Nuclear Energy Density Functionals for Astrophysical Applications

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Prelude

Nuclear models required for astrophysical applications (e.g. stellar nucleosynthesis, core-collapse supernova, neutron stars) should be:

- **versatile**: applicable to compute various properties (equation of state, transport properties, reaction rates, etc.) of various systems (nuclei, nuclear matter) under various conditions/phases
- **thermodynamically consistent**: avoid spurious instabilities
- **as microscopic as possible**: make reliable extrapolations
- **numerically tractable**: systematic calculations over a wide range of temperatures, pressures, compositions, magnetic fields.

The nuclear energy density functional theory appears to be currently the most suitable approach for astrophysical applications.

Duguet, Lect. Notes Phys. 879 (Springer-Verlag, 2014), p. 293

Dobaczewski & Nazarewicz, in ”50 years of Nuclear BCS” (WSP, 2013), pp.40-60

Route to phenomenological functionals

For simplicity, we consider **semilocal functionals** obtained from **generalized Skyrme effective interactions**

$$
\begin{aligned}
v_{ij} &= t_0(1+x_0P_\sigma)\delta(\boldsymbol{r}_{ij}) + \frac{1}{2}t_1(1+x_1P_\sigma)\frac{1}{\hbar^2}\left[p_{ij}^2\,\delta(\boldsymbol{r}_{ij}) + \delta(\boldsymbol{r}_{ij})\,p_{ij}^2\right] \\
&+ t_2(1+x_2P_\sigma)\frac{1}{\hbar^2}\boldsymbol{p}_{ij}.\delta(\boldsymbol{r}_{ij})\,\boldsymbol{p}_{ij} + \frac{1}{6}t_3(1+x_3P_\sigma)n(\boldsymbol{r})^\alpha\,\delta(\boldsymbol{r}_{ij}) \\
&+ \frac{1}{2}\,t_4(1+x_4P_\sigma)\frac{1}{\hbar^2}\left\{p_{ij}^2\,n(\boldsymbol{r})^\beta\,\delta(\boldsymbol{r}_{ij}) + \delta(\boldsymbol{r}_{ij})\,n(\boldsymbol{r})^\beta\,p_{ij}^2\right\} \\
&+ t_5(1+x_5P_\sigma)\frac{1}{\hbar^2}\boldsymbol{p}_{ij}\cdot n(\boldsymbol{r})^\gamma\,\delta(\boldsymbol{r}_{ij})\,\boldsymbol{p}_{ij} \\
&+ \frac{\mathrm{i}}{\hbar^2}W_0(\boldsymbol{\sigma_i}+\boldsymbol{\sigma_j})\cdot\boldsymbol{p}_{ij}\times\delta(\boldsymbol{r}_{ij})\,\boldsymbol{p}_{ij} + \frac{\mathrm{i}}{\hbar^2}W_1(\boldsymbol{\sigma}_i+\boldsymbol{\sigma}_j)\cdot\boldsymbol{p}_{ij}\times(n_{qi}+n_{qj})^\nu\delta(\boldsymbol{r}_{ij})\,\boldsymbol{p}_{ij}
\end{aligned}
$$

$$
\textbf{pairing}\ v_{ij}^\pi = \frac{1}{2}(1+P_\sigma)v^\pi[n_n(\boldsymbol{r}), n_p(\boldsymbol{r}), \nabla n_n(\boldsymbol{r}), \nabla n_p(\boldsymbol{r})]\delta(\boldsymbol{r}_{ij})
$$

$\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$, $\boldsymbol{r} = (\boldsymbol{r}_i + \boldsymbol{r}_j)/2$, $\boldsymbol{p}_{ij} = -\mathrm{i}\hbar(\boldsymbol{\nabla}_i - \boldsymbol{\nabla}_j)/2$ is the relative momentum, and P_σ is the two-body spin-exchange operator.

The parameters t_i, x_i, α, β, γ, ν, W_i are fitted to experimental and/or microscopic nuclear data.

Why not fitting directly the functional?

The cancellation of self-interaction errors implies that the coupling coefficients in the functional cannot be completely freely adjusted.
Chamel, Phys. Rev. C 82, 061307(R) (2010).

Let us consider the simple functional $\mathcal{E} = C\,(n_n + n_p)^2$.

- A single nucleon interacts with itself: $\mathcal{E} = C|\varphi(\boldsymbol{r},\sigma)|^4 \neq 0$.
- $\mathcal{E}$ must contain time-odd densities (the nucleon is spin-polarized):

$$\mathcal{E} = C\,(n_n + n_p)^2 - C\,(s_n + s_p)^2 \text{ with } s_{n/p} = n^{\uparrow}_{n/p} - n^{\downarrow}_{n/p}$$

Functionals constructed from effective interactions are free from *one-particle* self-interactions errors but

- they still contain many-particle self-interaction errors
  Bender, Duguet, Lacroix, Phys. Rev. C 79, 044319 (2009).
- they induce additional relations between coupling coefficients.
  Dobaczewski&Dudek, Phys.Rev. C52, 1827 (1995);55, 3177(E) (1997).

Nuclear uncertainties

Phenomenological functionals cannot be uniquely defined due to experimental and theoretical uncertainties.

How to quantify these uncertainties?

The energy per nucleon of nuclear matter at $T = 0$ around saturation density n_0 and for asymmetry $\eta = (n_n - n_p)/n$, is usually written as

$$e(n,\eta) = e_0(n) + S(n)\eta^2 + o\left(\eta^4\right) \text{ where}$$

$$e_0(n) = a_v + \frac{K_v}{18}\epsilon^2 - \frac{K'}{162}\epsilon^3 + o\left(\epsilon^4\right) \text{ with } \epsilon = (n - n_0)/n_0$$

$$S(n) = J + \frac{L}{3}\epsilon + \frac{K_{sym}}{18}\epsilon^2 + o\left(\epsilon^3\right) \text{ is the symmetry energy}$$

The lack of knowledge is embedded in a_v, K_v, K', etc.

In order to make meaningful comparisons, functionals corresponding to different values of these parameters should be **fitted using the same protocole**.

Brussels-Montreal Skyrme functionals (BSk)

For application to extreme astrophysical environments, functionals should reproduce **global properties of both finite nuclei and infinite homogeneous nuclear matter**.

Experimental data:

- nuclear masses with $Z, N \geq 8$
- nuclear charge radii
- symmetry energy $29 \leq J \leq 32$ MeV
- incompressibility $K_v = 240 \pm 10$ MeV (ISGMR)
  Colò et al., Phys.Rev.C70, 024307 (2004).

Many-body calculations using realistic interactions:

- equation of state of pure neutron matter
- $^1S_0$ pairing gaps in nuclear matter
- effective masses in nuclear matter

Chamel et al., Acta Phys. Pol. B46, 349(2015)

Phenomenological corrections for atomic nuclei

For atomic nuclei, we add the following corrections to the HFB energy:

- Wigner energy

$$E_W = V_W \exp\left\{ -\lambda\left(\frac{N-Z}{A}\right)^2 \right\} + V'_W |N-Z| \exp\left\{ -\left(\frac{A}{A_0}\right)^2 \right\}$$

$V_W \sim -2$ MeV, $V'_W \sim 1$ MeV, $\lambda \sim 300$ MeV, $A_0 \sim 20$

- rotational and vibrational spurious collective energy

$$E_{\rm coll} = E_{\rm rot}^{\rm crank}\Big\{ b\ \tanh(c|\beta_2|) + d|\beta_2|\ \exp\{-l(|\beta_2| - \beta_2^0)^2\} \Big\}$$

This latter correction was shown to be in good agreement with calculations using 5D collective Hamiltonian.
Goriely, Chamel, Pearson, Phys.Rev.C82,035804(2010).

In this way, these collective effects do not contaminate the parameters (≤ 20) of the functional.

Brussels-Montreal Skyrme functionals

- **fit to realistic $^1S_0$ pairing gaps (no self-energy)** (BSk16-17)
  Chamel, Goriely, Pearson, Nucl.Phys.A812,72 (2008)
  Goriely, Chamel, Pearson, PRL102,152503 (2009).
  Chamel, Phys. Rev. C 82, 014313 (2010).
- **removal of spurious spin-isospin instabilities** (BSk18)
  Chamel, Goriely, Pearson, Phys.Rev.C80,065804(2009)
  Chamel & Goriely, Phys. Rev. C 82, 045804 (2010).
- **fit to realistic neutron-matter equations of state** (BSk19-21)
  Goriely, Chamel, Pearson, Phys.Rev.C82,035804(2010)
- **fit to different symmetry energies** (BSk22-26)
  Goriely, Chamel, Pearson, Phys.Rev.C88,024308(2013)
- **optimal fit of the 2012 AME with standard Skyrme** (BSk27*)
  Goriely, Chamel, Pearson, Phys.Rev.C88,061302(R)(2013)
- **generalized spin-orbit coupling** (BSk28-29)
  Goriely, Nucl.Phys.A933,68(2015).
- **fit to realistic $^1S_0$ pairing gaps with self-energy** (BSk30-32)
  Goriely, Chamel, Pearson, Phys.Rev. C93,034337(2016).

Empirical pairing energy density functionals

The pairing functional is generally assumed to be **local** and very often parametrized as

$$E_{\rm pair} = \int d^3r\, \mathcal{E}_{\rm pair}(\boldsymbol{r})\,, \qquad \mathcal{E}_{\rm pair} = \frac{1}{4}\sum_{q=n,p} v^{\pi q}[n_n, n_p]\widetilde{n}_q^2$$

$$v^{\pi q}[n_n, n_p] = V_\Lambda^{\pi q}\left(1 - \eta_q \left(\frac{n}{n_0}\right)^{\alpha_q}\right)$$

with a suitable **cutoff** prescription (regularization).
Bertsch & Esbensen, Ann. Phys. 209, 327 (1991).

Drawbacks

- $V_\Lambda^{\pi q}$ must be refitted for any change in the cutoff.
- experimental data do not allow for an unambiguous determination of η_q and α_q.
- not enough flexibility to fit pairing gaps in nuclei and neutron matter, as required for reliable calculations of superfluidity in neutron-star crusts.

Pairing functionals from nuclear-matter calculations

Instead, we **fit *exactly* realistic ^{1}S$_0$ pairing gaps** $\Delta_q(n_n, n_p)$ in infinite homogeneous nuclear matter for each densities n_n and n_p.
Chamel, Phys. Rev. C 82, 014313 (2010)

$$v_\Lambda^{\pi q} = -\frac{8\pi^2}{\sqrt{\mu_q}}\left(\frac{\hbar^2}{2M_q^*}\right)^{3/2}\left[2\log\left(\frac{2\mu_q}{\Delta_q}\right) + \Lambda\left(\frac{\varepsilon_\Lambda}{\mu_q}\right)\right]^{-1}$$

$$\Lambda(x) = \log(16x) + 2\sqrt{1+x} - 2\log\left(1+\sqrt{1+x}\right) - 4$$

$$\mu_q = \frac{\hbar^2}{2M_q^*}(3\pi^2 n_q)^{2/3}$$

Regularization: s.p. energy cutoff ε_Λ above the Fermi level.

- **no free parameters** apart from the cutoff
- **automatic renormalization** of $v_\Lambda^{\pi q}$ with ε_Λ

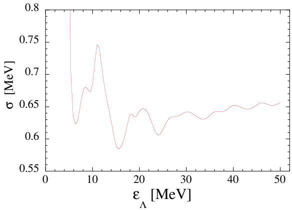
Pairing cutoff and experimental phase shifts

In the limit of vanishing density, the pairing strength

$$v^{\pi q}[n_n, n_p \to 0] = -\frac{4\pi^2}{\sqrt{\varepsilon_\Lambda}} \left(\frac{\hbar^2}{2M_q}\right)^{3/2}$$

should coincide with the bare force in the $^1S_0$ channel.

A fit to the **experimental $^1S_0$ NN phase shifts** yields $\varepsilon_\Lambda \sim 7 - 8$ MeV.
Esbensen et al., Phys. Rev. C 56, 3054 (1997).

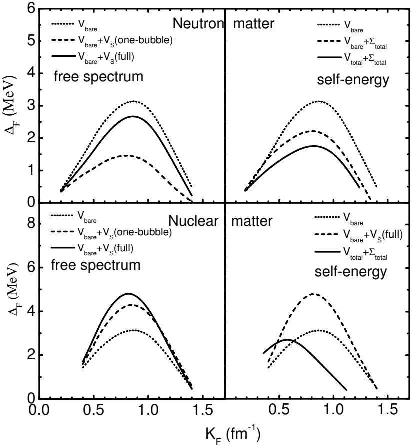


The fit to nuclear masses leads to a non monotonic dependence of the rms error on the cutoff.
Chamel et al., in "50 Years of Nuclear BCS" (World Scientific Publishing Company, 2013), pp.284-296

For the functionals BSk16-BS29, optimum mass fits were obtained with $\varepsilon_\Lambda \sim 16$ MeV, while we found $\varepsilon_\Lambda \sim 6.5$ MeV for BSk30-32.

$^1S_0$ pairing gaps in neutron and symmetric matter

For consistency, we considered the gaps obtained from extended BHF calculations since effective masses as well as equations of state have been also calculated with this approach.



For comparison, we fitted functionals to different approximations for the gaps:

- **BCS**: BSk16
- **polarization+free spectrum**: BSk17-BSk29
- **polarization+self-energy**: BSk30-32.

Cao et al., Phys.Rev.C74,064301(2006)

Other contributions to pairing in finite nuclei

Pairing in finite nuclei is not expected to be the same as in infinite nuclear matter because of

- **Coulomb and charge symmetry breaking effects**,
- **polarization effects in odd nuclei**,
- **coupling to surface vibrations**.

In an attempt to account for these effects, we include an additional phenomenological term in the pairing interaction (only for BSk30-32)

$$v^{\pi\, q} \to v^{\pi\, q} + \kappa_q |\nabla n|^2$$

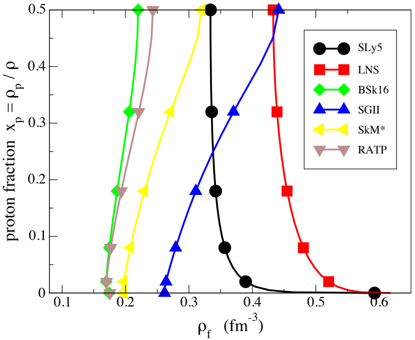
and we introduce renormalization factors $f_q^{\pm}$

$$v^{\pi\, q} \longrightarrow f_q^{\pm} v^{\pi\, q}$$

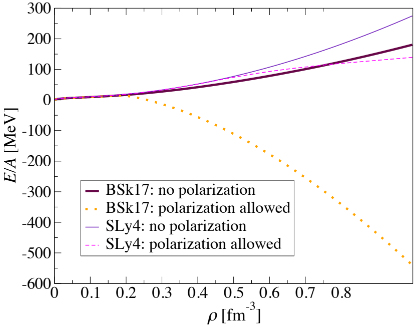
Parameters were determined by fitting nuclear masses. Typically $f_q^{\pm} \simeq 1 - 1.2$ and $f_q^{-} > f_q^{+}$, and $\kappa_q < 0$.

Ferromagnetic instability

Unlike microscopic calculations, conventional Skyrme functionals predict a ferromagnetic transition in nuclear matter



Margueron et al.,
J.Phys.G36(2009),125102.



Chamel et al.,
Phys.Rev.C80(2009),065804.

This instability can strongly affect the neutrino propagation in hot dense nuclear matter and leads to a collapse of neutron stars

Stability of unpolarized matter restored

The ferromagnetic instability at $T = 0$ can be completely removed by **adding new terms** in the standard Skyrme interaction (BSk18)

$$\frac{1}{2}\, t_4(1 + x_4 P_\sigma)\frac{1}{\hbar^2}\left\{p_{ij}^2\, n(\boldsymbol{r})^\beta\, \delta(\boldsymbol{r}_{ij}) + \delta(\boldsymbol{r}_{ij})\, n(\boldsymbol{r})^\beta\, p_{ij}^2\right\}$$

$$+t_5(1 + x_5 P_\sigma)\frac{1}{\hbar^2}\boldsymbol{p}_{ij}.n(\boldsymbol{r})^\gamma\, \delta(\boldsymbol{r}_{ij})\, \boldsymbol{p}_{ij}$$

Chamel, Goriely, Pearson, Phys.Rev.C80(2009),065804.

Dropping the J^2 terms and their associated time-odd parts (>BSk19)

- removes spin and spin-isospin instabilities at any $T \geq 0$
- prevents an anomalous behavior of the entropy
  Rios,Polls, Vidana, Phys. Rev. C 71, 055802 (2005)
- considerably improves the values of Landau parameters (especially G_0') and the sum rules
- but also leads to unrealistic effective masses in polarized matter

Chamel & Goriely, Phys.Rev.C82, 045804 (2010)

Landau parameters and the J^2 terms

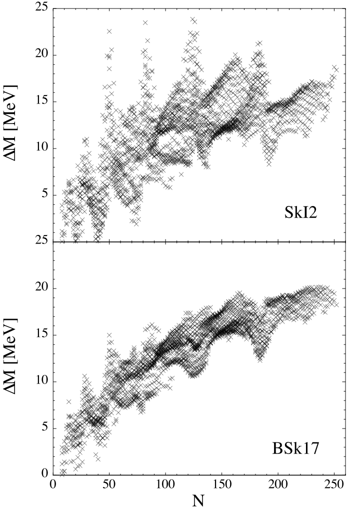
Landau parameters for Skyrme forces fitted without the J^2 terms. Values in parenthesis were obtained by dropping the time-odd couterparts of the form $\boldsymbol{s} \cdot \boldsymbol{T}$.

	G_0	G_0'	G_0^{NeuM}
SGII	0.01 (0.62)	0.51 (0.93)	-0.07 (1.19)
SLy4	1.11 (1.39)	-0.13 (0.90)	0.11 (1.27)
SkI1	-8.74 (1.09)	3.17 (0.90)	-5.57 (1.10)
SkI2	-1.18 (1.35)	0.77 (0.90)	-1.08 (1.24)
SkI3	0.57 (1.90)	0.20 (0.85)	-0.19 (1.35)
SkI4	-2.81 (1.77)	1.38 (0.88)	-2.03 (1.40)
SkI5	0.28 (1.79)	0.30 (0.85)	-0.31 (1.30)
SkO	-4.08 (0.48)	1.61 (0.98)	-3.17 (0.97)
LNS	0.83 (0.32)	0.14 (0.92)	0.59 (0.91)
Microscopic	0.83	1.22	0.77

$\boldsymbol{s} \cdot \boldsymbol{T}$ terms can be cancelled by fine-tuning a tensor interaction, but this leads to other instabilities.

Chamel & Goriely, Phys.Rev.C82, 045804 (2010)

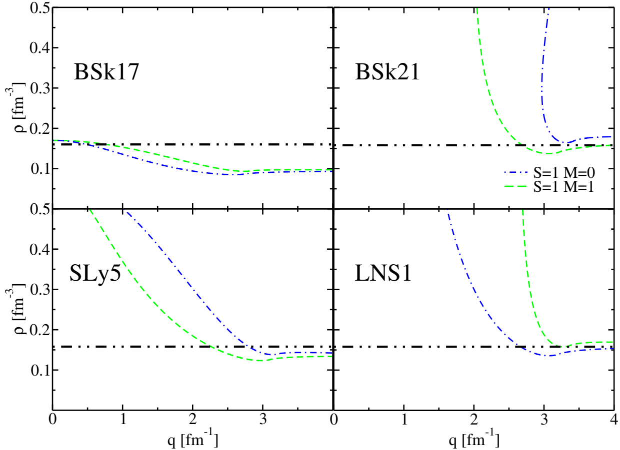
Impact of the J^2 terms



Warning:
Adding (SkI2) or removing (BSk17) a posteriori the J^2 terms without refitting the functional can induce large errors on masses!
Chamel & Goriely, Phys.Rev.C82, 045804 (2010)

Spin and spin-isospin instabilities

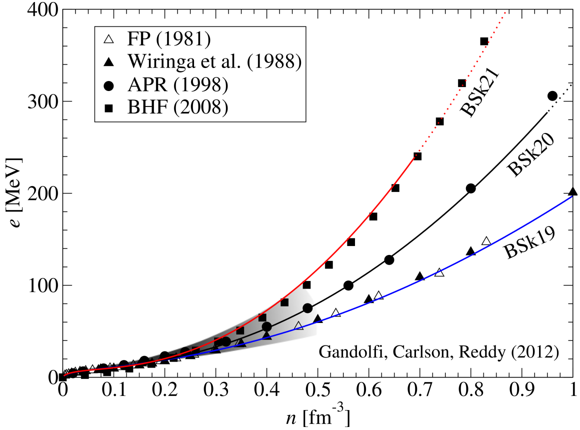
Although functionals >BSk18 are devoid of spurious long-wavelength instabilities, finite-size instabilities can still arise: e.g. neutron matter



Pastore et al., Phys.Rev.C90, 025804 (2014)

Neutron-matter equation of state

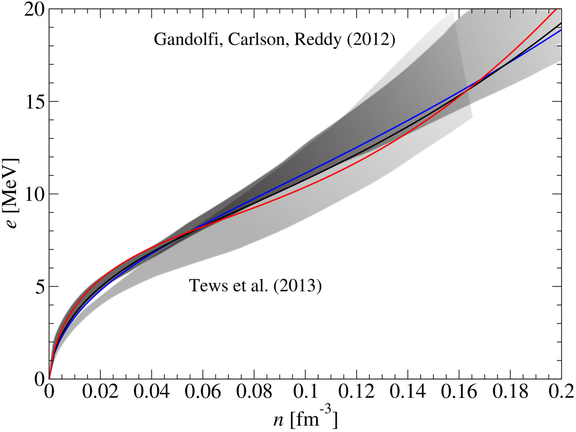
BSk19, BSk20 and BSk21 were fitted to realistic neutron-matter equations of state with different of degrees of stiffness:



Goriely, Chamel, Pearson, Phys. Rev. C 82, 035804 (2010).

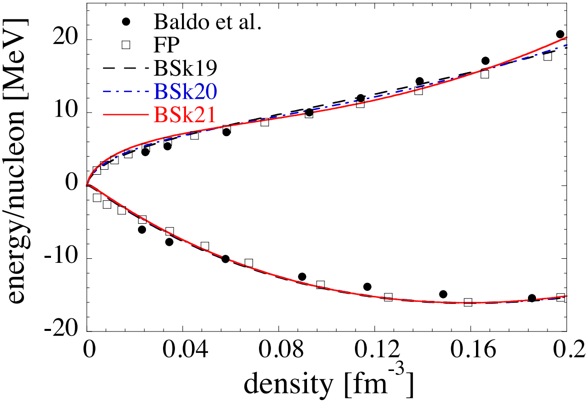
Neutron-matter equation of state at low densities

All three functionals yield similar equations of state at subsaturation densities consistent with ab initio calculations:



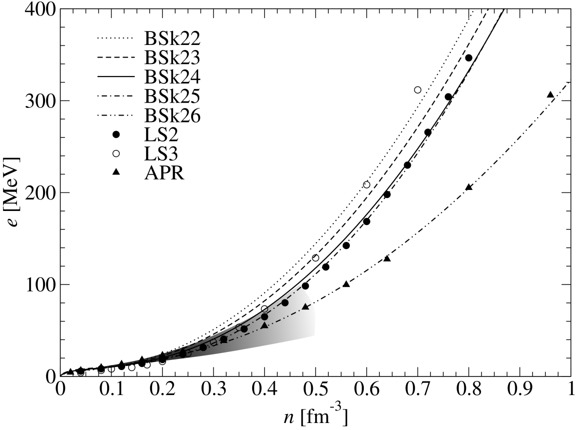
Nuclear-matter equation of state

These functionals are also in excellent agreement with BHF calculations in symmetric nuclear matter (as the BCPM functional):



Symmetry energy

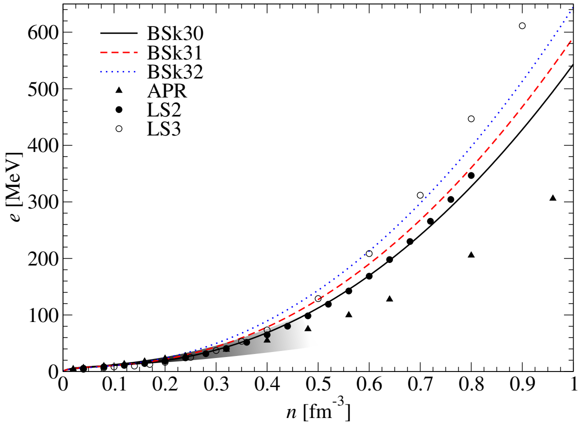
The functionals BSk22-26 were fitted to realistic neutron-matter equations of state but with different values for $J = 29 - 32$ MeV:



Goriely, Chamel, Pearson, Phys.Rev.C 88, 024308 (2013).

Symmetry energy, spin-orbit, pairing

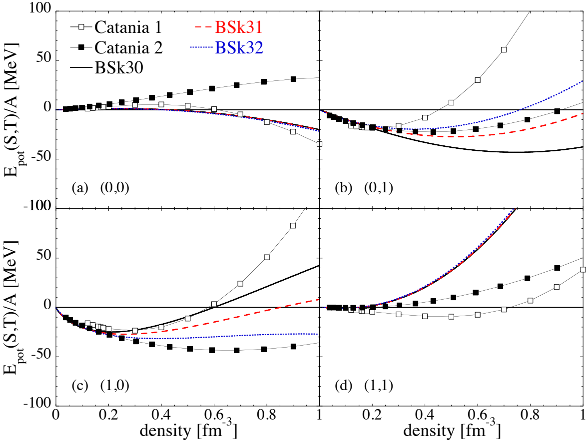
The functionals BSk30-32 were fitted to realistic pairing gaps and include improved spin-orbit coupling but with different values for $J = 30 - 32$ MeV:



Goriely, Chamel, Pearson, Phys.Rev.C 93,034337 (2016).

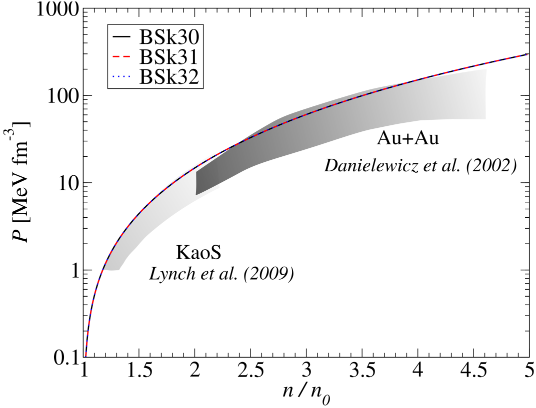
Potential energy in spin-isospin channels

These functionals are compatible with the potential energy in the different (S,T) channels, as predicted by BHF calculations:



Empirical constraints from heavy-ion collisions

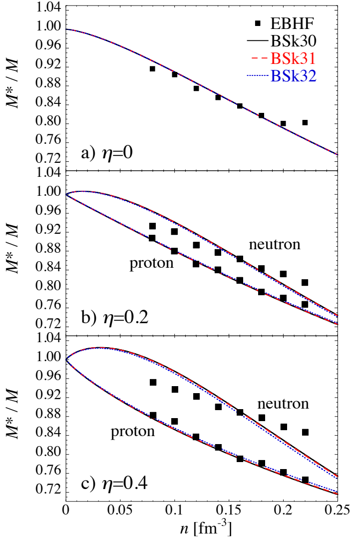
Our functionals are also consistent with empirical constraints inferred from heavy-ion collisions:



Danielewicz et al., Science 298, 1592 (2002)

Lynch et al., Prog. Part. Nuc. Phys.62, 427 (2009)

Nucleon effective masses in nuclear matter



Conventional Skyrme functionals usually predict a wrong splitting of effective masses.

Effective masses from BSk30-32 are consistent with

- isovector giant dipole resonances in finite nuclei,
- many-body calculations in asymmetric nuclear matter.

Chamel, Goriely, Pearson, Phys.Rev.C80,065804(2009)

EBHF calculations from *Cao et al.,Phys.Rev.C73,014313(2006)*.

Properties of finite nuclei

Fits to the 2353 measured masses with Z, $N > 8$ from the 2012 AME

	HFB-30	HFB-31	HFB-32
$\sigma(M)$ [MeV]	0.573	0.571	0.586
$\bar{\epsilon}(M)$ [MeV]	0.003	-0.004	-0.007
$\sigma(S_n)$ [MeV]	0.474	0.464	0.489
$\bar{\epsilon}(S_n)$ [MeV]	-0.008	0.000	-0.007
$\sigma(Q_\beta)$ [MeV]	0.589	0.578	0.601
$\bar{\epsilon}(Q_\beta)$ [MeV]	0.009	0.006	-0.004
$\sigma(R_c)$ [fm]	0.026	0.027	0.027
$\bar{\epsilon}(R_c)$ [fm]	0.001	0.002	0.000
$\sigma_{\rm mod}(26\ \theta)$[fm]	0.009	0.005	0.012
$\theta(^{208}\mathrm{Pb})$[fm]	0.133	0.151	0.170

Goriely, Chamel, Pearson, Phys.Rev. C93,034337(2016).

Conclusions

- Nuclear astrophysical applications require the determination of various **microscopic inputs**.
- These can be computed using the **nuclear energy density functional theory**.
- The **BSk functionals** were fitted using the **same protocole** to a wealth of experimental data and N-body calculations, spanning the current lack of knowledge of nuclear physics.
- In this way, the impact of nuclear observables on astrophysical phenomena can be consistently assessed.

- Nuclear properties (masses, radii, etc.) available on BRUSLIB `http://www.astro.ulb.ac.be/bruslib/`
- Unified equations of state for neutron stars (see A. Fantina's talk)

Nonlocal (Gogny) and relativistic functionals were also developed:
Goriely et al., Eur. Phys. J. A 52, 202 (2016)
Pena Arteaga, Goriely, Chamel, Eur. Phys. J. A 52, 320 (2016)