Energy density functional based on a finite-range potential and its implementation on axial HFB solver

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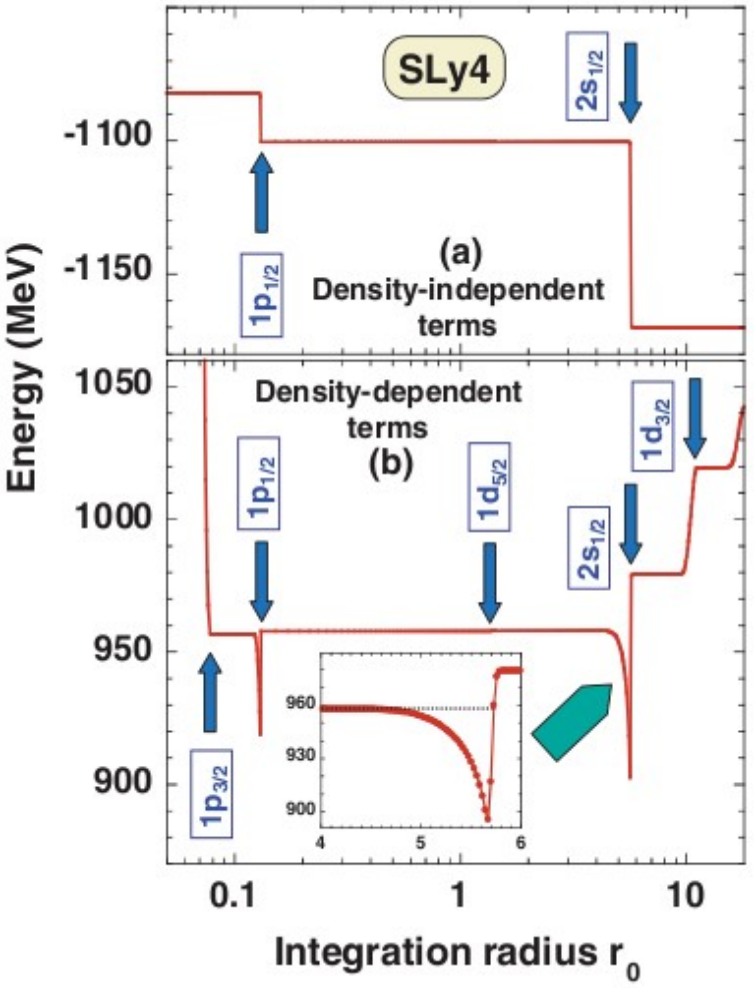
Nuclear DFT

- The nuclear DFT is the only microscopic theory which can be applied throughout the entire nuclear chart
- Important ingredient of nuclear DFT is the symmetry breaking (e.g. particle number, rotational symmetry, etc.) which can be used to introduce correlations
- In principle symmetries broken on the mean-field level should be restored with projection
- Density dependent term, appearing in most of the EDFs, is troublesome with projection. It causes non-analytic behavior of the energy kernels and other unwanted features
- For purpose of multi-reference calculations, an EDF without density dependence, based on an effective NN-force, is required.
- One possible approach is an EDF based on a finite range pseudopotential

Particle number projected energy of Skyrme terms. J. Dobaczewski, et. al., PRC 76 054315 (2007)



Finite range EDF

- First introduced at F. Raimondi, et.al, J. Phys. G 41, 055112 (2014)
- The form of the regularized finite range potential is

$$\mathcal{V}_j^{(n)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = \left(W_j^{(n)}\hat{1}_\sigma\hat{1}_\tau + B_j^{(n)}\hat{1}_\tau\hat{P}^\sigma - H_j^{(n)}\hat{1}_\sigma\hat{P}^\tau - M_j^{(n)}\hat{P}^\sigma\hat{P}^\tau\right) \times \hat{O}_j^{(n)}(\mathbf{k}_{12},\mathbf{k}_{34})\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{24})g_a(\mathbf{r}_{12})$$

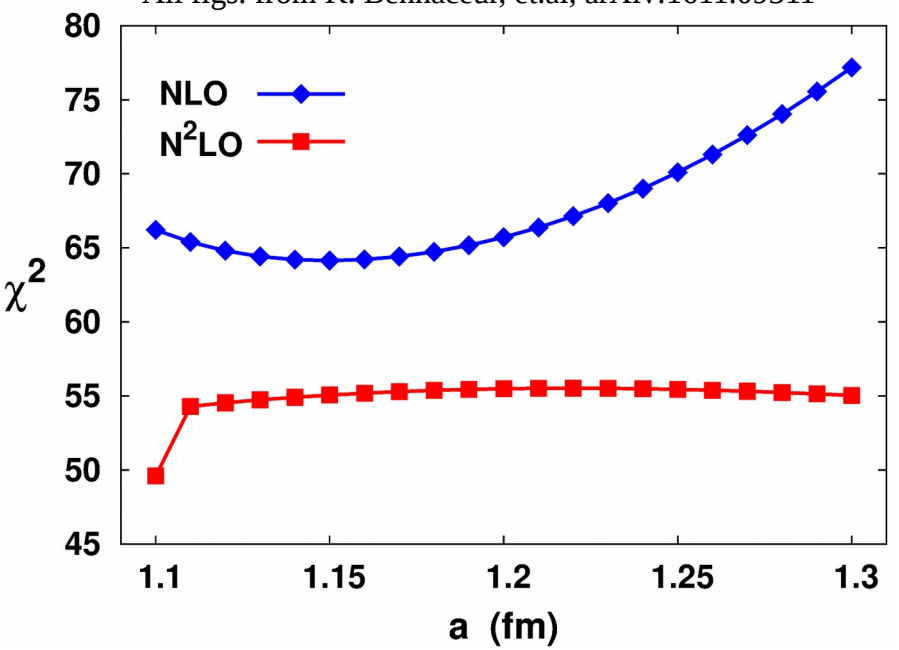
where $g_a(\boldsymbol{r})$ is a Gaussian with length scale a. Term $\hat{O}^{(n)}$ contains relative momentum operators $\boldsymbol{k}$ of the order n, with n = 0,2,4,6

- For each order of n, the potential contains adjustable parameters $W_j^{(n)}$, $B_j^{(n)}$, $H_j^{(n)}$, and $M_j^{(n)}$.
- This potential is used as a generator for the EDF for both, particle-hole and particle-particle channels
- In addition a contact spin-orbit term has been introduced
- First set of optimized parameters published recently: K. Bennaceur, A. Idini, J. Dobaczewski, P. Dobaczewski, M. Kortelainen, and F. Raimondi, arXiv:1611.09311 (2016). Optimization at spherical HFB level
- Optimization data set contained masses of spherical nuclei, radii, pairing gap, and some constraints on infinite nuclear matter. A zero range two-body term was introduced to obtain better pairing channel properties
- Sensitivity analysis was done for obtained parameters

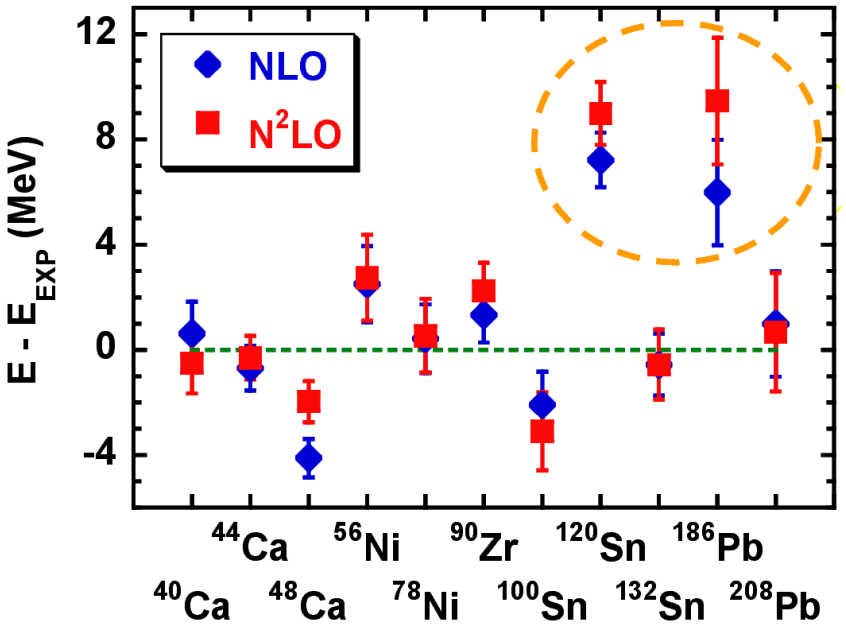
Results from the first optimization

- At N2LO level, the χ^2 depends only weakly on the length scale *a*
- For spherical doubly-magic nuclei binding energy is usually rather well reproduced
- At mid-shell, small effective mass deteriorates predicted binding energies
- For deformed nuclei, propagated uncertainties become larger

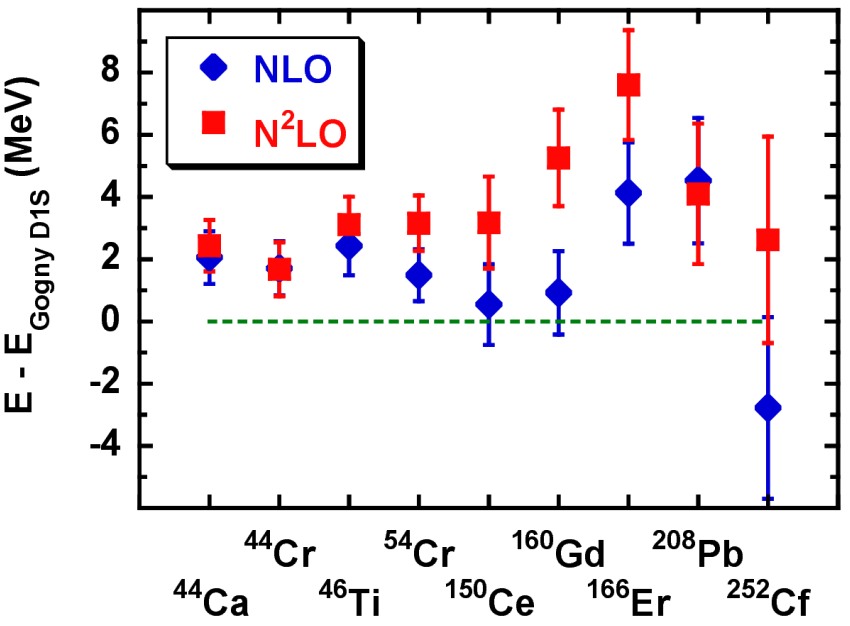
All figs. from K. Bennaceur, et.al, arXiv:1611.09311



Binding energies with propagated errors compared to experimental values



Binding energies with propagated errors compared to Gogny D1S



Parameterization

Table 3. The NLO and N^{2}LO coupling constants of local pseudopotentials (3) and (7) regularized at $a = 1.15\,\mathrm{fm}$. (in $\mathrm{MeV\,fm}^{n+3}$) shown together with their statistical errors.

Order	Coupling Constant	NLO REG2c.161026	N^{2}LO REG4c.161026
$n=0$	$W_1^{(0)}$	41.678375±0.6	3121.637124±1.5
	$B_1^{(0)}$	−1405.790048±4.3	−4884.029523±1.8
	$H_1^{(0)}$	202.879894±4.1	3688.310059±2.9
	$M_1^{(0)}$	−2460.684507±6.7	−5661.028710±2.8
$n=2$	$W_1^{(2)}$	−79.747992±4.2	547.802973±1.9
	$B_1^{(2)}$	73.112729±1.4	−319.513120±1.3
	$H_1^{(2)}$	−681.295790±3.2	−134.164127±0.3
	$M_1^{(2)}$	−48.161707±5.1	−318.407541±0.6
$n=4$	$W_1^{(4)}$		2019.945667±2.2
	$B_1^{(4)}$		−2365.956384±1.6
	$H_1^{(4)}$		2310.445509±1.8
	$M_1^{(4)}$		−2117.509518±4.0
	W_{SO}	177.076480±4.7	174.786236±5.1

In addition a contact term

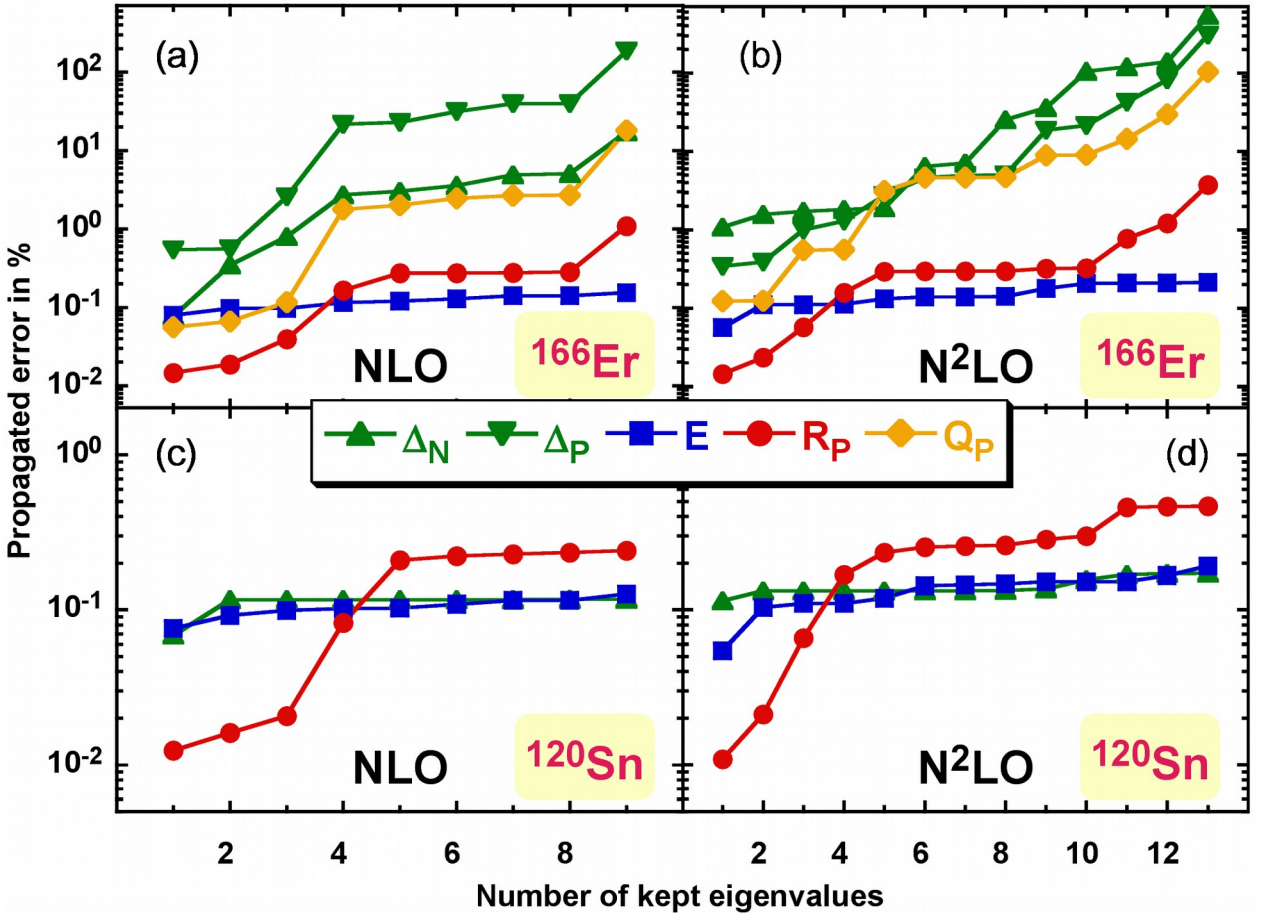
$$\mathcal{V}_\delta(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = t_0\left(1+x_0\hat{P}^\sigma\right)\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{24})\delta(\mathbf{r}_{12})$$

with $x_0 = 1$, $t_0 = 1000$ MeV fm^3.

Propagated error and deformed nucleus

- A closer inspection shows that propagated error for some observables in deformed ^{166}Er becomes large
- Current input data can not constrain parameters which are strongly connected to these observables
- Future EDF parameter optimization done at deformed HFB level should fix some of these issues
- This optimization can be carried out with newly developed HFB code called HFBtemp
- Use POUNDerS algorithm for parameter optimization

Propagated error as function of number of eigenvalues kept when computing covariance matrix. K. Bennaceur, et.al, arXiv:1611.09311



HFBtemp code

- Development HFBtemp nuclear DFT code started a few years ago.
- The goal is to build a modular HFB code, in which one could freely combine various basis (axial, 3D Cartesian, ...) with various EDFs (Skyrme, finite range, ...), and later with other components (FAM-QRPA, PNP, AMP, …)
- Code design allows various symmetry breaking schemes
- Coding is done with c++ (2011 standard). Many external libraries used (Eigen, boost, yaml-cpp)
- Uses a lot of template programming structures. Even the used elementary scalar type is a template parameter
- Inheritance allows to reuse many components
- Documentation with doxygen. This gives nice html and LaTeX documentation of the code
- The structure of the code aims to clarity and modularity (with some expense of CPU time and memory use)
- Design motto “CPU time is cheap, human time is expensive”

Benchmark of Skyrme EDF

- Skyrme EDF benchmarks well to HFBTHO (v2.00). HFBTHO was also benchmarked very well to HOSPHE and HFODD in CPC 184 (2013) 1592.
- Currently code contains axial and 3D Cartesian harmonic oscillator bases. The same Skyrme EDF module works for both cases

56Ni, SLy4, no Coulomb, no pairing, 16 shells

	HFBTHO	HFBtemp (axial)
E(tot)	-617.292118	-617.292118
E(kin)	1032.067336	1032.067333
Rms radius	3.616269	3.616269

24Mg, SLy4, no Coulomb, with pairing, 5 shells

	HFBTHO	HFBtemp (axial)	HFBtemp (3D)
E(tot)	-221.190506	-221.190505	-221.190505
E(kin)	408.593335	408.593334	408.593333
E(pair)	-7.386960	-7.386958	-7.386956
Delta(n)	1.737435	1.737435	1.737435
Q2 tot [b]	0.621284	0.621284	0.621284
Rms radius	2.908357	2.908357	2.908357

Coulomb

- For the purpose of the finite range EDF, a robust Coulomb method is required, which should manage without excessive amount of mesh points
- The Coulomb Green function method, as used in the HFODD, seems to be ideal for the task
- The direct Coulomb field can be calculated as

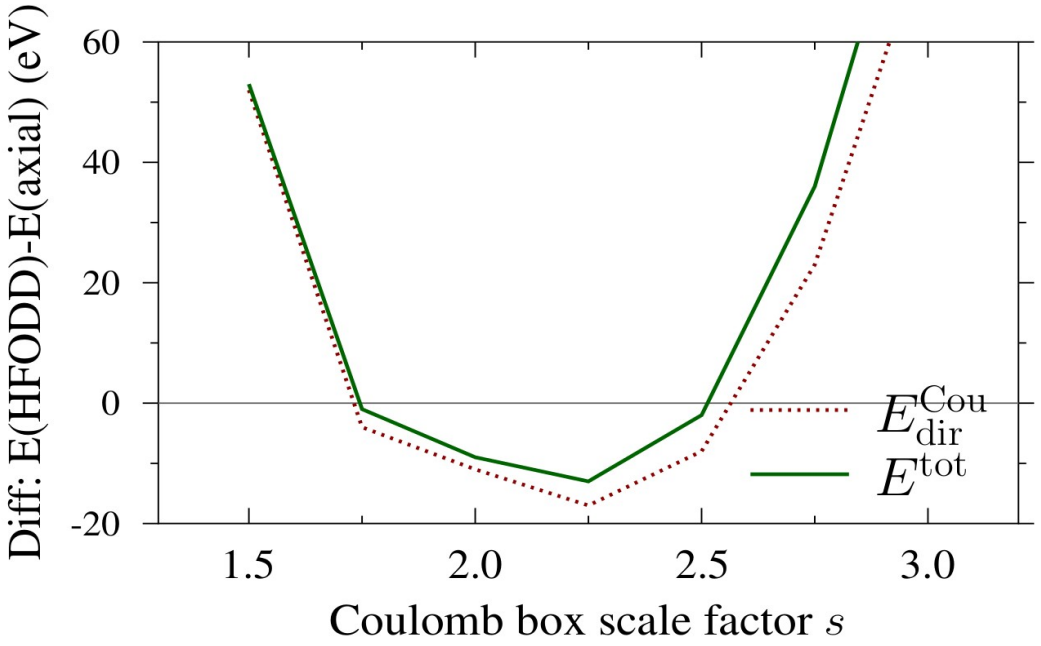
$$U^{\mathrm{Coul}}(\boldsymbol{r}) = e^2 \int_V d^3\boldsymbol{r}'\, G_D(\boldsymbol{r},\boldsymbol{r}')\rho_p(\boldsymbol{r}') - \frac{1}{4\pi}\oint_S d^2s'\, \frac{\partial G_D(\boldsymbol{r},\boldsymbol{r}')}{\partial n'}\, U^{\mathrm{Coul}}(\boldsymbol{r}').$$

From J.Dobaczewski, J.Dudek CPC 102 (1997) 166

where G_D is the Dirichlet Green function

- Similarly as with HFODD, Coulomb term effectively corresponds to Fourier transformation of the proton density (to avoid singularity at $\boldsymbol{r} = \boldsymbol{r}'$)
- Surface term includes at the moment monopole and quadrupole terms
- So far, Coulomb has been implemented only for axial case. Template specialization for 3D case is still to be done

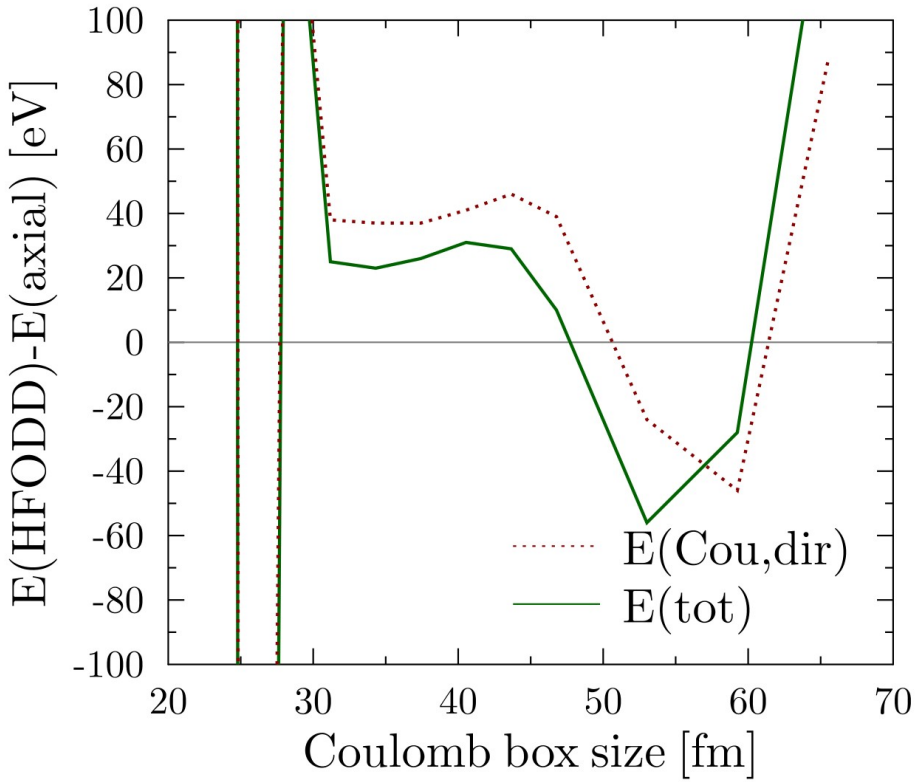
Coulomb: Benchmark to HFODD



^{16}O, N_{sh}=8, SLy4. Coulomb box size:

$r_{\rm max} = s \times 13.157\,{\rm fm}$, $z_{\rm max} = s \times 13.081\,{\rm fm}$

Mesh points: 24×48, k_{max}: 60



24Mg, SLy4, Nsh = 8, deformation β = 0.402

k_{max} = 80, mesh points: 24x24

- Direct Coulomb term benchmarks to HFODD very nicely

Finite range EDF, implementation

- The local version of the finite range potential is implemented in a similar manner to tensor-hypercontraction method (see R.M. Parrish, et.al, PRL 111, 132505 (2013)), with exception that auxiliary basis is not used, and potential is instead directly evaluated
- The exchange part of Hamiltonian can be calculated from matrix product

$$h^{\mathrm{ex}} = X^{\dagger}\left(V \circ \left(X \rho X^{\dagger}\right)\right) X$$

where ρ is the density matrix in configuration space, *X* is the matrix containing basis functions in the mesh, *V* is the interaction in the coordinate space, and circle denotes Hadamart product

- Direct part and pairing part can be also computed in this framework
- The product

$$\rho\left(\boldsymbol{x}, \boldsymbol{x}'\right) = X \rho X^{\dagger}$$

is a density matrix in coordinate space

- The local finite range potential has been implemented on HFBtemp for axial case
- All in all, relatively fast computation of *h*. Downside: large memory usage

Benchmark of finite range EDF

44Ca, 10 shells, N2LO potential + contact delta and spin-orbit terms. No Coulomb

	HFODD	HFBtemp
E(tot)	-461.901891	-461.901891
E(kin)	769.915053	769.915053
E(finite range)	-1963.846263	−1963.846264
E(pair)	-10.694950	-10.694950
E(contact)	742.724270	742.724270
Pairing gap (n)	3.115393	3.115393
RMS radius	3.4038	3.403800

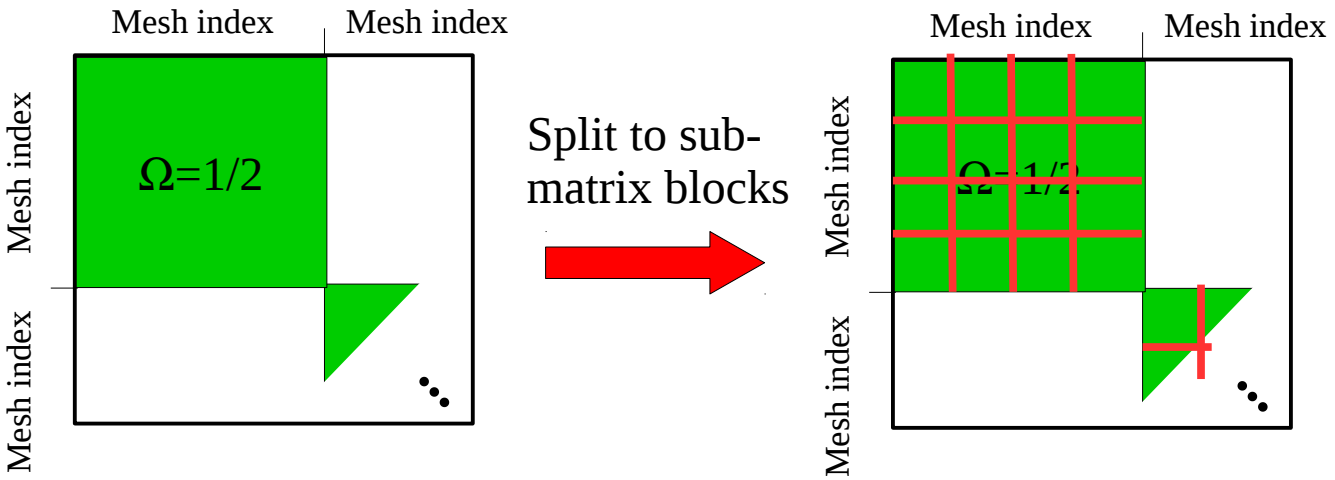
46Ti, 10 shells, NLO potential + contact delta and spin-orbit terms. With Coulomb

	HFODD	HFBtemp
E(tot)	-403.457828	-403.455844
E(kin)	786.562411	786.557953
E(finite range)	-3112.537801	−3112.51592
E(Coul, direct)	93.874908	93.874696
E(Coul, exchange)	-8.846136	-8.844310

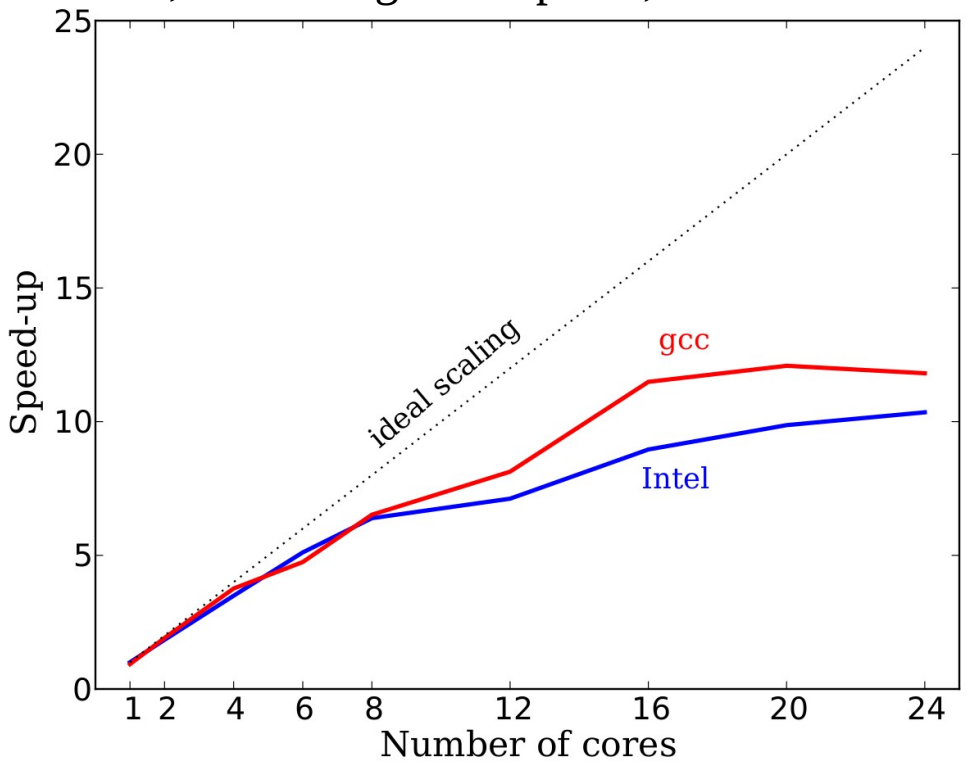
Precision of the Coulomb exchange term presently the most limiting factor when benchmarking to HFODD

OpenMP parallelization of HFBtemp

- Most of the CPU time in a HFB iteration is used when applying exchange or pairing part of the interaction to the coordinate space density matrix or pairing tensor
- OpenMP parallelization has been implemented on most time-critical parts of the code.
- Due to large matrices, the size of the CPU cache memory becomes a limiting factor for parallelization → Split matrices to sub-matrix blocks
- Gives rather good scaling up to ~16 cores
- Typical CPU time for one HFB iteration with NLO potential, 16 shells, and 32x32=1024 mesh points is ~330 s with one Haswell core.
- For large scale calculation, a hybrid MPI/OpenMP scheme is implemented to calculate multiple nuclei



Speed-up: 16 shells, 32x32 mesh split to 8 sub-blocks, Intel and gcc compilers, Haswell cores



Conclusions and future plans

- The goal is to obtain an EDF based on a finite range pseudopotential, applicable for multi-reference DFT calculations
- The first set of parameters was optimized at spherical HFB level. Gives rather good description of most spherical nuclei. However, uncertainties with deformed nuclei seem to be larger

Finite range EDF future plans

- Address the problem of low effective mass
- Optimize model parameters at deformed HFB level by using HFBtemp
- Large scale mass table survey

HFBtemp code development

- Combine with POUNDerS algorithm to run the parameter optimization
- Implement Coulomb for 3D case
- Complete finite amplitude method QRPA module implementation