Nuclear Energy Density Functionals for Astrophysical Simulations of Compact Stars

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Models of dense matter required to compute all the necessary inputs to astrophysical simulations of compact 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 $T$, $P$, composition, $B$.

The nuclear energy density functional theory appears to be the most suitable approach.
Outline

1. Nuclear energy density functional theory
   ▶ Brief overview
   ▶ Mean-field methods with effective interactions

2. Brussels-Montreal nuclear energy density functionals
   ▶ Fitting protocol
   ▶ Recent developments towards more realistic functionals
Nuclear energy density functional theory in a nutshell

The energy $E$ of a nuclear system ($q = n, p$ for neutrons, protons) is expressed as a (universal) functional of

\[ n_q(r, \sigma; r', \sigma') = \langle \Psi | c_q(r' \sigma')^\dagger c_q(r \sigma) | \Psi \rangle \]

\[ \tilde{n}_q(r, \sigma; r', \sigma') = -\sigma' \langle \Psi | c_q(r' - \sigma') c_q(r \sigma) | \Psi \rangle, \]

where $c_q(r \sigma)^\dagger$ and $c_q(r \sigma)$ are the creation and destruction operators for nucleon $q$ at position $r$ with spin $\sigma = \pm 1$.

In turn, these matrices are expressed in terms of independent quasiparticle wavefunctions $\varphi_{1k}^{(q)}(r)$ and $\varphi_{2k}^{(q)}(r)$ as

\[ n_q(r, \sigma; r', \sigma') = \sum_{k(q)} \varphi_{2k}^{(q)}(r, \sigma) \varphi_{2k}^{(q)}(r', \sigma')^* \]

\[ \tilde{n}_q(r, \sigma; r', \sigma') = -\sum_{k(q)} \varphi_{2k}^{(q)}(r, \sigma) \varphi_{1k}^{(q)}(r', \sigma')^* = -\sum_k \varphi_{1k}^{(q)}(r, \sigma) \varphi_{2k}^{(q)}(r', \sigma')^*. \]

The **exact ground-state energy** is obtained by minimizing the functional $E[n_q(r, \sigma; r', \sigma'), \tilde{n}_q(r, \sigma; r', \sigma')]$ under the constraint of fixed nucleon numbers (and completeness relations on $\varphi_{1k}^{(q)}(r)$ and $\varphi_{2k}^{(q)}(r)$).
Nuclear energy density functional theory in a nut shell

For simplicity, the functional is usually written in a **semilocal form** as

\[
E = \int \mathcal{E} \left[ n_q(r), \nabla n_q(r), \tau_q(r), J_q(r), \tilde{n}_q(r) \right] \, d^3r
\]

where

\[
n_q(r) = \sum_{\sigma=\pm 1} n_q(r, \sigma; r, \sigma)
\]

\[
\tau_q(r) = \sum_{\sigma=\pm 1} \int d^3r' \, \delta(r - r') \nabla \cdot \nabla' n_q(r, \sigma; r', \sigma)
\]

\[
J_q(r) = -i \sum_{\sigma, \sigma' = \pm 1} \int d^3r' \, \delta(r - r') \nabla n_q(r, \sigma; r', \sigma') \times \sigma_{\sigma'\sigma}
\]

\[
\tilde{n}_q(r) = \sum_{\sigma=\pm 1} \tilde{n}_q(r, \sigma; r, \sigma)
\]

and \(\sigma_{\sigma\sigma'}\) denotes the Pauli spin matrices.

*Duguet, Lecture Notes in Physics 879 (Springer-Verlag, 2014), p. 293*

*Dobaczewski & Nazarewicz, in "50 years of Nuclear BCS" (World Scientific Publishing, 2013), pp.40-60*
Nuclear energy density functional theory in a nutshell

Minimizing $E \left[ \varphi^{(q)}_{1k}(r), \varphi^{(q)}_{2k}(r) \right]$ under the constraint of fixed nucleon numbers leads to the Hartree-Fock-Bogoliubov equations:

$$
\sum_{\sigma'} \begin{pmatrix}
  h_q(r)_{\sigma \sigma'} & \Delta_q(r)\delta_{\sigma \sigma'} \\
  \Delta_q(r)\delta_{\sigma \sigma'} & -h_q(r)_{\sigma \sigma'}
\end{pmatrix}
\begin{pmatrix}
  \varphi^{(q)}_{1k}(r, \sigma') \\
  \varphi^{(q)}_{2k}(r, \sigma')
\end{pmatrix} = E_k
\begin{pmatrix}
  \varphi^{(q)}_{1k}(r, \sigma) \\
  \varphi^{(q)}_{2k}(r, \sigma)
\end{pmatrix}
$$

$h_q(r)_{\sigma \sigma'} \equiv -\nabla \cdot \frac{\delta E}{\delta \tau_q(r)} \nabla \delta_{\sigma \sigma'} + \frac{\delta E}{\delta n_q(r)} \delta_{\sigma \sigma'} - i \frac{\delta E}{\delta J_q(r)} \cdot \nabla \times \sigma_{\sigma' \sigma} - \mu_q \delta_{\sigma \sigma'}$,

$\mu_q$ are the nucleon chemical potentials,

$\Delta_q(r) \equiv \frac{\delta E}{\delta \tilde{n}_q(r)}$ is called the pair potential or the pairing field.

With suitable boundary conditions, these equations can describe nuclei, neutron-star crusts, homogeneous nuclear matter as in the core of neutron stars, superfluid vortices, etc.
Effective nuclear energy density functional

- **In principle, the nuclear functional could be inferred from realistic interactions** (i.e. fitted to experimental NN phase shifts) using many-body methods

\[
\mathcal{E} = \frac{\hbar^2}{2M} (\tau_n + \tau_p) + A(n_n, n_p) + B(n_n, n_p)\tau_n + B(n_p, n_n)\tau_p
\]

\[
+ C(n_n, n_p)(\nabla n_n)^2 + C(n_p, n_n)(\nabla n_p)^2 + D(n_n, n_p)(\nabla n_n) \cdot (\nabla n_p)
\]

+ Coulomb, spin-orbit and pairing

*Drut, Furnstahl and Platter, Prog. Part. Nucl. Phys. 64 (2010) 120.*

- **But this is a very difficult task** so in practice, phenomenological functionals are employed.

*Bender, Heenen and Reinhard, Rev. Mod. Phys. 75, 121 (2003).*

*Bulgac in “50 years of Nuclear BCS” (World Scientific Publishing, 2013), pp. 100-110*
Skyrme effective nucleon-nucleon interactions

Functionals can be constructed from **Skyrme effective interactions** in the “mean-field” approximation

\[ v_{ij} = t_0 (1 + x_0 P_\sigma) \delta(r_{ij}) + \frac{1}{6} t_3 (1 + x_3 P_\sigma) n(r)^\alpha \delta(r_{ij}) \]

\[ + \frac{1}{2} t_1 (1 + x_1 P_\sigma) \frac{1}{\hbar^2} \left[ p_{ij}^2 \delta(r_{ij}) + \delta(r_{ij}) p_{ij}^2 \right] + t_2 (1 + x_2 P_\sigma) \frac{1}{\hbar^2} p_{ij} \cdot \delta(r_{ij}) p_{ij} \]

\[ + \frac{i}{\hbar^2} W_0 (\sigma_i + \sigma_j) \cdot p_{ij} \times \delta(r_{ij}) p_{ij} + \frac{1}{2} (1 + P_\sigma) v^\pi (r) \delta(r_{ij}) \]

\[ r_{ij} = r_i - r_j, \quad r = (r_i + r_j)/2, \quad p_{ij} = -i\hbar (\nabla_i - \nabla_j)/2 \]

is the relative momentum, and \( P_\sigma \) is the two-body spin-exchange operator.

The parameters must be fitted to experimental and/or microscopic nuclear data.
Why not fitting directly the functional?

Let us consider a functional of the form

\[ E = \frac{\hbar^2}{2M} (\tau_n + \tau_p) + A(n_n, n_p) + B(n_n, n_p)\tau_n + B(n_p, n_n)\tau_p \]
\[ + C(n_n, n_p)(\nabla n_n)^2 + C(n_p, n_n)(\nabla n_p)^2 + D(n_n, n_p)(\nabla n_n) \cdot (\nabla n_p) \]

In the one-particle limit, the potential energy calculated with such a functional does not vanish: the particle interacts with itself!

Extra terms must be added depending on the spin (kinetic) densities

\[ s_q(r) = \sum_{\sigma, \sigma' = \pm 1} n_q(r, \sigma; r, \sigma') \langle \sigma' | \hat{\sigma} | \sigma \rangle \]
\[ T_{q\mu}(r) = \sum_{\sigma, \sigma' = \pm 1} \int d^3 r' \delta(r - r') \nabla \cdot \nabla' n_q(r, \sigma; r', \sigma') \langle \sigma' | \hat{\sigma}_\mu | \sigma \rangle \]

The cancellation of self-interaction errors implies that the coupling coefficients in the functional cannot be completely freely adjusted.

Nuclear uncertainties

How to quantify nuclear 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

$$e(n, \eta) = e_0(n) + S(n)\eta^2 + o(\eta^4)$$

where

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

with $\epsilon = (n - n_0)/n_0$

$$S(n) = J + \frac{L}{3} \epsilon + \frac{K_{sym}}{18} \epsilon^2 + o(\epsilon^3)$$

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 protocol.
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)

**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
- stability against spin and spin-isospin fluctuations

Phenomenological corrections for atomic nuclei

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

- Wigner energy

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

\( V_W \sim -2 \text{ MeV}, \ V'_W \sim 1 \text{ MeV}, \ \lambda \sim 300 \text{ MeV}, \ A_0 \sim 20 \)

- rotational and vibrational spurious collective energy

\[ E_{\text{coll}} = E_{\text{crank}}^{\text{rot}} \left\{ b \ \tanh(c |\beta_2|) + d |\beta_2| \ \exp\left\{ -l( |\beta_2| - \beta_0^2 \right)^2 \right\} \right\} \]

This latter correction was shown to be in good agreement with calculations using 5D collective Hamiltonian.


In this way, these collective effects do not contaminate the parameters (\( \leq 20 \)) of the functional.
Brussels-Montreal Skyrme functionals

- **fit to realistic $^1S_0$ pairing gaps (no self-energy)** (BSk16-17)
  - Goriely, Chamel, Pearson, PRL102,152503 (2009).

- **removal of spurious spin-isospin instabilities** (BSk18)

- **fit to realistic neutron-matter equations of state** (BSk19-21)

- **fit to different symmetry energies** (BSk22-26)

- **optimal fit of the 2012 AME - rms 0.512 MeV** (BSk27*)

- **generalized spin-orbit coupling** (BSk28-29)

- **fit to realistic $^1S_0$ pairing gaps with self-energy** (BSk30-32)
Empirical pairing energy density functionals

The pairing functional is generally assumed to be \textbf{local} and very often parametrized as

\[ E_{\text{pair}} = \int d^3 r \, \varepsilon_{\text{pair}}(r), \quad \varepsilon_{\text{pair}} = \frac{1}{4} \sum_{q=n,p} V^{\pi q}[n_n, n_p] \bar{n}_q^2 \]

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

with a suitable \textbf{cutoff} prescription (regularization). \cite{Bertsch1991}.

\( V_{\pi q}^\Lambda \) is usually fitted to the average gap in \(^{120}\text{Sn}\). However, this does not allow for an unambiguous determination of \( \eta_q \) and \( \alpha_q \). Systematic studies of nuclei seem to favor \( \eta_q \sim 0.5 \) and \( 0.5 \lesssim \alpha_q \lesssim 1 \).

Drawbacks for astrophysical applications

This kind of functionals do not have enough flexibility to fit realistic pairing gaps in finite nuclei and in infinite nuclear matter.
Pairing functionals from nuclear-matter calculations

Instead of postulating a specific form for $v^{\pi q}[n_n, n_p]$, we fit exactly realistic $^1S_0$ pairing gaps $\Delta_q(n_n, n_p)$ in infinite homogeneous nuclear matter for each densities $n_n$ and $n_p$.

Inverting the HFB equations in nuclear matter for a given pairing gap function $\Delta_q$ thus yields (s.p. energy cutoff $\varepsilon_\Lambda$ above the Fermi level):

$$v^{\pi q} = -8\pi^2 \left( \frac{\hbar^2}{2M_q^*} \right)^{3/2} \left( \int_0^{\mu_q+\varepsilon_\Lambda} \frac{\sqrt{\varepsilon}d\varepsilon}{\sqrt{(\varepsilon - \mu_q)^2 + \Delta_q^2}} \right)^{-1}$$

$$\frac{\hbar^2}{2M_q^*} = \frac{\delta E}{\delta \tau_q}$$

Analytical expression of the pairing strength

In the “weak-coupling approximation” \( \Delta_q \ll \mu_q \) and \( \Delta_q \ll \varepsilon_\Lambda \),

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

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

\[
\mu_q = \frac{\hbar^2}{2M^*_q} \left( 3\pi^2 n_q \right)^{2/3}
\]


- **one-to-one correspondence** between pairing in nuclei and homogeneous nuclear matter
- **no free parameters** apart from the cutoff
- **automatic renormalization** of the pairing strength with \( \varepsilon_\Lambda \)
Pairing cutoff and experimental phase shifts

In the limit of vanishing density, the pairing strength

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

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. 


The fit to nuclear masses leads to a non monotonic dependence of the rms error on the cutoff.

\textit{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.
For comparison, we fitted functionals to different approximations for the gaps:

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

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)

\[ v^\pi q \rightarrow v^\pi q + \kappa_q |\nabla n|^2 \]

and we introduce renormalization factors \( f_q^{\pm} \)

\[ v^\pi q \rightarrow f_q^{\pm} v^\pi q \]

Parameters were determined by fitting nuclear masses. Typically \( f_q^{\pm} \approx 1 - 1.2 \) 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.,

Chamel et al.,

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)

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

$$+ t_5 (1 + x_5 P_\sigma) \frac{1}{\hbar^2} p_{ij} \cdot n(r)^\gamma \delta(r_{ij}) p_{ij}$$


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
- considerably improves the values of Landau parameters (especially $G'_0$) and the sum rules
- but also leads to unrealistic effective masses in polarized matter

Spin and spin-isospin instabilities

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

$\rho$ [fm$^{-3}$]

BSk17

BSk21

SLy5

LNS1

$q$ [fm$^{-1}$]

$S=1$ $M=0$

$S=1$ $M=1$

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

Neutron-matter equation of state at low densities

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

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

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:

Empirical constraints from heavy-ion collisions

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

\[ P \text{ [MeV fm}^{-3}\text{]} \]

- BSk30
- BSk31
- BSk32

\[ n / n_0 \]

\[ 1 \quad 1.5 \quad 2 \quad 2.5 \quad 3 \quad 3.5 \quad 4 \quad 4.5 \quad 5 \]

The values for the symmetry energy $J$ and its slope $L$ obtained with our functionals are compatible with various experimental constraints.

Figure adapted from Kolomeitsev et al. (2016).
Conventional Skyrme functionals like SLy 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.

This could be achieved using generalized Skyrme interactions with $t_4$ and $t_5$ terms.

*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

<table>
<thead>
<tr>
<th>Property</th>
<th>HFB-30</th>
<th>HFB-31</th>
<th>HFB-32</th>
</tr>
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<tbody>
<tr>
<td>$\sigma_{\text{mod}}(M)$ [MeV]</td>
<td>0.564</td>
<td>0.561</td>
<td>0.576</td>
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<tr>
<td>$\sigma(M)$ [MeV]</td>
<td>0.573</td>
<td>0.571</td>
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<td>$\bar{\epsilon}(M)$ [MeV]</td>
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</tr>
<tr>
<td>$\sigma(S_n)$ [MeV]</td>
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<td>0.464</td>
<td>0.489</td>
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<tr>
<td>$\bar{\epsilon}(S_n)$ [MeV]</td>
<td>-0.008</td>
<td>0.000</td>
<td>-0.007</td>
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<tr>
<td>$\sigma(Q_\beta)$ [MeV]</td>
<td>0.589</td>
<td>0.578</td>
<td>0.601</td>
</tr>
<tr>
<td>$\bar{\epsilon}(Q_\beta)$ [MeV]</td>
<td>0.009</td>
<td>0.006</td>
<td>-0.004</td>
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<tr>
<td>$\sigma(R_c)$ [fm]</td>
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<td>0.027</td>
<td>0.027</td>
</tr>
<tr>
<td>$\bar{\epsilon}(R_c)$ [fm]</td>
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<td>0.002</td>
<td>0.000</td>
</tr>
<tr>
<td>$\sigma_{\text{mod}}(26\theta)$[fm]</td>
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<td>0.005</td>
<td>0.012</td>
</tr>
<tr>
<td>$\theta(208\text{Pb})$[fm]</td>
<td>0.133</td>
<td>0.151</td>
<td>0.170</td>
</tr>
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</table>


The popular SLy functional fits the data from the 2003 AME (even-even nuclei) with an error of 5.1 MeV

Conclusions

- Astrophysical simulations of compact stars require the determination of various microscopic inputs.
- This can be achieved using the nuclear energy density functional theory.
- The BSk functionals were fitted using the same protocol 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 at BRUSLIB

- Unified equations of state for neutron stars (see A. Fantina’s talk)

Nonlocal (Gogny) and relativistic functionals were also developed: