Zawartość informacyjna nowej obserwabli

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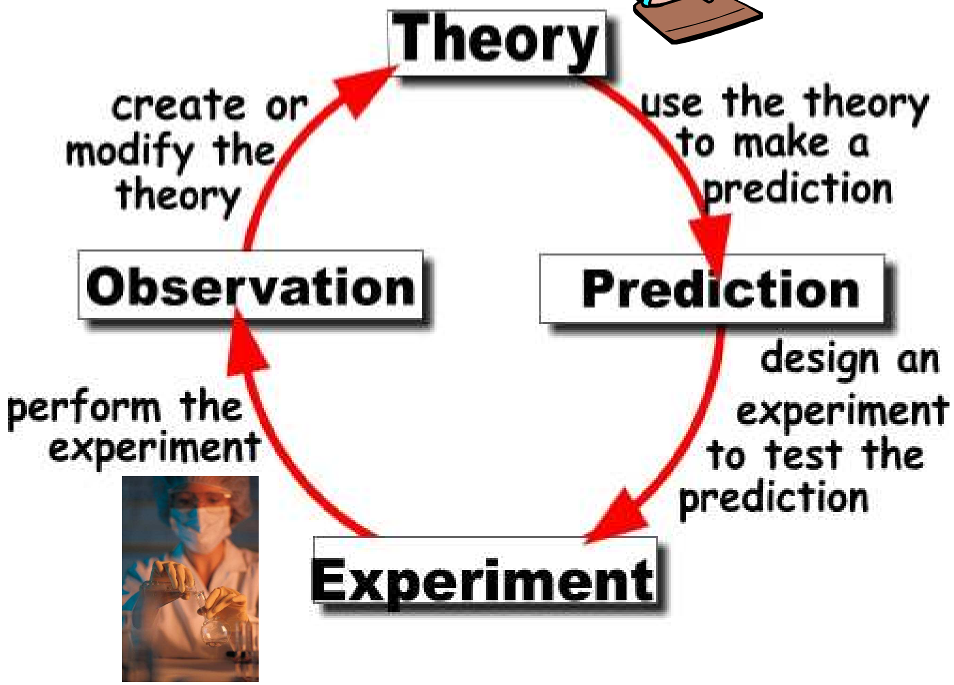
UW, 19 grudnia, 2011

Scientific method

The scientific method uses objective experimentation to predict, verify, or refute, an assertion made by a theory. Based on the results of the experiment(s), the theory is modified. The process of predict, verify or refute is repeated, continually testing and modifying the theory until the theory fits all possible experimental observations. Then the theory is considered a scientific law.



Jądra atomowe komunikują się z nami przy pomocy różnych obserwabli. Niektóre łatwo zmierzyć, inne wymagają ogromnego wysiłku, nowych technik i ogromnych kosztów. Tematem seminarium będzie zawartość informacyjna i użyteczność nowej obserwabli, w kontekście aktualnych modeli teoretycznych. Pokażę również, w jaki sposób mozna skwantyfikować pojęcie korelacji pomiędzy różnymi obserwablami i jak oszacowac systematyczny i statystyczny błąd teorii, która zawiera parametry dopasowane do doświadczenia.

Konkretne przykłady:

- Związek pomiędzy skórą neutronową a polaryzowalnością dipolową
- Teoretyczne przewidywania linii oderwania neutronu
- Równanie stanu gwiazdy materii jądrowej i równanie Tolmana-Oppenheimera-Volkoffa gwiazdy neutronowej).

Characteristics of good theory:

- Predictive power
- Robust extrapolations
- Validation of data
- Short- and long-term guidance

Systematic errors (due to incorrect assumptions/poor modeling)

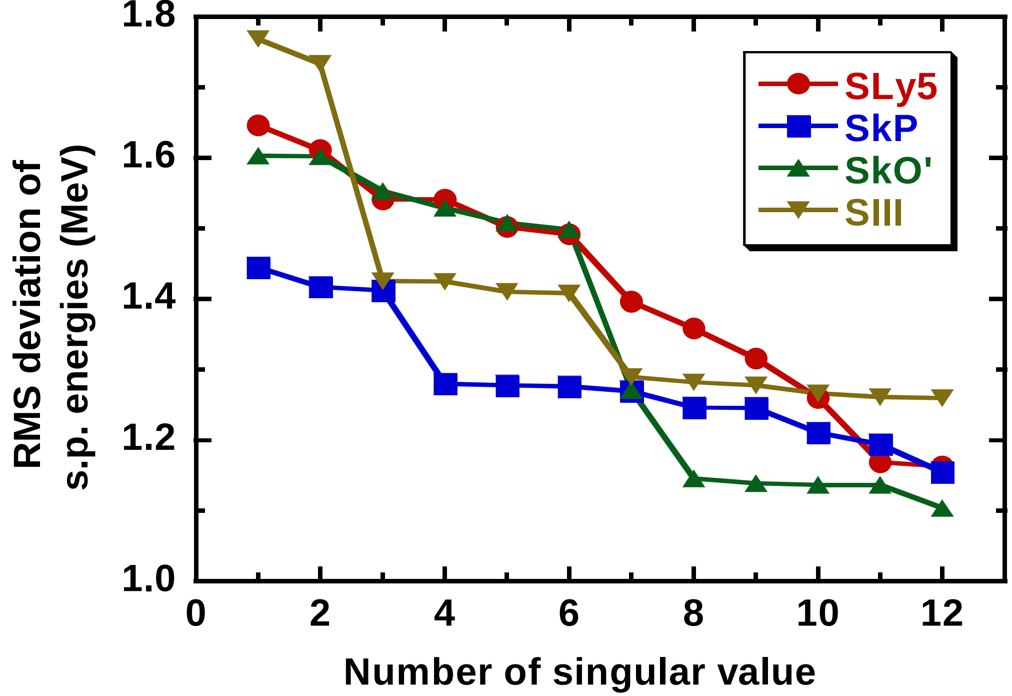
Statistical errors (optimization and numerical errors)

Early attempts to employ statistical methods of linear-regression and error analysis have been revived recently and been applied to determine the correlations between model parameters, parameter uncertainties, and the errors of calculated observables. This is essential for providing predictive capability and extrapolability, and estimate the theoretical uncertainties.

- G.F. Bertsch et al., Phys. Rev. C 71, 054311 (2005).
- M. Kortelainen et al., Phys. Rev. C 77, 064307 (2008).
- J. Toivanen et al., Phys. Rev. C 78, 034306 (2008).
- P. Klüpfel et al., Phys. Rev. C 79, 034310 (2009).
- P.-G. Reinhard and W. Nazarewicz, Phys Rev. C 81, 051303 (R) (2010)
- M . Kortelainen et al., Phys. Rev. C 82, 024313 (2010)
- J. Dudek et al., Int. J. Mod. Phys. E 19, 652 (2010).

Examples of some DFT-based work

M . Kortelainen et al., Phys. Rev. C 77, 064307 (2008)



Based on:

P.G. Reinhard and WN, Phys. Rev. C 81, 051303 (R) (2010)

To what extent is a new observable independent of existing ones and what new information does it bring in? Without any preconceived knowledge, all different observables are independent of each other and can usefully inform theory. On the other extreme, new data would be redundant if our theoretical model were perfect. Reality lies in between.

Consider a model described by coupling constants $\mathbf{p} = (p_1, \ldots, p_F)$
Any predicted expectation value of an observable is a function of these parameters. Since the number of parameters is much smaller than the number of observables, there *must exist correlations* between computed quantities. Moreover, since the model space has been optimized to a limited set of observables, there may also exist correlations between model parameters.

How to confine the model space to a *physically reasonable* domain?

Statistical methods of linear-regression and error analysis

$$\chi^2(\mathbf{p}) = \sum_{\mathcal{O}} \left(\frac{\mathcal{O}^{(\mathrm{th})}(\mathbf{p}) - \mathcal{O}^{(\mathrm{exp})}}{\Delta \mathcal{O}} \right)^2$$

Objective function

Expected uncertainties

fit-observables
(may include pseudo-data)

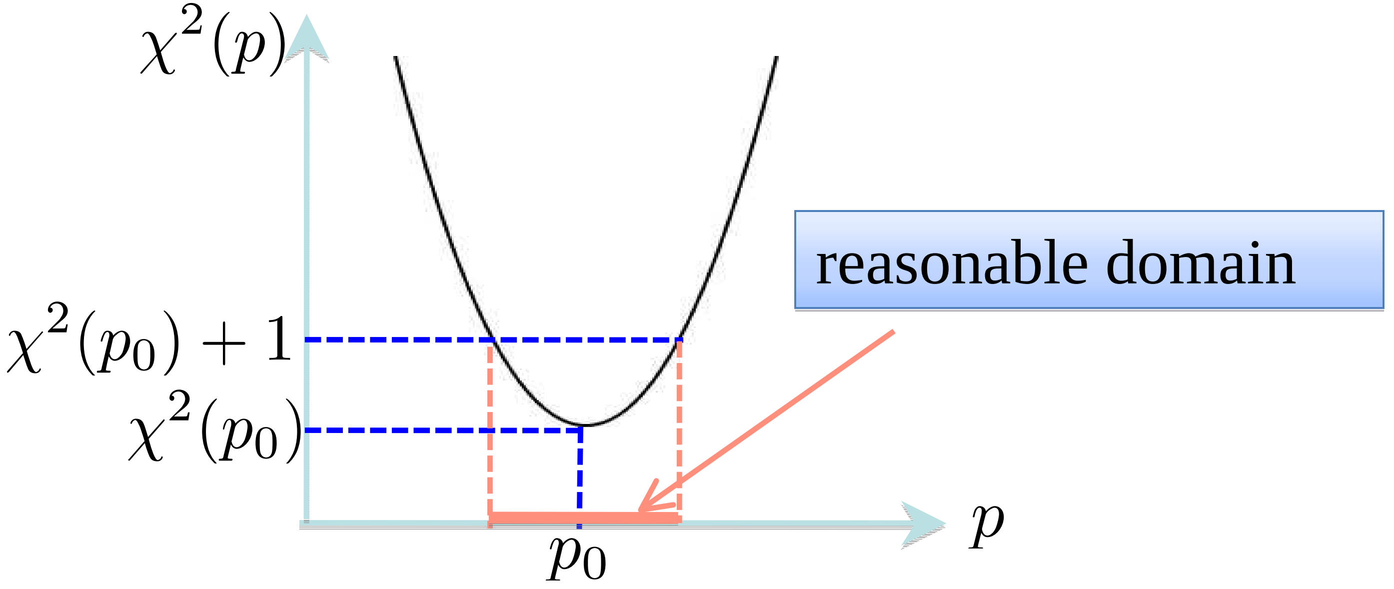
Consider a model described by coupling constants $\mathbf{p} = (p_1, ..., p_F)$

The optimum parameter set $\mathbf{p}_0 : \quad \chi^2(\mathbf{p}_0) = \chi^2_{\min} = \text{minimal.}$

$$\chi^2(\mathbf{p}) - \chi^2_{\min} \approx \sum_{i,j=1}^{F} (p_i - p_{i,0}) \mathcal{M}_{ij} (p_j - p_{j,0}), \quad \mathcal{M}_{ij} = \partial_{p_i} \partial_{p_j} \chi^2 \Big|_{\mathbf{p}_0}$$

The reasonable domain is defined as that multitude of parameters around minimum that fall inside the covariance ellipsoid :

$$(\mathbf{p} - \mathbf{p}_0) \hat{\mathcal{M}} (\mathbf{p} - \mathbf{p}_0) \leq 1$$



Statistical uncertainty in variable A:

$$\overline{\Delta A^2} = \sum_{ij} \partial_{p_i} A (\hat{M}^{-1})_{ij} \partial_{p_j} A, \quad \partial_{p_i} A = \partial_{p_i} A \Big|_{\mathbf{p}_C}$$

Correlation between variables A and B:

$$\overline{\Delta A \, \Delta B} = \sum_{ij} \partial_{p_i} A (\hat{M}^{-1})_{ij} \partial_{p_j} B$$

Product-moment correlation coefficient between two observables/variables A and B:

$$c_{AB} = \frac{\overline{\Delta A \, \Delta B}}{\sqrt{\overline{\Delta A^2} \; \overline{\Delta B^2}}}$$

=1: full alignment/correlation
=0: not aligned/statistically independent

How to estimate systematic (model) error?

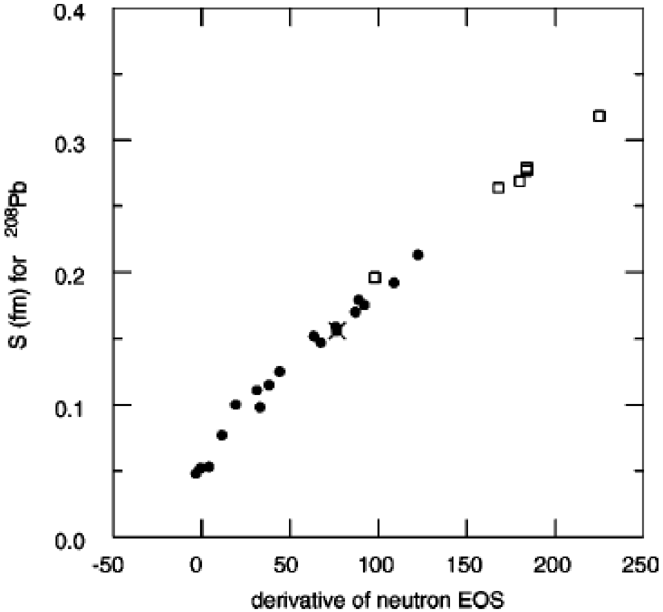
Take a set of reasonable models M_i

Make a prediction $O(M_i)$

Compute average and variation within this set

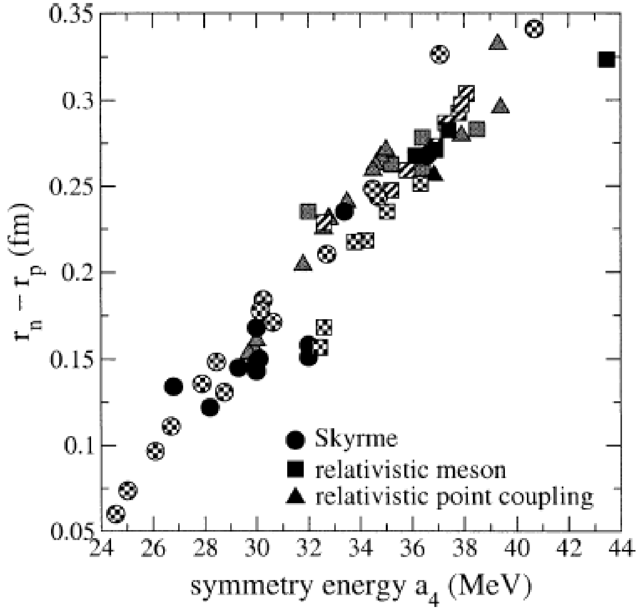
$$C_{AB}^{\mathrm{models}} = \frac{|\overline{\Delta A\, \Delta B}|_M}{\sqrt{(\overline{\Delta A^2)})_M\ (\overline{\Delta B^2})_M}}$$

Various correlations reported…

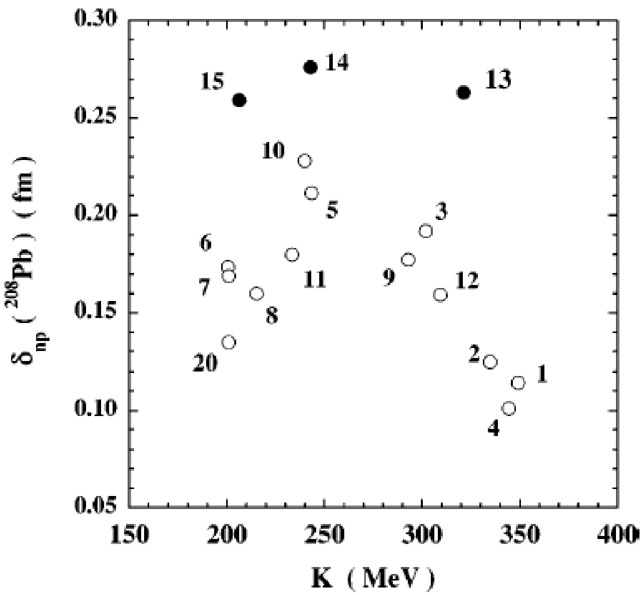


Typel and Brown, Phys. Rev. C 64, 027302 (2001)

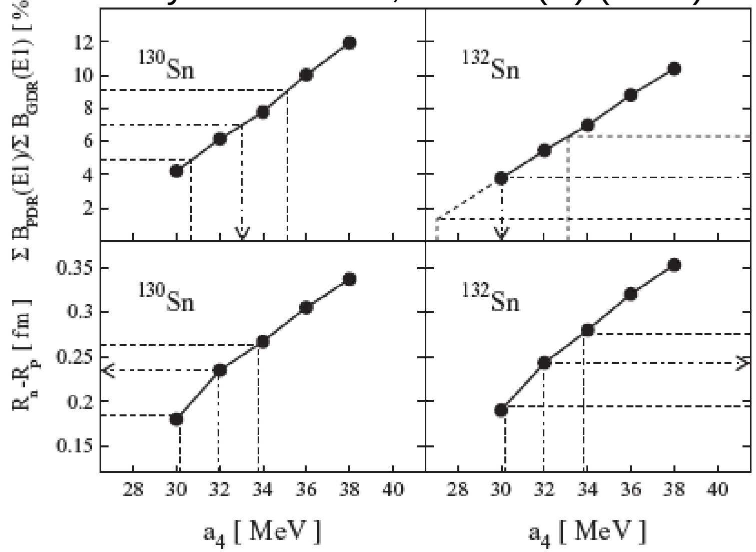
Furnstahl, Nucl. Phys. A 706, 85 (2002)



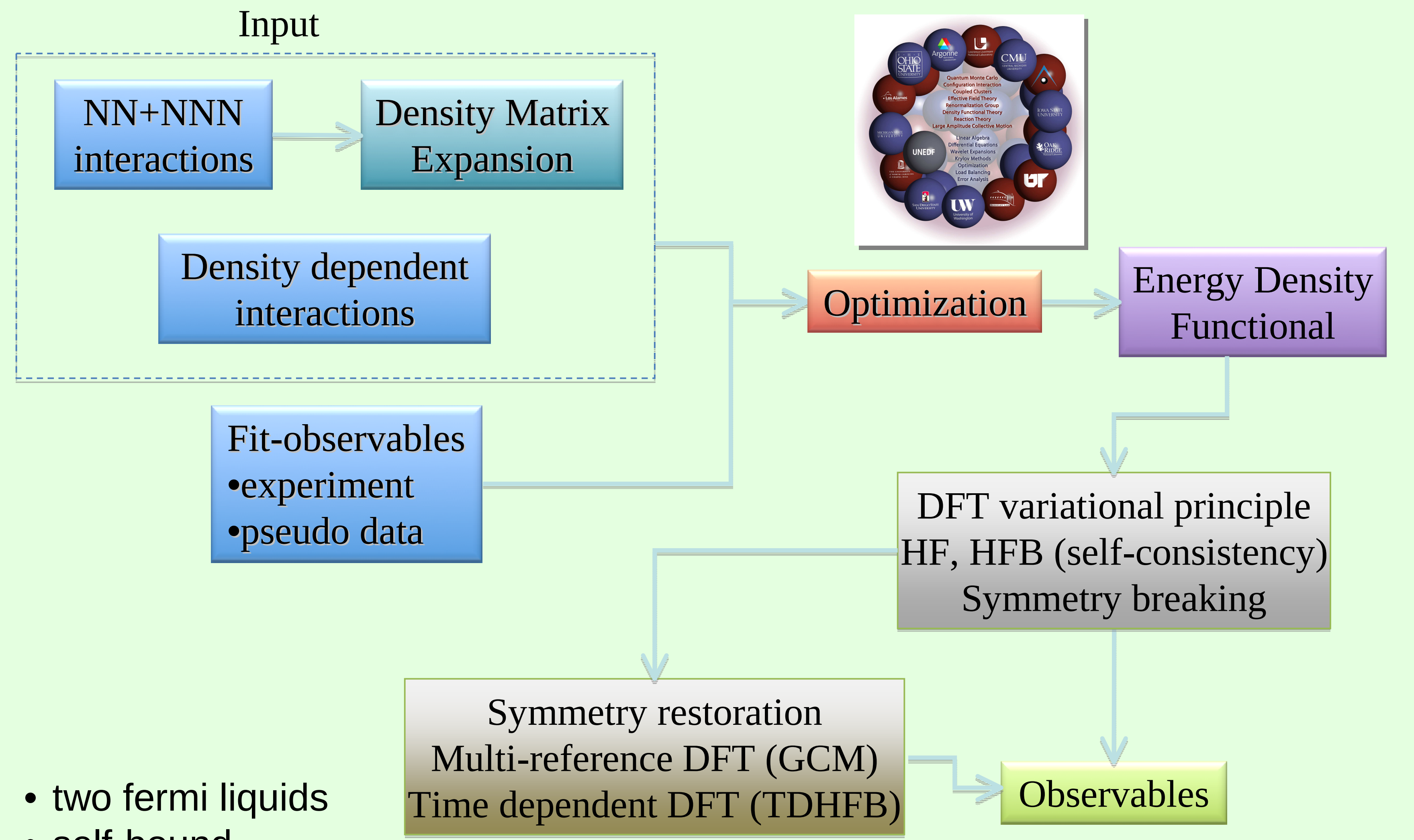
Yoshida and Sagawa, Phys. Rev. C 69, 024318 (2004)



Klimkiewicz et al., Phys. Rev. C 76, 051603(R) (2007)



Nuclear Density Functional Theory and Extensions



- two fermi liquids
- self-bound
- superfluid (ph and pp channels)
- self-consistent mean-fields
- broken-symmetry generalized product states

- Direct comparison with experiment
- Pseudo-data for reactions and astrophysics

The model used: DFT (EDF + fitting protocol)

The fit-observables embrace nuclear bulk properties (binding energies, surface thicknesses, charge radii, spin-orbit splittings, and pairing gaps) for selected semi-magic nuclei which are proven to allow a reasonable DFT description.

SV-min Skyrme functional

P. Klüpfel et al, Phys. Rev. C79, 034310 (2009)

force	K	m^*/m	a_{sym}	a'_{sym}	κ	ρ_{eq}	E/A
SV-min	222	0.95	30.7	93	0.08	0.1610	-15.91
$\pm$	8	0.15	1.4	89	0.40	0.0013	0.06

RMF-δ-t RMF functional

Includes isoscalar scalar, vector, isovector vector, tensor couplings of vector fields, isovector scalar field with mass 980 MeV, and the Coulomb field; the density dependence is modeled only by non-linear couplings of the scalar field. Since the resulting NMP of this model (K=197MeV, a_{sym}=38MeV, m*/m=0.59) strongly deviate from the accepted values, we use this model only to discuss the robustness of our certain predictions and to illustrate the model dependence of the statistical analysis.

Quantities of interest…

bulk equilibrium symmetry energy

$$a_{\rm sym} = \frac{\partial^2}{\partial I^2}\frac{E}{A}\Big|_{\rho=\rho_{\rm eq.}}, \qquad I = \frac{\rho_n - \rho_p}{\rho_n + \rho_p}$$

symmetry energy at surface density

$$a_{\rm sym}(\rm surface) = a_{\rm sym} - 0.08\frac{\partial}{\partial\rho}a_{\rm sym}$$

slope of binding energy of neutron matter

$$\frac{\partial}{\partial\rho}\frac{E_{\rm neut}}{A}\Big|_{\rho=0.1{\rm fm}^{-3}}$$

dipole polarizability

$$\alpha_D = 2\sum_{n\in{\rm RPA}}\frac{1}{E_n}|\langle\Phi_n|\hat{D}|\Phi_0\rangle|^2$$

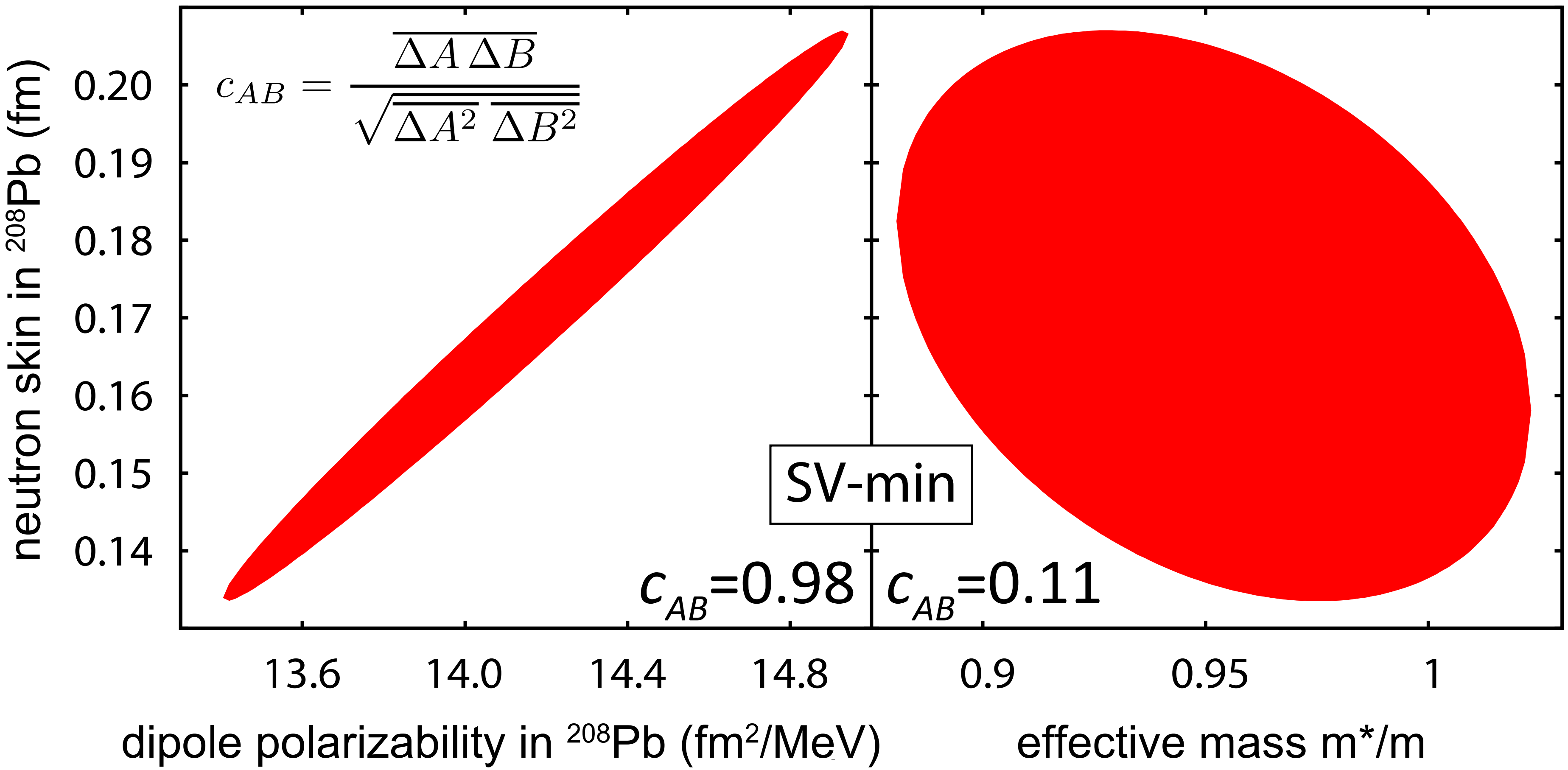
low-energy dipole strength

$$B(E1,{\rm PDR}) = \sum_{n,E_n<E_{\rm max}} B(E1,n)$$

neutron skin

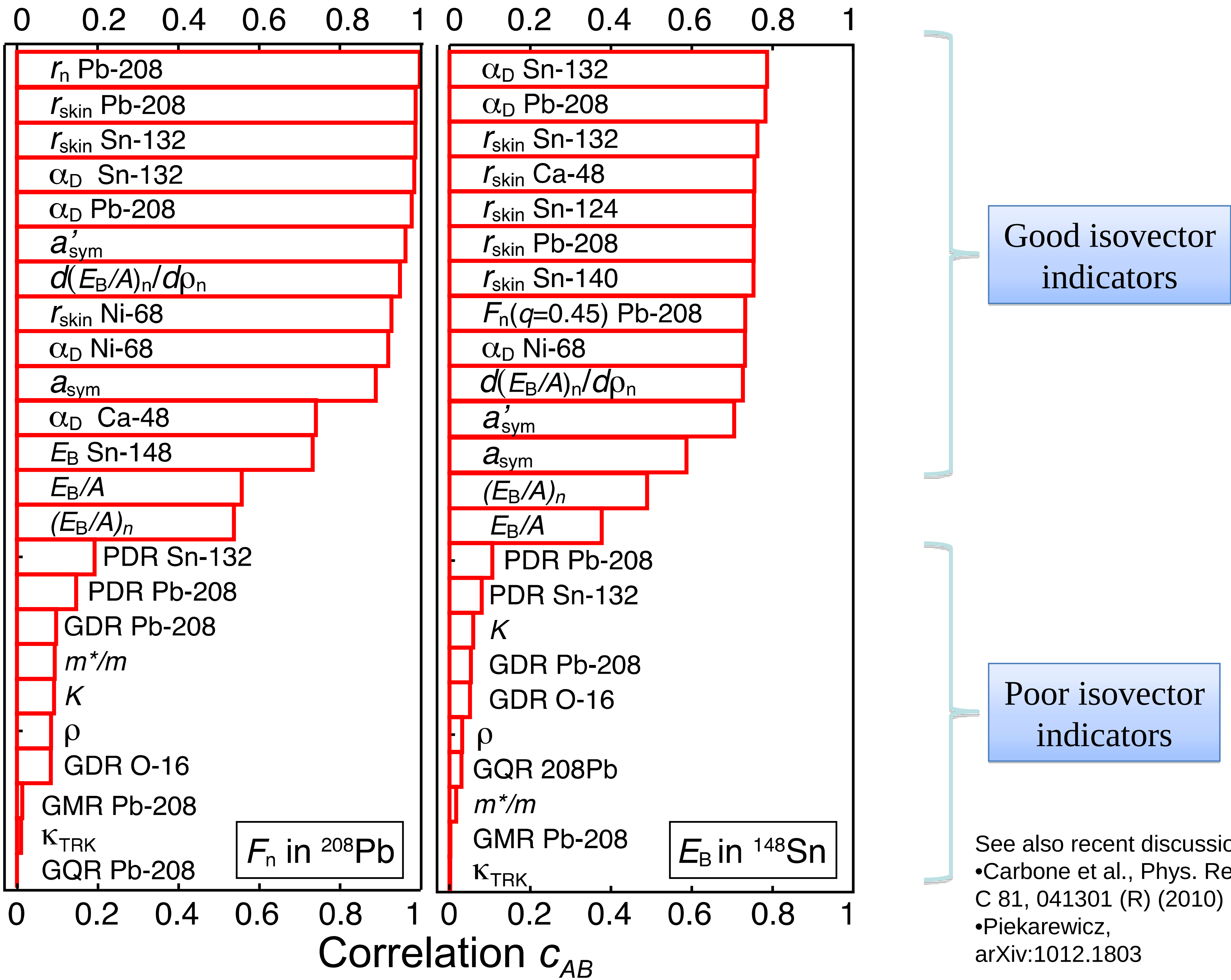
$$r_{\rm skin} = r_n^{\rm rms} - r_p^{\rm rms}$$

An example…



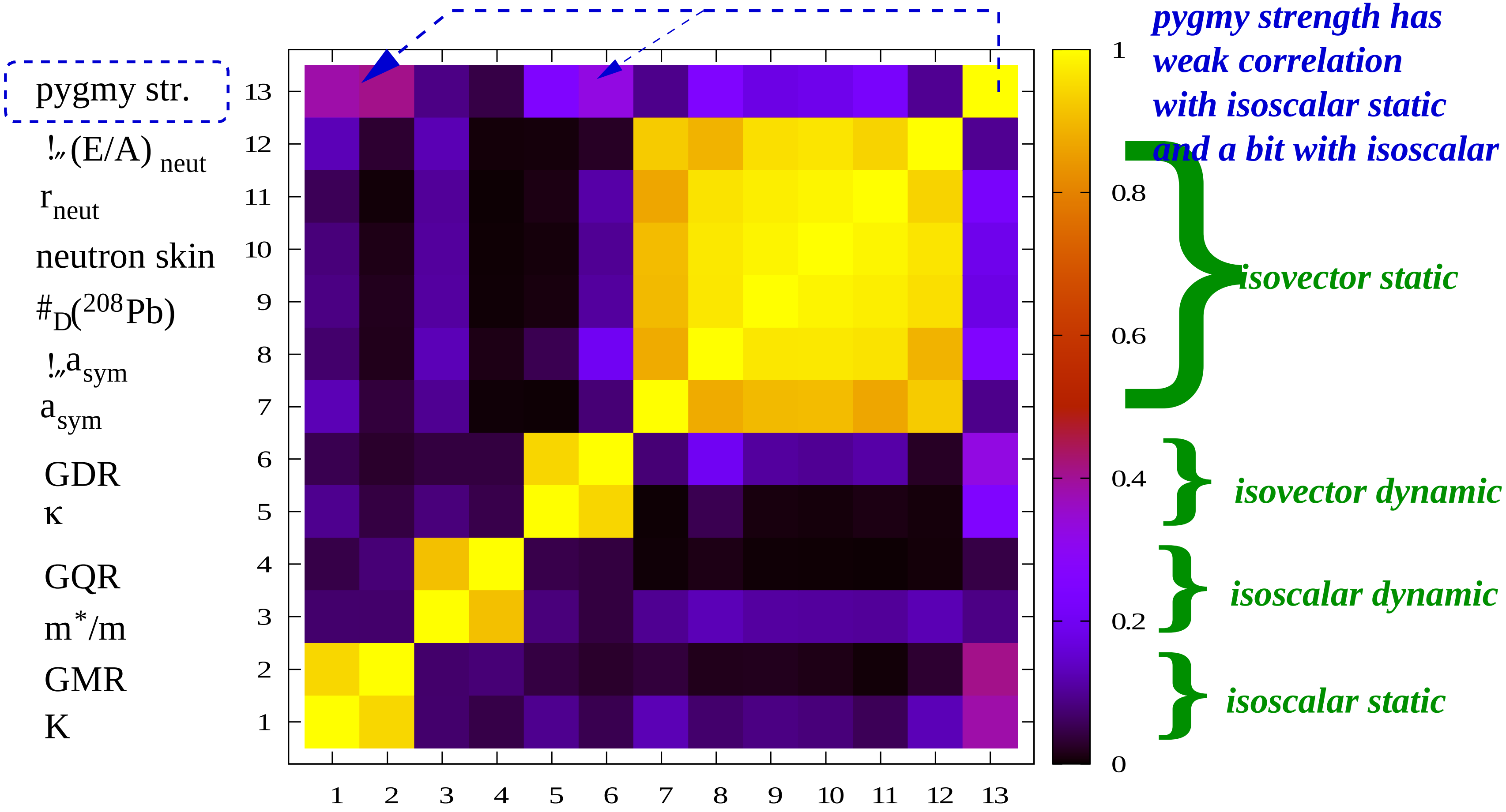
$\alpha_D(\mathrm{exp}) = 13.3 \pm 1.4\,\mathrm{fm}^2/\mathrm{MeV}$ A.Veyssiere et al., Nucl. Phys. A 159, 561 (1970)

$\alpha_D(\mathrm{fit}) \approx 13.6\,\mathrm{fm}^2/\mathrm{MeV}$ E. Lipparini and S. Stringari, Phys. Rep. 175, 103 (1989)



See also recent discussion
•Carbone et al., Phys. Rev. C 81, 041301 (R) (2010)
•Piekarewicz, arXiv:1012.1803

Covariance analysis – matrix of mutual correlations



each giant resonance is uniquely correlated with one nuclear matter property

a_{sym} (isoscalar static) correlated to polarizability

the 4 blocks of basic bulk properties are well separated

UNEDF0 functional optimization

PHYSICAL REVIEW C **82**, 024313 (2010)

Nuclear energy density optimization

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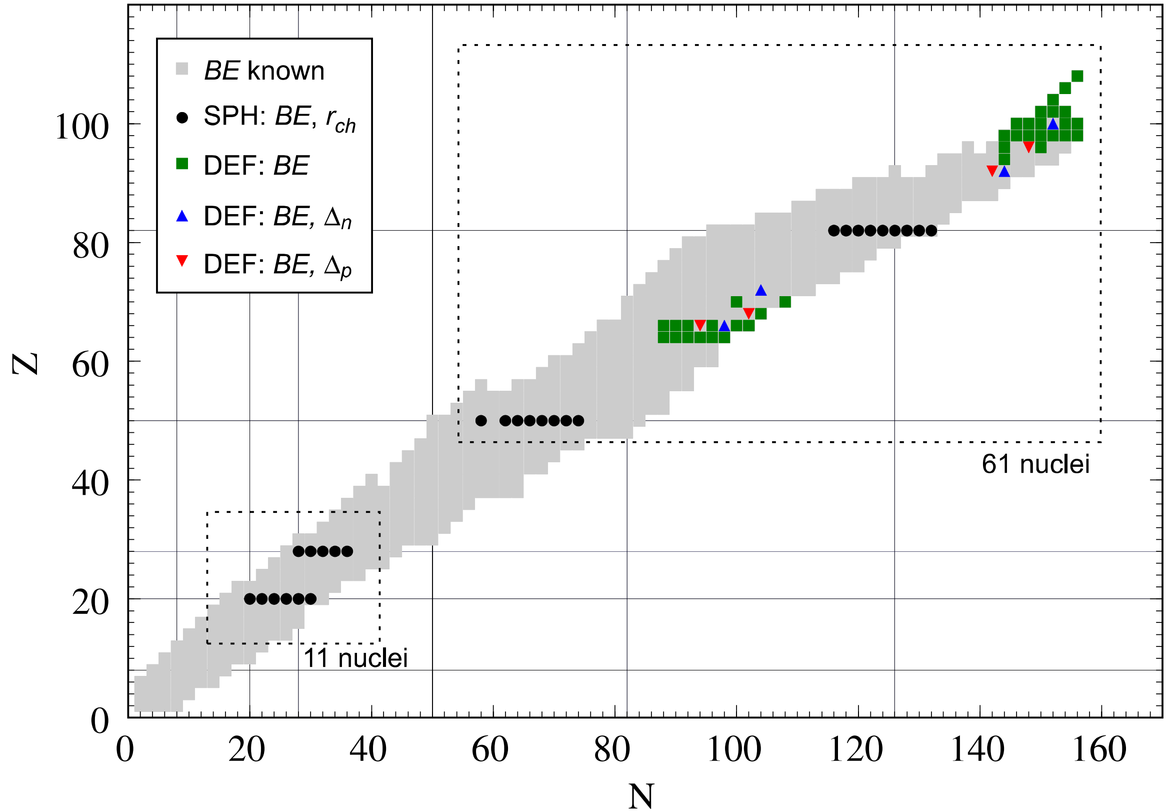
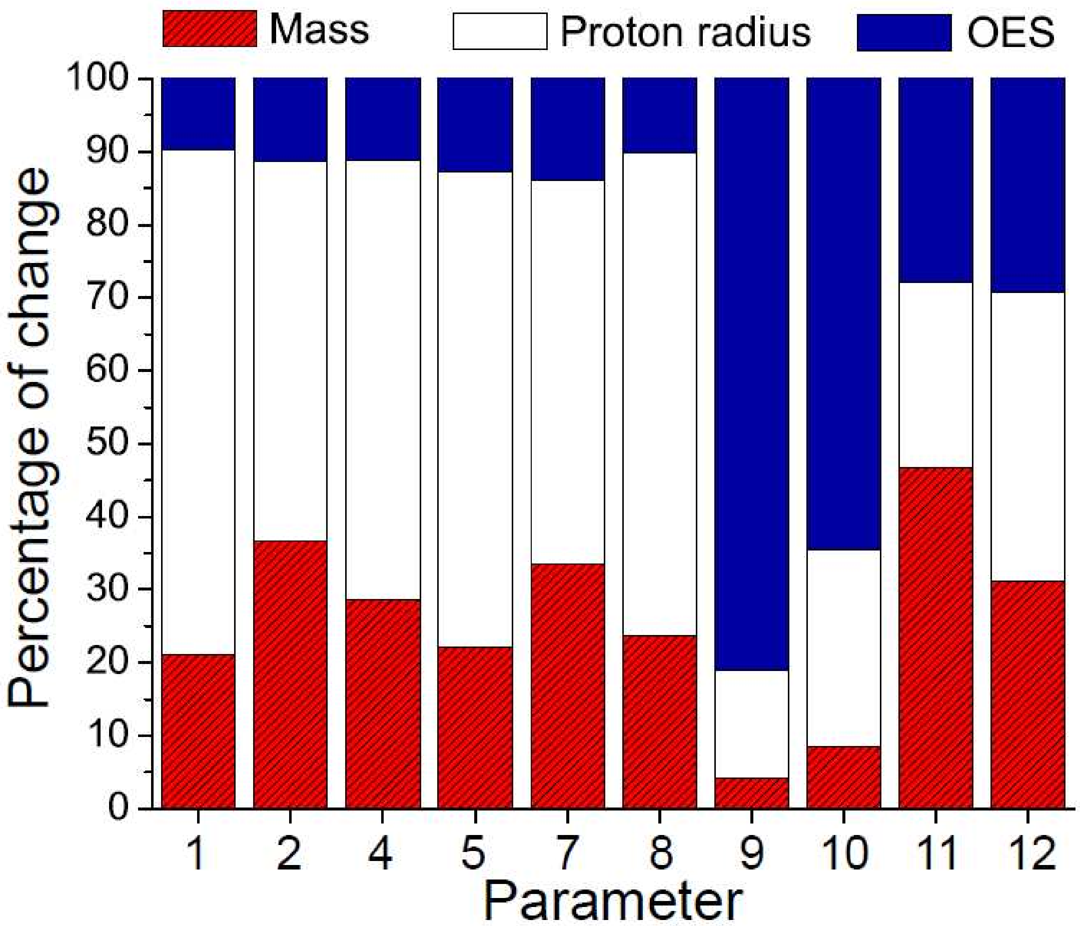
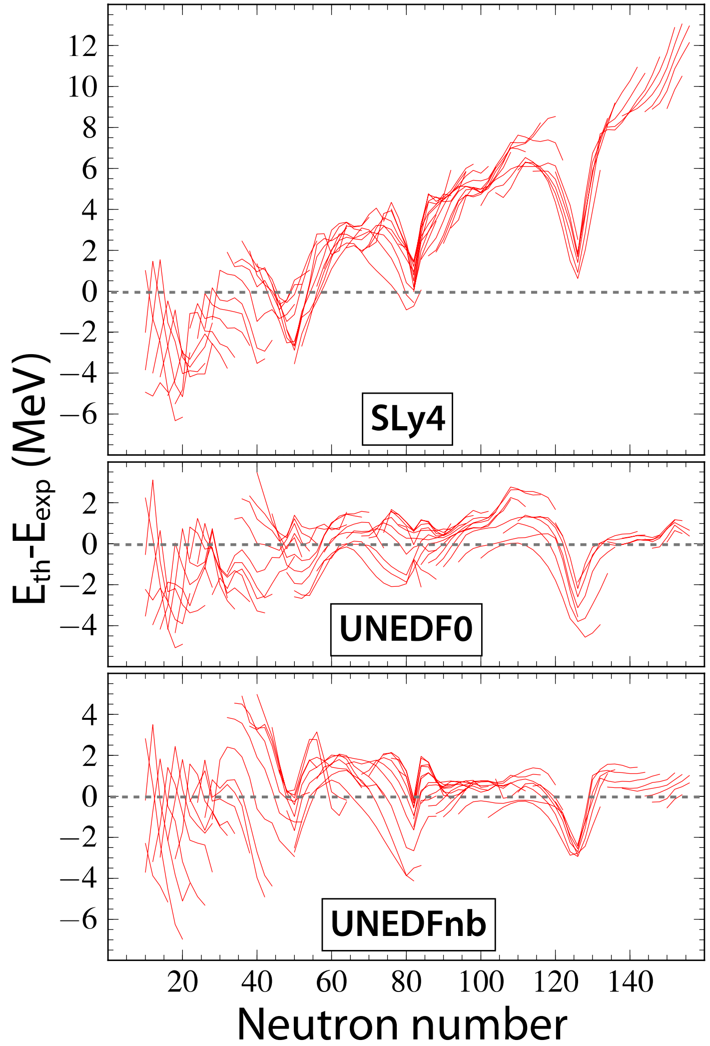


fit-observables

Assessing the impact of parameters on observables





Quality Control

Integral to any scientific project is the verification of methods and codes, the estimation of uncertainties, and assessment.

Verification and Validation

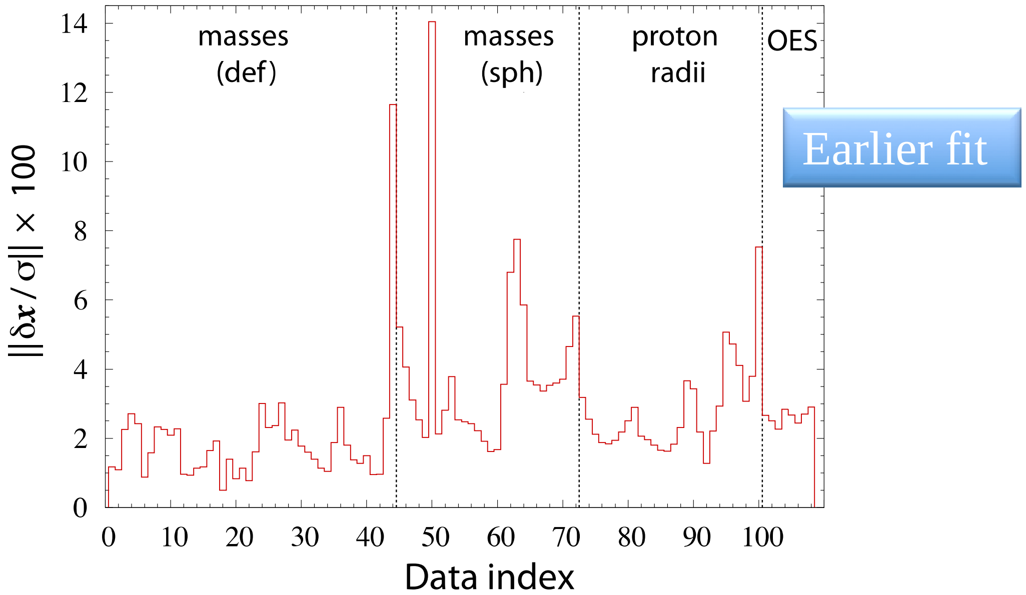
- Cross-check of different methods and codes
- Benchmarking

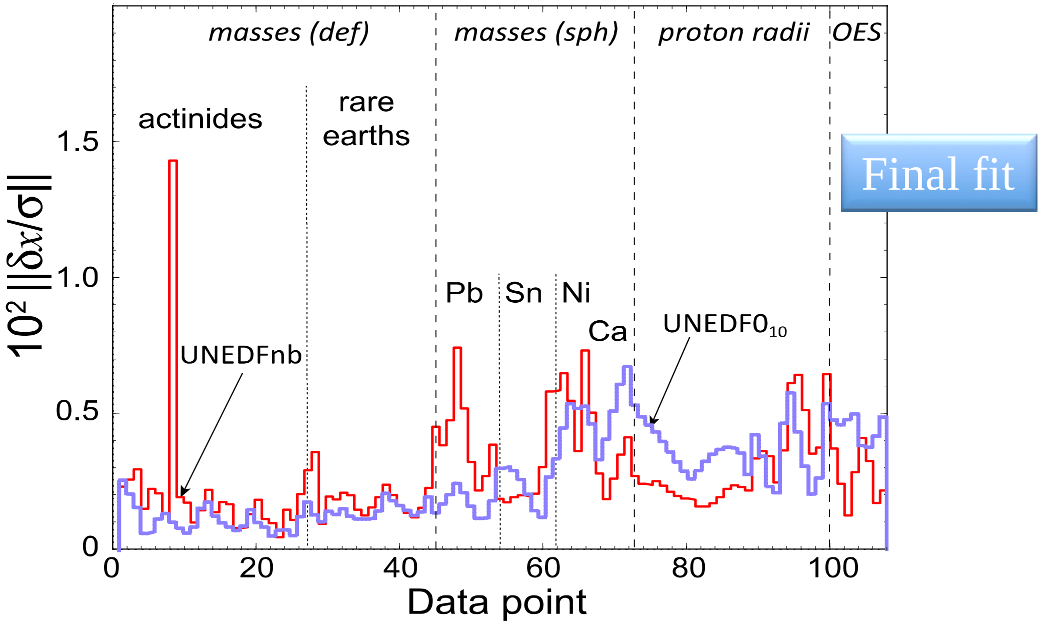
Uncertainty Quantification and Error Analysis

- Tools for correlation analysis to estimate errors and significance
- Uncertainty analysis

Assessment

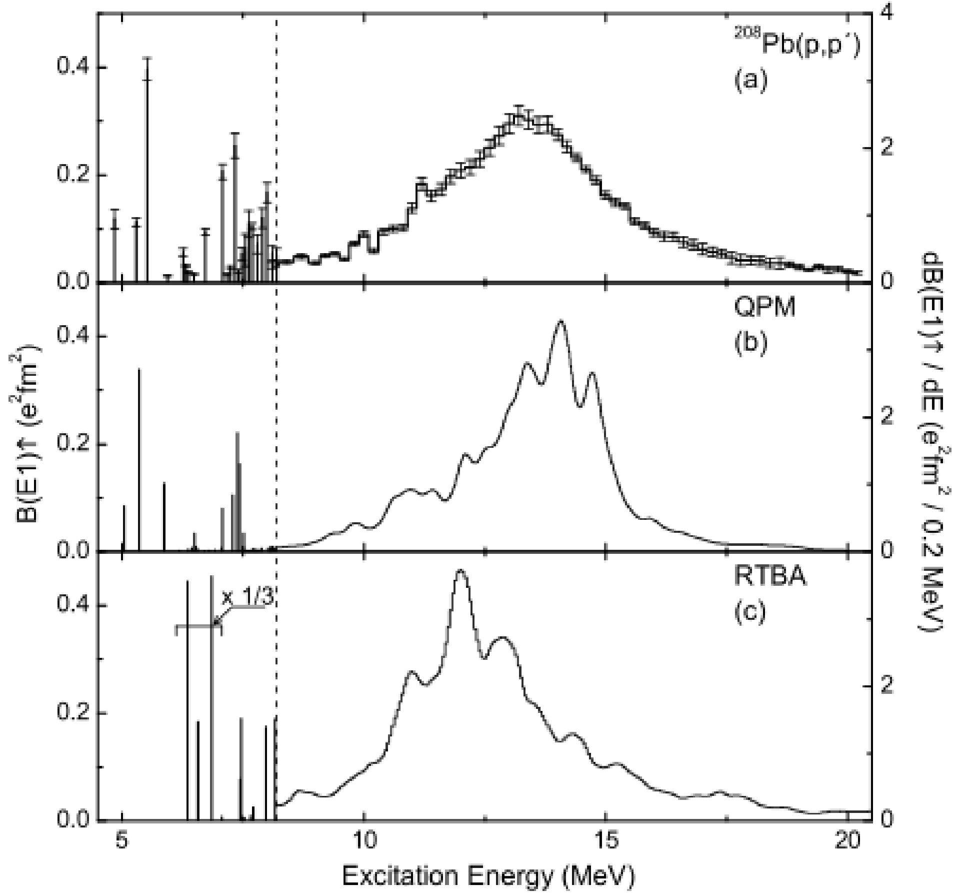
- Development and application of statistical tools
- Analysis of experimental data significance

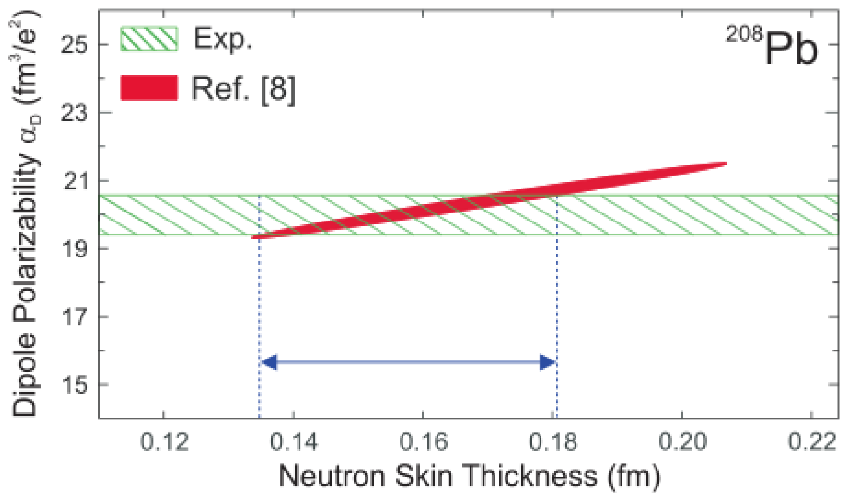




Neutron skins

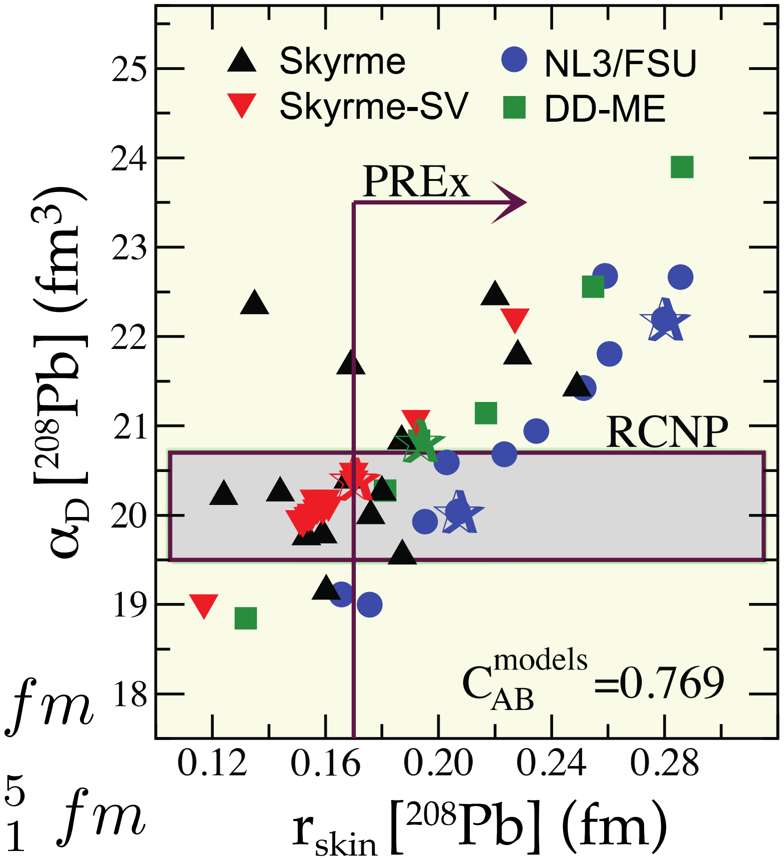
Tamii et al., Complete electric dipole response and the neutron skin in ^{208}Pb, Phys. Rev. Lett. 107, 062502 (2011)

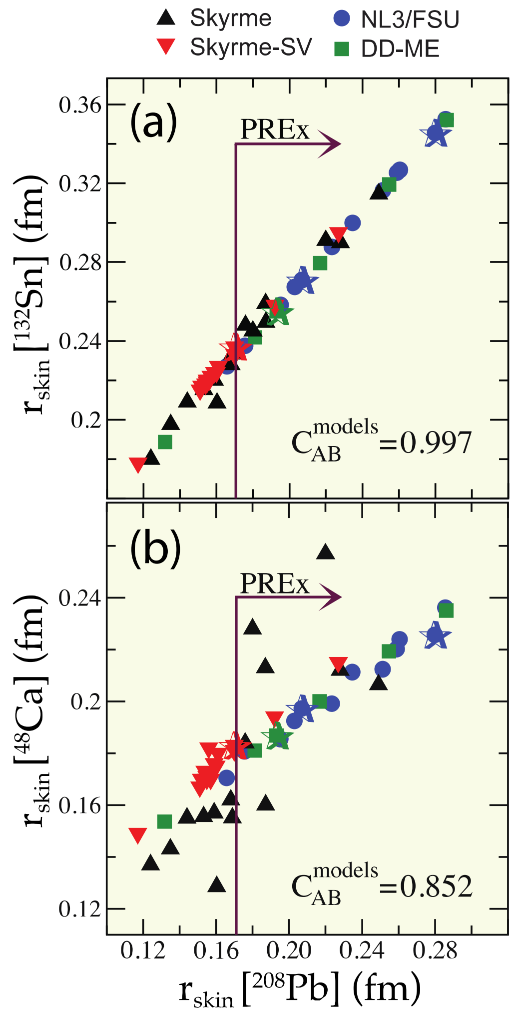




Piekarewicz et al., to be submitted

	$\alpha_D[^{208}\text{Pb}]$			$r_{skin}[^{132}\text{Sn}]$			$r_{skin}[^{48}\text{Ca}]$		
Model	C_{AB}^{model}	Slope	Intercept	C_{AB}^{model}	Slope	Intercept	C_{AB}^{model}	Slope	Intercept
Skyrme	0.9959	29.0847	15.5290	0.9992	1.0568	0.0555	0.9768	0.5989	0.0798
DD-ME	0.9939	31.9907	14.5206	1.0000	1.0575	0.0500	0.9997	0.5272	0.0849
NL3/FSU	0.9941	29.8864	13.9692	0.9999	1.0429	0.0547	0.9868	0.5028	0.0897





PREX: $0.34^{+0.15}_{-0.17}\ fm$

Tamii: $0.156^{+0.025}_{-0.021}\ fm$

Theory: $0.168 \pm 0.022\ fm$

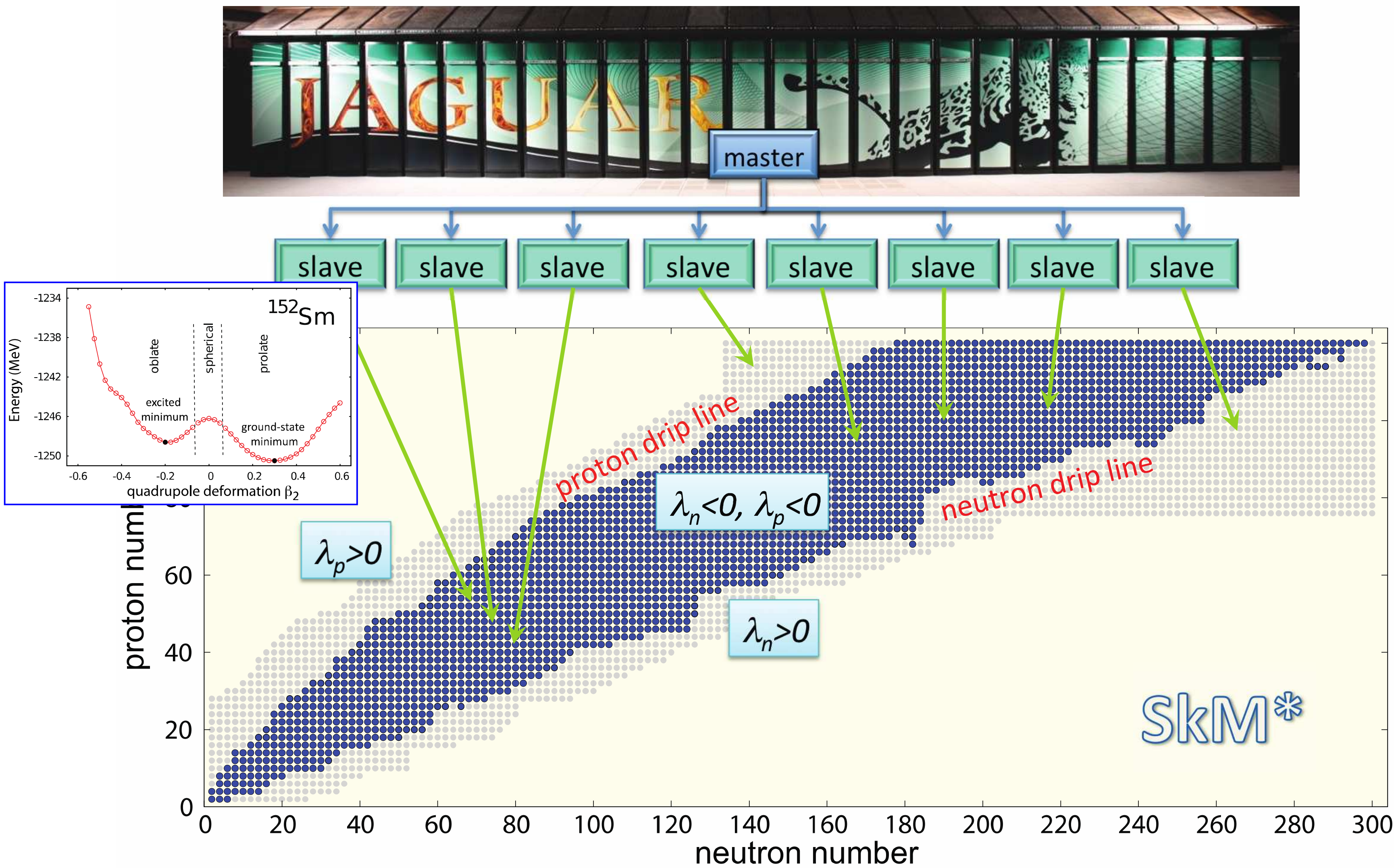
Assessing impact of new measurements

We also carried out calculations with a new EDF obtained by a new fit where the neutron-rich nuclei have been given more weight (a factor 2 to 3 for the three outermost neutron-rich isotopes in most chains). The purpose of this exercise is to simulate the expected increased amount of data on neutron-rich nuclei.

While the correlations seem to change very little, the extrapolation uncertainties in neutron observables shrink by a factor of 1.5–2.0. For instance, with this new functional, the predicted neutron skin in ^{208}Pb is 0.191(0.024) fm, as compared to the SV-min value of 0.170(0.037) fm. This exercise demonstrates that detailed conclusions of the statistical analysis depend on a chosen model and a selected set of fit observables.

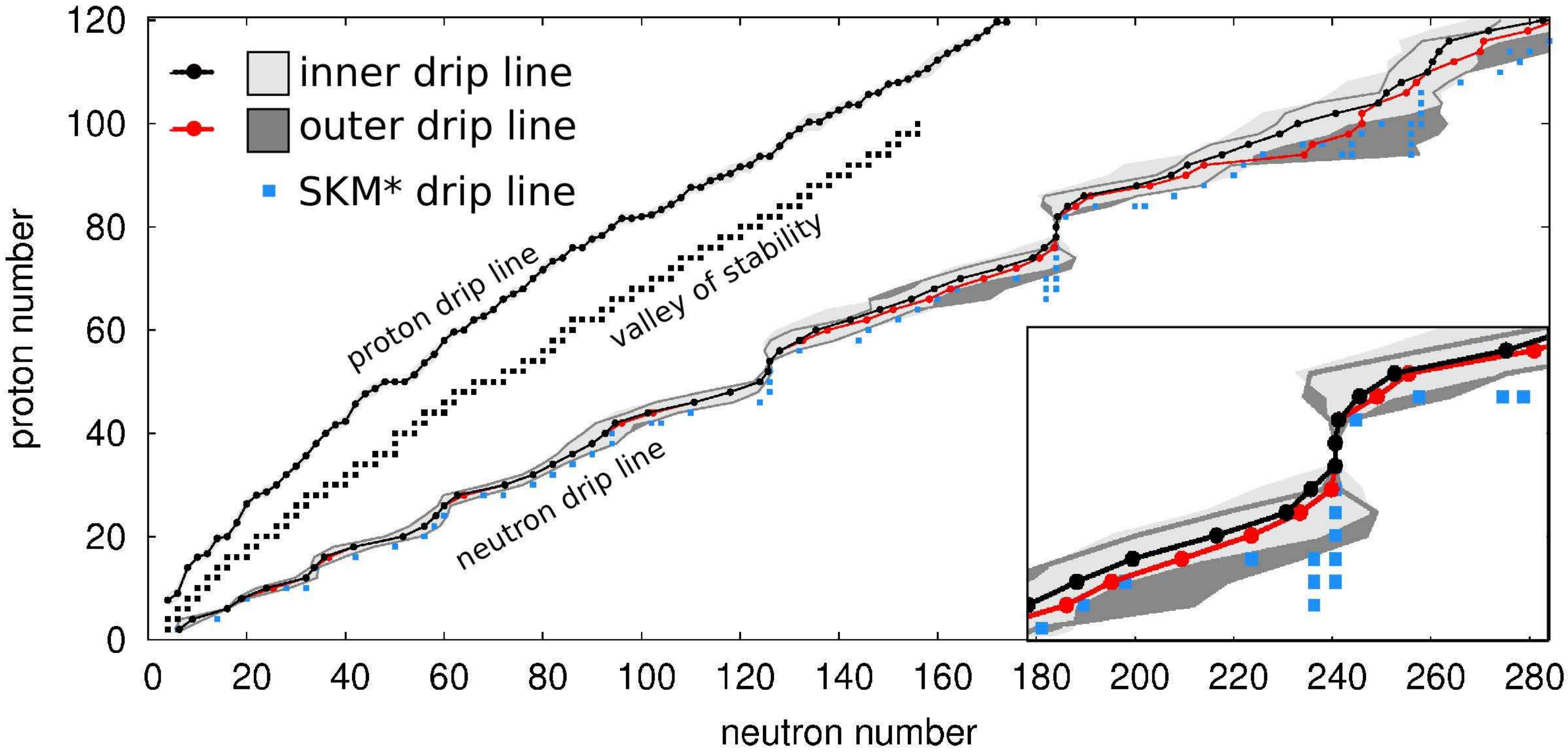
Example: Large Scale Mass Table Calculations

HFB+LN mass table, HFBTHO

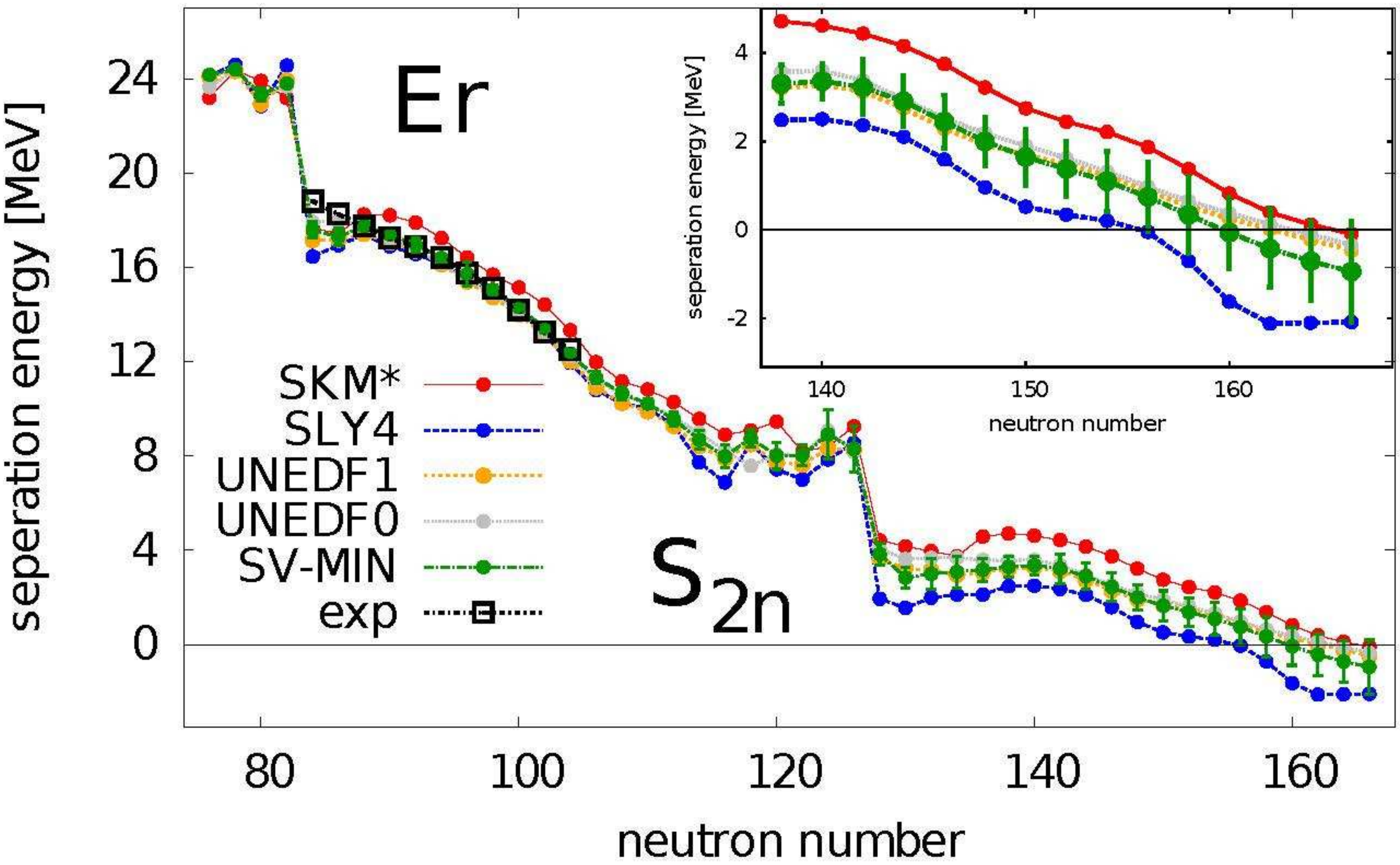


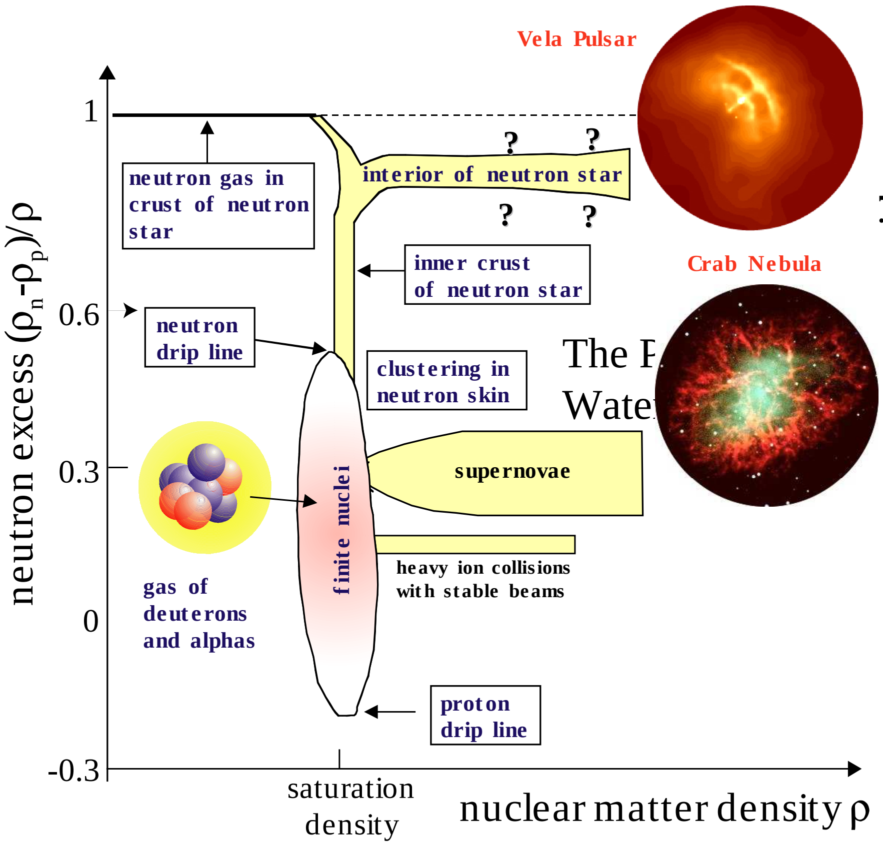
- ➲ 5,000 even-even nuclei, 250,000 HFB runs, 9,060 processors – about 2 CPU hours
- ➲ Full mass table: 20,000 nuclei, 12M configurations — full JAGUAR

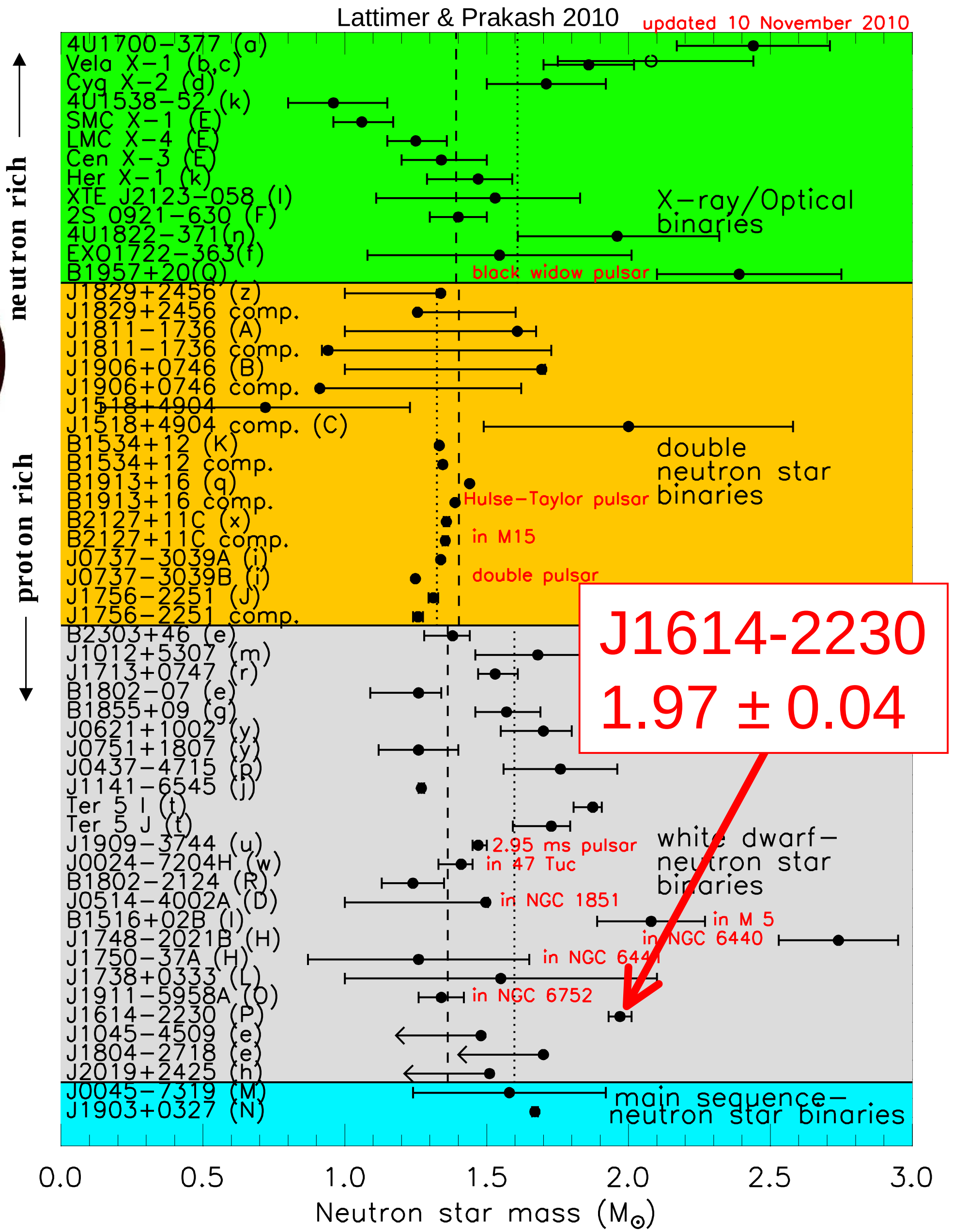
J. Erler et al., in preparation



J. Erler et al., in preparation

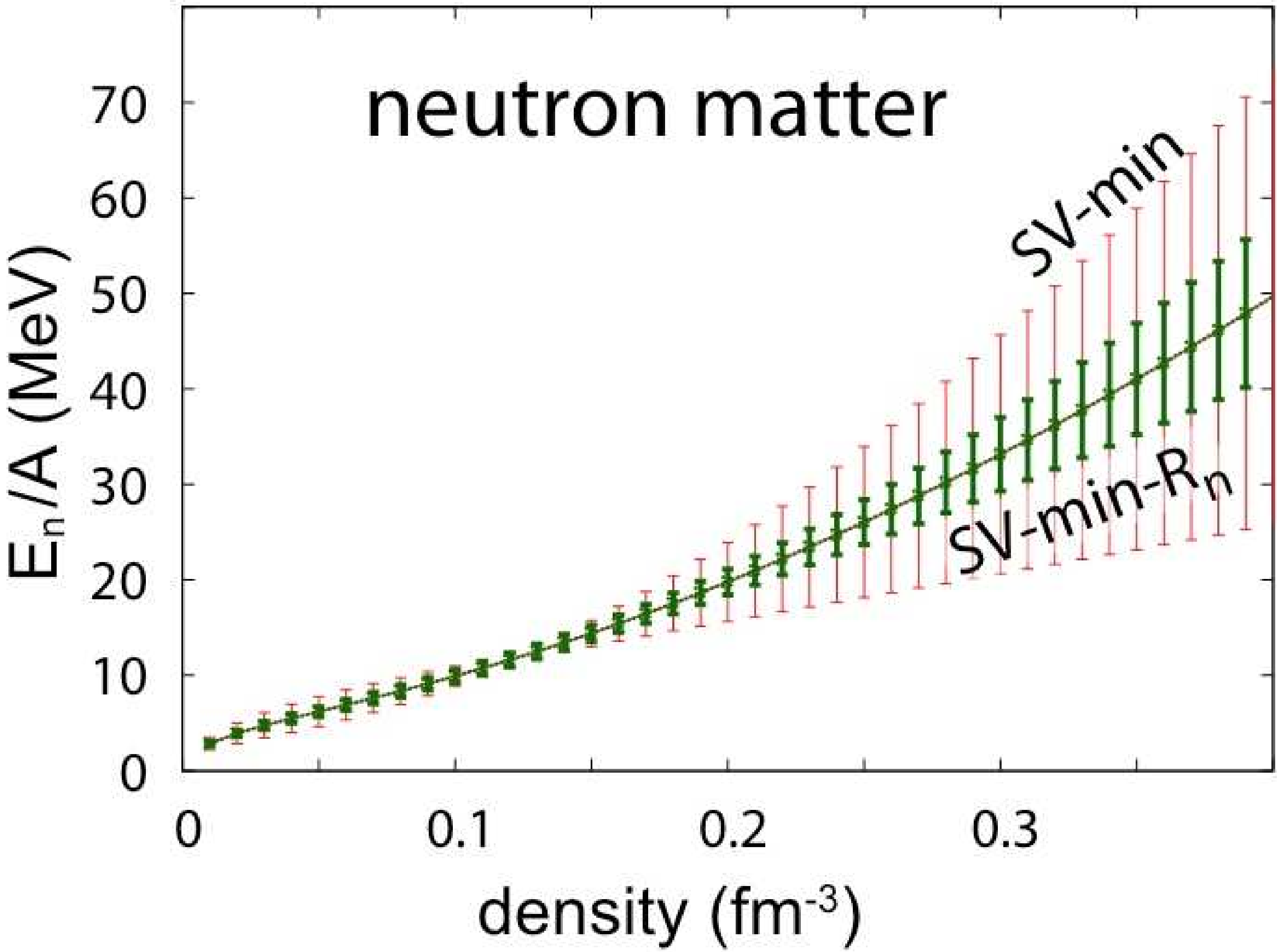


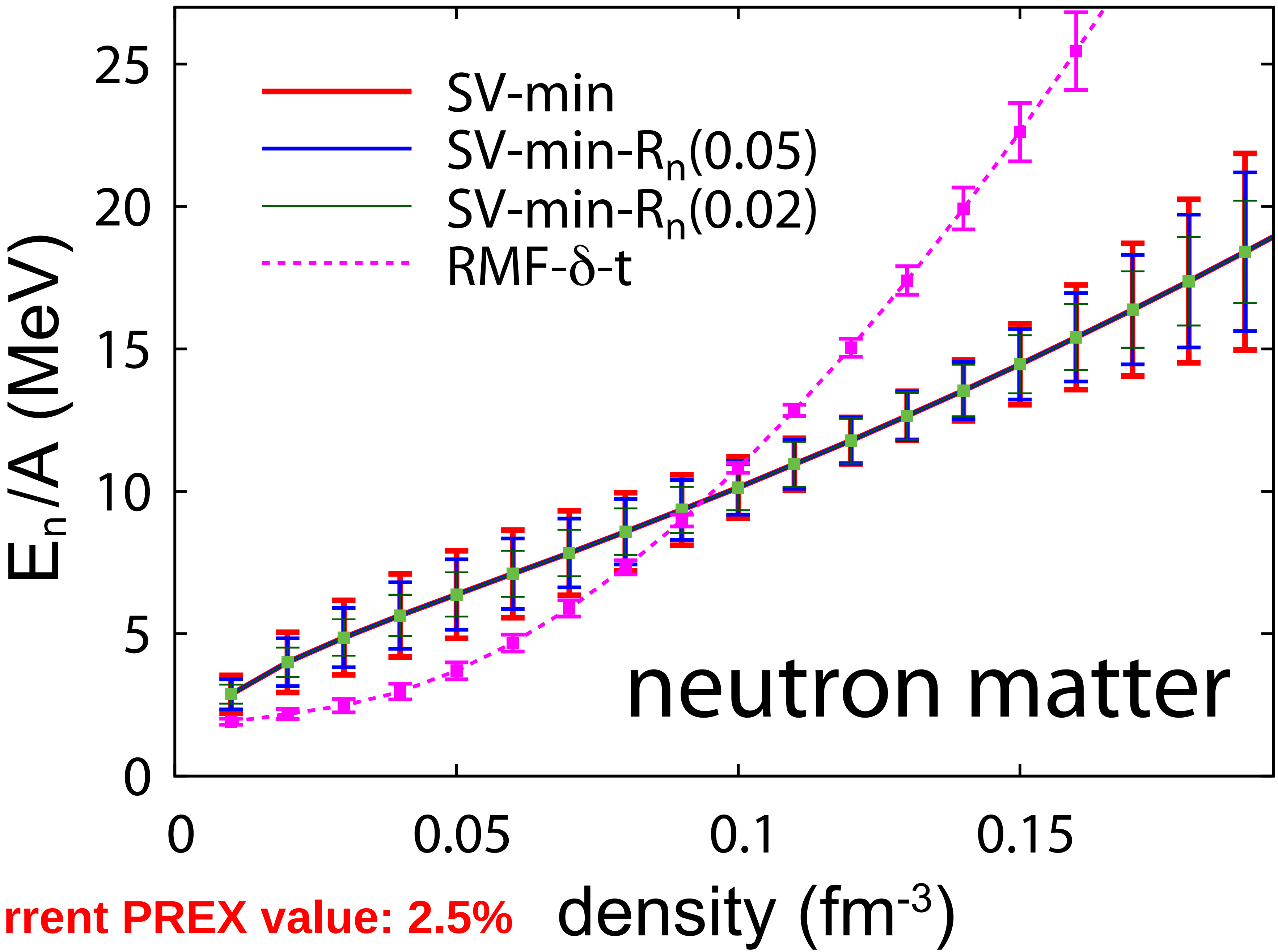




EOS for the nucleonic matter of such a heavy neutron star indicate that the density at its center must be roughly five times that of ordinary nuclei.

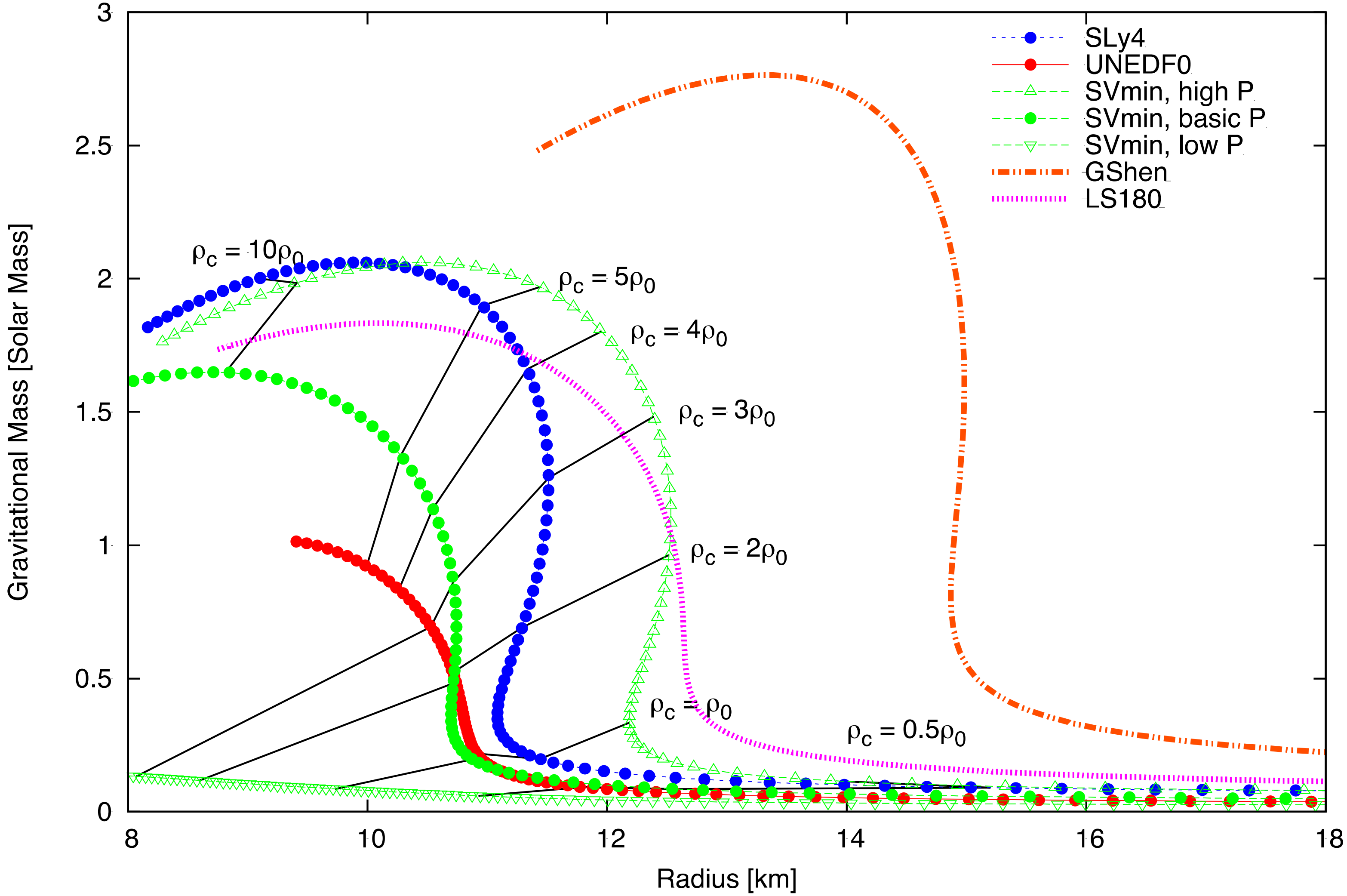
To estimate the impact of precise experimental determination of neutron skin, we generated a new functional SV-min-R_n by adding the value of neutron radius in 208Pb, r_n=5.61 fm, with an adopted error 0.02 fm, to the set of fit observables. With this new functional, calculated uncertainties on isovector indicators shrink by about a factor of two.





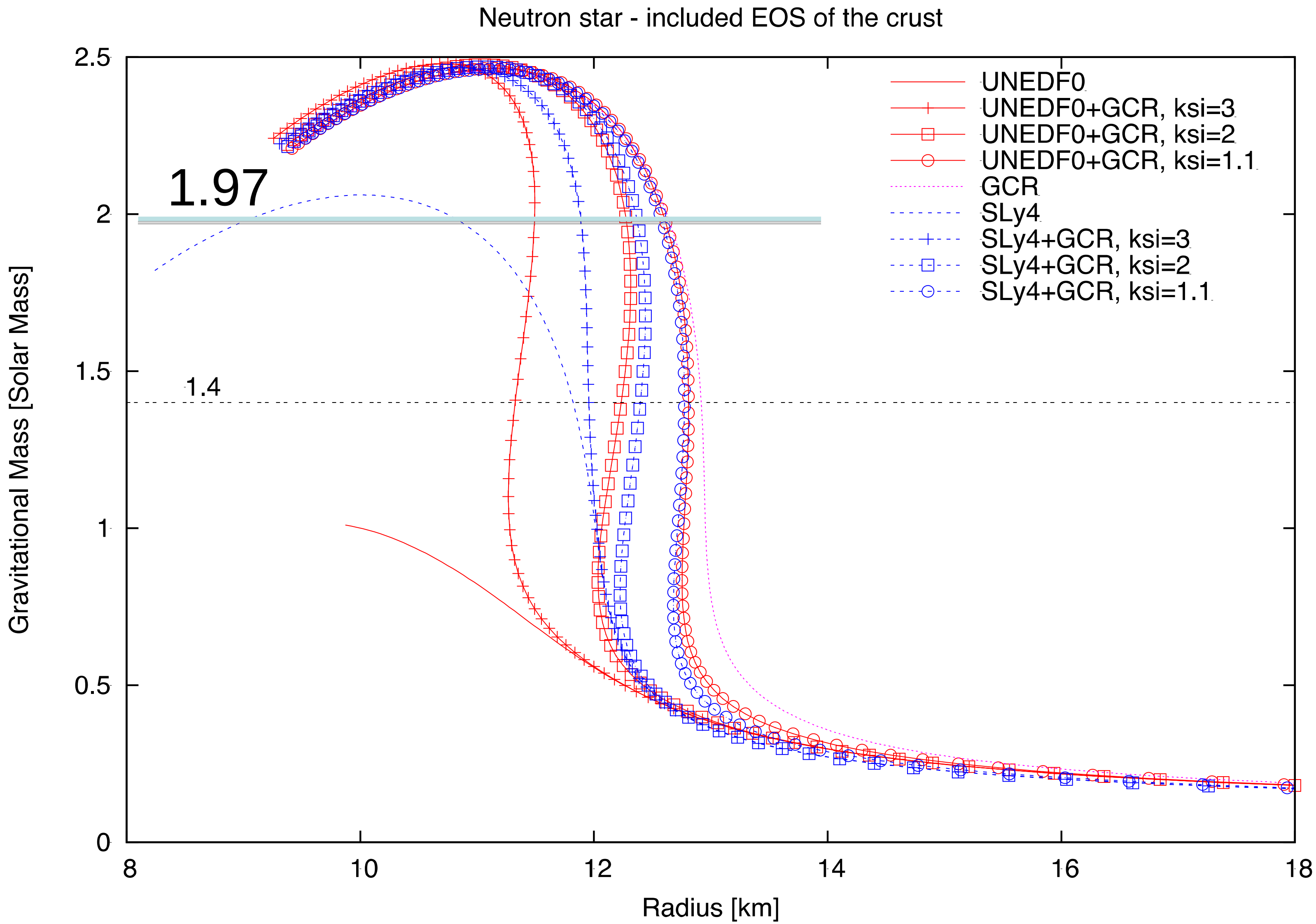
Current PREX value: 2.5%

Rafalski, Erlel, Horowitz, WN, in preparation



Tolman–Oppenheimer–Volkoff (TOV) equation:

$$\frac{dP(r)}{dr} = -\frac{G}{r^2}\left[\rho(r) + \frac{P(r)}{c^2}\right]\left[M(r) + 4\pi r^3 \frac{P(r)}{c^2}\right]\left[1 - \frac{2GM(r)}{c^2 r}\right]^{-1}$$



Neutron star - included EOS of the crust
Gravitational Mass [Solar Mass]
Radius [km]
1.97
1.4
UNEDF0
UNEDF0+GCR, ksi=3
UNEDF0+GCR, ksi=2
UNEDF0+GCR, ksi=1.1
GCR
SLy4
SLy4+GCR, ksi=3
SLy4+GCR, ksi=2
SLy4+GCR, ksi=1.1
0
0.5
1
1.5
2
2.5
8
10
12
14
16
18

PHYSICAL REVIEW A 83, 040001 (2011): Editorial: Uncertainty Estimates

The purpose of this Editorial is to discuss the importance of including uncertainty estimates in papers involving theoretical calculations of physical quantities.

It is not unusual for manuscripts on theoretical work to be submitted without uncertainty estimates for numerical results. In contrast, papers presenting the results of laboratory measurements would usually not be considered acceptable for publication in Physical Review A without a detailed discussion of the uncertainties involved in the measurements. For example, a graphical presentation of data is always accompanied by error bars for the data points. The determination of these error bars is often the most difficult part of the measurement. Without them, it is impossible to tell whether or not bumps and irregularities in the data are real physical effects, or artifacts of the measurement. Even papers reporting the observation of entirely new phenomena need to contain enough information to convince the reader that the effect being reported is real. The standards become much more rigorous for papers claiming high accuracy.

The question is to what extent can the same high standards be applied to papers reporting the results of theoretical calculations. It is all too often the case that the numerical results are presented without uncertainty estimates. Authors sometimes say that it is difficult to arrive at error estimates. Should this be considered an adequate reason for omitting them? In order to answer this question, we need to consider the goals and objectives of the theoretical (or computational) work being done.

(…) there is a broad class of papers where estimates of theoretical uncertainties can and should be made. Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances:

1. If the authors claim high accuracy, or improvements on the accuracy of previous work.

2. If the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements.

3. If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

These guidelines have been used on a case-by-case basis for the past two years. Authors have adapted well to this, resulting in papers of greater interest and significance for our readers.

Summary

We propose to use a statistical least-squares analysis to identify the impact of new observables, quantify correlations between predicted observables, and assess uncertainties of theoretical predictions.

Theory must recognize the importance of quantifying the accuracy of predictions. Theory is developing new statistical tools to deliver uncertainty quantification and error analysis for theoretical studies as well as for the assessment of new experimental data. Such technologies are virtually unknown in the low-energy nuclear theory community presently, and are essential as new theories and computational tools are explicitly intended to be applied to entirely new nuclear systems and conditions that *are not accessible to experiment.*