# New approaches to build a nuclear energy density functional

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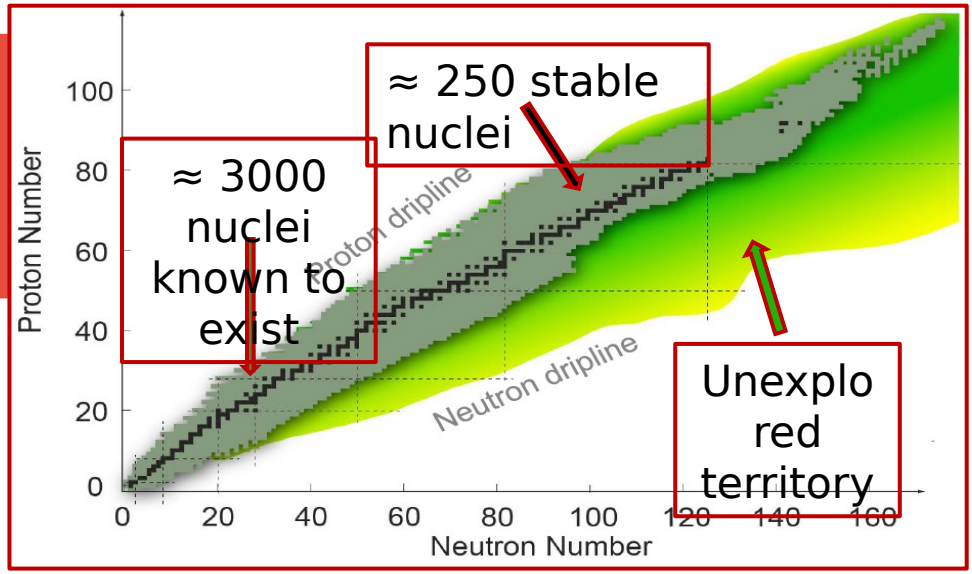
# Table of contents

# Motivation




## Current EDFs:

- are firmly **grounded on DFT**
- constitute our **best tool** for the description of nuclear **ground state** masses, radii, deformation,... as well as of **collective excitations**
- applicable to the **whole nuclear chart**
- are **phenomenological**
- large **extrapolation errors** difficult to **quantify**
- **not based** on a solid **systematic** theoretical **framework** for **improvement**

# Motivation

**New avenues** must be **explored** in order to **improve** current **EDFs** (here our attempts)**:**

→ **Inverse Kohn Sham method:** starting from reference densities (experiment or ab initio), it is in principle possible to derive the Kohn-Sham potential ($V_{KS}$). From its knowledge the EDF could be found by functional integration.

G. Accorto, P. Brandolini, F. Marino, A. Porro, A. Scalesi, G. Colò, X. Roca-Maza, and E. Vigezzi «*First step in the nuclear inverse Kohn-Sham problem: From densities to potentials*», Phys. Rev. C **101**, 024315 (2020)

A. Liardi, F. Marino, G. Colò, X. Roca-Maza, and E. Vigezzi «*Complete solution to the inverse Kohn-Sham problem: From the density to the energy*», Phys. Rev. C 105, 034309 (2022)

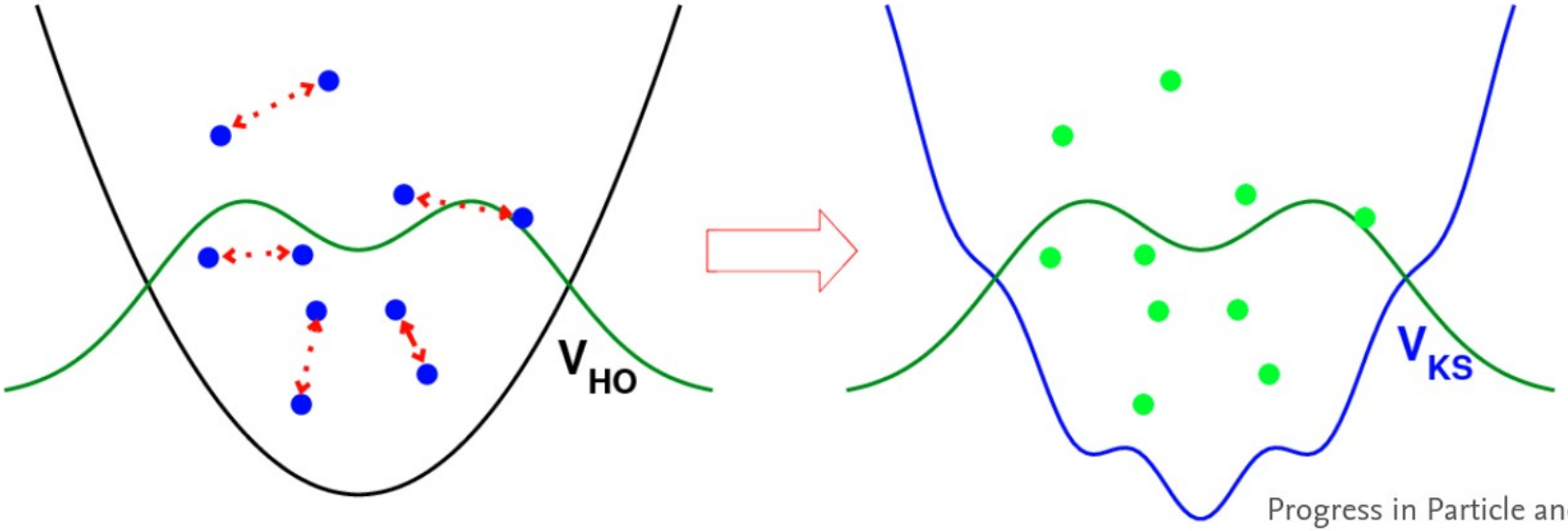
→ **Jacob's ladder**: systematic way of improving EDFs based on ab initio calculations[1] of artificial systems, without resorting on phenomenology or ad-hoc information.

F. Marino, C. Barbieri, A. Carbone, G. Colò, A. Lovato, F. Pederiva, X. Roca-Maza, and E. Vigezzi, «*Nuclear energy density functionals grounded in ab initio calculations*», Phys. Rev. C 104, 024315 (2021)

[1]Other attempts exist but attempts so far were of limited success [J. Dobaczewski, J. Phys. G 43, 04LT01 (2016), G. Salvioni, et al. J. Phys. G 47, 085107 (2020)]

# Kohn-Sham (KS) method

**KS method → most practical way to implement DFT.** Based on the idea that solving the problem of the interacting system under study is equivalent of solving a system of independent particles subject to an effective potential, provided the density is the same.

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Volume 64, Issue 1, January 2010, Pages 120-168

# Kohn-Sham equations

KS orbitals

$$\rho(\vec{r}) = \sum_{i}^{N_{\text{orb}}} |\phi_i(\vec{r})|^2. \qquad (1)$$

In addition, it is assumed that the kinetic energy $T$ has the same form as in the independent particle case. Then, the EDF is written as

$$E[\rho] = \sum_i \int d^3r\, \phi_i^*(\vec{r}) \left(-\frac{\hbar^2}{2m}\right) \nabla^2 \phi_i(\vec{r}) + F[\rho], \qquad (2)$$

and its minimization leads to the well-known Kohn-Sham equations of the type

(= U in the following slides)

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{\delta F[\rho]}{\delta \rho}\right) \phi_i(\vec{r}) = \varepsilon_i \phi_i(\vec{r}), \qquad (3)$$

KS potential (well defined up to a constant shift)

# Inverse Kohn-Sham (Sph. Sym.): ρ → $V_{KS}$

**van Leeuwen and Baerends (vLB) method** [Phys. Rev. A 49, 2421 (1994)]

KS potential

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2mr^2}+U(r)\right]u_i(r)=\varepsilon_i u_i(r),$$

$$U(r)=\frac{1}{4\pi r^2\rho(r)}\sum_{i=0}^{N_{\text{orb}}}\left[n_i u_i(r)\left(\frac{\hbar^2}{2m}\frac{d^2}{dr^2}-U_l\right)u_i+\varepsilon_i n_i u_i^2\right].$$

Algebraic manipulation: multiply by $n_i u_i(r)$ on both sides, summing over i, and dividing by $4\pi r^2\rho(r)$

**Iterative algorithm vLB:**

ρ ↔ target density

$$U^{(k+1)}(r)=\frac{1}{4\pi r^2\tilde{\rho}(r)}\sum_{i=0}^{N_{\text{orb}}}\left[n_i u_i^{(k)}(r)\left(\frac{\hbar^2}{2m}\frac{d^2}{dr^2}-U_l\right)u_i^{(k)}+\varepsilon_i n_i\left(u_i^{(k)}\right)^2\right]=\frac{\rho^{(k)}(r)}{\tilde{\rho}(r)}U^{(k)}(r).$$

In regions where the density at the kth step is larger than the target density the potential is increased in absolute value → make sense for repulsive U but not for attractive U

$$U^{k+1}(r)=U^{(k)}(r)+\gamma\frac{\rho^{(k)}(r)-\tilde{\rho}(r)}{\tilde{\rho}(r)}$$

# Inverse Kohn-Sham: ρ → $V_{KS}$

**Constrained variational (CV) method** [D. S. Jensen and A. Wasserman, Int. J. Quantum Chem. 118, e25425 (2018)]

**Minimization** of the **non-interacting kinetic energy** with the **constraint** that the orbitals are **orthonormal** [Lagrange multiplier $\boldsymbol{\varepsilon_{ij}}$] and that the density must coincide with the **target density** [Lagrange multiplier **U(r)**]

$$J[\{\phi_i\}; U(\vec{r}), \{\varepsilon_{ij}\}] = T_s[\{\phi_i\}] + \int d^3r\, U(\vec{r})\rho(\vec{r}) - \sum_{i=1}^{N_{\text{orb}}} \sum_{j=1}^{i} \varepsilon_{ij} \int d^3r\, \phi_i^*(\vec{r})\phi_j(\vec{r}),$$

$$\delta J[\{\phi_i\}; U(\vec{r}), \{\varepsilon_{ij}\}] = 0.$$

# Tests using SkX HF densities as input

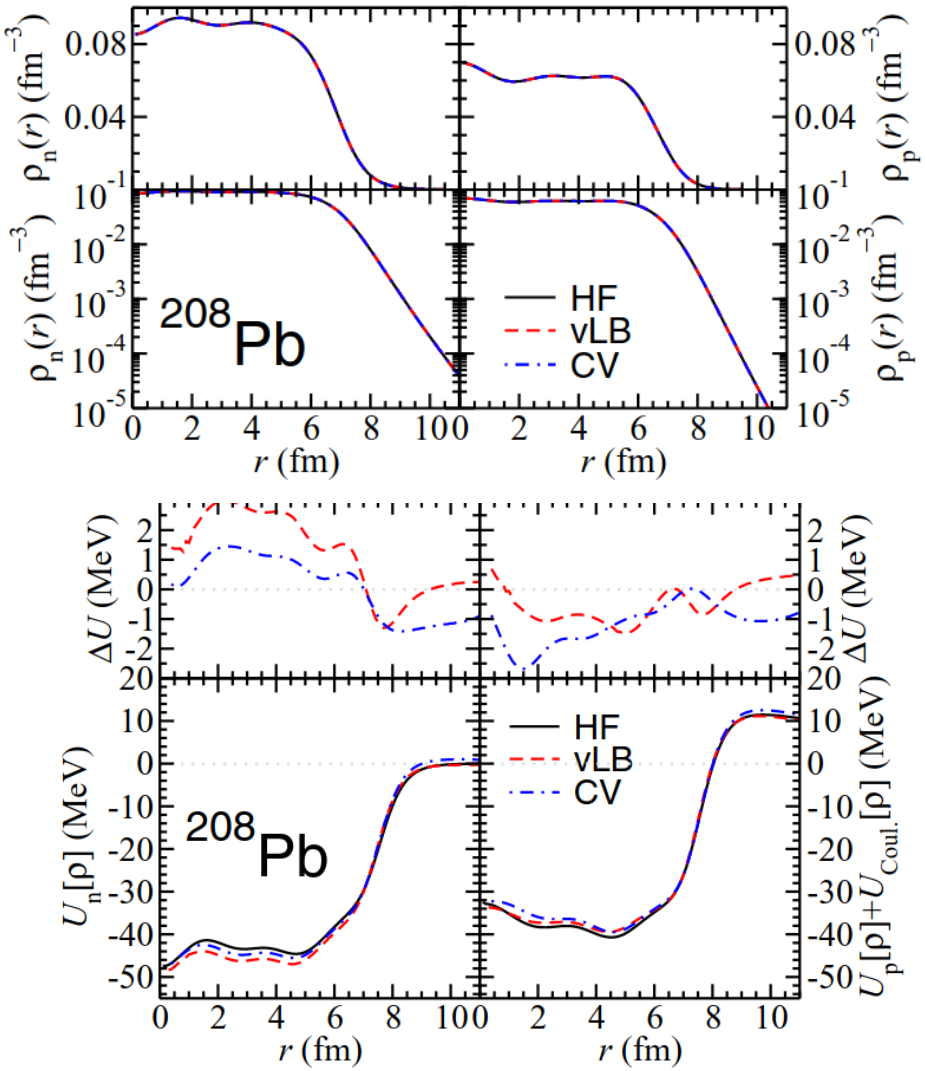
We **assume** that the **KS potential** is a function of **space coordinates** through the dependence on the **local densities** only (APPROX).

**Energy** of the **last occupied orbital →** neutron/proton separation energy. It provides a **unique way** to set the **absolute** value of the **KS potential** (= asymptotic for large ***r*** )

The absolute value of the resulting **difference** U with respect to the HF potentials is **smaller** than **2.5 MeV** both for protons and neutrons

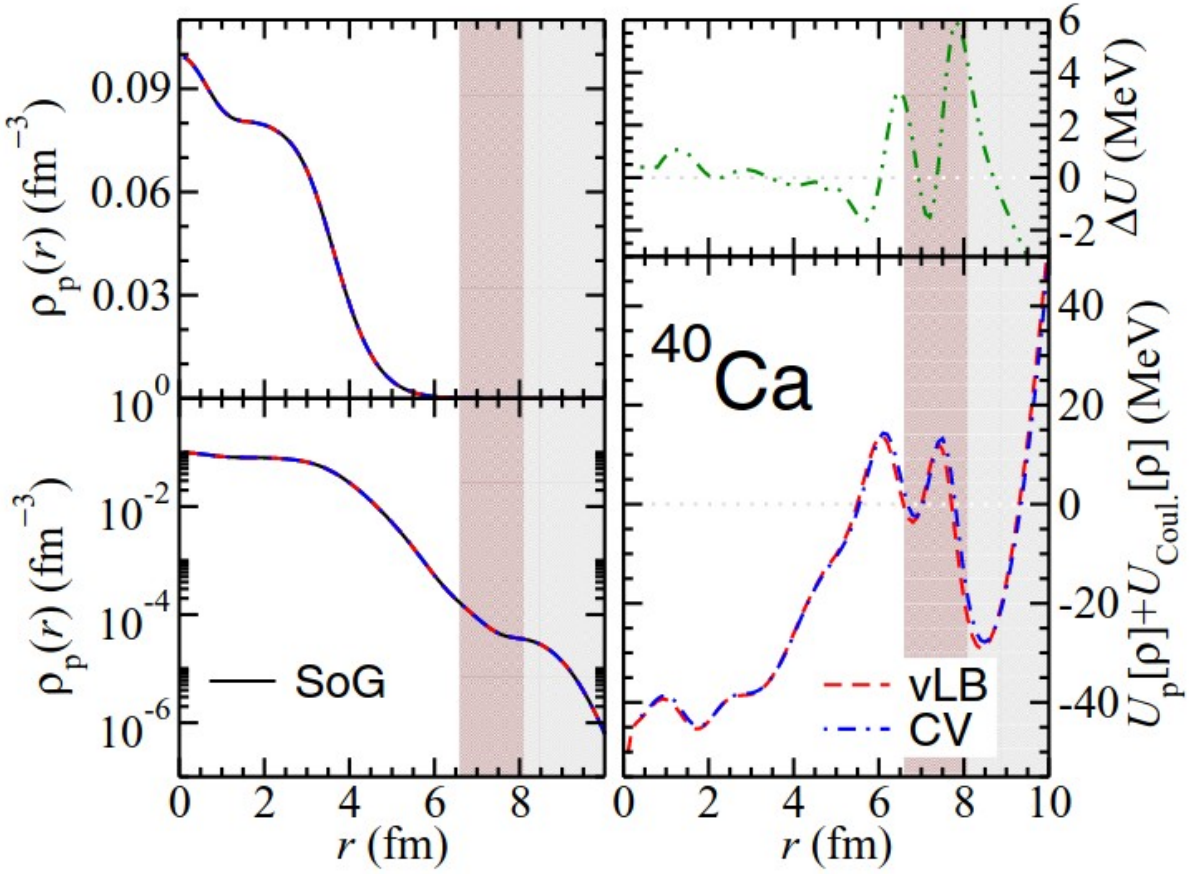
**Spin-orbit is neglected** but has no relevant influence (it is well known that spin-orbit shifts do not affect wave functions and densities, as a rule)

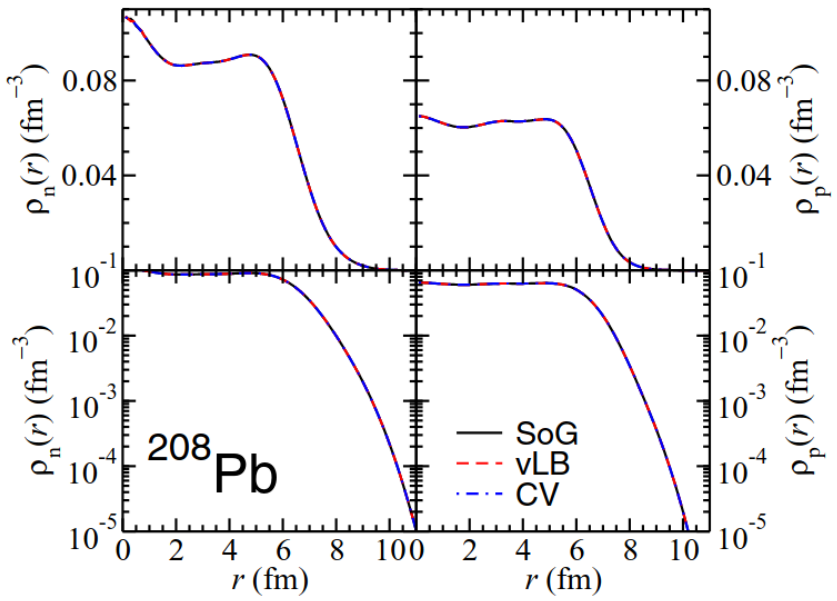
**HF** contains some effects due to the effective mass **m∗/m < 1** while **IKS** assumes **m∗/m = 1**.

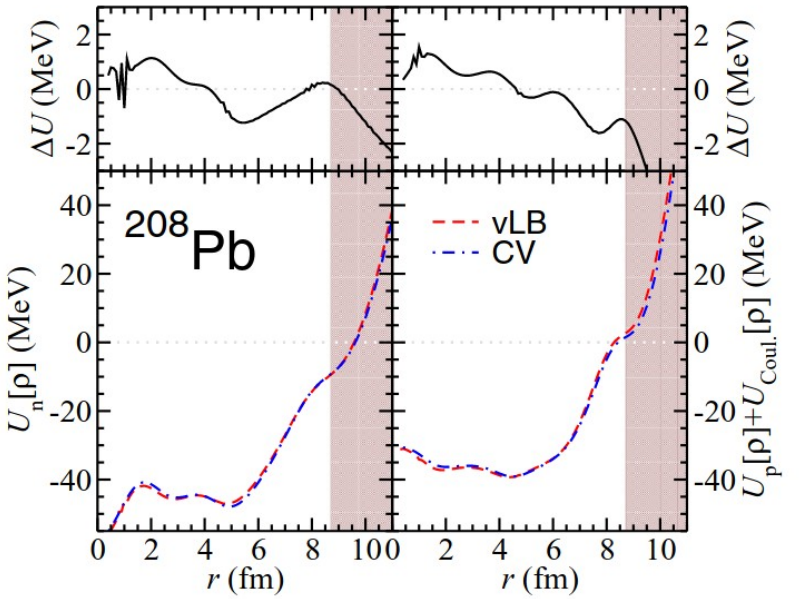


# IKS potential form experimental densities

**Experimental densities** parametrized as sum of gaussians[1] (GoS)




[1] H. D. Vries, C. D. Jager, and C. D. Vries, At. Data Nucl. Data Tables 36, 495 (1987)

# IKS: from ρ to E[ρ]

Once the **Kohn-Sham potential** is known **along a path of densities**, then the corresponding change in the energy functional can be reconstructed (**E[ρ] from functional integration**)

**Notation:**

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v_{\mathrm{KS}}\right)\phi_i = \epsilon_i\phi_i,$$

$$v_{KS} = v[\rho] + v_{\mathrm{ext}}.$$

$$F[\rho_B] - F[\rho_A] = \int_A^B dt \int d^3r\, v([\rho_t(\mathbf{r})], \mathbf{r})\frac{d\rho_t(\mathbf{r})}{dt}.$$

Used to produce the density path

**Density path can be freely chosen:** for example a volume conserving scaling of r→ λr of the density. Equivalent to perturb the system with $v_{\mathrm{ext},\mu}(r) = \mu r^2$

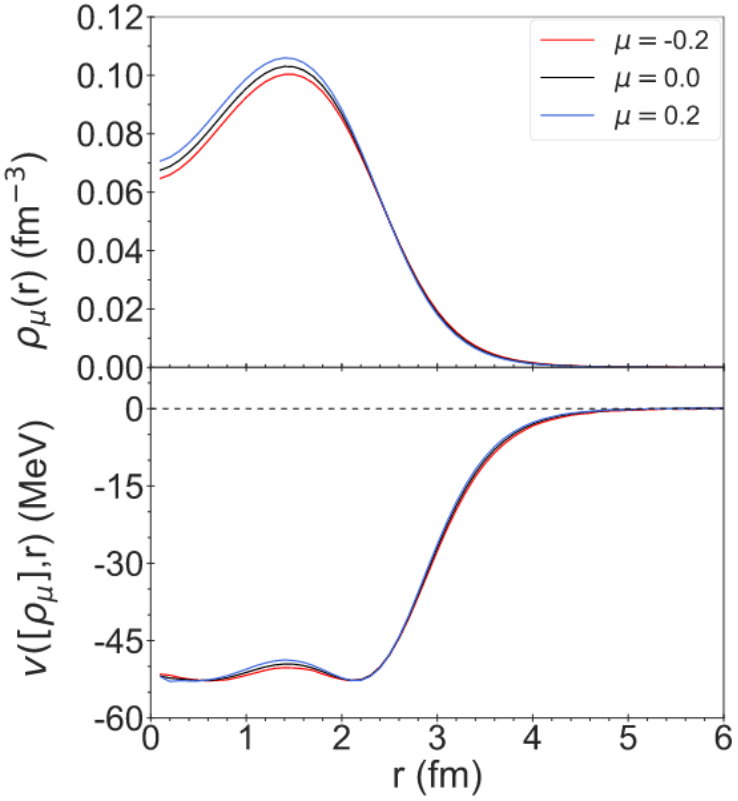
**Checking our procedure:** energy conservation ΔE=0

$$\Delta T = -\int_A^B dt \int d\mathbf{r}\, v_{\mathrm{KS}}([\rho_t(\mathbf{r})], \mathbf{r})\frac{d\rho_t(\mathbf{r})}{dt}.$$

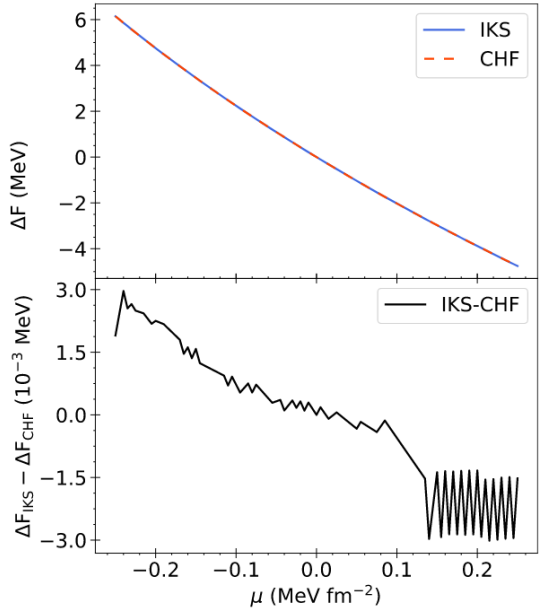
*J. Chem. Theory Comput.* **2009,** *5,* 699–707

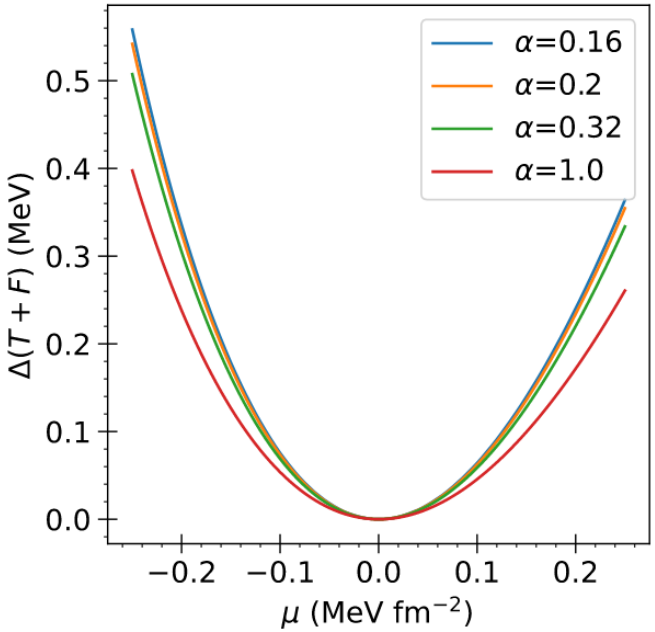
# Theoretical test: from ρ to E[ρ]

**Constrained HF** calculations with a **Skyrme** ($t_0$,$t_3$) for different values of μ (external potential) as a benchmark




From potential (U) to potential energy (F) differences




**Distinguish exponent of the $t_3$ in $E_{Skyrme}[\rho]$**

# Conclusions IKS:

→ **IKS** has been **used** in **electronic DFT** and **recently** in **nuclear DFT** (also by the Zagreb+Tokyo groups)

→ We have shown the **feasibility** of our **method** in **simple cases** (e.g. neglecting spin densities, spherical symmetry,...)

→ We have shown that **current experimental densities cannot be used** to obtain the **IKS potential**.

→ To **reconstruct E[ρ]** one would need a **benchmark density along a parametrized path** (e.g. qualitatively g.s. density and the GMR transition density).

→ Hence, **ab initio** calculations could **foster** our recent investigations and allow for a **more realistic application** of the **IKS in nuclear physics**.

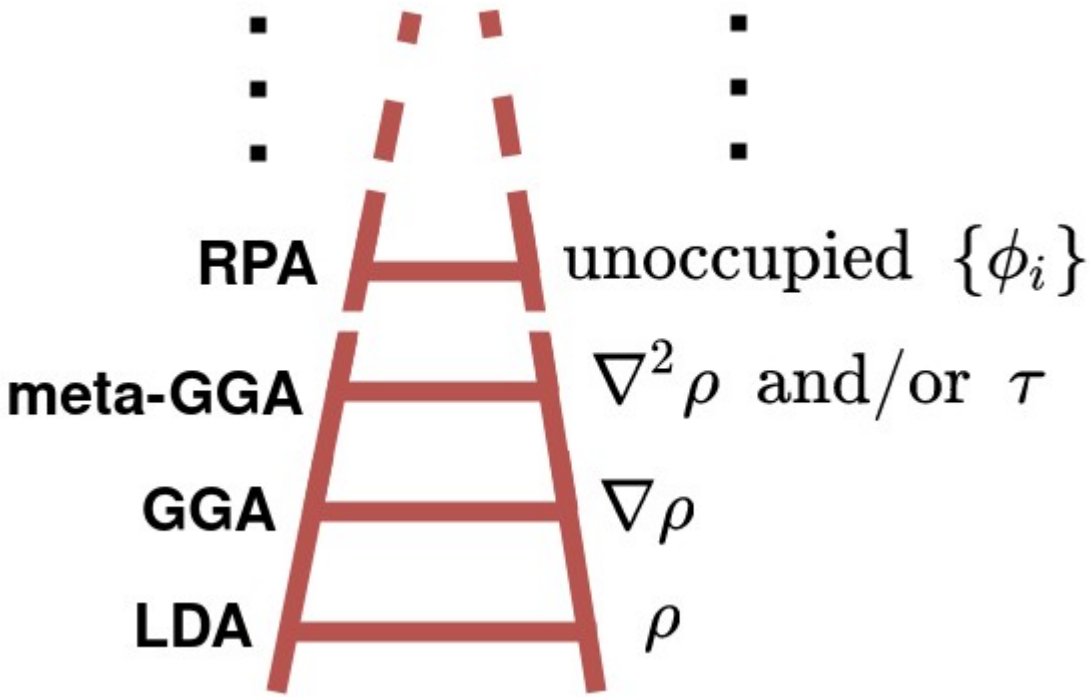
# Jacob's ladder to systematically build an EDF

**LDA:** proven by unpolarized[1] and polarized infinite matter

**GGA:** proven by perturbed infinite matter[2]

**Meta-GGA:** second order gradient terms such as τ. Proven by m*.

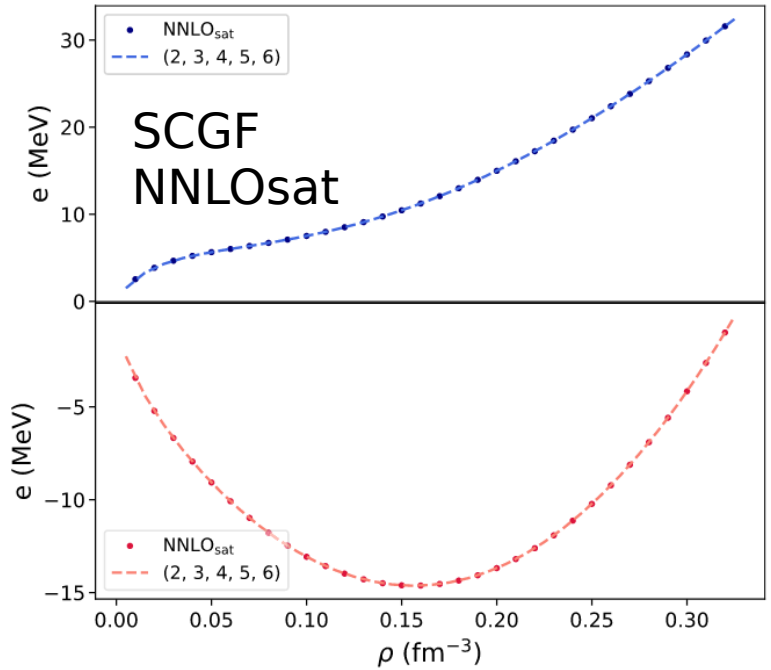
**Improved Meta-GGA:** spin-orbit. Proven by neutron and neutron-proton drops.




We aim at **extending the predictive power** of current EDFs by devising a **non-empirical EDF**, constructed on the basis of **Quantum Monte Carlo** and **Self-consistent Green Function** calculations of **artificial systems**.

1 F. Marino, C. Barbieri, A. Carbone, G. Colò, A. Lovato, F. Pederiva, X. Roca-Maza, and E. Vigezzi, «*Nuclear energy density functionals grounded in ab initio calculations*», Phys. Rev. C 104, 024315 (2021)
2 Work in progress. F Marino et al.

# LDA-EDF



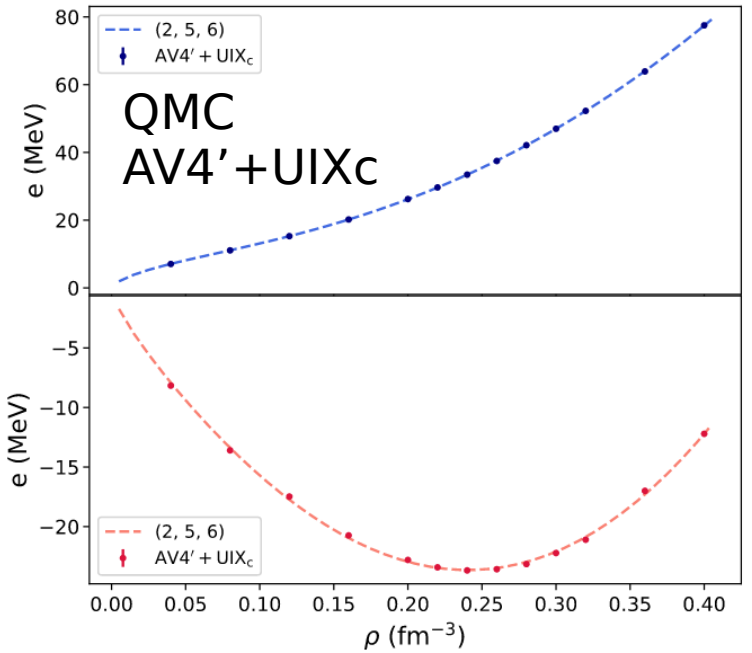



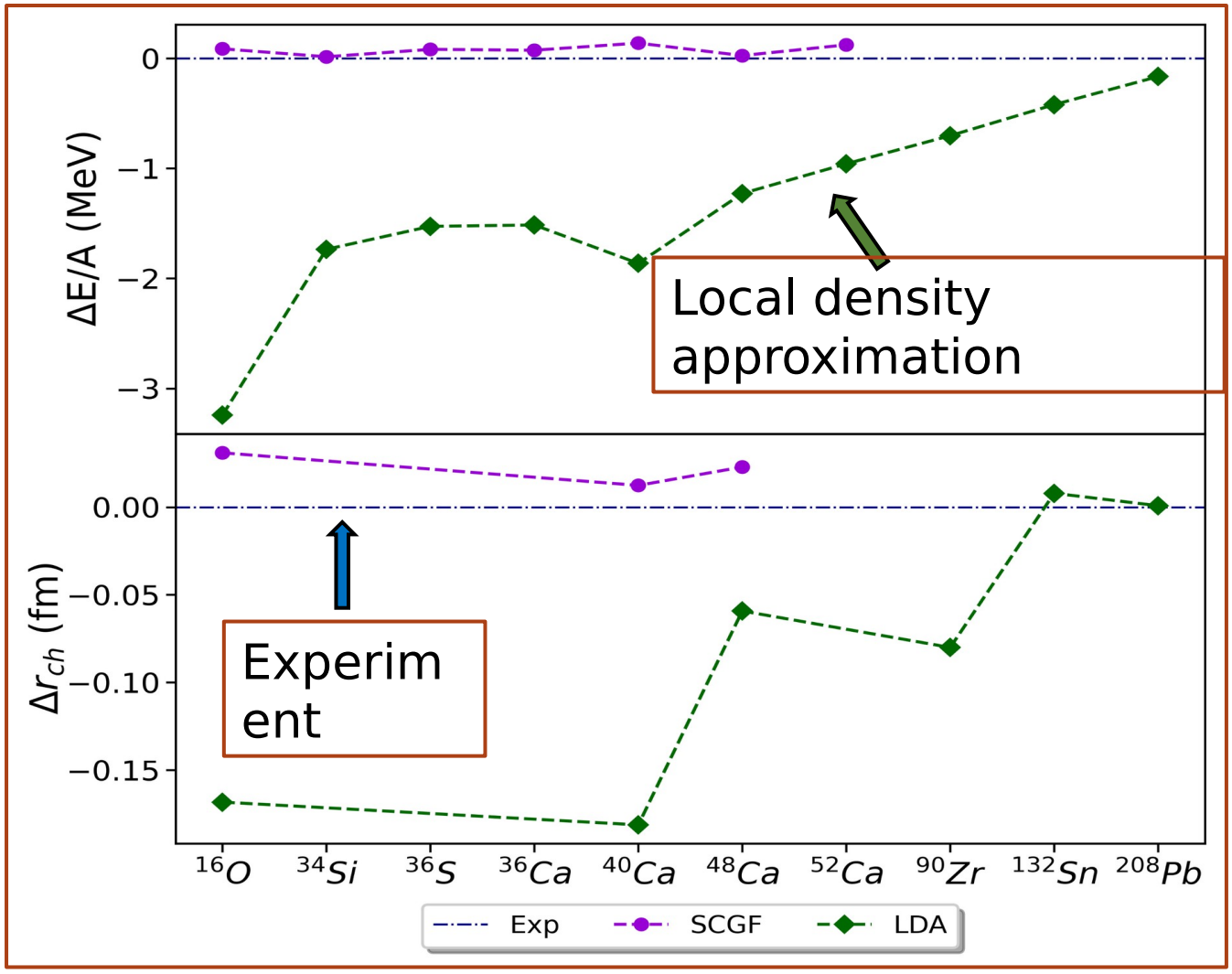

TABLE III. Coefficients of the optimal polynomial parametrizations (23) of the NNLO$_{sat}$ and AV4′ + UIX$_c$ EoS. The exponents $\gamma$ and the corresponding parameters $c_{\gamma,0}$ and $c_{\gamma,1}$ are reported.

| | $\gamma$ | $c_{\gamma,0}$ (MeV fm$^{3\gamma}$) | $c_{\gamma,1}$ (MeV fm$^{3\gamma}$) |
|---|---|---|---|
| NNLO$_{sat}$ | 2/3 | −182.41 | 16.93 |
| | 1 | 252.54 | 920.29 |
| | 4/3 | −501.04 | −4026.38 |
| | 5/3 | 63.80 | 6440.50 |
| | 2 | 669.42 | −3646.52 |
| AV4′ + UIX$_c$ | 2/3 | −131.94 | 81.04 |
| | 5/3 | −578.00 | 64.04 |
| | 2 | 901.30 | 48.97 |

$$v(\rho,\beta) = \sum_{\gamma=1/3\ldots6/3} c_\gamma(\beta)\rho^\gamma = \sum_{\gamma=1/3\ldots6/3} [c_{\gamma,0} + c_{\gamma,1}\beta^2]\rho^\gamma$$

**Checking optimal density dependencies** (exponents and coefficients) of two Hamiltonians and **providing best parametrizations**.

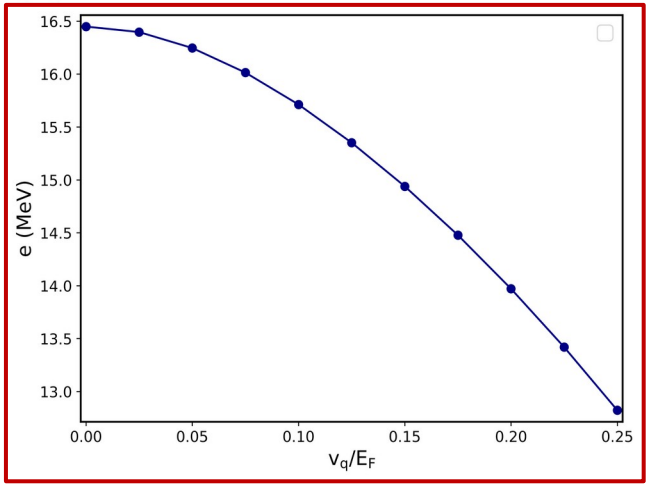
# LDA-EDF in finite nuclei



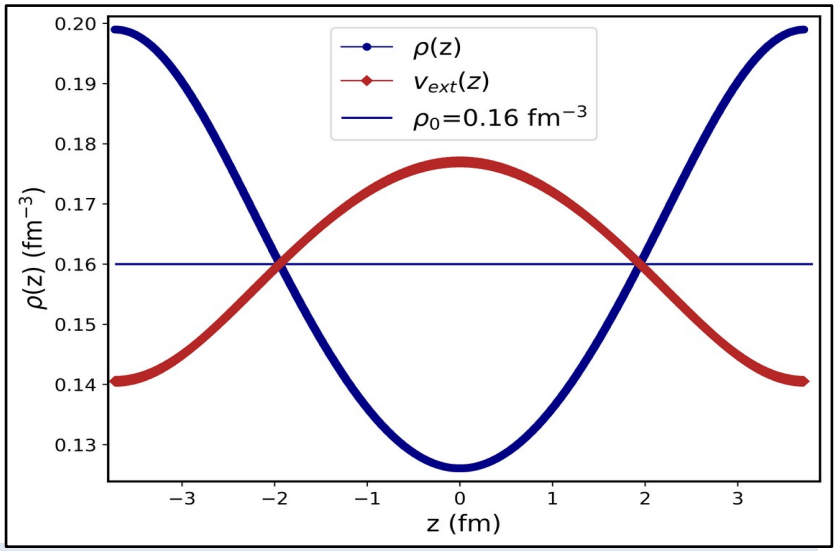
# Linear response (χ)

Solve the **Schrodinger** equation of a **finite** number of **particles** under the **action of an external potential** (v cos(qr)) **in a box** with **periodic boundary conditions** in **QMC, SCGF** and **EDF**.

$$\frac{E[v]}{N} - \frac{E_0}{N} = \frac{v_q^2}{\rho_0}\chi(q)$$

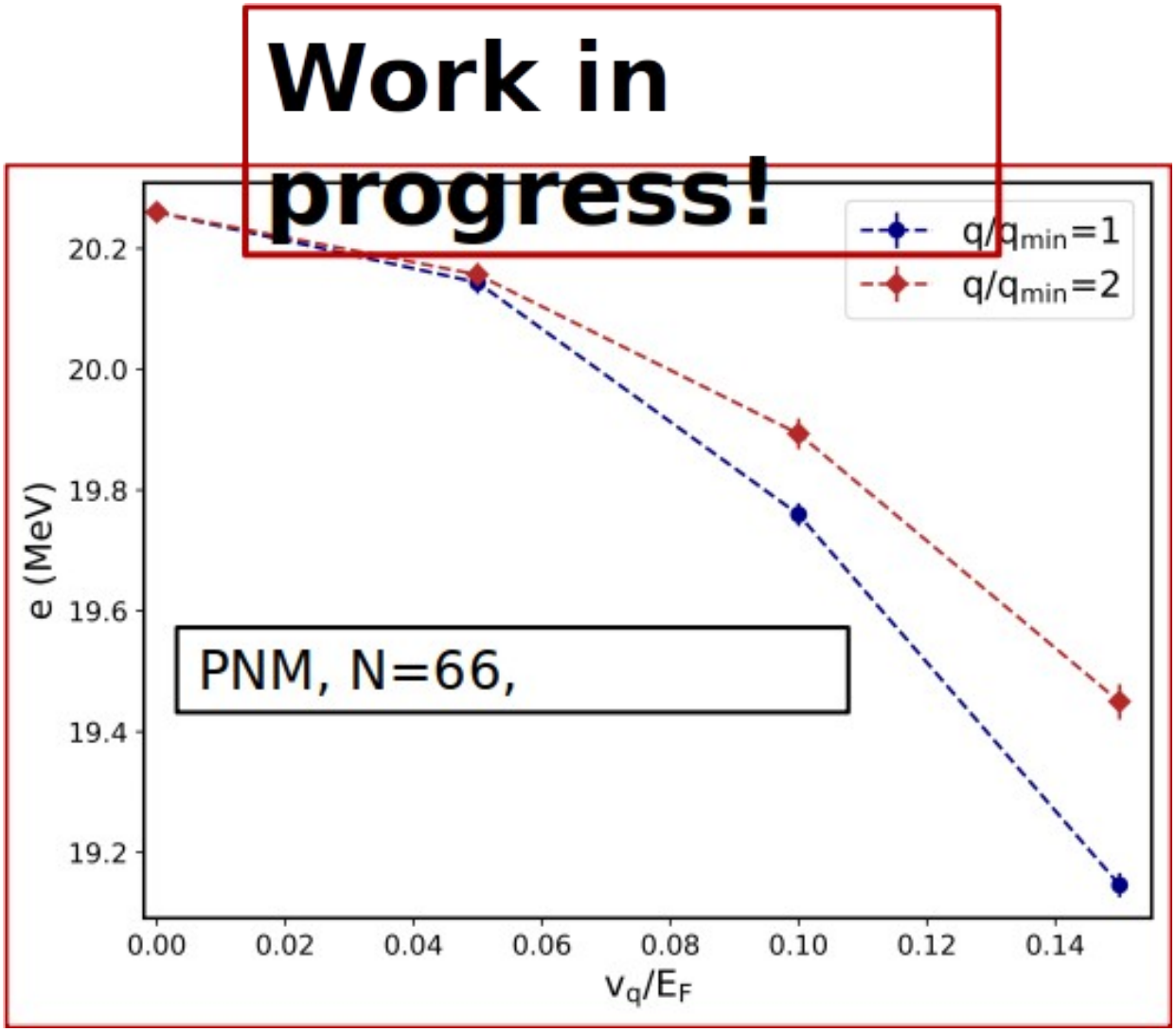



$$\rho(\mathbf{x}) = \rho_0 + 2v_{\mathbf{q}}\chi_{\mathbf{q}}\cos(\mathbf{q}\cdot\mathbf{x})$$




**Fix gradient** terms of the **EDF** from **QMC/SCGF** results of energy variation (v,q). (actually: no need to explicitly calculate χ)

# QMC results AV4’ + UIXc



# Conlcusions and perspectives

→ We are developing a **ladder** of ***ab initio*-constrained** nuclear EDFs (main person F. Marino)

→ The first rung (**local density approximation**) has been implemented (known to be deficient in nuclei)

→ Gradient terms are currently being constrained on **response of nuclear matter** (from QMC and SCGF) to a weak static perturbation

→ Near-term goals are completing the gradient approximation and **applying** the new EDFs to ground state and collective states (RPA)

# Collaborators

**Students:**

| | |
|---|---|
| - G. Accorto (Bachelor & Master Milano, PhD Zagreb) | IKS |
| - **F. Marino** (Bachelor & Master Milano, PhD Milano) | IKS, Jacob's ladder |
| - A. Porro (Bacelor Milano, Master & PhD CEA) | IKS |
| - A. Scalesi (Bachelor & Master Milano, PhD CEA-IRFU) | IKS |
| - A. Liardi (Master Student @ Cambridge) | IKS |

**Senior scientists:**

| | |
|---|---|
| - G. Colò, X. Roca-Maza and | DFT |
| C. Barbieri (U. Milano and INFN Milano) | SCGF |
| - A. Lovato (INFN Trento) | QMC |
| - F. Pederiva (U. Trento, INFN-TIPFA) | QMC |
| - E. Vigezzi (INFN Milano) | DFT |