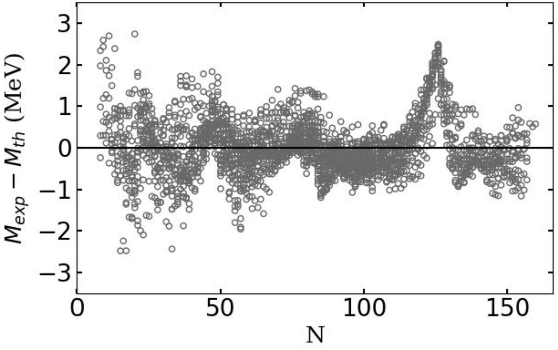
Root-mean-square (rms) deviation and mean deviation calculated from the sum over: $O_{exp} - O_{th}$

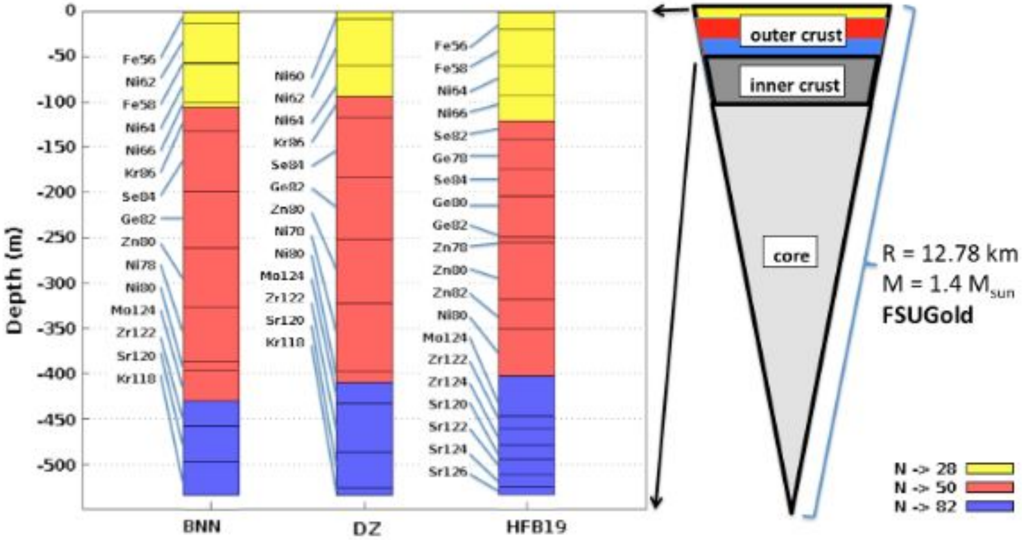
σ (M) = 0.631 MeV

ε (M) = -0.041 MeV

σ (R_C) = 0.0250 MeV

ε (R_C) = -0.0045 MeV





ig. 4. Composition of a canonical 1.4 $M_\odot$ neutron star with a 12.78 km radius as redicted by three mass models: "BNN-world", DZ, and HFB19.

Figure from: J. Piekarewicz & R. Utama, Acta Phys. Pol. B 47, 659 (2016)

The BSkG functionals

BSkG1

EPJA **57**, 333 (2021)

Skyrme-Hartree-Fock-Bogoliubov mass models on a 3D mesh: effect of triaxial shape

Guillaume Scamps[1,a], **Stephane Goriely**[1], **Erik Olsen**[1], **Michael Bender**[2], **Wouter Ryssens**[1,3]

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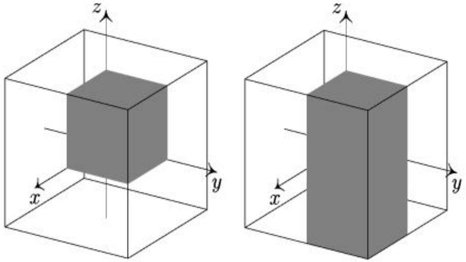

The BSk**G** functionals

BSk**G**1

EPJA **57**, 333 (2021)

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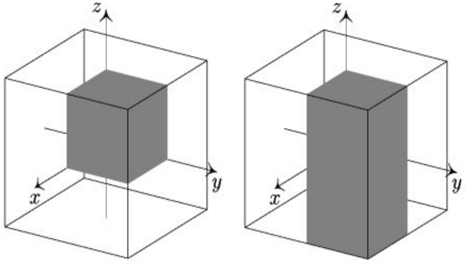
[3] Center for Theoretical Physics, Sloane Physics Laboratory, Yale University, New Haven, CT 06520, USA

- Brussels-Skyrme-on-the-**grid** (BSkG);
- HFB code based coordinate space in 3D mesh -> **MOCCa** code (Ryssens et. al., EPJA 55, 93 (2019));
- better control of numerical accuracy;

Modular **C**ranking **C**ode = MOCCa

HFB solver at **3D coordinate-space on Lagrangian mesh** from
W. Ryssens et al,
[W. Ryssens PhD Thesis, ULB (2016).]



HFB solver

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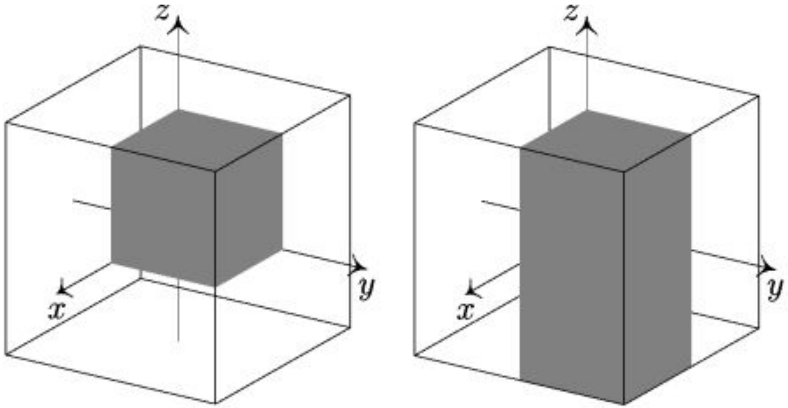

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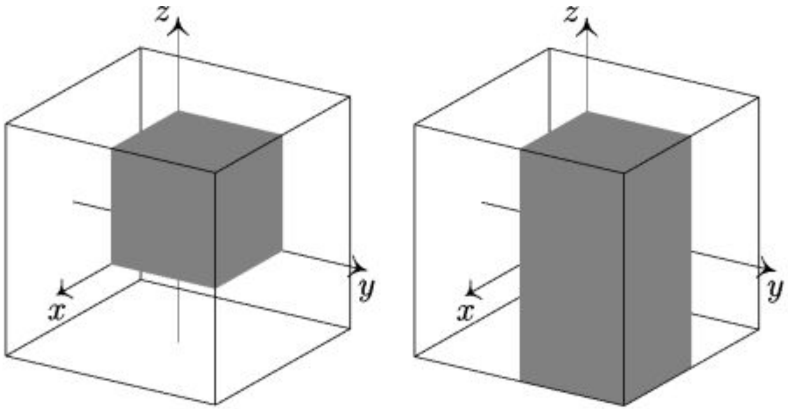
HFB solver

Modular **C**ranking **C**ode = MOCCa

HFB solver at **3D coordinate-space on Lagrangian mesh** from W. Ryssens et al, W. R. PhD Thesis, ULB (2016).



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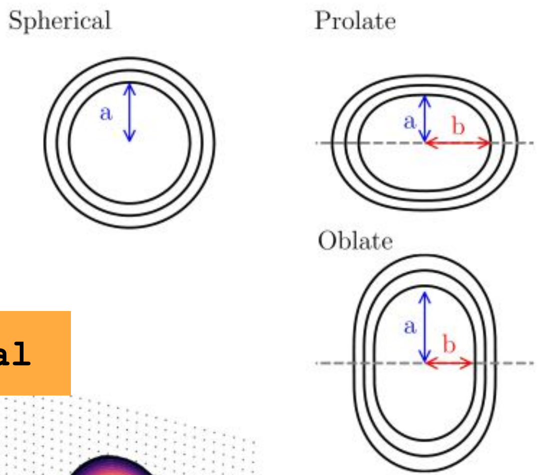
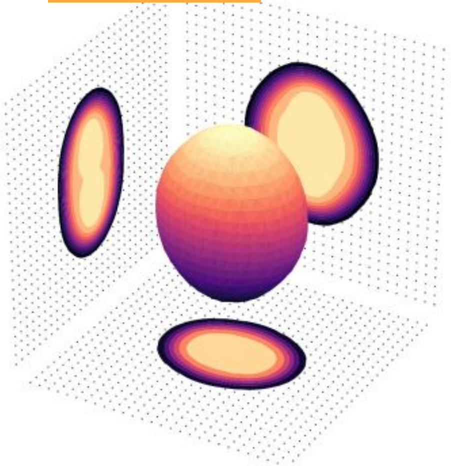
Nuclear shapes



Triaxal



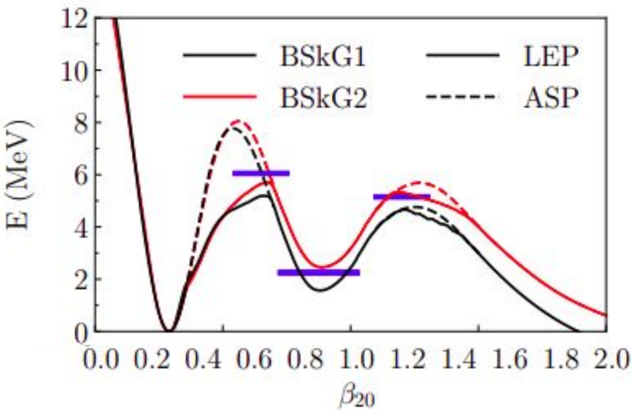
The BSk**G** functionals

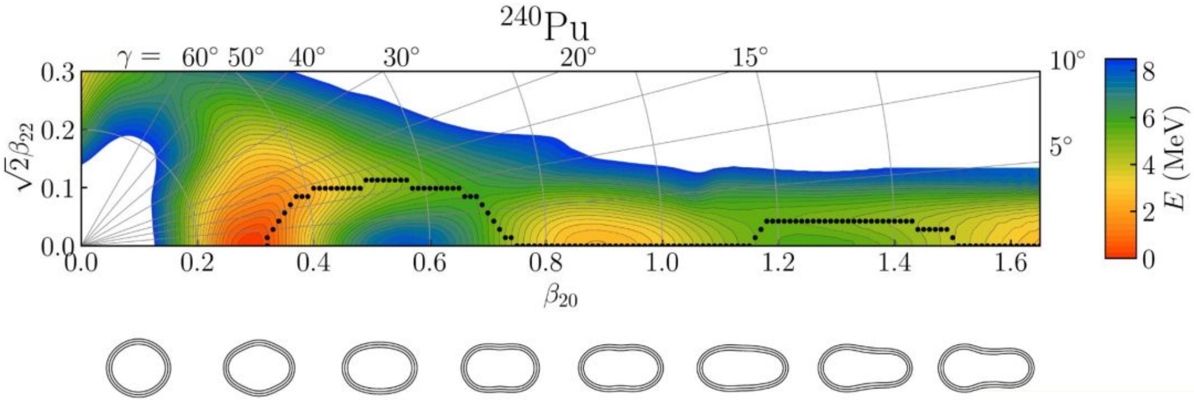
BSk**G**2:
fission properties

Skyrme-Hartree-Fock-Bogoliubov mass models on a 3D mesh. IIb. Fission properties of BSkG2.

Wouter Ryssens [a,1], Guillaume Scamps [1,2], Stephane Goriely [1], Michael Bender [3]

arXiv: 2302.03097





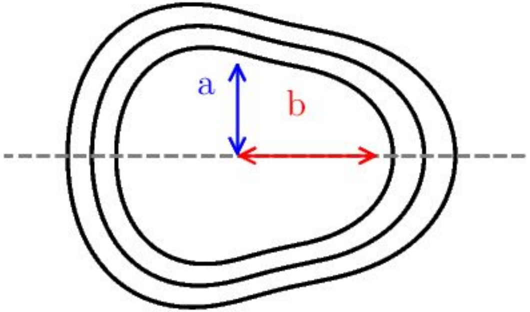
ASP = Axial Symmetric Path
LEP = Low Energy Path

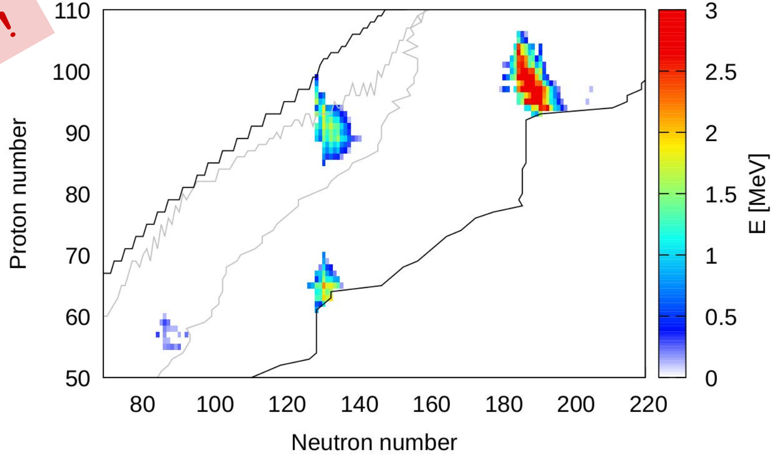
The BSkG3 mass model

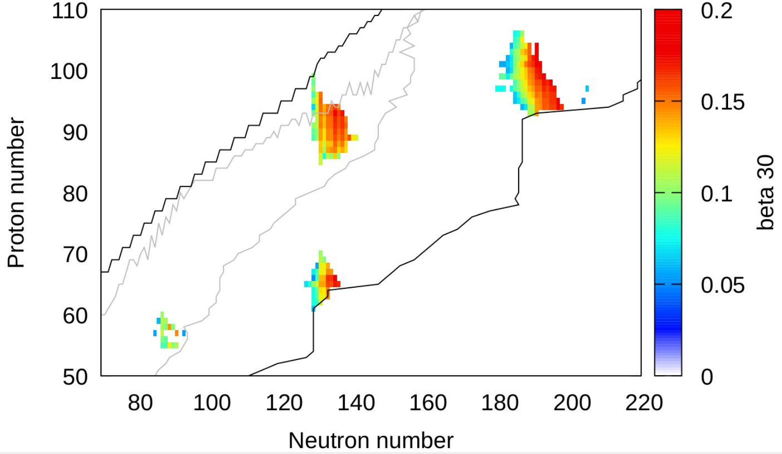
Octupole shapes in ground state

PRELIMINARY!

Reflection-asymmetric (RA)







The BSk**G** functionals

Brussels-Skyrme-on-the-**grid** (BSkG)

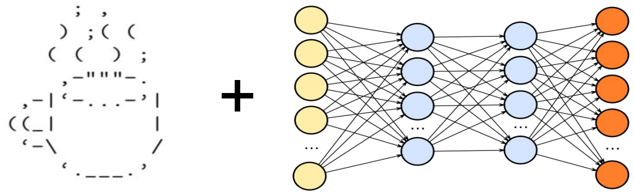
EPJA **57**, 333 (2021)

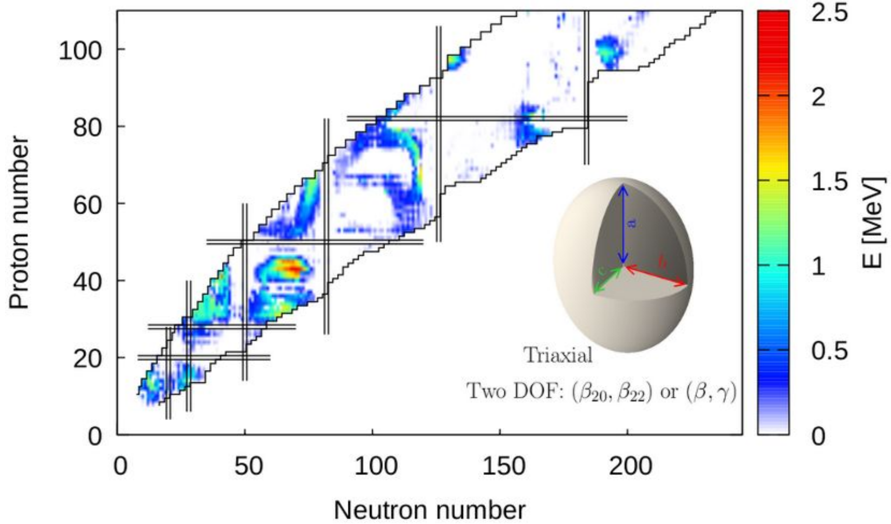
EPJA **58**, 246 (2022)

- HFB code based coordinate space in 3D mesh -> MOCCa code (Ryssens et. al., EPJA 55, 93 (2019));

- better control of numerical accuracy;
- allow **triaxial deformation**.
- *machine learning* to accelerate the fit.

- **Allows for time-reversal symmetry breaking.** No more Equal Filling Approximation (EFA).
- Incorporated information on the **fission properties** of twelve actinide nuclei in the fitting protocol.





The BSk**G** functionals

BSkG2

EPJA **58**, 246 (2022)

Skyrme–Hartree–Fock–Bogoliubov mass models on a 3D mesh: II. Time-reversal symmetry breaking

Wouter Ryssens[1,a], **Guillaume Scamps**[1,2], **Stephane Goriely**[1], **Michael Bender**[3]

[1] Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles, Campus de la Plaine CP 226, 1050 Brussels, Belgium
[2] Department of Physics, University of Washington, Seattle, WA 98195-1560, USA
[3] Université de Lyon, Université Claude Bernard Lyon 1, CNRS / IN2P3, IP2I Lyon, UMR 5822, 69622 Villeurbanne, France

- **Allows for time-reversal symmetry breaking.**
  Inclusion of '*time-odd*' terms in the Skyrme EDF.
  No more Equal Filling Approximation (EFA).

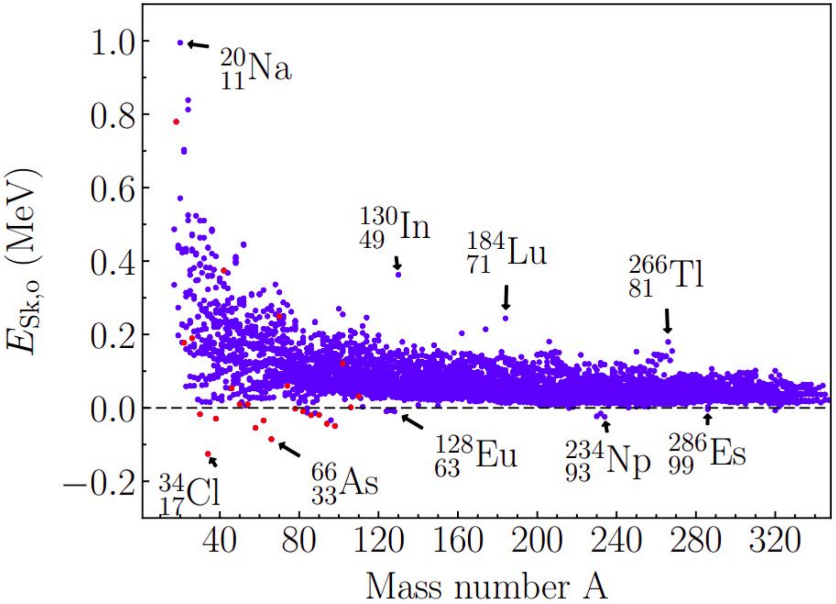
- Incorporated information on the **fission properties** of twelve actinide nuclei in the fitting protocol.

Access to more observables:
- magnetic moments;
- rotational bands.

The BSkG3 mass model

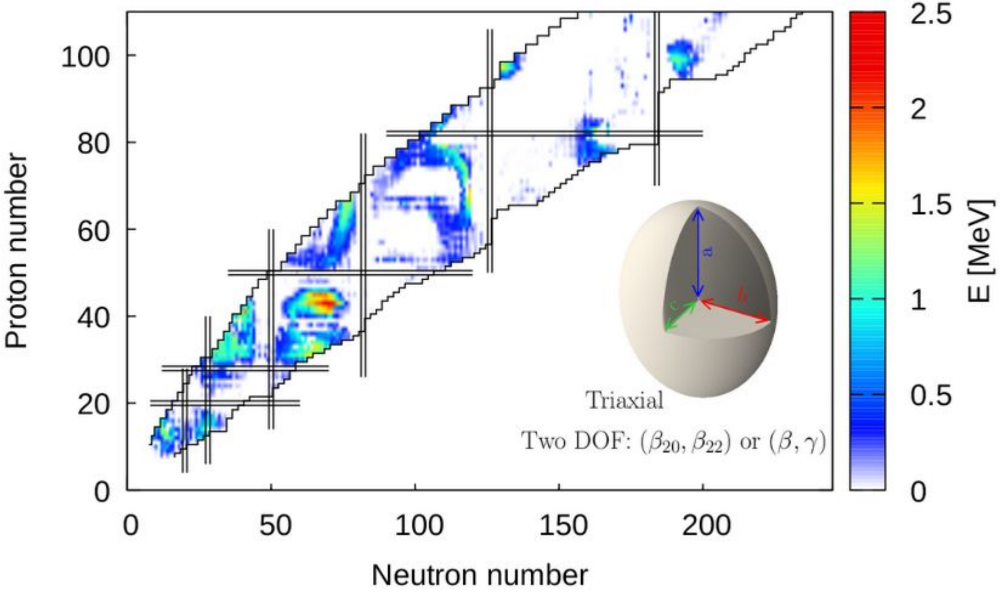
- **Allows for time-reversal symmetry breaking.** Inclusion of ‘*time-odd*’ terms in the Skyrme EDF - instead of Equal Filling Approximation (EFA) of previous model.

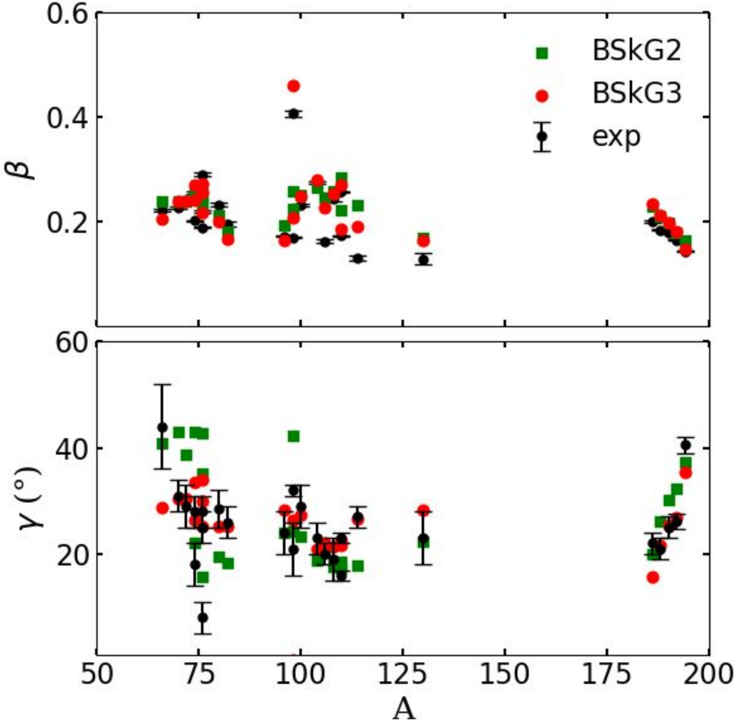
- Incorporated information on the **fission properties** of twelve actinide nuclei in the fitting protocol.



The BSkG3 mass model

Deformation

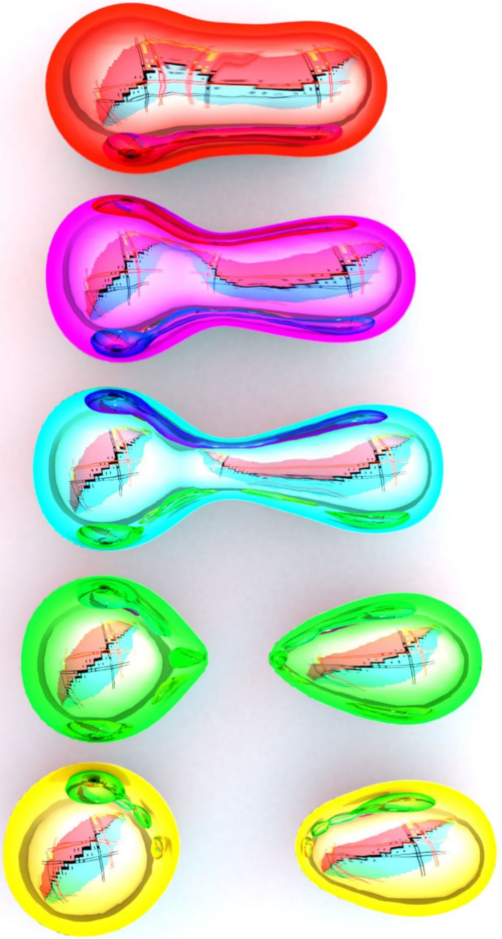




Binding energy difference between **unrestricted** calculations and calculations **restricted** to axial quadrupole deformation with BSkG1.

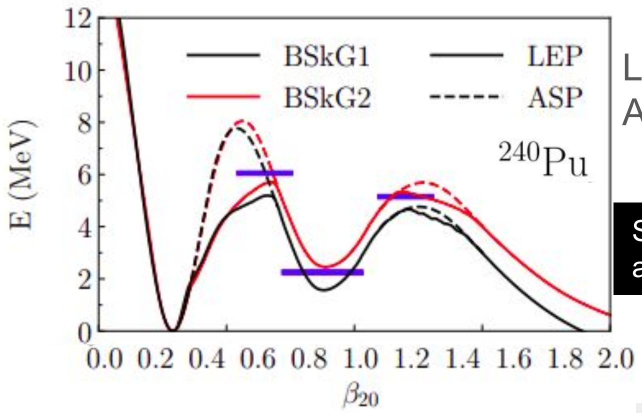
Quadrupole **deformation** (top) and **triaxiality** angle (bottom) for BSkG2 (green), BSkG3(red) and experimental data (black).

The BSkG3 mass model



Fission barriers

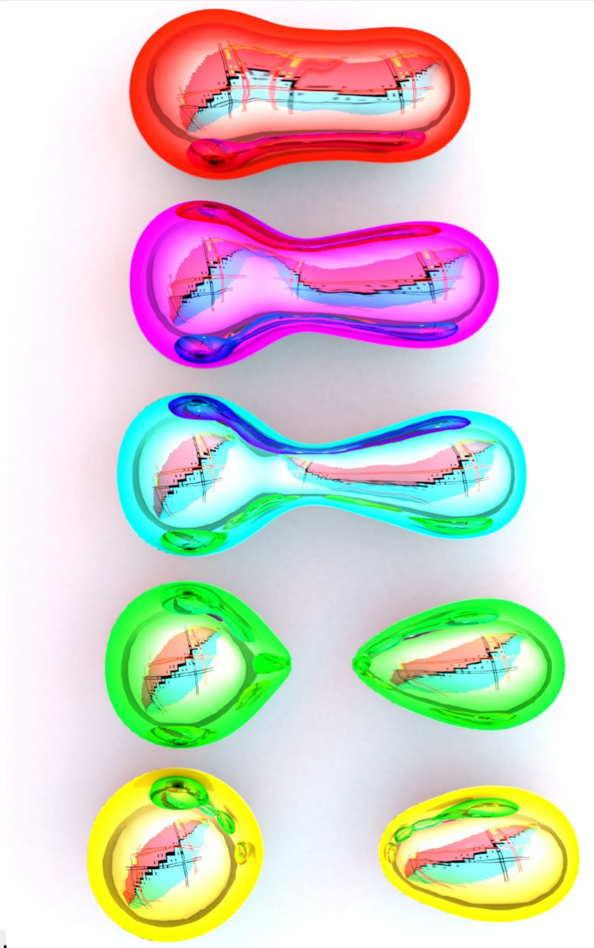
Primary (E_I), secondary (E_{II}) ***fission barrier*** heights and fission isomer excitation energies (E_{iso}) of actinide nuclei.



LEP = Low Energy Path
ASP = Axial Symmetric Path

See W. Ryssens et al. arXiv: 2302.03097

The BSkG3 mass model



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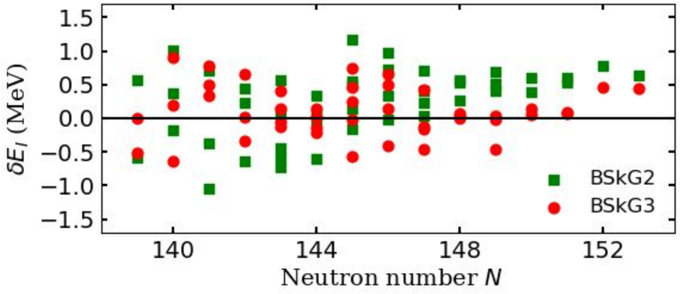
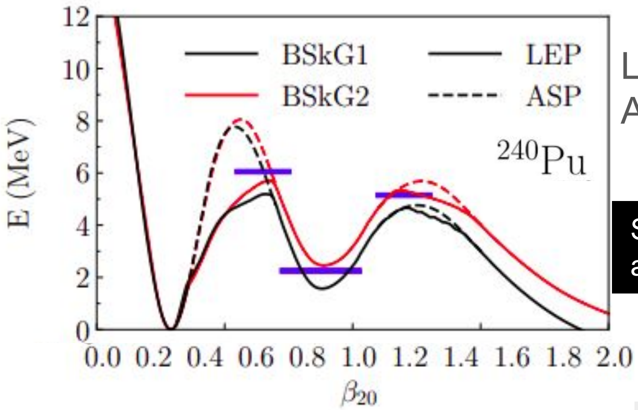


σ (E_I) = 0.33 MeV

ε (E_I) = +0.05 MeV



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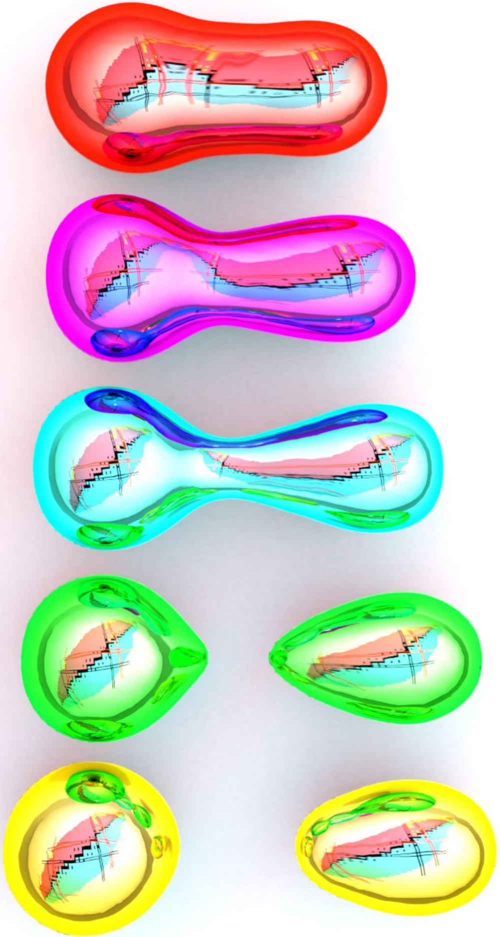
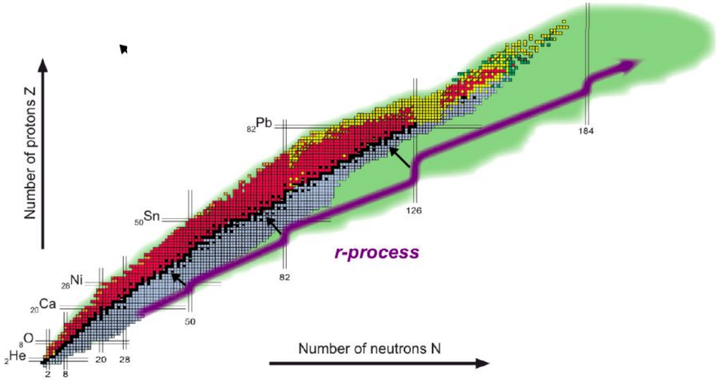
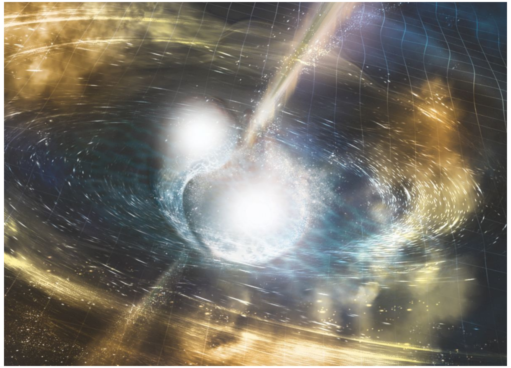
The BSkG3 mass model



Fission barriers



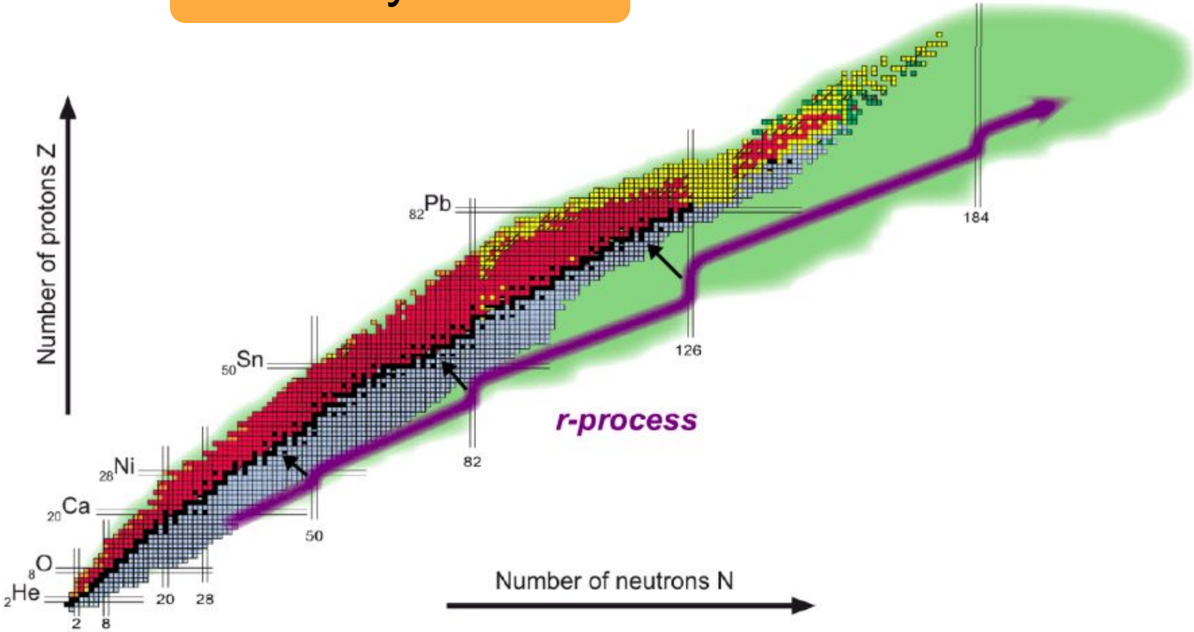
Fission properties impact several aspects of the r-process such as:



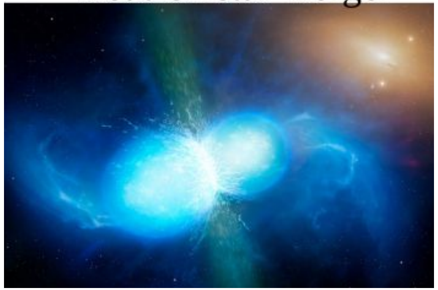
- **"fission recycling"**;
- the **r-process abundances** in the 110 ≤ A ≤ 170 region;
- the production of cosmic chronometers such as Th and U;
- the **heating rate of kilonovae**.

Motivation

Nucleosynthesis



Neutron star merger



Supernova explosion

Description of **nuclear masses** and **fission** paths in *experimentally unknown* regions.

The BSkG3 interaction

Pairing:

$$E_{\mathrm{pair}} = \frac{1}{4} \sum_{q=p,n} \int d^3\mathbf{r}\, g_q(\rho_n, \rho_p) \tilde{\rho}_q^*(\mathbf{r}) \tilde{\rho}_q(\mathbf{r}) \,,$$

Different from BSkG1 and BSkG2

$$g_q(\rho_n, \rho_p) = V_q(\rho_n, \rho_p) \left[1 + \kappa_q (\nabla \rho_0)^2\right]$$

The BSkG3 interaction

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$$g_q(\rho_n, \rho_p) = V_q(\rho_n, \rho_p) \left[1 + \kappa_q (\nabla \rho_0)^2 \right]$$

Designed to match the pairing gaps in INM deduced from *ab-initio* calculations.

L. G. Cao et al., PRC, 73, 014313, 2006.
Brueckner calculations with realistic
two-body and three-body forces
and account for self-energy corrections.

The BSkG3 interaction

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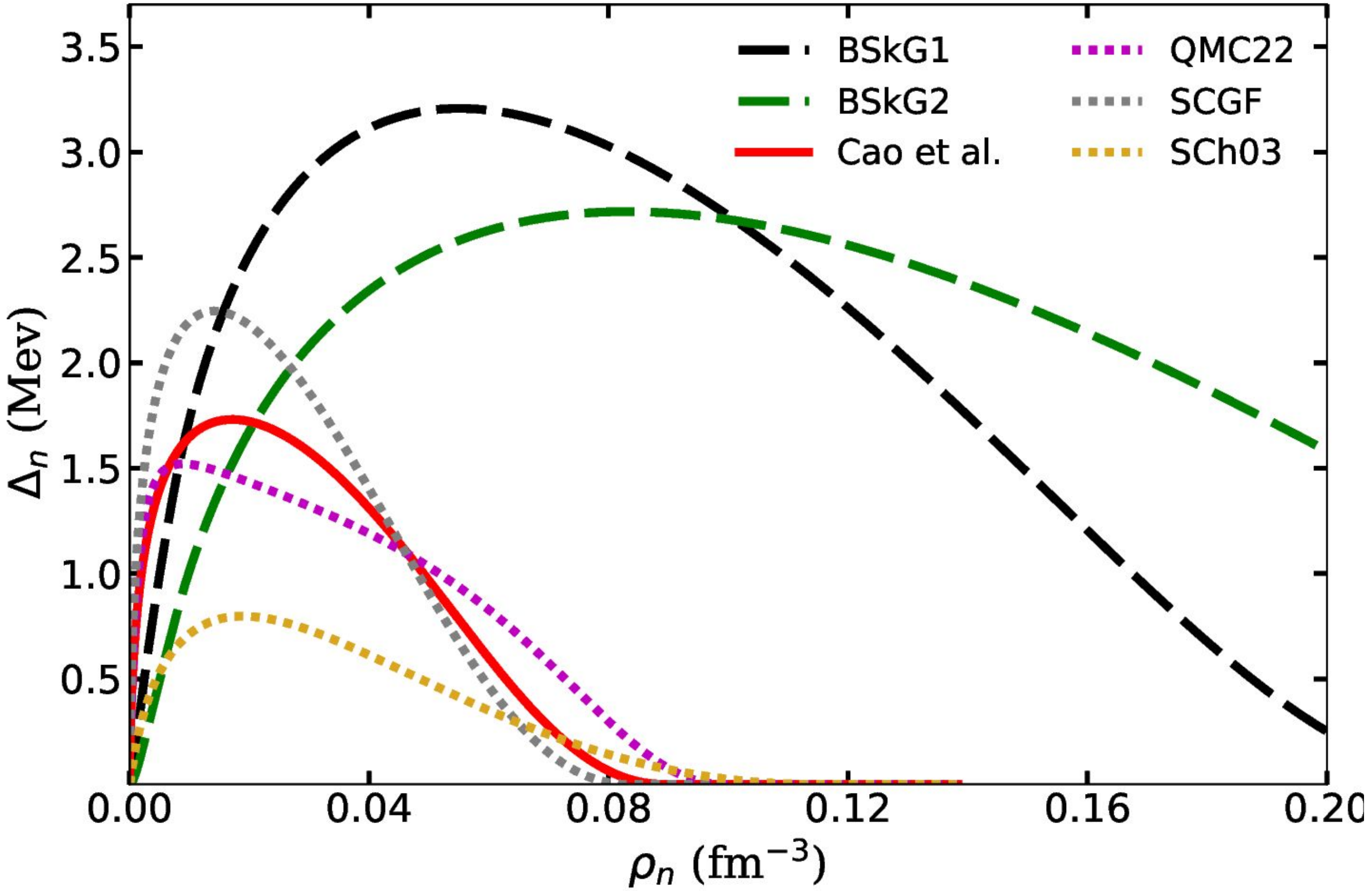
Designed to match the pairing gaps in INM deduced from *ab-initio* calculations.

L. G. Cao et al., PRC, 73, 014313, 2006.
Brueckner calculations with realistic two-body and three-body forces and account for self-energy corrections.

- Parameters $\kappa_{n/p}$ **adjusted** to reproduce **experimental** neutron and proton **pairing** gaps.
- $\kappa_{n/p}$ **vanish at INM** since it multiplies the density gradients.

The BSkG3 interaction

Pairing:

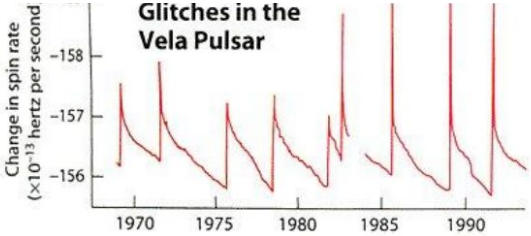


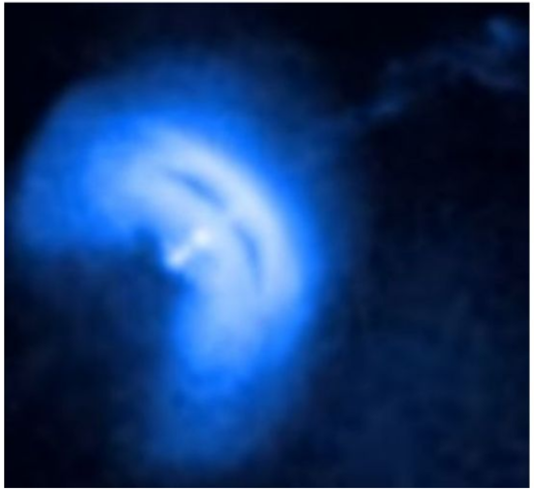
The BSkG3 interaction

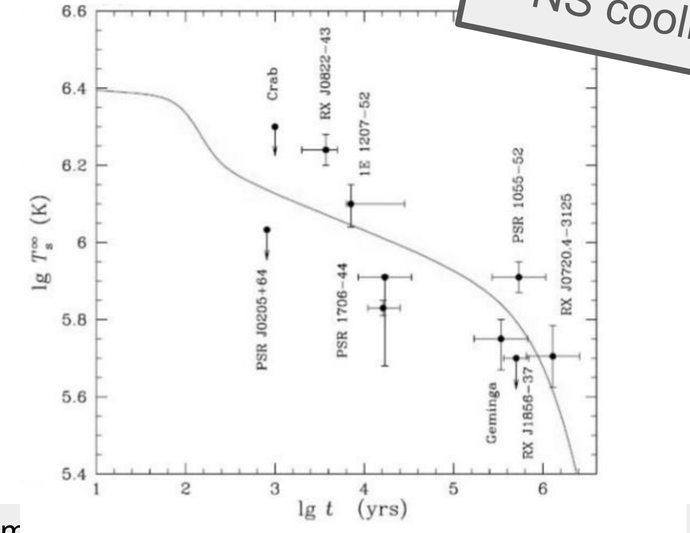
Pairing:

Important to describe **superfluids** in NSs.

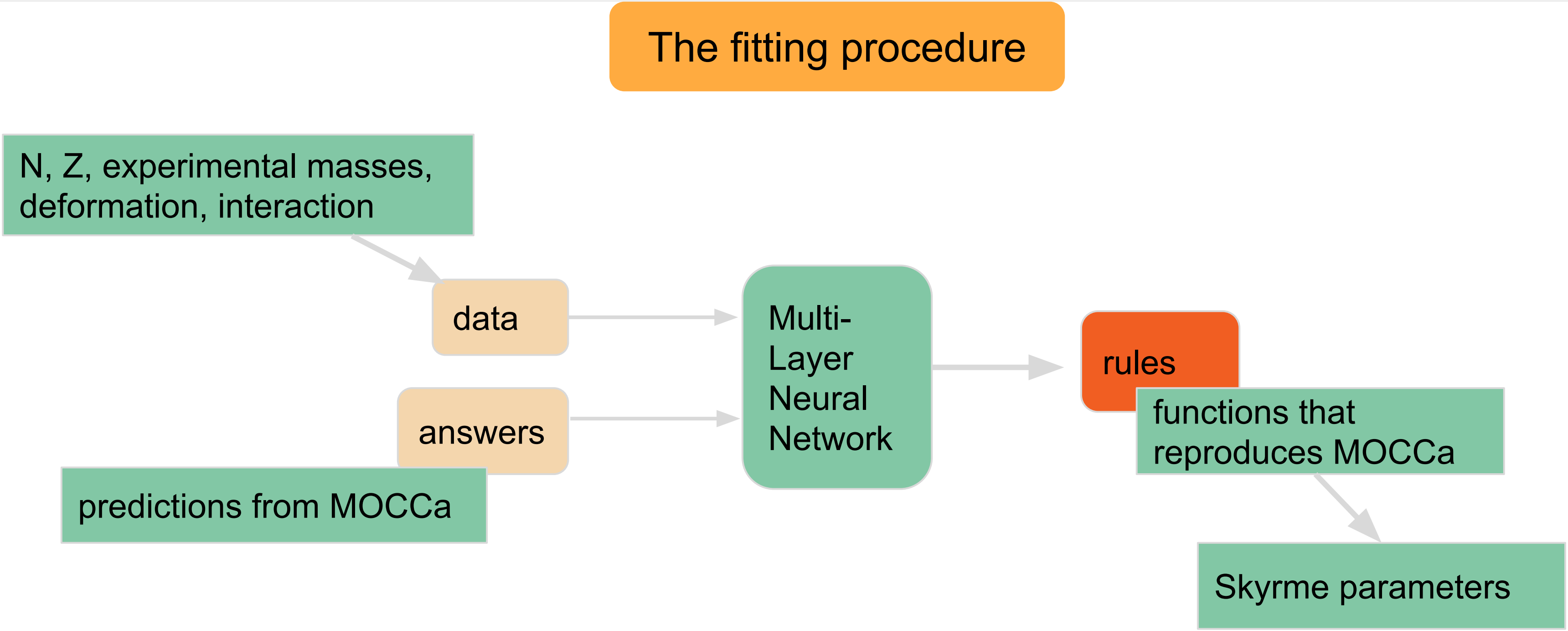
NS cooling







workflow



The fitting procedure

N, Z, experimental masses, deformation, interaction

data

answers

predictions from MOCCa

Multi-Layer Neural Network

rules

functions that reproduces MOCCa

Skyrme parameters

How to describe an atomic nucleus?

macroscopic description, e.g., LDM: liquid drop model

ab-initio: from the bare nucleon-nucleon interaction.

How to describe an atomic nucleus?

macroscopic description, e.g., LDM: liquid drop model.

too simple.
(usually with no shell structure, neutron skin, pairing correlations...)

ab-initio: from the bare nucleon-nucleon interaction.

not (yet) feasible to describe thousands of nuclei along the nuclear chart.

A good compromise:

Energy density functional (EDF): an effective description of nuclei based on one-body densities.

Allows for predictions across the entire nuclear chart, firmly founded on a **microscopic description** of the nucleus.