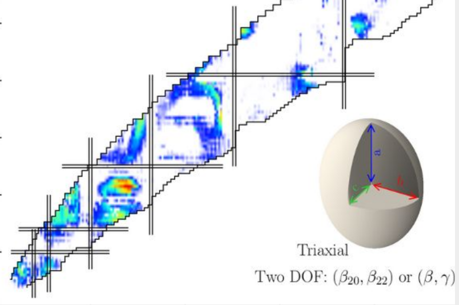
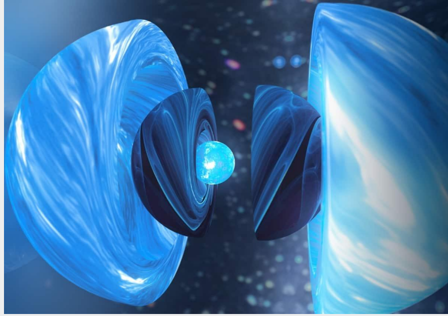




Constructing nuclear functionals for neutron stars and nucleosynthesis applications

Guilherme Grams,
Wouter Ryssens, Guillaume Scamps,
Stephane Goriely and Nicolas Chamel
Astronomy and Astrophysics Institute (IAA) - ULB

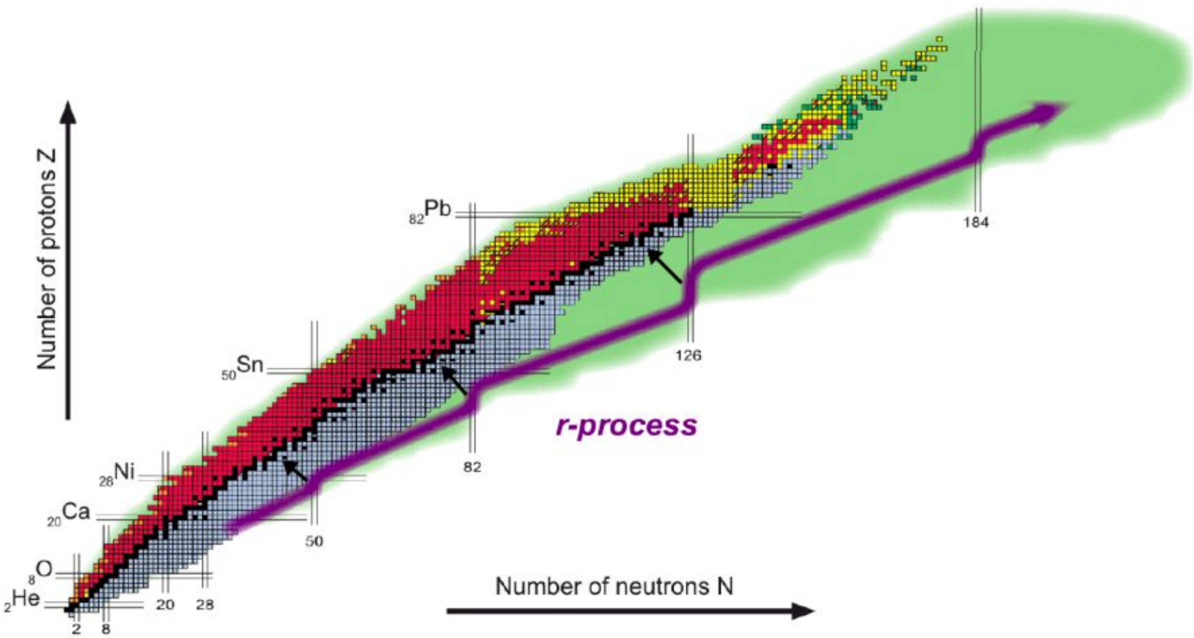
UNIVERSITÉ LIBRE DE BRUXELLES

QMBC 2023 in memory of Peter Schuck,
Orsay - 23/03/23

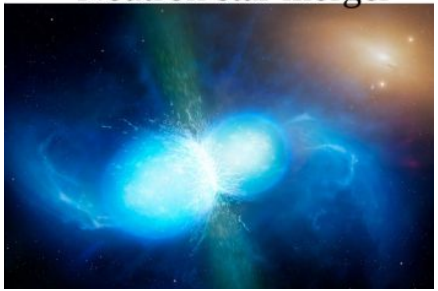
IAA bruxelles

Motivation

Nucleosynthesis



Neutron star merger

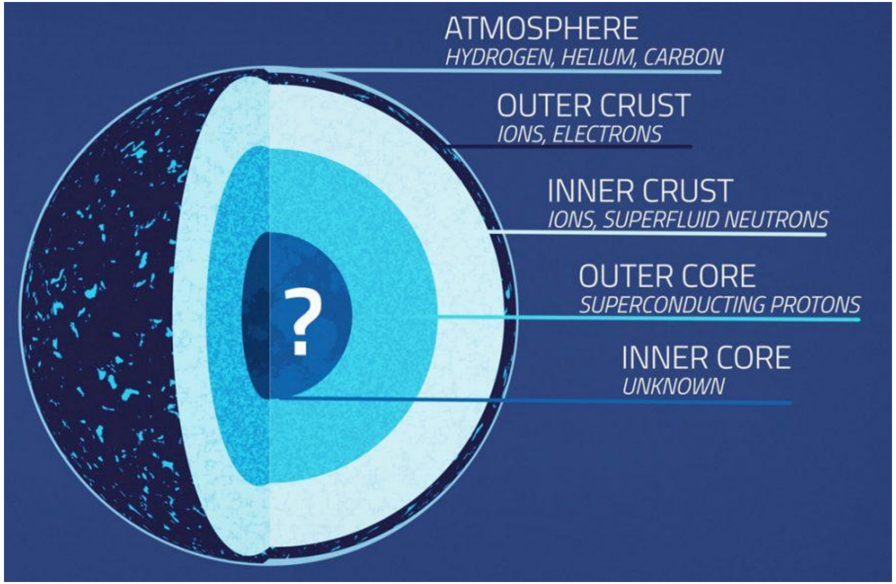


Supernova explosion

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

Motivation

Neutron star physics



Nuclear physics inputs:

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

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

The road to here

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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]

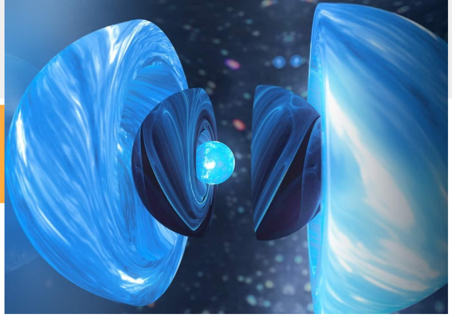
[1]*Institut d'Astronomie et d'Astrophysique, CP-226, Université Libre de Bruxelles, 1050 Brussels, Belgium*
[2]*Département de Physique, Université de Montréal, Montréal (Québec), H3C 3J7 Canada*

The BSks functionals

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.

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**.

See N. Chamel and V. Allard talks.

The road to here

Brussels
mass models

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

F. TONDEUR
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Received 2 December 1977

HFB-1 mass model
BSk-1 nuclear force

A Hartree–Fock–Bogoliubov mass formula

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New BSk**G** family:

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

Received: 7 September 2021 / Accepted: 26 November 2021

The BSkG functionals

BSkG1

EPJA **57**, 333 (2021)

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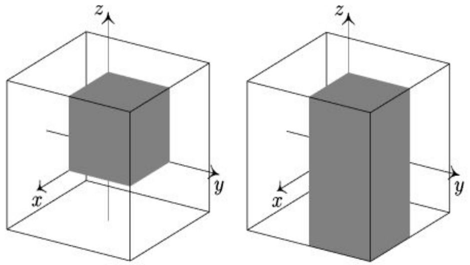
- Brussels-Skyrme-on-the-**grid** (BSkG);



The BSkG functionals

BSkG1

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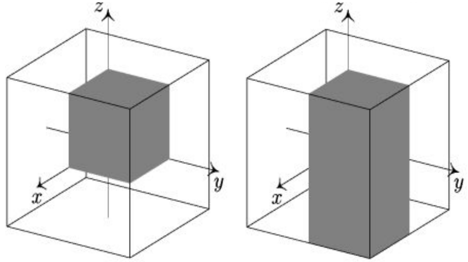
[3] Center for Theoretical Physics, Sloane Physics Laboratory, Yale University, New Haven, CT 06520, USA

- 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).]



The BSkG functionals

BSk**G**1

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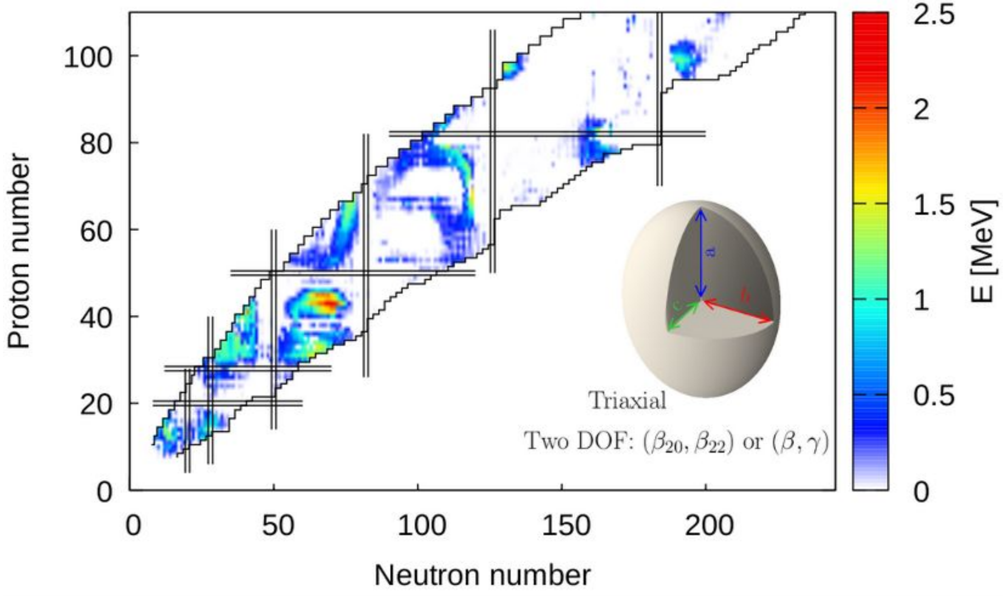
- better control of numerical accuracy;
- allow **triaxial deformation**.



The BSkG functionals

BSk**G**1

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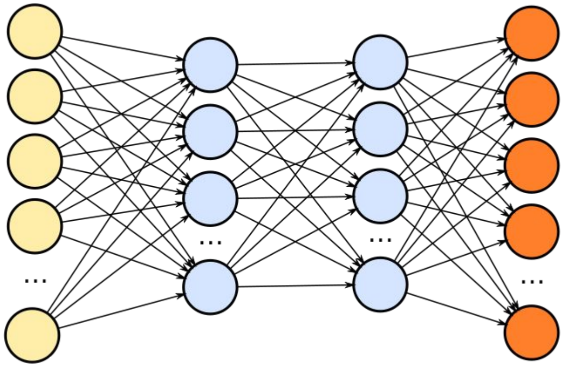
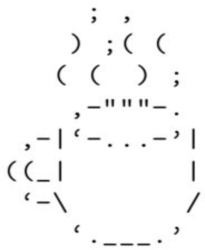
- Brussels-Skyrme-on-the-**grid** (BSkG);
- HFB code based coordinate space in 3D mesh -> MOCCa code (Ryssens et. al., EPJA 55, 93 (2019));
- better control of numerical accuracy;
- allow **triaxial deformation**.
- *machine learning* to accelerate the fit.

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





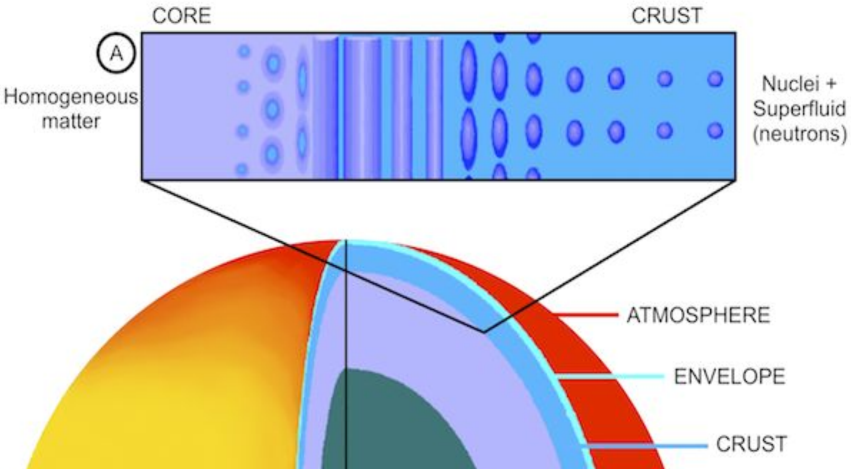
The BSkG3 functional

Astrophysics interest.

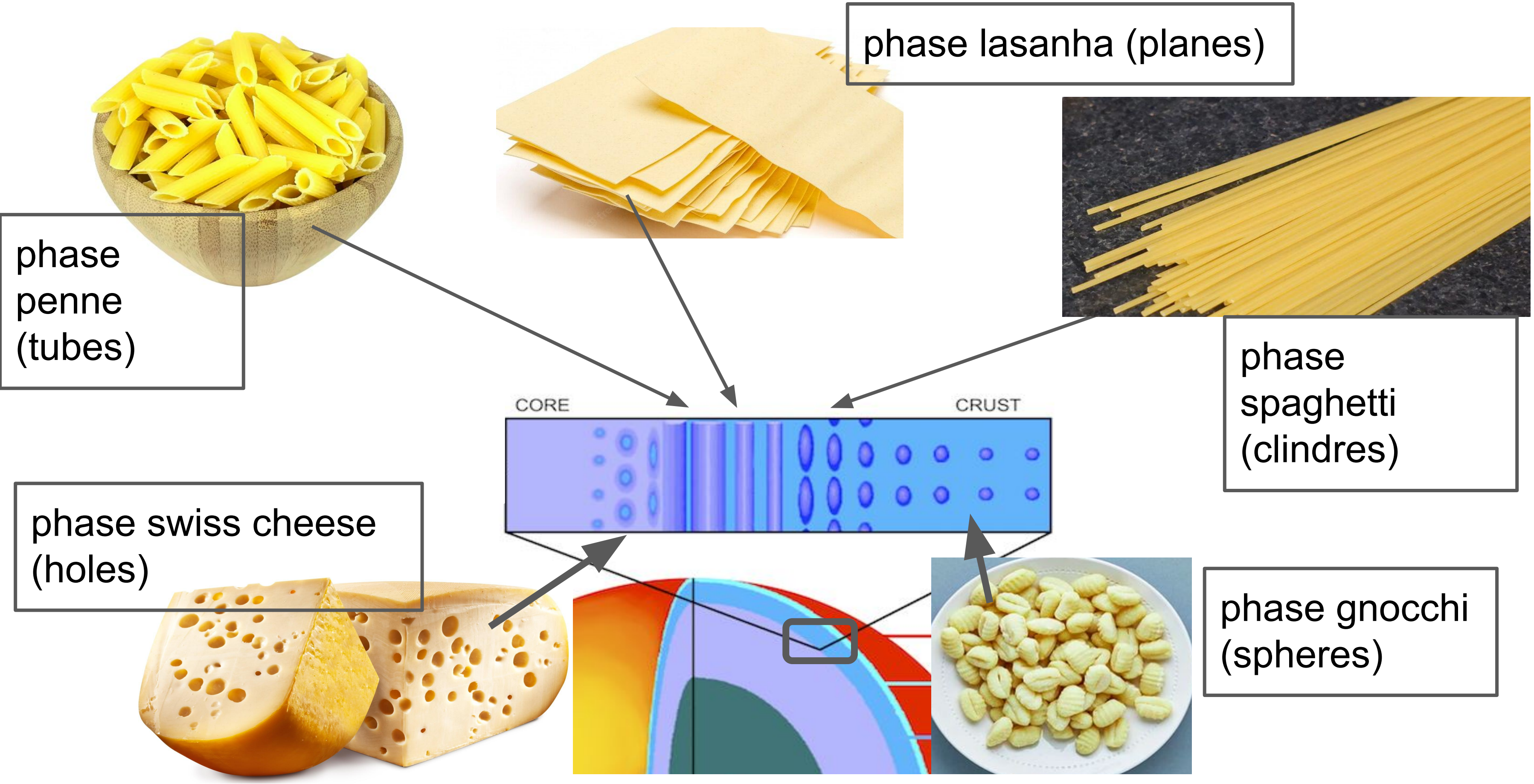
- Improves the description of **masses** of nuclei in NS **outer-crust**.
- Nuclear **deformations** are important at the deep layers of the NS inner-crust, where **pasta phases** could be formed.

From BSkG series

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



Pasta phases : see talk of N. Shchechilin.



The BSkG3 functional

Connects the best features of Brussels functionals.

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;
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Not present in previous BSkG models.

From BSkG series

- 3D coordinate-space on Lagrangian mesh (high numerical accuracy);
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The BSkG3 mass model

Reproduction of known nuclear masses.

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

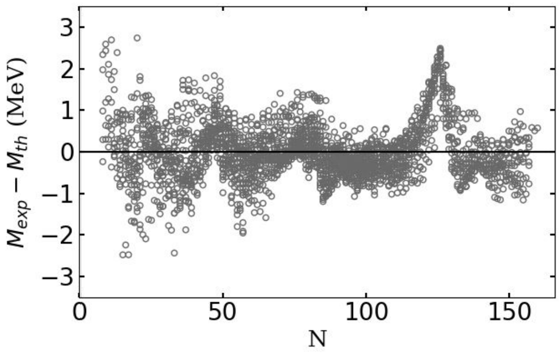
σ (M) = 0.681 MeV

ε (M) = -0.041 MeV

σ (R_C) = 0.0250 MeV
ε (R_C) = -0.0045 MeV

PRELIMINARY!

All 2457 nuclei in the AME2020 nuclear chart.



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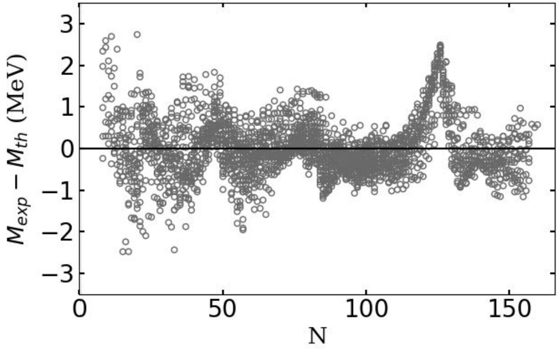
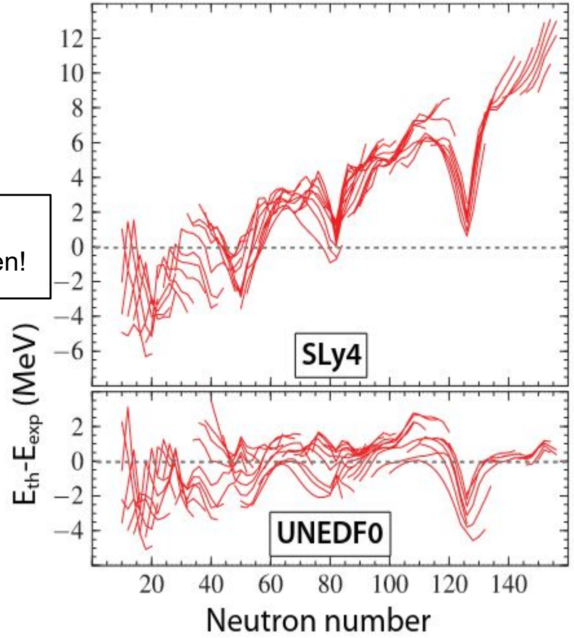


Comparison:

BSkG2
σ (M) = 0.678 MeV
BSkG1
σ (M) = 0.741 MeV

SLy4
σ (M) = 4.80 MeV
UNEDF0
σ (M) = 1.45 MeV

Just 520 even-even!



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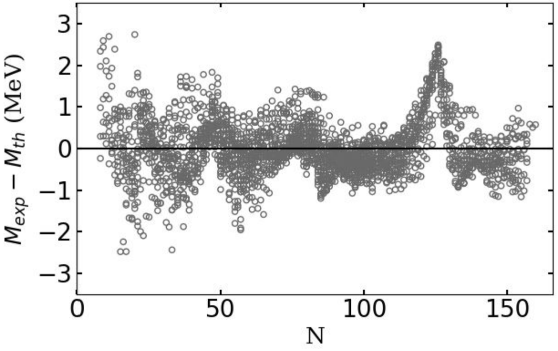


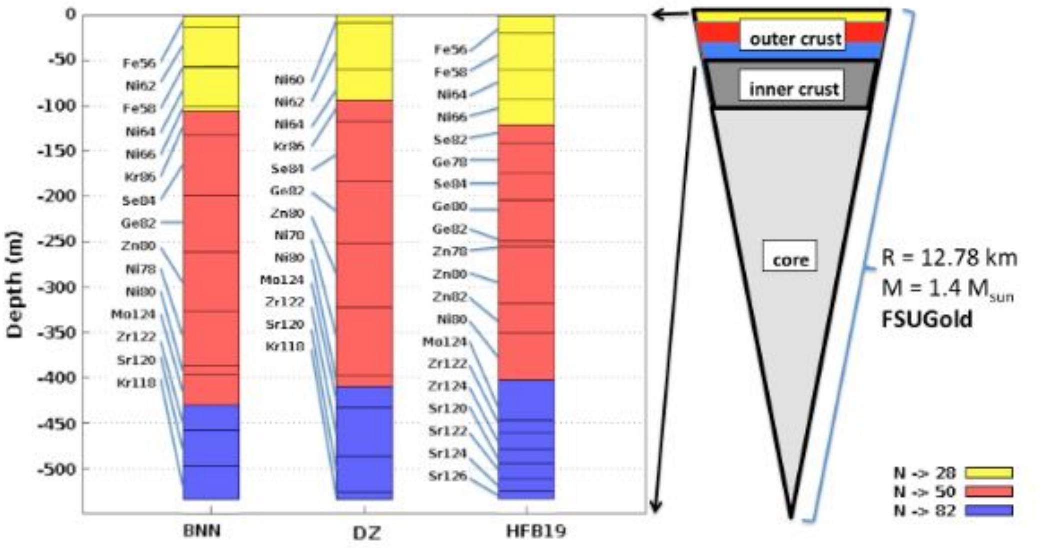
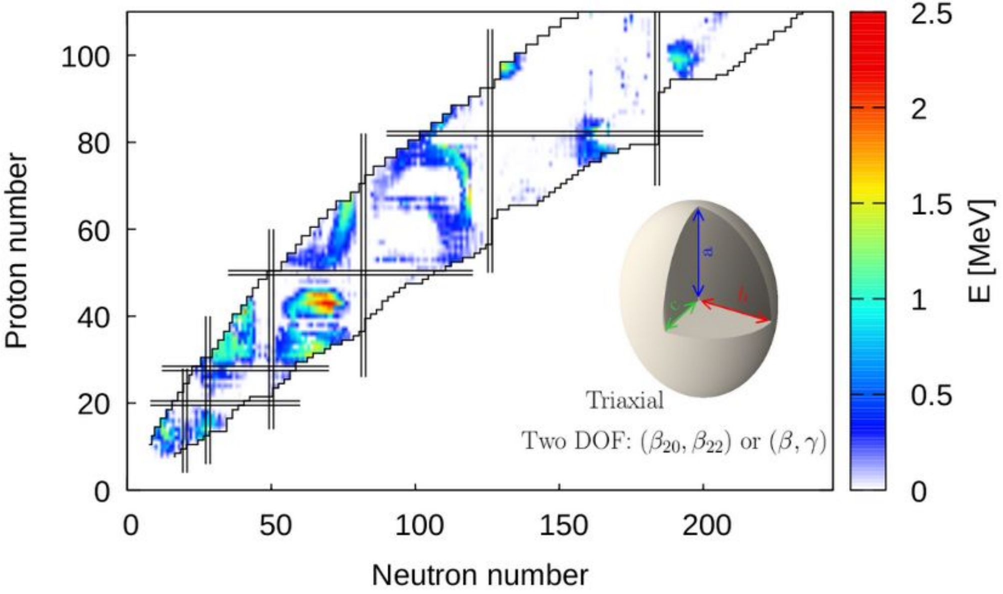


Fig. 4. Composition of a canonical 1.4 $M_\odot$ neutron star with a 12.78 km radius as predicted by three mass models: "BNN-world", DZ, and HFB19.

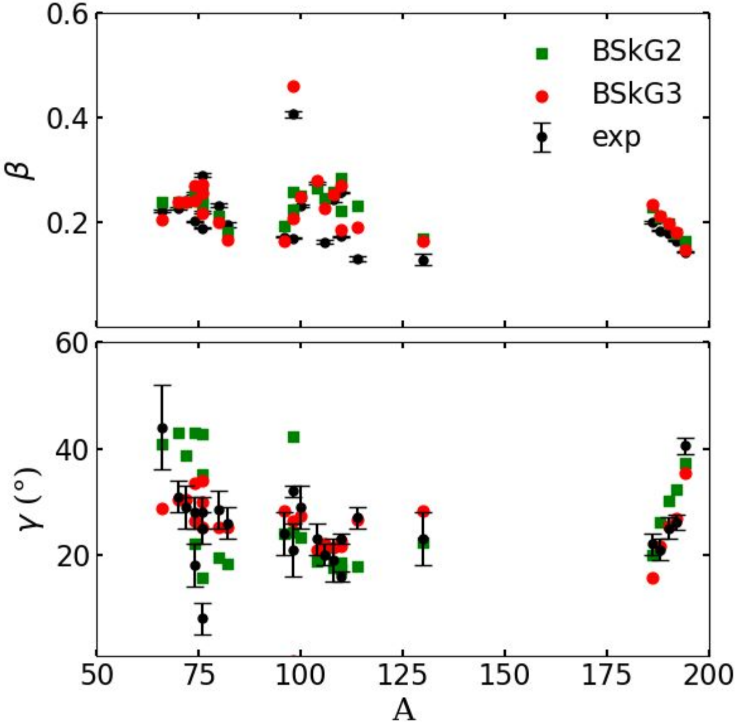
Figure from: J. Piekarewicz & R. Utama, Acta Phys. Pol. B 47, 659 (2016)

The BSkG3 mass model

Deformation

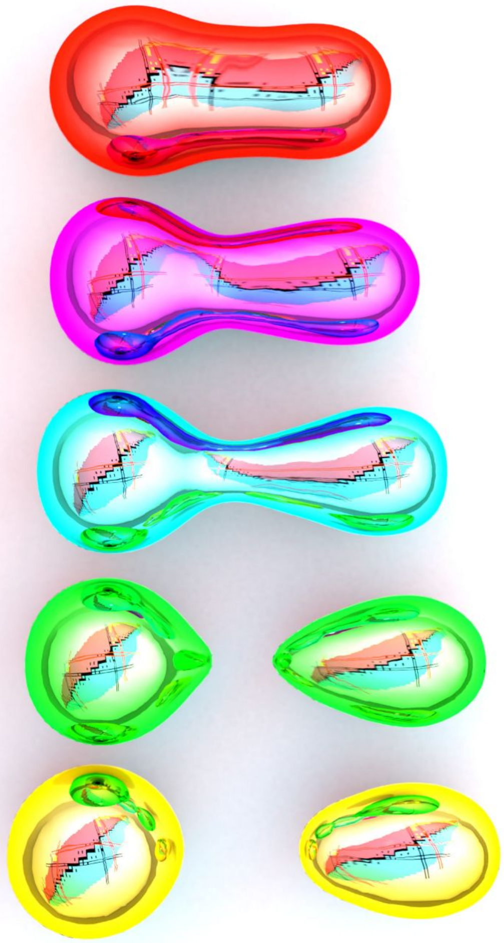


Binding energy difference between **unrestricted** calculations and calculations **restricted** to axial quadrupole deformation with BSkG1.



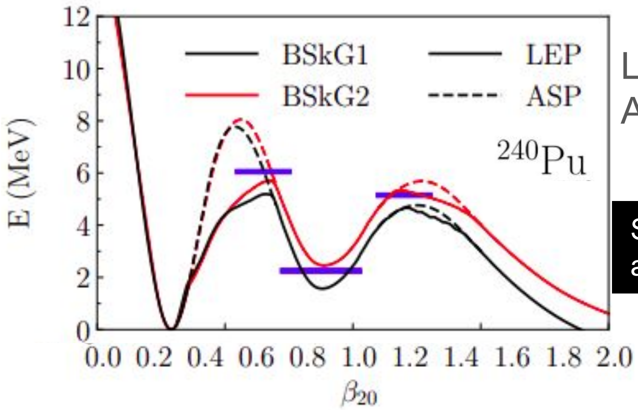
Quadrupole **deformation** (top) and **triaxiality** angle (bottom) for BSkG2 (green), BSkG3(red) and experimental data (black).

The BSkG3 mass model



Fission barriers

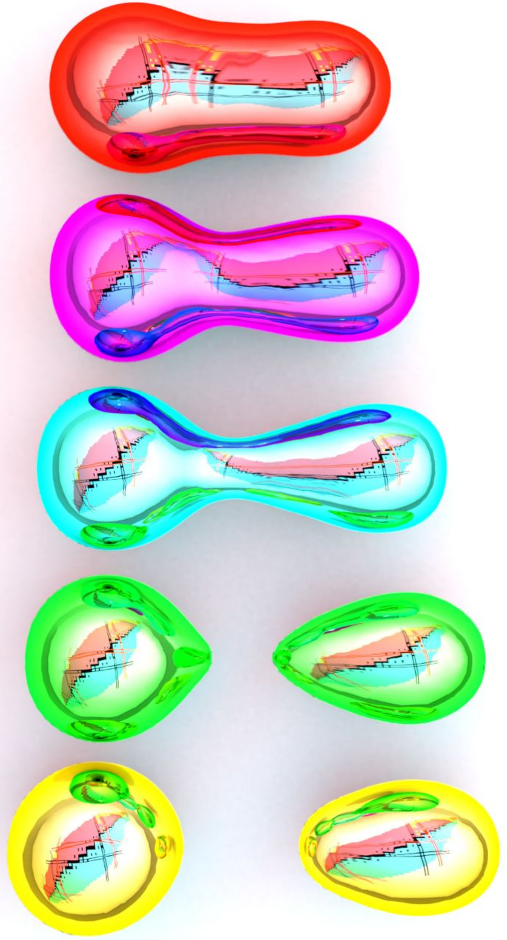
Primary (E_I), secondary (E_{II}) ***fission barrier*** heights and fission isomer excitation energies (E_{iso}) of actinide nuclei.



LEP = Low Energy Path
ASP = Axial Symmetric Path

See W. Ryssens et al.
arXiv: 2302.03097

The BSkG3 mass model



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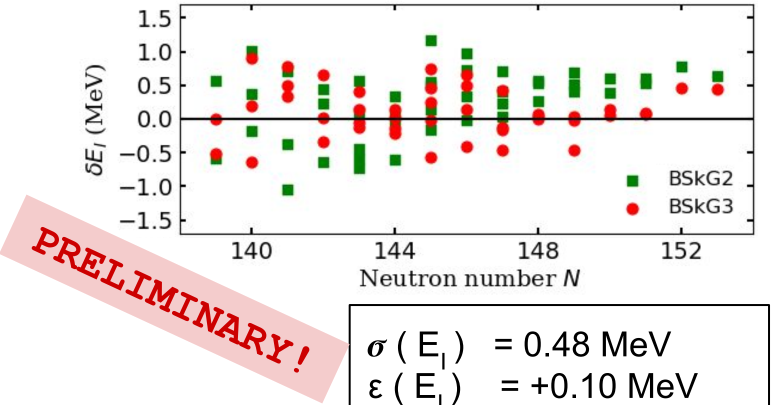
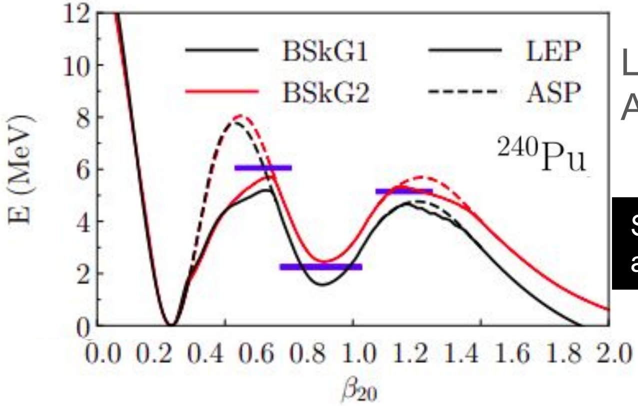


σ (E_I) = 0.48 MeV
ε (E_I) = +0.10 MeV



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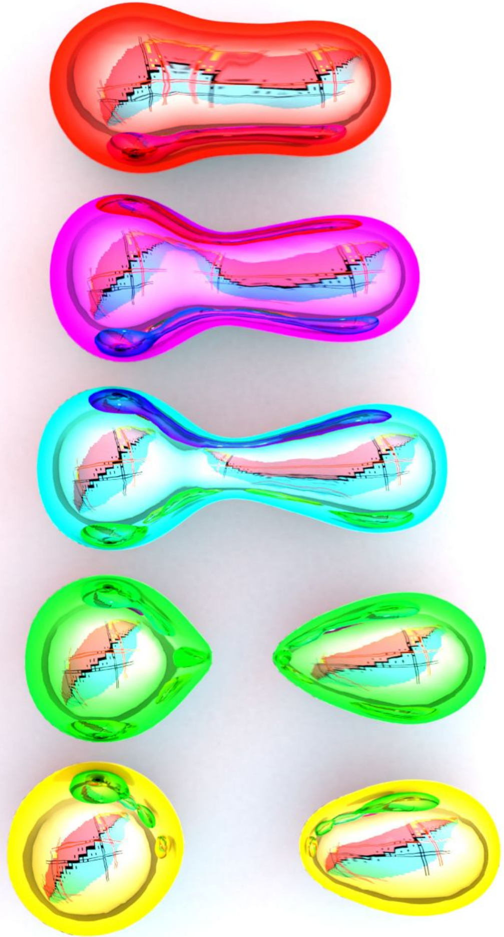
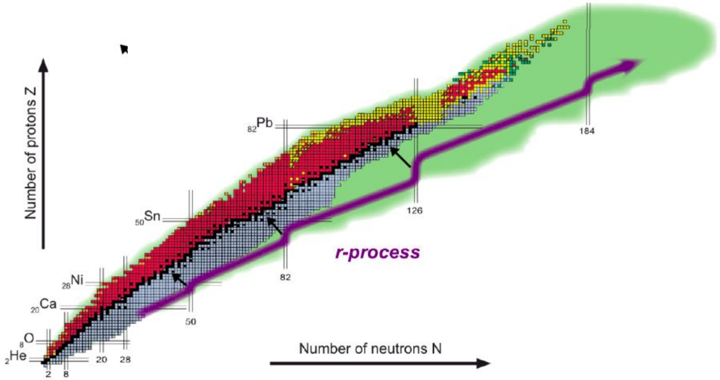
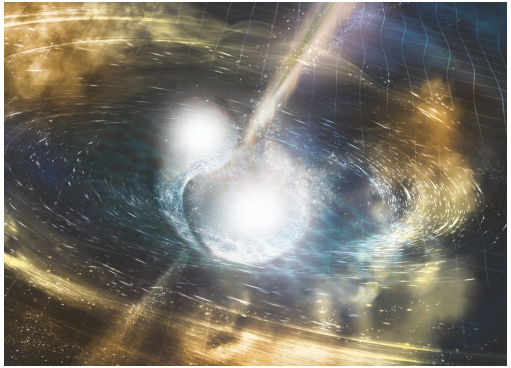
The BSkG3 mass model



Fission barriers



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



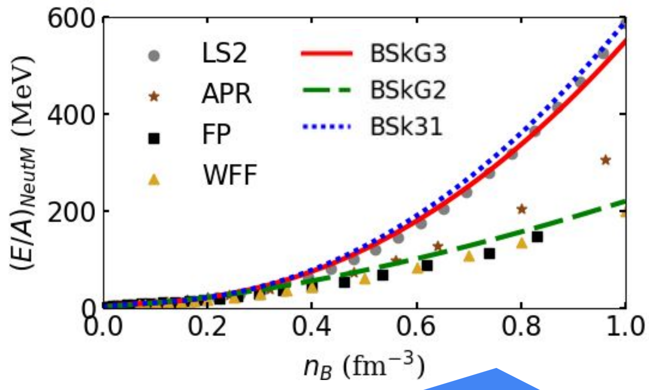
- **"fission recycling"**;
- the **r-process abundances** in the 110 ≤ A ≤ 170 region;
- the production of cosmic chronometers such as Th and U;
- the **heating rate of kilonovae**.

The BSkG3 interaction

Neutron matter (NeutM) energy

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

Neutron matter energy



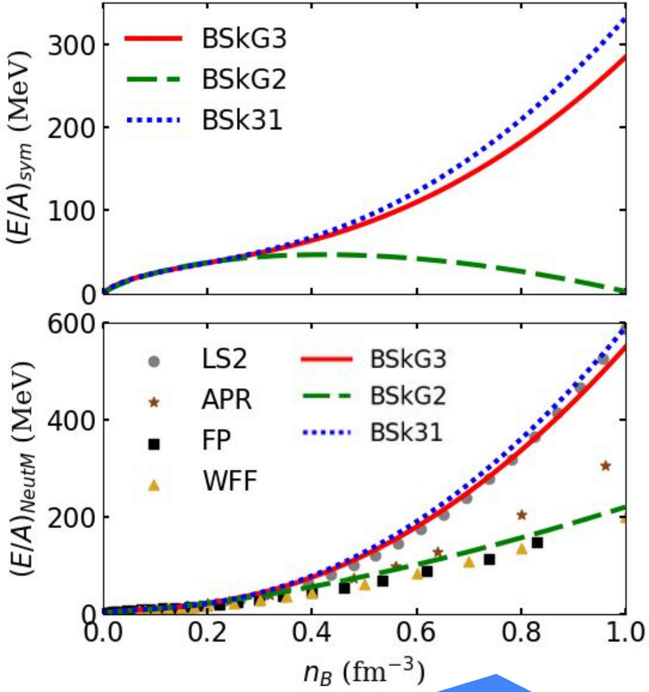
important for describing massive neutron star

The BSkG3 interaction

Neutron matter (NeutM) & symmetry energy

Symmetry energy: $e_{NeutM} - e_{SM}$

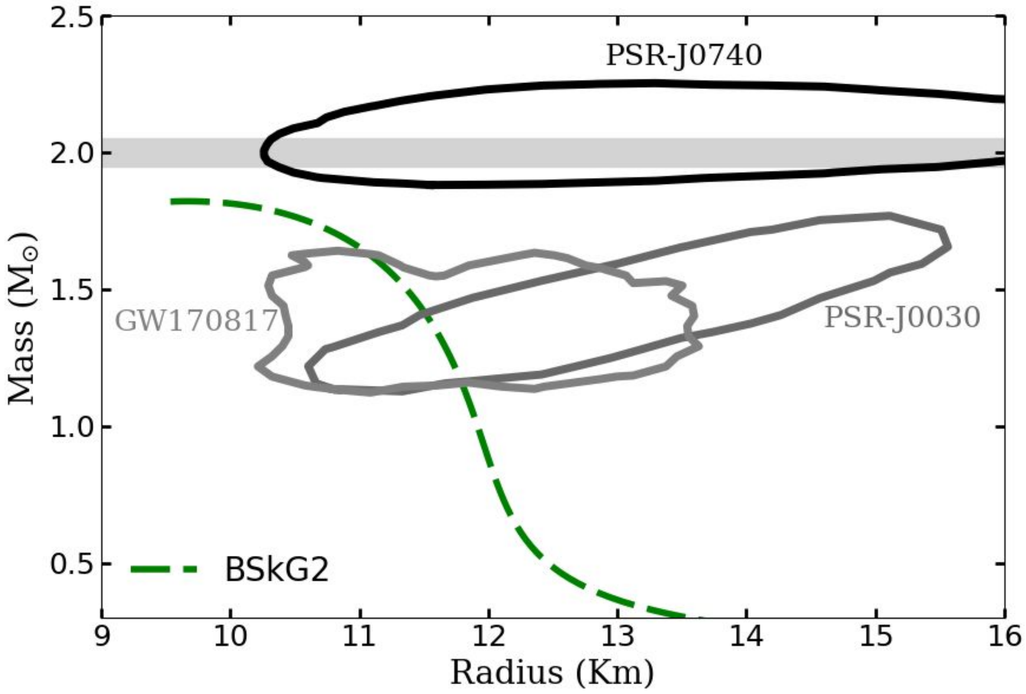
Neutron matter energy



important for describing massive neutron star

The BSkG3 interaction

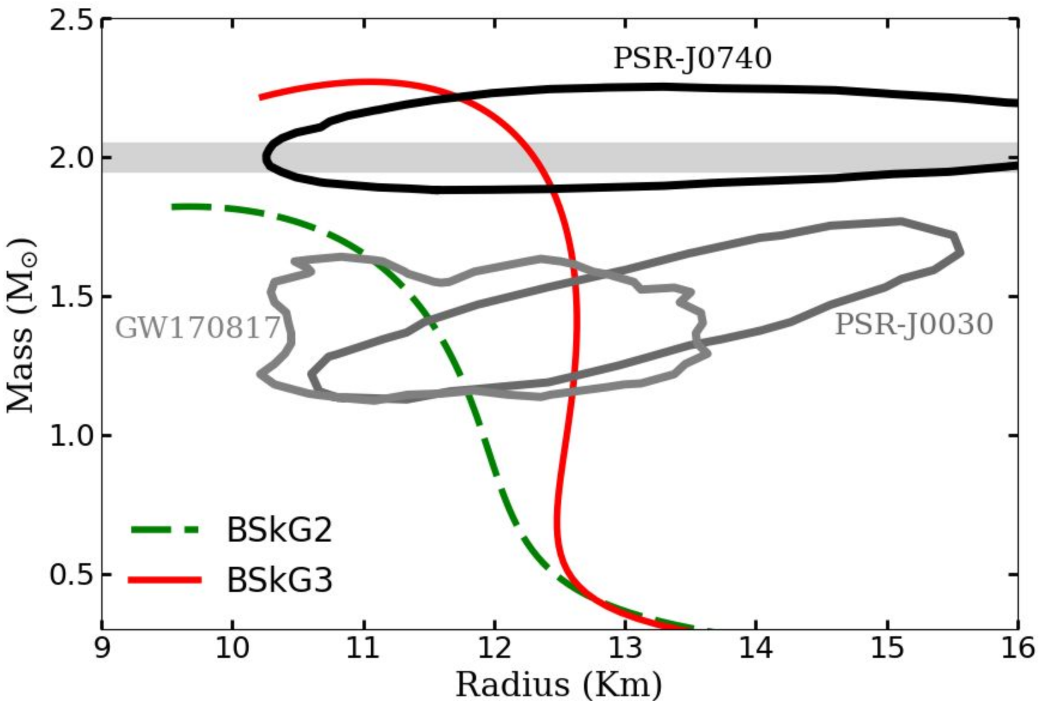
nuclear EoS → **TOV equations** (General Relativity) → Neutron star properties



BSkG2 does not reproduce massive pulsars

The BSkG3 interaction

Neutron star properties



$R_{1.4}$ = 12.6 km

M_{max} = 2.3 Msun
R_{Mmax} = 11.1 km

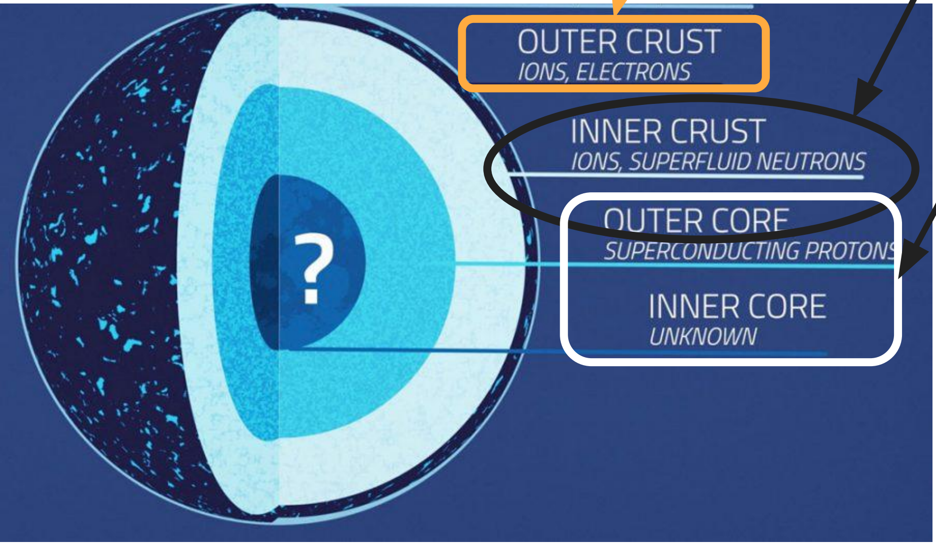
M_{dUrca} = 1.5 Msun
n_{dUrca} = 0.43 fm^{-3}

Summary

Root-mean-square on experimental masses and fission barriers:

σ (M) < 800 KeV

σ (E_I) < 500 KeV



- new **pairing** prescription with self-energy corrections (important for neutron and proton **superfluids** in NS **crust and core**);

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

The road ahead:

- systematic exploration of symmetry energy;
- move to finite temperature EoS;
- Fine-tune time-odd terms.

Acknowledgements

I thank:

- My collaborators: Wouter Ryssens, Guillaume Scamps, Stephane Goriely and Nicolas Chamel.
- The computational resources provided by the *Consortium des Équipements de Calcul Intensif* (CECI).
- The funding agencies FNRS and FWO.
- The EVEREST and MANASLU EOS projects.

- **Thank you for the attention!**

extra slides

The BSkG3 functional

Skyrme EDF

Standard Skyrme used in BSkG1 and BSkG2

Energy

Coupling constants

Local densities ρ and kinetic density τ of a HFB state

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

The BSkG3 functional

Skyrme EDF

Standard Skyrme used in BSkG1 and BSkG2

Energy

Coupling constants

Local densities ρ and kinetic density τ of a HFB state

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

Extended Skyrme used in BSkG3

$$E^{\text{BSkG3}} = C_1(\rho)\rho^2 + C_2(\rho)\rho\tau + C_3(\rho)\nabla\rho\nabla\rho + \ldots$$

$$C_2(\rho) = C_2(t_1, x_1, t_2, x_2) + C_2(t_4, x_4)\rho^\beta + C_2(t_5, x_5)\rho^\gamma$$

where t1,x1,...,t5,x5 are Skyrme parameters.

Ingredients of the mass model

We represent an atomic nucleus with N neutrons and Z protons with a many-body state of the Bogoliubov type, whose total energy E_{tot} we define as:

$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{corr}} . \tag{1}$$

We call E_{HFB} the mean-field energy and E_{corr} is a set of corrections that account (approximately) for correlations that cannot be captured by single mean-field reference state constructed from separate neutron and proton orbitals. More precisely, the mean-field energy consists of five parts:

$$E_{\text{HFB}} = E_{\text{kin}} + E_{\text{Sk}} + E_{\text{pair}} + E_{\text{Coul}} + E_{\text{cm}}^{(1)} , \tag{2}$$

which are, respectively, the kinetic, Skyrme, pairing and the Coulomb energy and the one-body part of the centre-of-mass correction [24]. The correction energy E_{corr} is written in terms of three parts:

$$E_{\text{corr}} = E_{\text{rot}} + E_{\text{cm}}^{(2)} + E_{\text{W}} , \tag{3}$$

$$E_{\text{Sk}} = \int d^3\mathbf{r} \sum_{t=0,1} \left[\mathcal{E}_{t,\text{e}}(\mathbf{r}) + \mathcal{E}_{t,\text{o}}(\mathbf{r})\right] ,$$

$$\begin{aligned}
\mathcal{E}_{t,\text{e}}(\mathbf{r}) = {} & C_t^{\rho\rho}(\rho_0)\, \rho_t^2(\mathbf{r}) + C_t^{\rho\tau}(\rho_0)\, \rho_t(\mathbf{r})\, \tau_t(\mathbf{r}) \\
& + C_t^{\rho\nabla J} \rho_t(\mathbf{r})\, \boldsymbol{\nabla} \cdot \mathbf{J}_t(\mathbf{r}) \\
& + C_t^{\rho\Delta\rho}\, \rho_t(\mathbf{r})\, \Delta\rho_t(\mathbf{r}) \\
& + C_t^{\nabla\rho\nabla\rho}(\rho_0)\, \boldsymbol{\nabla}\rho_t(\mathbf{r}) \cdot \boldsymbol{\nabla}\rho_t(\mathbf{r}) \\
& + C_t^{\rho\nabla\rho\nabla\rho}(\rho_0)\, \rho_t(\mathbf{r}) \boldsymbol{\nabla}\rho_0(\mathbf{r}) \cdot \boldsymbol{\nabla}\rho_t(\mathbf{r})
\end{aligned} \tag{6}$$

$$\begin{aligned}
\mathcal{E}_{t,\text{o}}(\mathbf{r}) = {} & C_t^{ss}(\rho_0)\, \mathbf{s}_t(\mathbf{r}) \cdot \mathbf{s}_t(\mathbf{r}) + C_t^{jj}(\rho_0)\, \mathbf{j}_t(\mathbf{r}) \cdot \mathbf{j}_t(\mathbf{r}) \\
& + C_t^{j\nabla s}\, \mathbf{j}_t(\mathbf{r}) \cdot \nabla \times \mathbf{s}_t(\mathbf{r}) .
\end{aligned} \tag{7}$$

$$\begin{aligned}
C_t^{\rho\tau}(\rho_0) = {} & +\frac{1}{2} C_{0t}^{+}(t_1, x_1) + \frac{1}{2} C_{0t}^{-}(t_2, x_2) \\
& + \frac{1}{2} C_{0t}^{+}(t_4, x_4)\rho_0^{\beta} + \frac{1}{2} C_{0t}^{-}(t_5, x_5)\rho_0^{\gamma} ,
\end{aligned} \tag{8}$$

$$C_t^{\nabla\rho\nabla\rho}(\rho_0) = +\frac{3}{8} C_{0t}^{+}(t_4, x_4)\rho_0^{\beta} - \frac{1}{8} C_{0t}^{-}(t_5, x_5)\rho_0^{\gamma} , \tag{9}$$

$$C_t^{\rho\nabla\rho\nabla\rho}(\rho_0) = -\frac{1}{2} C_{0t}^{+}(t_4, x_4)\rho_0^{\beta-1} . \tag{10}$$

The BSkG3 interaction

Pairing interaction:

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

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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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.

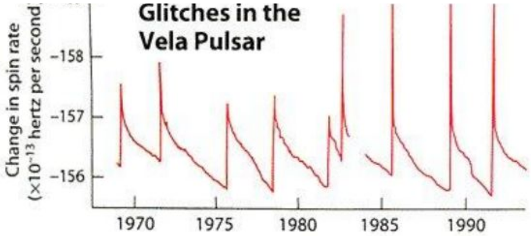
$$g_q(\rho_n, \rho_p) = V_q(\rho_n, \rho_p) \left[1 + \kappa_q (\nabla \rho_0)^2\right]$$

- 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.

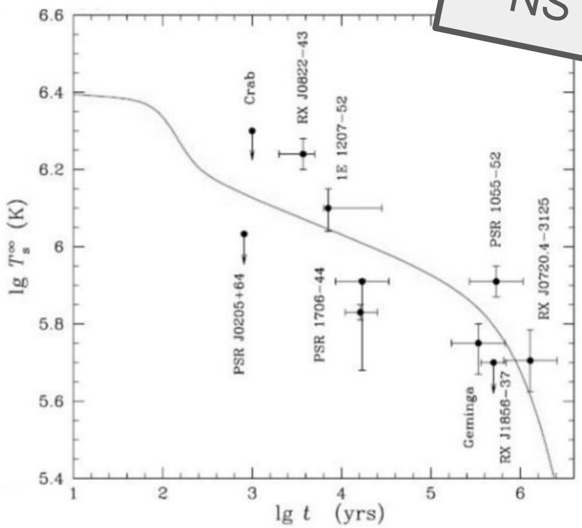
The BSkG3 interaction

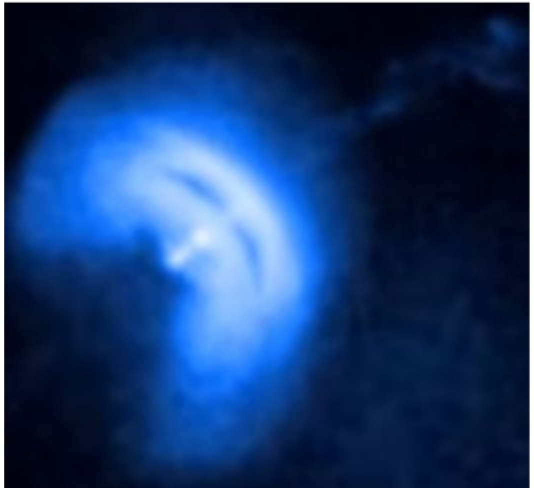
Pairing interaction:

Important to describe **superfluids** in NSs.



NS cooling

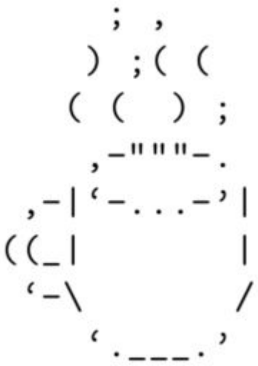




The BSkG3 functional

The fitting procedure

MOCCa



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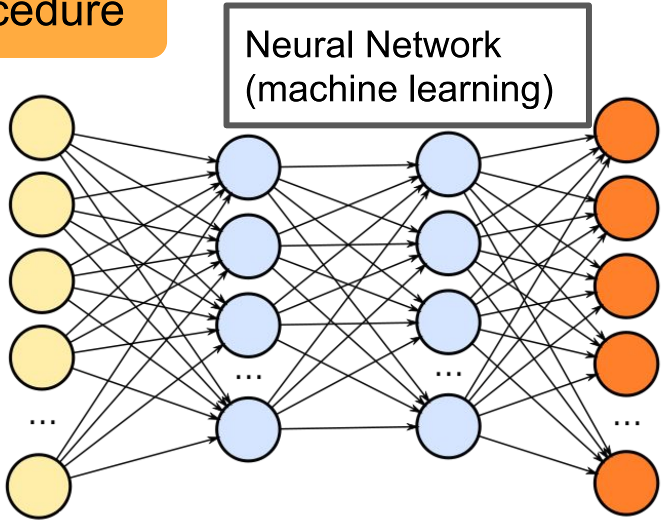


- **Fitted to experimental masses, charge radii, proton and neutron pairing gaps,**

- **constrain infinite nuclear matter properties.**

Deformed nuclei are important to describe **pasta configurations in NS**

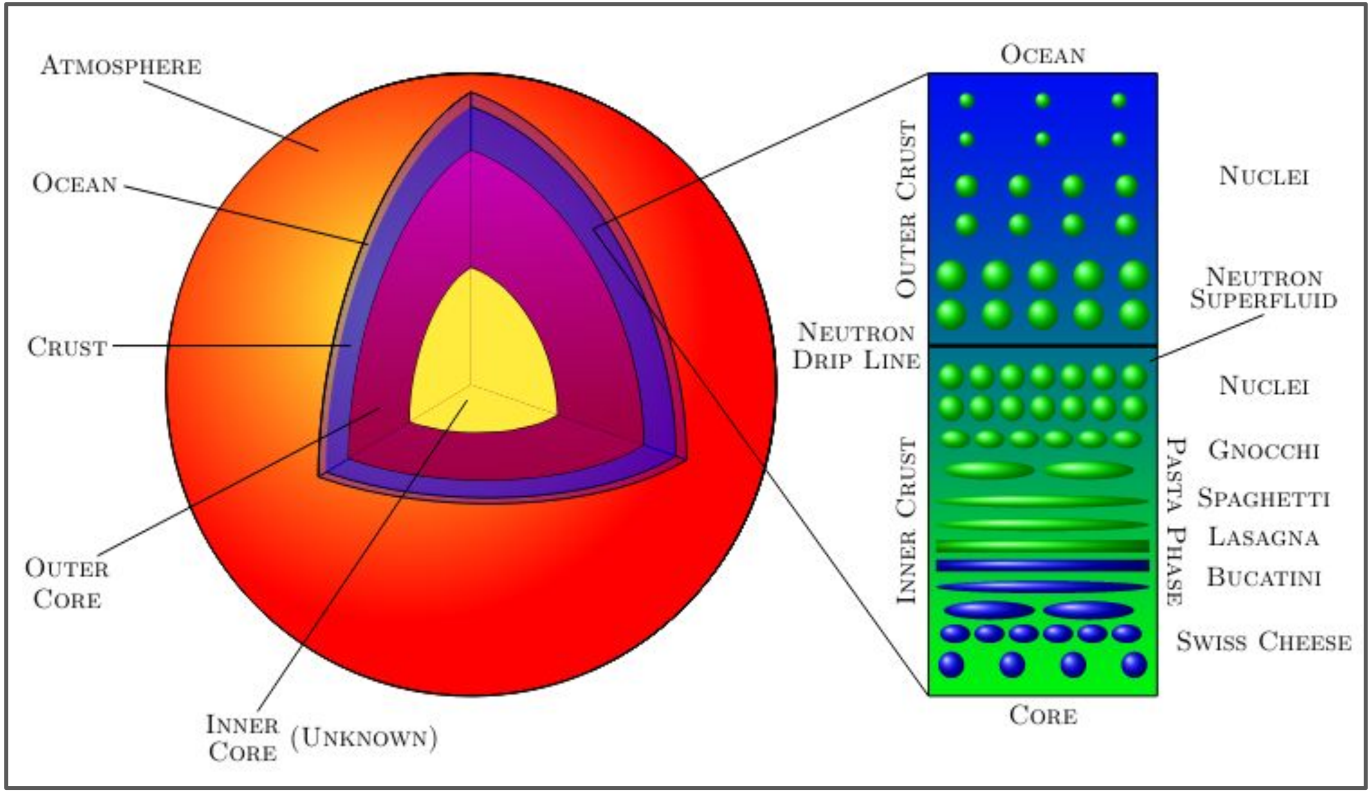
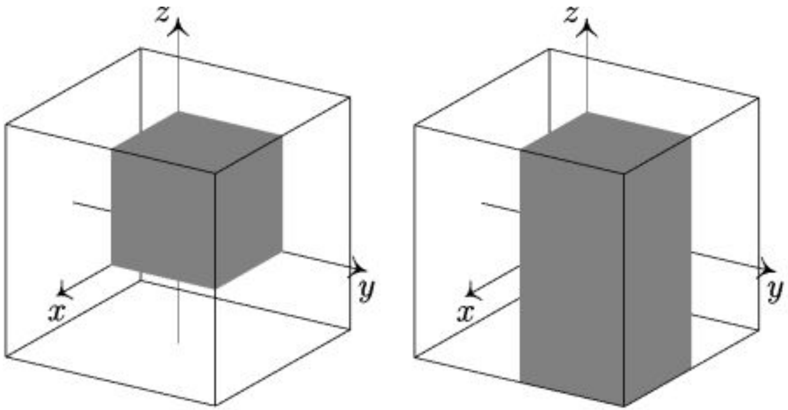


Figure from: Javier F. Acevedo et al JCAP 03, 038 (2020).

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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HFB solver

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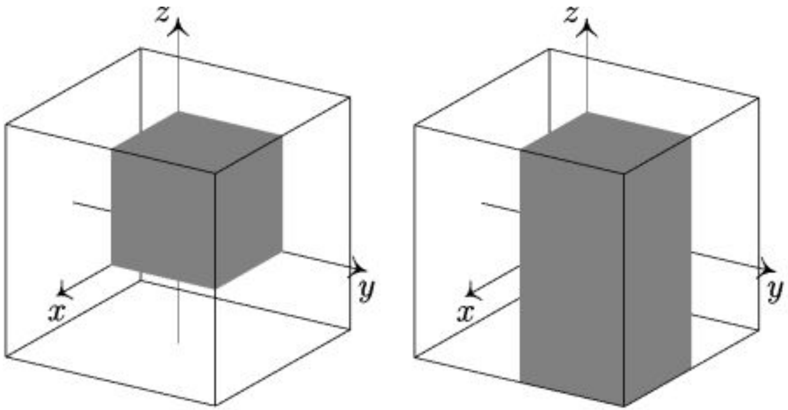
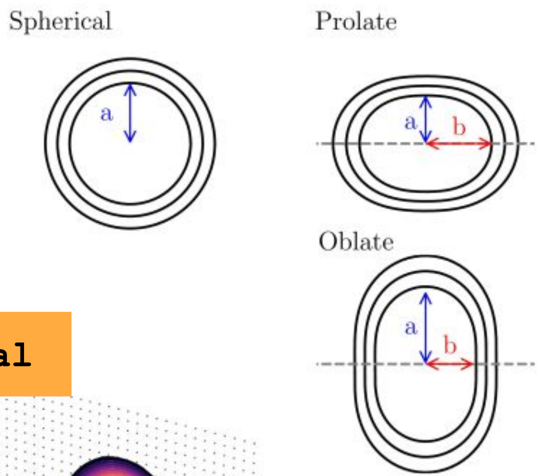
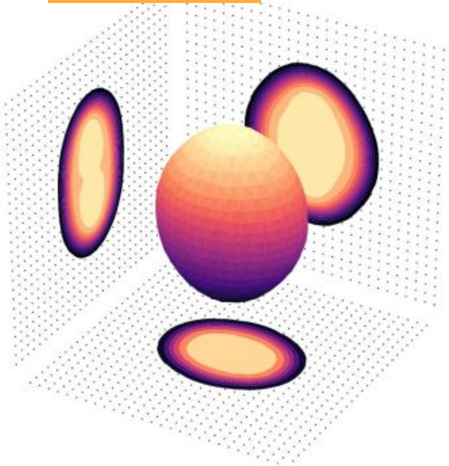


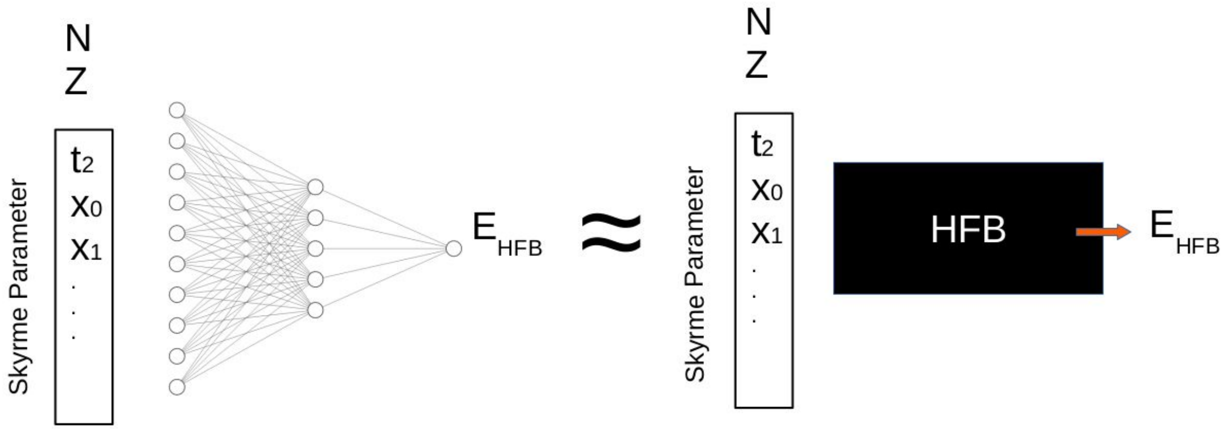
Nuclear shapes



Triaxal



Machine learning method to fit



1. Create a **dataset of MOCCa results.**

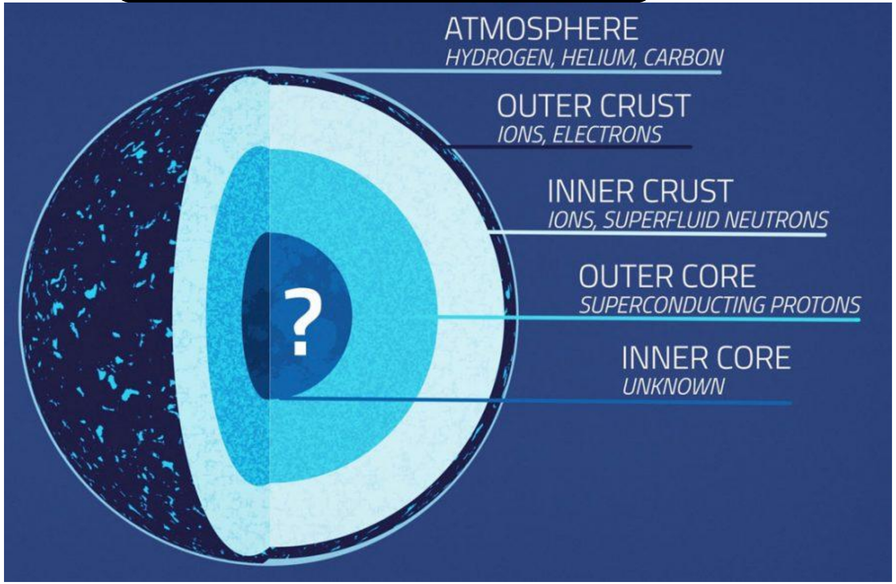
2. Adjust a **machine learning system** to create an **emulator of the HFB solver**.
3. Adjust the mass model parameters using the emulator.

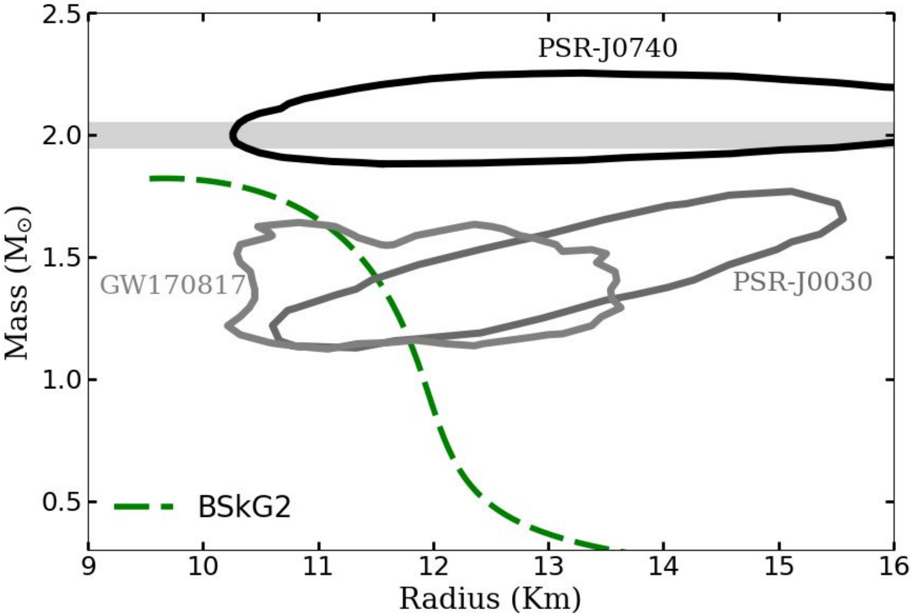
   Machine learning prediction for one nucleus ~ a few seconds.
   MOCCa predictions for one nucleus ~ 20 minutes.

4. **The mass table is computed with MOCCa.**

Motivation

Neutron star physics





Previous BSkG forces failed to reproduce massive neutrons stars.

The BSkG3 functional

The fitting procedure

1. Deduce INM equations, e.g., symmetry energy, energy per particle, compressibility, effective mass, etc.
   $J = J(t_2, x_0, x_1, \ldots)$, $K_V = K_V(t_2, x_0, x_1, \ldots)$, $m^*_{s/v} = m^*_{s/v}(t_2, x_0, x_1, \ldots)$,

2. Impose constraints in the INM; obtain Skyrme parameters from the fit.

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2. Impose constraints in the INM; obtain Skyrme parameters from the fit.

1. Novelty at BSkG3:
   impose constraint at **neutron matter energy** (NeutM) **at high density** (1 fm^{-3})
   E_{NeutM}(at 1 fm^{-3}) = $\mathbf{E_{NeutM}(t_4,t_5,\ldots,t_2,x_0,x_1, \ldots)}$ $\in$ [550 , 600 MeV].

2. Possible thanks to the **extended Skyrme** form which contains $\mathbf{t_4}$ and $\mathbf{t_5}$ terms (density dependent extension of $\mathbf{t_1}$ and $\mathbf{t_2}$).

3. Ensures a **stiff** neutron matter **equation of state** (essential for **neutron stars**).

The BSkG 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).

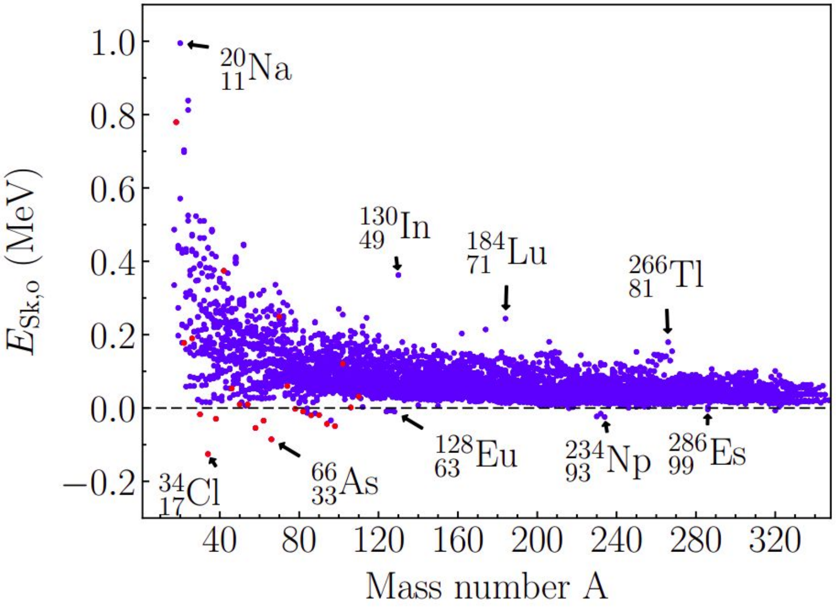
- Incorporated information on the **fission properties** of twelve actinide nuclei in the fitting protocol.

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.



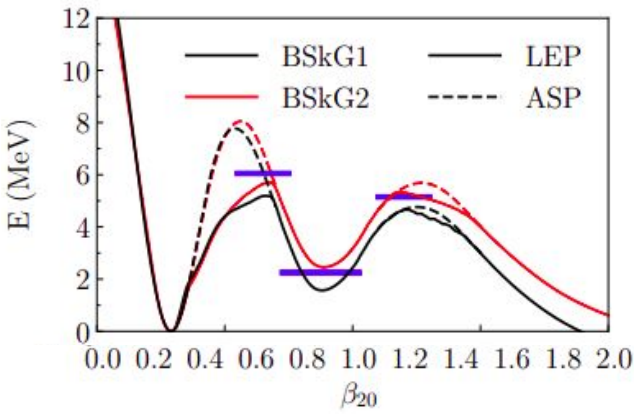
The BSkG functionals

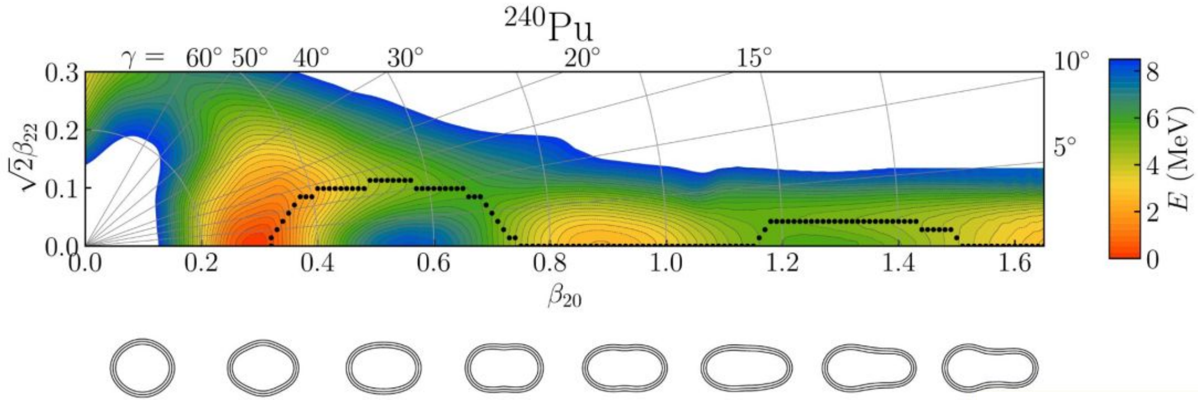
BSkG2:
fission properties

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





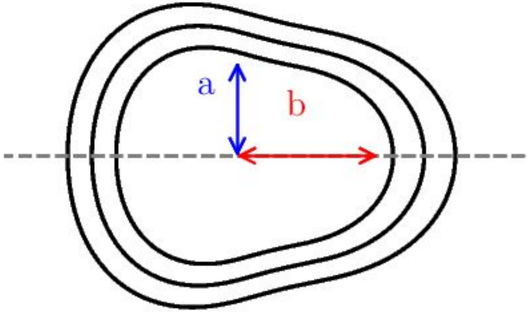
ASP = Axial Symmetric Path
LEP = Low Energy Path

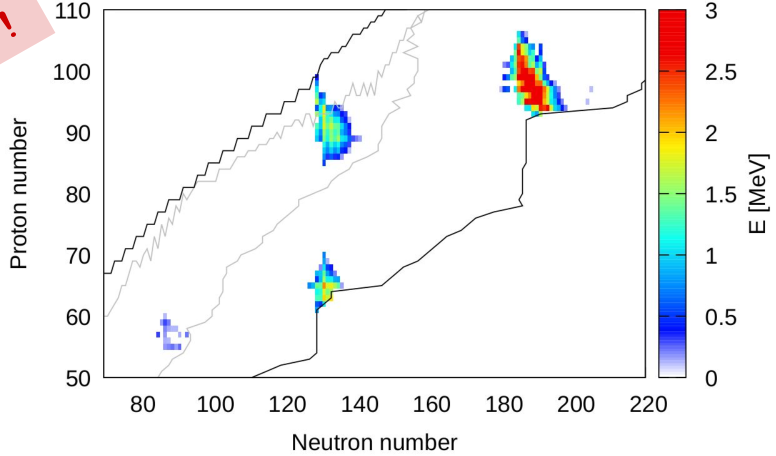
The BSkG3 mass model

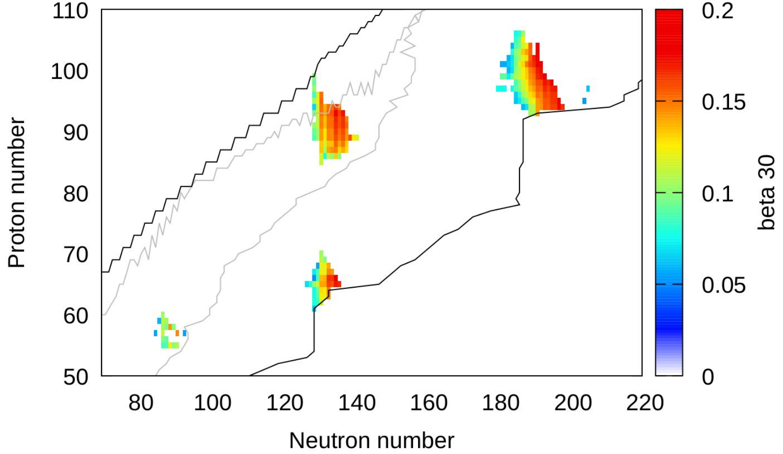
Octupole shapes in ground state

PRELIMINARY!

Reflection-asymmetric (RA)

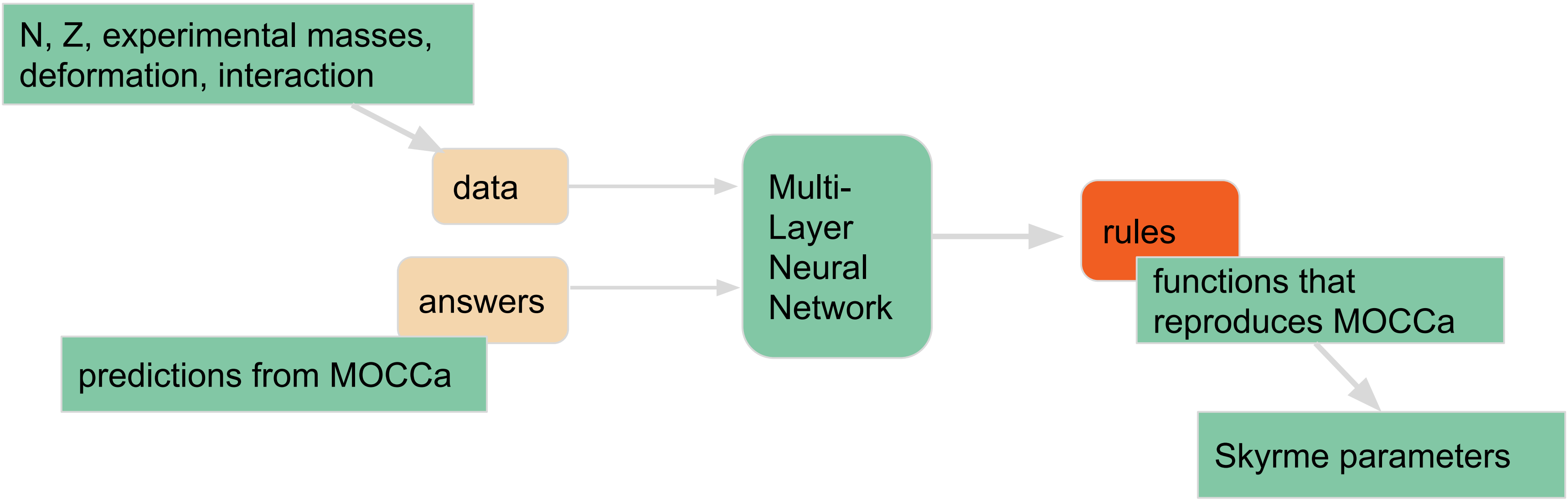






workflow

The fitting procedure



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.

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 nuclear force

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

- EDF to calculate self-consistently the nuclei binding energies.
- Skyrme nucleon-nucleon interaction + Hartree-Fock many-body method.
- **Fitted to a large number of experimental masses.**

- **Pairing** channel first computed with BCS approximation (Tondeur 1977). From HFB-1 models the **Bogoliubov** method is applied.
- **Constrained** on infinite **nuclear matter** properties (saturation density, symmetry energy, etc).
- Axial symmetry + harmonic oscillator basis.
- Equal Filling Approximation (EFA).

The road to here

Brussels mass models

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[d] *Institut Supérieur Industriel de Bruxelles, 1000 Brussels, Belgium*

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

New BSk**G** family:

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

Received: 7 September 2021 / Accepted: 26 November 2021

- BSkG1: coordinate space representation on a **3D mesh**, allows for **triaxial** nuclei. *Machine learning tools as emulator* for the parameter adjustment.
- BSkG2: **break time-reversal symmetry**: includes time-odd terms on EDF (no more EFA) + information on **fission barriers** included on the fit procedure.

Coordinate space representation opens the door for applications such **fission process** and **nuclear pasta** on *neutron stars* and *supernovae*.

The BSkG3 mass model

Skyrme-HFB on the Grid

- **Nuclear interaction** described by an extended **Skyrme force**;
- **Many body problem** solved with **Hartree-Fock-Bogoliubov approximation**.
- **3D coordinate space** representation. **Triaxial** deformation.

Difference from previous BSkGs to BSkG3:

The BSkG3 mass model

Skyrme-HFB on the Grid

- **Nuclear interaction** described by an extended **Skyrme force**;
- **Many body problem** solved with **Hartree-Fock-Bogoliubov approximation**.
- **3D coordinate space** representation. **Triaxial** deformation.

Difference from previous BSkGs to BSkG3:

Improvement on ***pairing*** channel.
Functional fitted to ab-initio calculations of pairing gaps with self-energy corrections.

Important for the neutron **superfluid** present on **neutron star inner-crust**.

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*
(Received 20 January 2016; published 31 March 2016)

The BSkG3 mass model

Skyrme-HFB on the Grid

- **Nuclear interaction** described by an extended **Skyrme force**;
- **Many body problem** solved with **Hartree-Fock-Bogoliubov approximation**.
- **3D coordinate space** representation. **Triaxial** deformation.

Difference from previous BSkGs to BSkG3:

Two extra density depend terms on EDF.
Already present on BSk-18 to BSk-32, it helps to obtain a ***stiff neutron matter equation of state***, and maintained a good reproduction of experimental masses.

PHYSICAL REVIEW C **80**, 065804 (2009)

Further explorations of Skyrme-Hartree-Fock-Bogoliubov mass formulas. XI. Stabilizing neutron stars against a ferromagnetic collapse

N. Chamel,[1] S. Goriely,[1] and J. M. Pearson[2]
[1]*Institut d'Astronomie et d'Astrophysique, CP226, Université Libre de Bruxelles, B-1050 Brussels, Belgium*
[2]*Département de Physique, Université de Montréal, Montréal, Québec H3C 3J7, Canada*
(Received 11 September 2009; published 17 December 2009)

We construct a new Hartree-Fock-Bogoliubov (HFB) mass model, labeled HFB-18, with a generalized Skyrme force. The additional terms that we have introduced into the force are density-dependent generalizations of the

PHYSICAL REVIEW C **82**, 035804 (2010)

Further explorations of Skyrme-Hartree-Fock-Bogoliubov mass formulas. XII. Stiffness and stability of neutron-star matter

S. Goriely,[1] N. Chamel,[1] and J. M. Pearson[2]
[1]*Institut d'Astronomie et d'Astrophysique, CP-226, Université Libre de Bruxelles, B-1050 Brussels, Belgium*
[2]*Département de Physique, Université de Montréal, Montréal (Québec), H3C 3J7 Canada*
(Received 10 June 2010; published 24 September 2010)

We construct three new Hartree-Fock-Bogoliubov (HFB) mass models, labeled HFB-19, HFB-20, and HFB-21,

The BSkG3 functional

Skyrme EDF

Standard Skyrme used in BSkG1 and BSkG2

Energy

Coupling constants

Local densities ρ and kinetic density τ of a HFB state

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

Extended Skyrme used in BSkG3

$$E^{BSkG3} = C_1(\rho)\rho^2 + C_2(\rho)\rho\tau + C_3(\rho)\nabla\rho\nabla\rho + \ldots$$

$$C_2(\rho) = C_2(t_1, x_1) + C_2^{\beta}(t_4, x_4)\rho^{\beta}$$

$$C_3(\rho) = C_3(t_2, x_2) + C_3^{\gamma}(t_5, x_5)\rho^{\gamma}$$