Fitting Energy Density Functionals for low-energy nuclear structure

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INT Program: Bayesian Methods in Nuclear Physics
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Lyon 1 CNRS IN2P3 Les deux infinis IPNL JYVÄSKYLÄN YLIOPISTO UNIVERSITY OF JYVÄSKYLÄ

People involved

- IPNL (Lyon): M. Bender, D. Davesne, R. Jodon, J. Meyer
- IRFU (Saclay): T. Duguet
- ULB (Bruxelles): P.H. Heenen, V. Hellemans
- University of York: J. Dobaczewski, A. Pastore
- University of Surrey: F. Raimondi, A. Idini

Mean-field models

- Stationary Schrödinger equation for A particles

$$\hat{H}\Psi = \left(\hat{T} + \hat{V}_2 + \hat{V}_3 + \ldots\right)\Psi = E_0\Psi$$

- Mean-field approximation, Hartree-Fock(-Bogolyubov)

$$E = \langle\Phi|\hat{H}_{\text{eff}}|\Phi\rangle \simeq E_0 = \langle\Psi|\hat{H}|\Psi\rangle$$

- Effective interaction $\hat{H}_{\text{eff}} = \hat{T} + \hat{V}_{\text{eff}}$

$$\hat{V}_{\text{eff}} = \hat{V}_{\text{eff}}(\mathbf{p}), \quad \mathbf{p} \in \mathbb{R}^n, \quad n \lesssim 10$$

Details don't matter but:

- HF(B) equations are non linear and are solved iteratively
- Can be very time consuming when many symmetries are broken
- Fit often done using only spherical nuclei or, at least, time even systems

Will the interaction give meaningful results when symmetries are broken ?

Resolution of the HF(B) equations

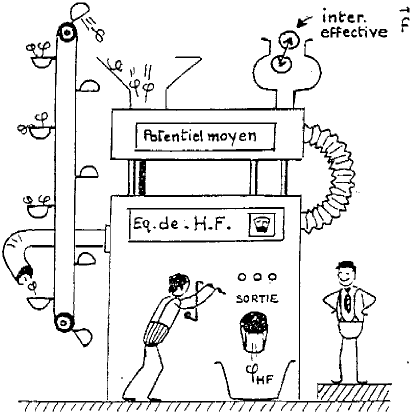


Figure : Picture by J. Dechargé, from “Approches de champ moyen et au-delà”, J.-F. Berger, École Joliot-Curie: “Les noyaux en pleine forme”, 1991.

- Calculations have to give finite numbers at the end...
- Parameters must be usable for nuclei not in the fit

Skyrme effective interactions

- Two-body term (with $x \equiv \mathbf{r}, s, q$) $\simeq$ SV interaction

$$\begin{aligned} V_2(x_1,x_2;x_3,x_4) = \Big[& t_0\left(\boldsymbol{\delta}^s + x_0\,\mathbf{P}^s\right) \\ & + \tfrac{1}{2}\,t_1\left(\boldsymbol{\delta}^s + x_1\,\mathbf{P}^s\right)\left(\hat{\mathbf{k}}_{12}^{*2} + \hat{\mathbf{k}}_{34}^{2}\right) \\ & + t_2\left(\boldsymbol{\delta}^s + x_2\,\mathbf{P}^s\right)\hat{\mathbf{k}}_{12}^{*}\cdot\hat{\mathbf{k}}_{34} \\ & + \mathrm{i}\,W_0\,\boldsymbol{\delta}^s\left(\hat{\boldsymbol{\sigma}}_{13} + \hat{\boldsymbol{\sigma}}_{24}\right)\cdot\left(\hat{\mathbf{k}}_{12}^{*}\times\hat{\mathbf{k}}_{34}\right)\Big] \\ & \times\delta(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_2-\mathbf{r}_4)\delta(\mathbf{r}_1-\mathbf{r}_2) \end{aligned}$$

- Two-body density dependent term $\simeq$ SLy interactions

$$\begin{aligned} & V_3(x_1,x_2;x_3,x_4) = \\ & \quad \tfrac{1}{6}\,t_3\left(\boldsymbol{\delta}^s + x_3\,\mathbf{P}^s\right)\rho_0^{\alpha}(\mathbf{r}_1)\delta(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_2-\mathbf{r}_4)\delta(\mathbf{r}_1-\mathbf{r}_2) \end{aligned}$$

$\Rightarrow$ 9 parameters to fit

How to fit the parameters of an effective interaction ?

It's simple !

- Choose a set relevant observables
- Use constraints to write a penalty function χ^2
- Minimize it...
- ... and, most likely, this will not lead to any useful result

Why ?

- Some parameters may be poorly constrained
- Some constraints may be impossible to satisfy simultaneously
- Problems (which you would not even think[1]) can occur

So you need to modify the χ^2

$\Rightarrow$ You don't know the χ^2 before you start to minimize it...

"Good judgement is the result of experience and experience the result of bad judgement."
– Mark Twain

Who seems to be very popular in this workshop...

[1] in your worst nightmares

What the χ^2 is made of?

Penalty function: $\chi^2 = \chi^2_{\text{inm}} + \chi^2_{\text{surf.}} + \chi^2_{\text{neut.}} + \chi^2_{\text{nuclei}} +$?

with

- Infinite nuclear matter properties

$$\chi^2_{\text{inm}} = \left(\frac{\rho_{\text{sat}}^{\text{calc.}} - \rho_{\text{sat}}}{\Delta \rho_{\text{sat}}} \right)^2 + \ldots$$

- Surface properties

$$\chi^2_{\text{surf.}} = \left(\frac{a_s^{\text{calc.}} - a_s}{\Delta a_s} \right)^2$$

- Neutrons matter: several points obtained from "exact" calculations (*ab initio* calculations)
- Nuclei: Binding energies, charge radii of doubly magic nuclei, single particle energies, ...

Minimization and post-fit analysis

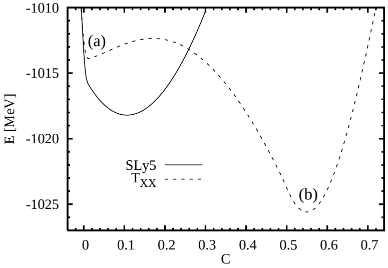
- Minimization:
  Nealder Mead, conjugated gradients, Pounders, ...
- Post-fit analysis:
  covariance matrix, correlations between parameters, statistical error bars
- But one usually assumes that
  - the χ^2 is smooth
  - ... or, at least, is defined everywhere

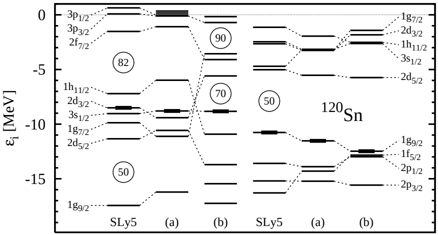
The χ^2 is not always smooth... (1)

Competition between different shell structures

$$C = \int \mathbf{J}_n \cdot \boldsymbol{\nabla} \rho_n \, \mathrm{d}^3 r$$

Constrained calculation →





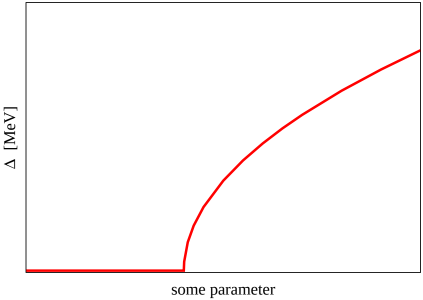
χ^2(masses, charge radii, ...)

may not be continuous !

:-(

The χ^2 is not always smooth... (2)

Pairing is a critical phenomenon...

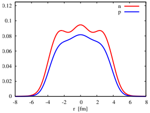


If Δ is zero, how to find the direction where it becomes finite ?

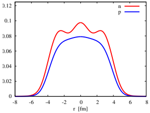
The χ^2 is not always even defined!

- Instabilities often experienced with the skyrme functionals
  - Ferromagnetic instabilities: (spin polarization) $n\uparrow$, $p\uparrow$
  - Isospin instabilities: neutron-proton *segregation*
  - Both: $n\uparrow$, $p\downarrow$

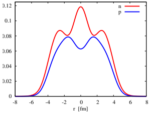
- Example: isospin instability in ^{48}Ca



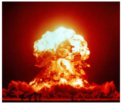
$C_1^{\Delta\rho} = 15$ MeV fm^5 $\sim$ SLy5



25 MeV fm^5



35 MeV fm^5



$\gtrsim 36$ MeV fm^5

T. Lesinski, K.B., T. Duguet, J. Meyer, PRC 74, 044315 (2006).

$C_1^{\Delta\rho}$ is just a combination of some parameters

Linear response – Stability criterium

Response of the system to a perturbation given by

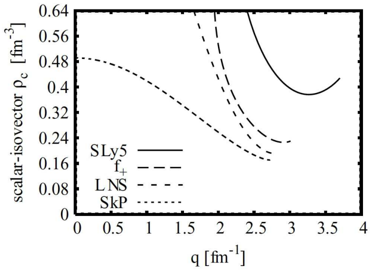
$$\mathcal{Q}^{(\alpha)} = \sum_a e^{i\mathbf{q}\cdot\mathbf{r}_a}\, \Theta_a^{(\alpha)},$$

$$\Theta_a^{\rm ss} = 1_a, \quad \Theta_a^{\rm vs} = \boldsymbol{\sigma}_a, \quad \Theta_a^{\rm sv} = \vec{\tau}_a, \quad \Theta_a^{\rm vv} = \boldsymbol{\sigma}_a \vec{\tau}_a$$

Response functions are given by

$$\chi^{(\alpha)}(\omega,\mathbf{q}) = \frac{1}{\Omega}\sum_n |\langle n|\mathcal{Q}^{(\alpha)}|0\rangle|^2 \left(\frac{1}{\omega - E_{n_0} + i\eta} - \frac{1}{\omega + E_{n_0} - i\eta}\right)$$

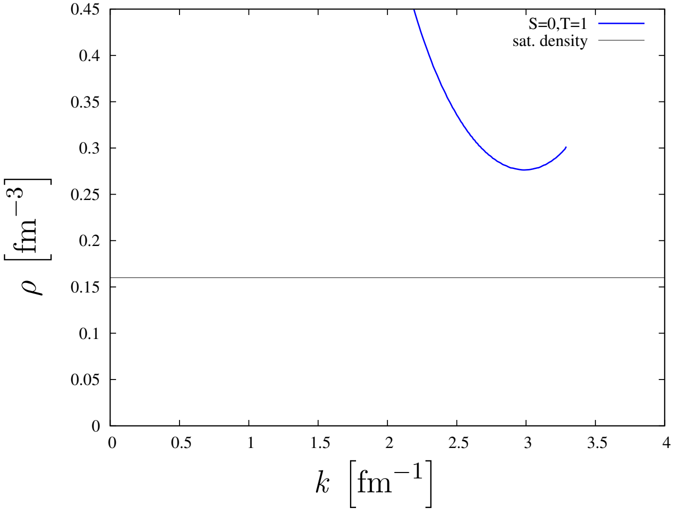
(Cf. C. Garcia–Recio *et al.*, Ann. of Phys. 214 (1992) 293–340)



- Predicts instabilities in finite size systems
- Easy to implement
- Negligible computation time

Linear response as a tool for diagnosis

Pole of the response at $E = 0$ $\equiv$ instability



- T. Lesinski, K.B., T. Duguet, J. Meyer, PRC 74, 044315 (2006);
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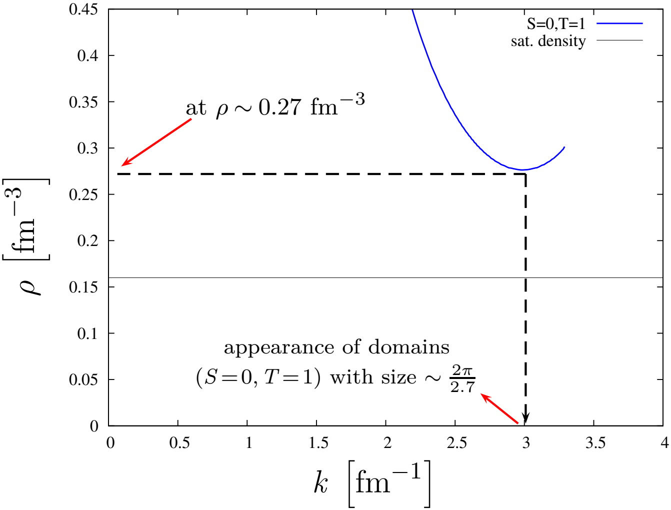

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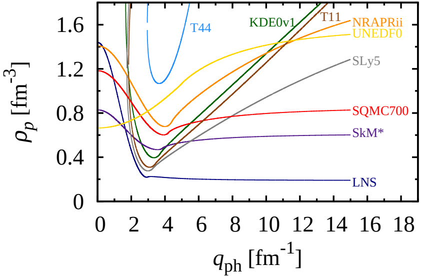
Attempt to define a stability criterium[2]

Study in the scalar-isoscalar channel ($S = 0, T = 1$) based on 9 different functionals



- The lowest density for which the response has a pole, $\rho_{\min}$, must be so that

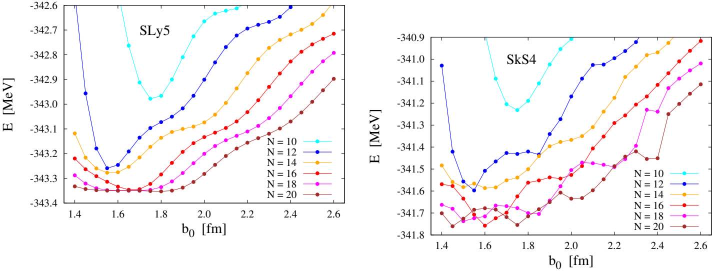
$$\rho_{\min} > 1.2 \times \rho_{\text{sat}}$$

- Other channels ?
- What if the criterium is too conservative ?

[2] V. Hellemans, A. Pastore, T. Duguet, K.B., D. Davesne, J. Meyer, M. Bender, P.-H. Heenen, PRC 88, 064323

Calculations on harmonic oscillator basis

- "Chaotic" behavior with the oscillator parameter b_0 and the size of the basis N



Calculations using the code HFBTHO

Fit of new interactions...

Stability must be enforced during the fit of the parameters !

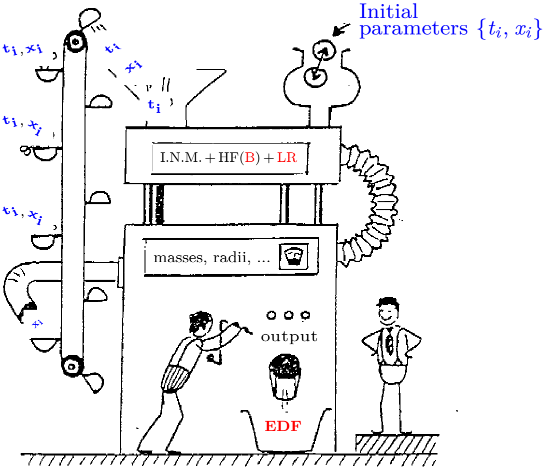


Figure : Adapted from the picture by J. Dechargé, from “Approches de champ moyen et au-delà”, J.-F. Berger, École Joliot-Curie, 1991.

New generation of Skyrme interaction: SLyMR1

- For some reasons, we decided to replace the density dep. term

$$V_{\rm dd} = \frac{t_3}{6}\left(1 + x_3 \hat{P}^{\sigma}\right)\rho_0^{\alpha}\,\delta(\mathbf{r})$$

- by

$$\begin{aligned}
V_{\rm 3b} &= u_0\,\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{23}) \\
&\quad + \frac{u_1}{2}\left(1 + y_1 \hat{P}^{\sigma}_{12}\right)\left[\mathbf{k}'^2_{12}\,\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{23}) + \delta(\mathbf{r}_{13})\delta(\mathbf{r}_{23})\,\mathbf{k}^2_{12}\right] \\
&\quad + u_2\left[1 + y_{21}\hat{P}^{\sigma}_{12} + y_{22}\left(\hat{P}^{\sigma}_{13} + \hat{P}^{\sigma}_{23}\right)\right]\mathbf{k}'_{12}\cdot\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{23})\mathbf{k}_{12} \\
V_{\rm 4b} &= v_0\,\delta(\mathbf{r}_{14})\delta(\mathbf{r}_{24})\delta(\mathbf{r}_{34})
\end{aligned}$$

More terms with gradients,
more chance to encounter instabilities

SLyMR1: the most constrained interaction ever

- 2- and 3-body terms + 4-body contact term (no ρ_0^α term)
- Used for the normal and pairing fields
- Infinite nuclear matter
  - ρ_{sat}, E/A, K_∞, m^*/m, J, L
  - Neutron matter equation of state
  - Constraints in spin channels and on the effective mass
- (Double magic) nuclei
  - Binding energy
  - Charge radii
  - Energy difference between 2 spin-orbit partners (in ^{208}Pb)
- Spherical semi-magic nuclei (^{44}Ca and ^{120}Sn)
  - Binding energy
  - Spectral gaps
- Linear response code fully functional
  - $\rho_{\mathrm{crit,min}} \geqslant 0.26\ \mathrm{fm}^{-3}$ in symmetric and neutron matter

First version: SLyMR1$_\beta$

par.	unit	p_i	Δp_i	$\Delta p_i / p_i$
t_0	MeV fm^3	-1229.79	94.95	7.7 %
t_1	MeV fm^5	838.80	223.25	26.6 %
t_2	MeV fm^5	-1333.04	604.87	45.4 %
u_0	MeV fm^6	4017.82	1485.84	37.0 %
u_1	MeV fm^8	-3820.19	2293.79	60.0 %
u_2	MeV fm^8	14578.51	5322.63	36.5 %
x_0		0.1695	0.2290	135.1 %
x_1		0.6598	0.2686	40.7 %
x_2		-1.1512	0.0999	8.7 %
y_1		1.2941	1.0130	78.3 %
y_{21}		-1.1201	0.0634	5.7 %
y_{22}		-0.0813	0.0212	26.1 %
W_0	MeV fm^5	97.780	18.337	18.8 %
v_0	MeV fm^9	-9371.16	33266.54	355.0 %

SLyMR1$_\beta$: correlations

	ρ_{sat}	E/A	K_∞	m^*/m	J	$\langle V \rangle_{pp}$
	0.154 fm^{-3}	-16.12 MeV	279 MeV	0.56	33.7 MeV	-2.75 MeV
ρ_{sat}	1.00	-0.24	-0.33	-0.00	0.03	-0.01
E/A		1.00	-0.43	0.18	-0.49	0.17
K_∞			1.00	0.29	-0.19	0.13
m^*/m				1.00	-0.17	0.19
J					1.00	-0.33
V_{pp}						1.00

- Bad features

$$K_\infty \searrow \ \Leftrightarrow \ m^*/m \searrow$$

$$m^*/m \searrow \ \Leftrightarrow \ \langle V \rangle_{pp} \nearrow$$

- m^*/m and $\langle V \rangle_{pp}$ are strongly correlated but the correlation coefficient is rather small (?)
- Going from $m^*/m = 0.56$ to 0.7 is a change of 25 %

Several problems with SLyMR1$_\beta$

- Four-body term poorly constrained
- Other ones not relevant for the present discussion

$\Rightarrow$ Improved penalty function: SLyMR1

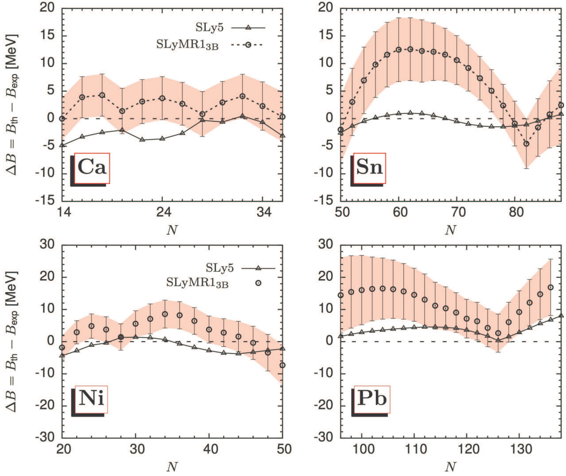
  - Slightly different constraints
  - 4-body term **disregarded**

SLyMR1: parameters

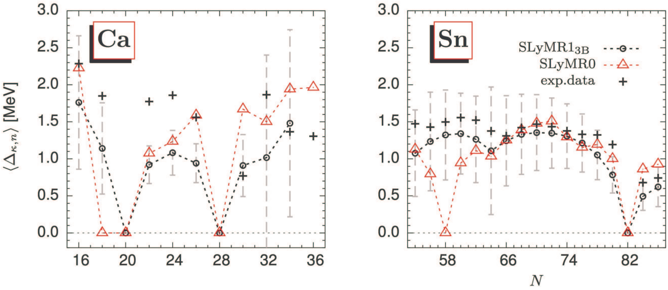
- Parameters

par.	unit	p_i	Δp_i	$\Delta p_i / p_i$	
t_0	MeV fm^3	-1249.47	94.95	7.4 %	(7.7 %)
t_1	MeV fm^5	943.83	223.25	18.4 %	(26.6 %)
t_2	MeV fm^5	-1141.47	604.87	52.3 %	(45.4 %)
u_0	MeV fm^6	3436.76	1485.84	37.7 %	(37.0 %)
u_1	MeV fm^8	-4471.94	2293.79	14.9 %	(60.0 %)
u_2	MeV fm^8	13596.13	5322.63	34.1 %	(36.5 %)
x_0		0.2182	0.2290	102.3 %	(135.1 %)
x_1		0.6306	0.2686	33.7 %	(40.7 %)
x_2		-1.1598	0.0999	7.8 %	(8.7 %)
y_1		0.9880	1.0130	78.7 %	(78.3 %)
y_{21}		-1.1253	0.0634	5.1 %	(5.7 %)
y_{22}		-0.0793	0.0212	26.3 %	(26.1 %)
W_0	MeV fm^5	124.647	18.337	18.7 %	(18.8 %)
v_0	MeV fm^9				(355.0 %)

SLyMR1: binding energies



SLyMR1: gaps



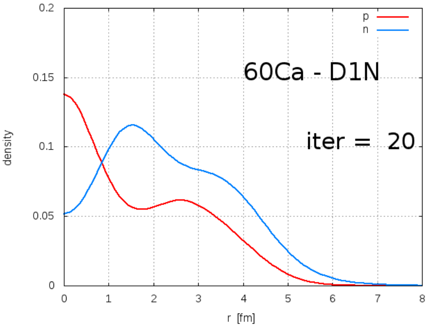
Ca
Sn
SLyMR1$_{3B}$
SLyMR0
exp.data
$\langle \Delta_{\kappa,n} \rangle$ [MeV]
N

Conclusions

- The construction of a penalty function is a dynamical process
- Constraints which are not simply related with observables are not trivial to handle
- What does the covariance matrix tell us when the problem is non linear ?
- What about systematic errors ?

Finite-range interactions free from finite-size instabilities ?

Very exotic ^{60}Ca nucleus using Gogny D1N interaction



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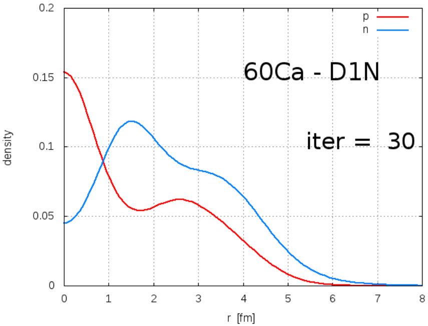

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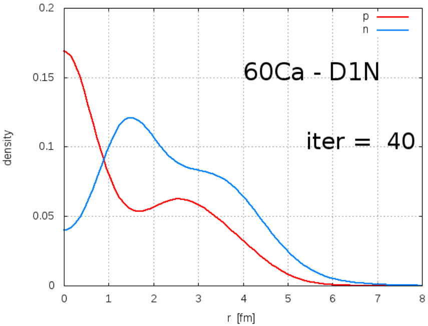

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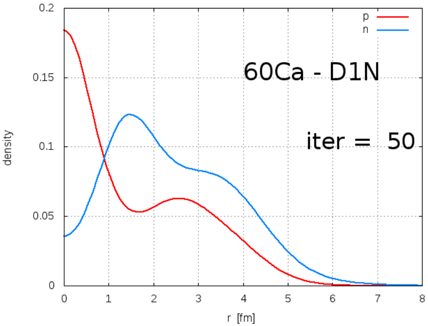

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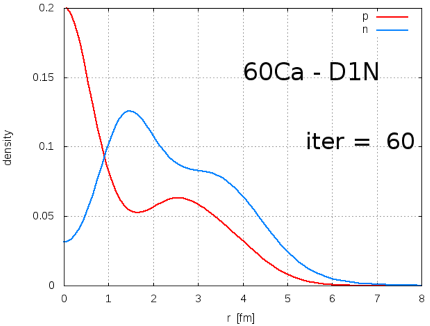

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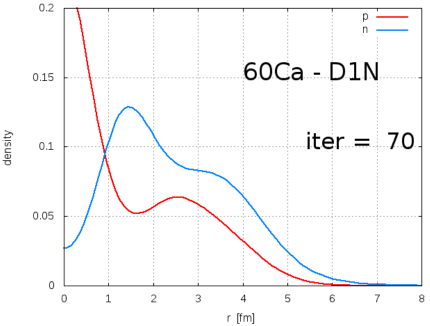

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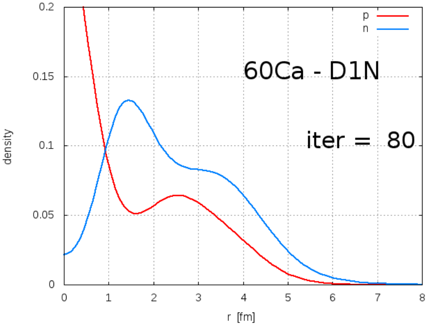

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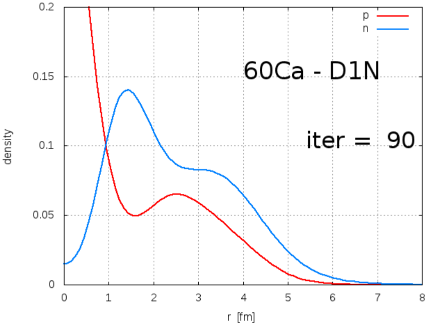

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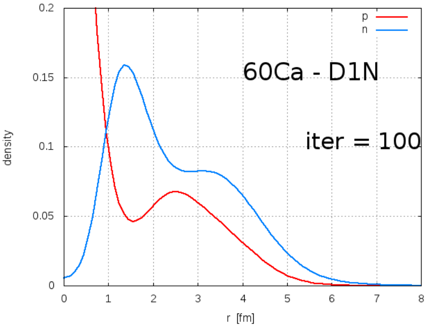

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