Nuclear charge and neutron radii and nuclear matter: correlation analysis

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INT Program INT-16-2a: Bayesian Methods in Nuclear Physics

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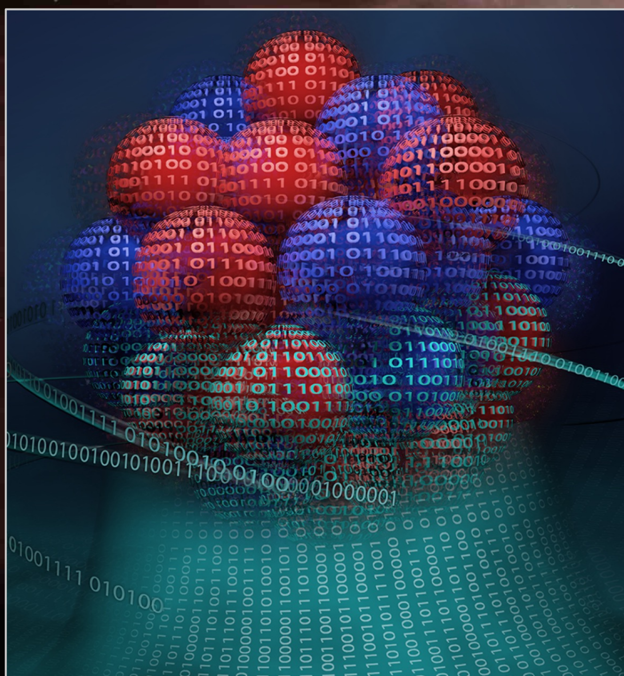


- Perspective
- Correlation analysis and model mixing (intra- and inter-model correlations)
- Proton-, neutron radii, skins, and nuclear matter properties
- Conclusions

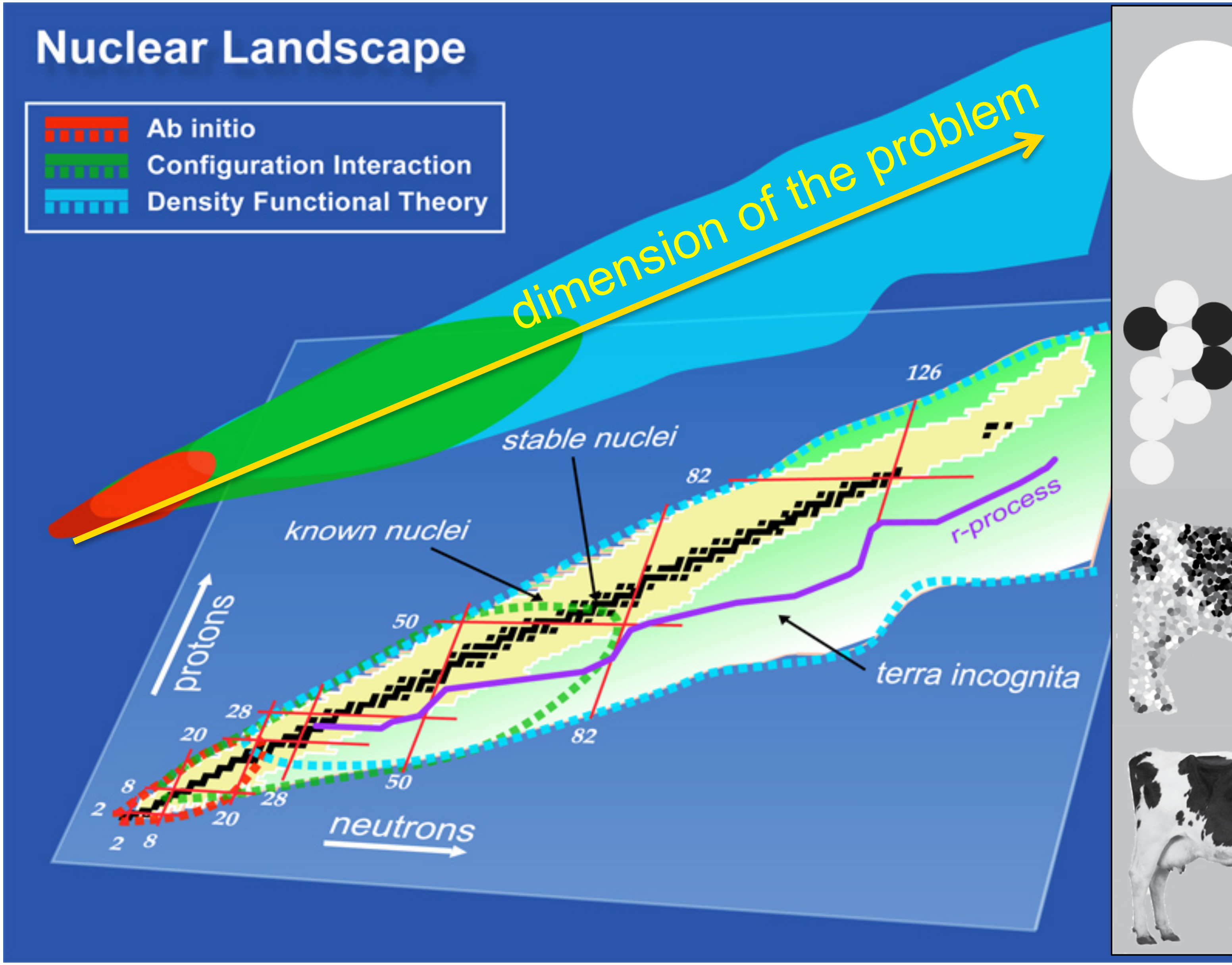
Classification of theories

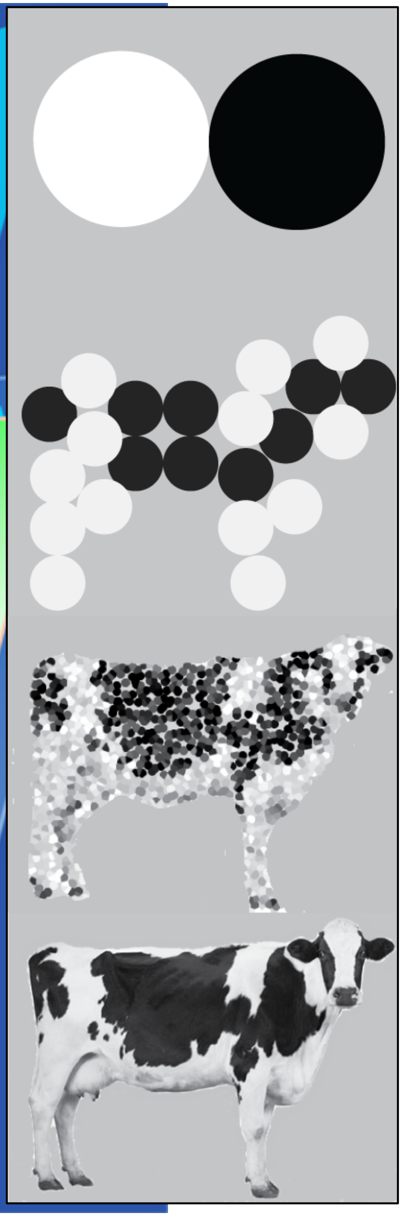
(according to Alexander I. Kitaigorodskii)

- A third rate theory explains after the event (postdictive, retrodictive)
- A second rate theory forbids
- A first rate theory predicts (predictive)

UQ is crucial to make this assessment

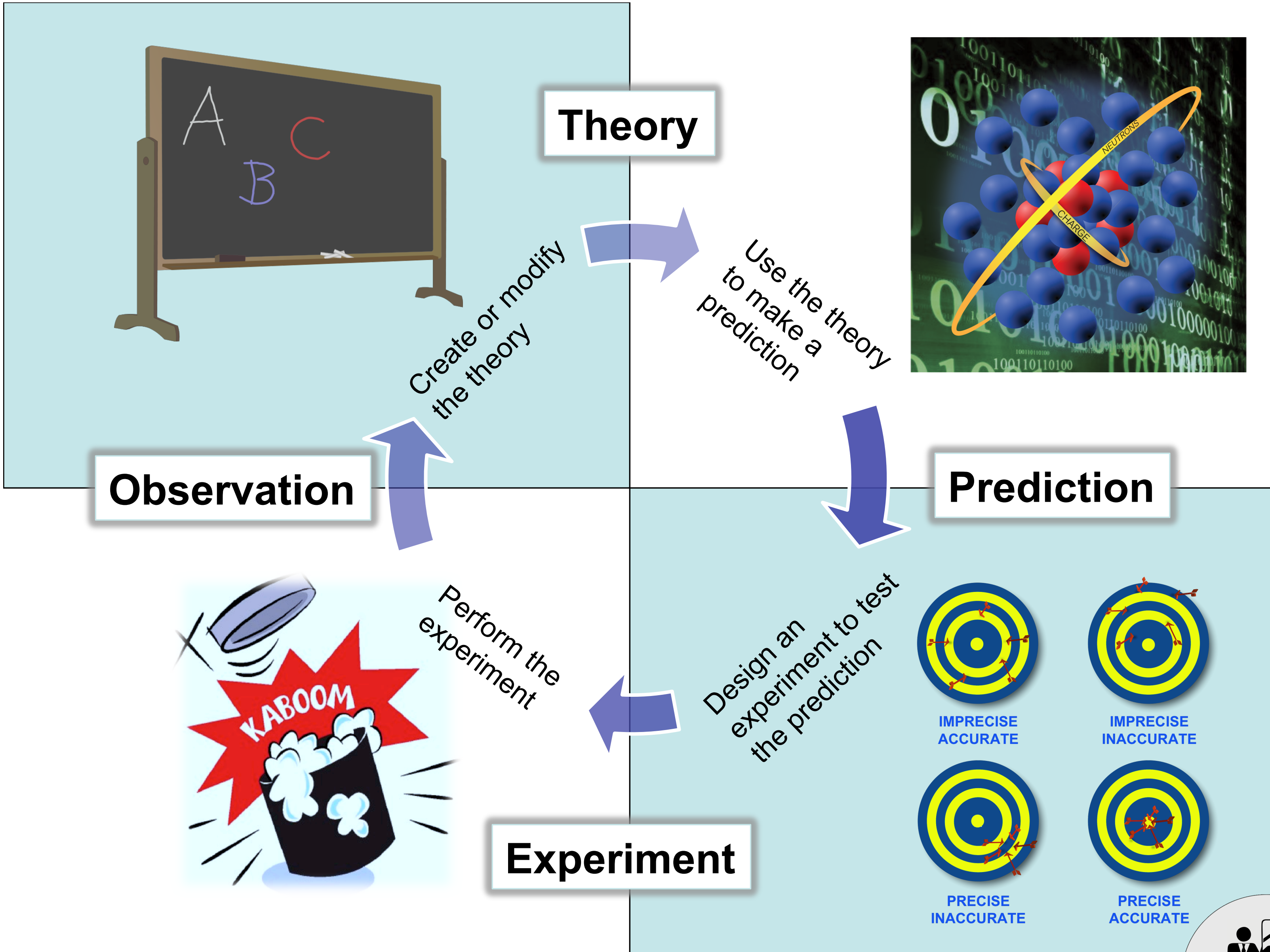
How to explain the nuclear landscape from the bottom up? **Theory roadmap**





The resolving power of a theoretical model should always be as low as reasonably possible for the question at hand

J. Phys. G 43, 044002 (2016)



Today's posterior is tomorrow's prior

Consider a model described by coupling constants $\boldsymbol{\theta}$ ={θ_1, $\theta_{2\ldots}$ θ_κ). Any predicted expectation value of an observable Y_i 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.

$$\chi^2(\boldsymbol{\theta}) = \sum_{i}^{n_y} \left(\frac{Y_i(\boldsymbol{\theta}) - Y_i(\exp)}{\sigma_i} \right)^2$$

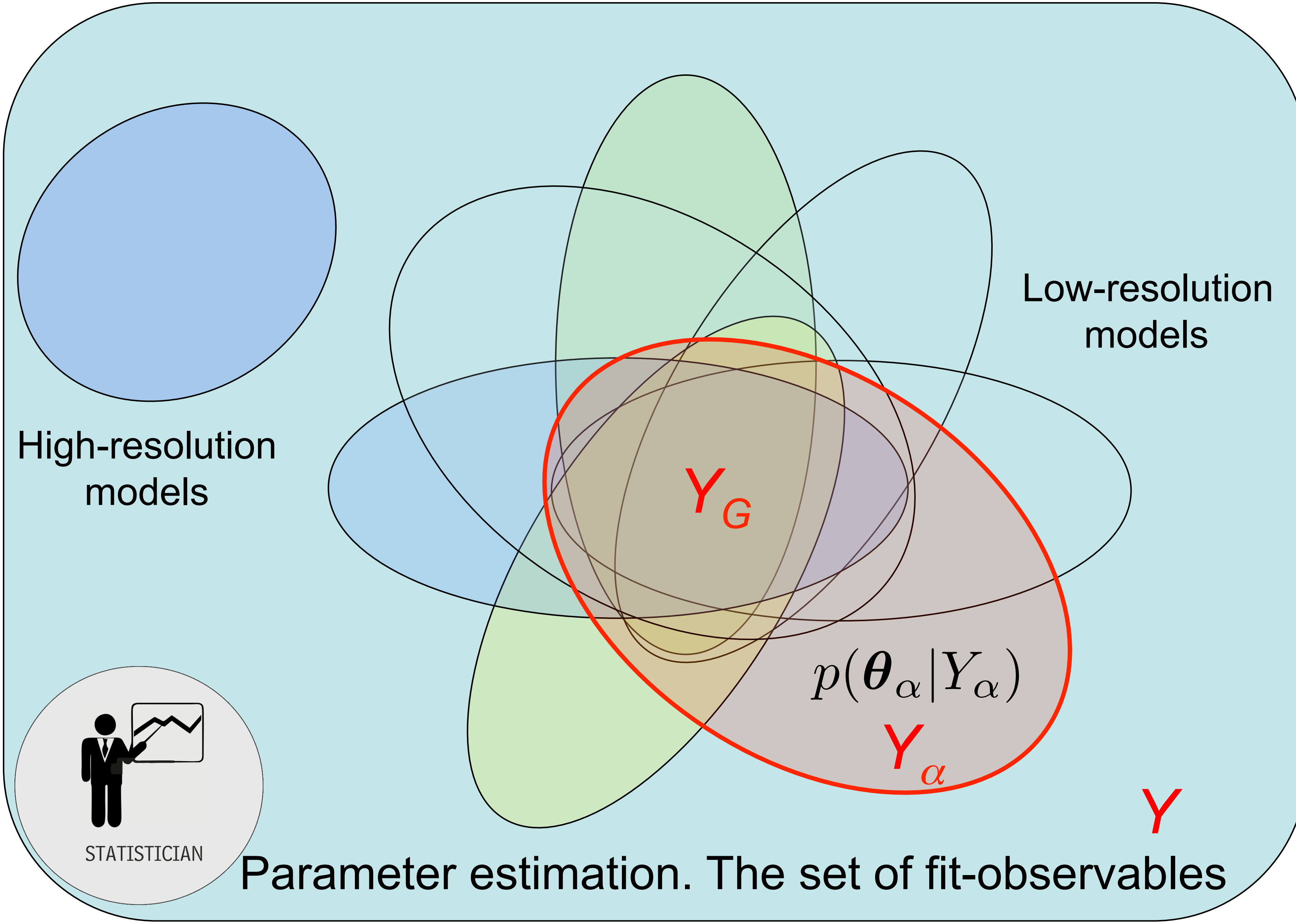
Objective function

Model predictions

Expected uncertainties

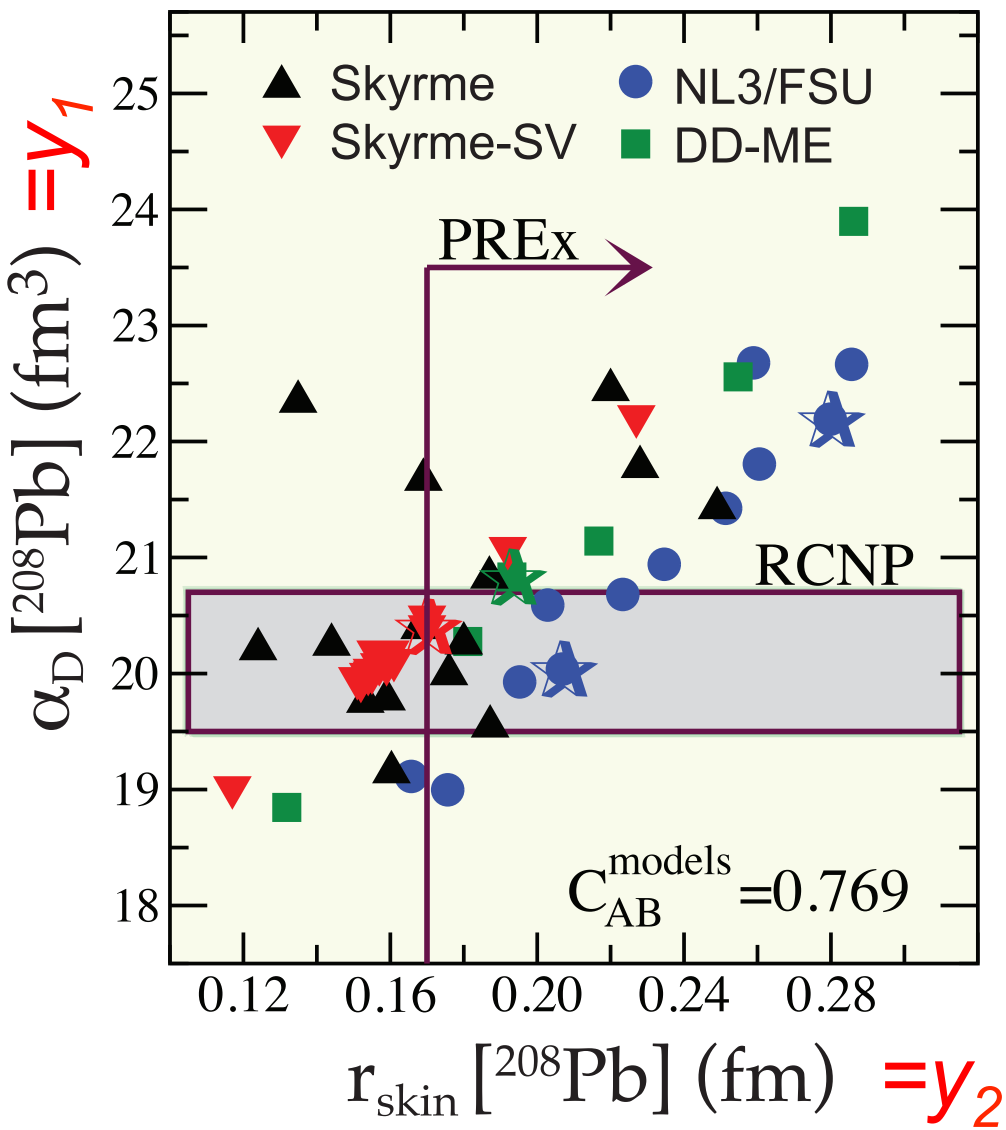
fit-observables
(may include pseudo-data)

How to quantify inter-model correlations?



Example of inter-model correlation analysis

J. Piekarewicz et al., Phys. Rev. C (1) 85, 041302(R) (2012)



	$\alpha_D[^{208}\mathrm{Pb}]$		
Model	C_{AB}^{model}	Slope	Intercept
Skyrme	0.9959	29.0847	15.5290
DD-ME	0.9939	31.9907	14.5206
NL3/FSU	0.9941	29.8864	13.9692

$$\hat{\boldsymbol{\theta}}(M_\alpha) \equiv \boldsymbol{\theta}(M_\alpha)_{\mathrm{MLE}}$$

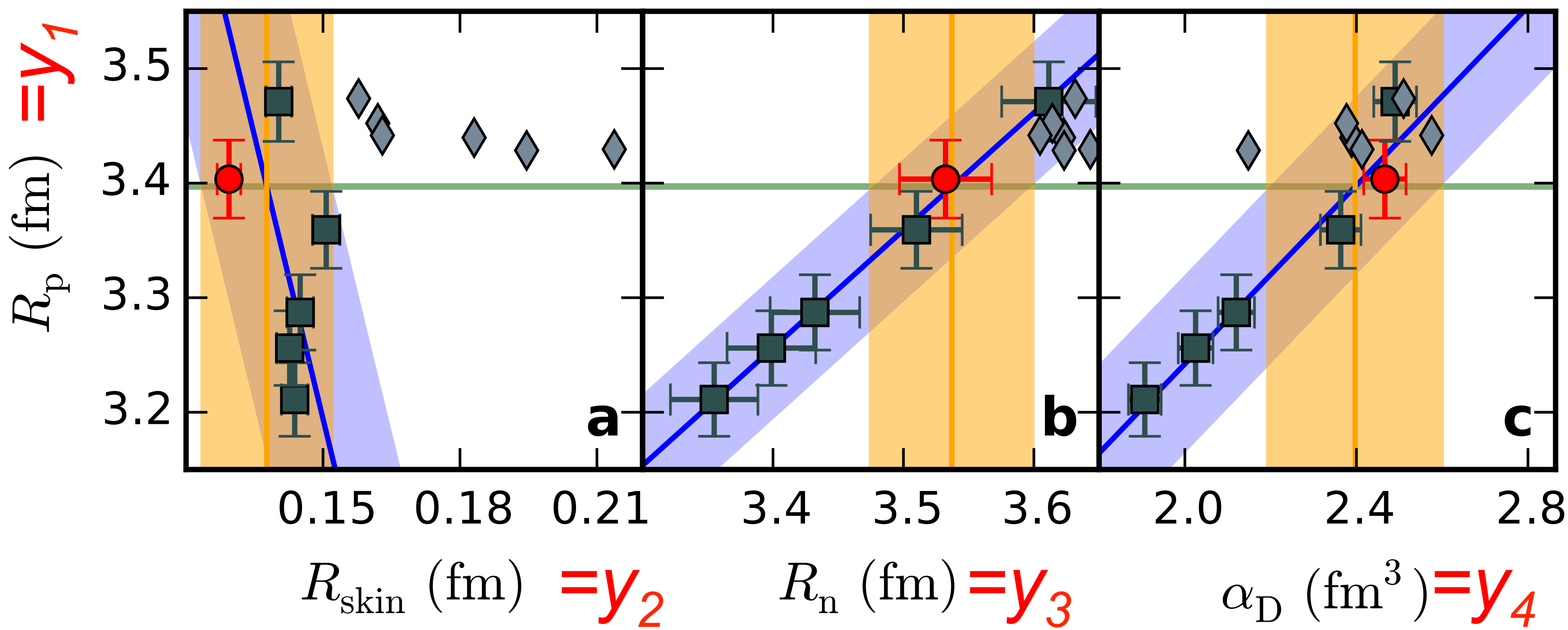
$$y_i[\hat{\boldsymbol{\theta}}(M_\alpha)]$$

Purpose:

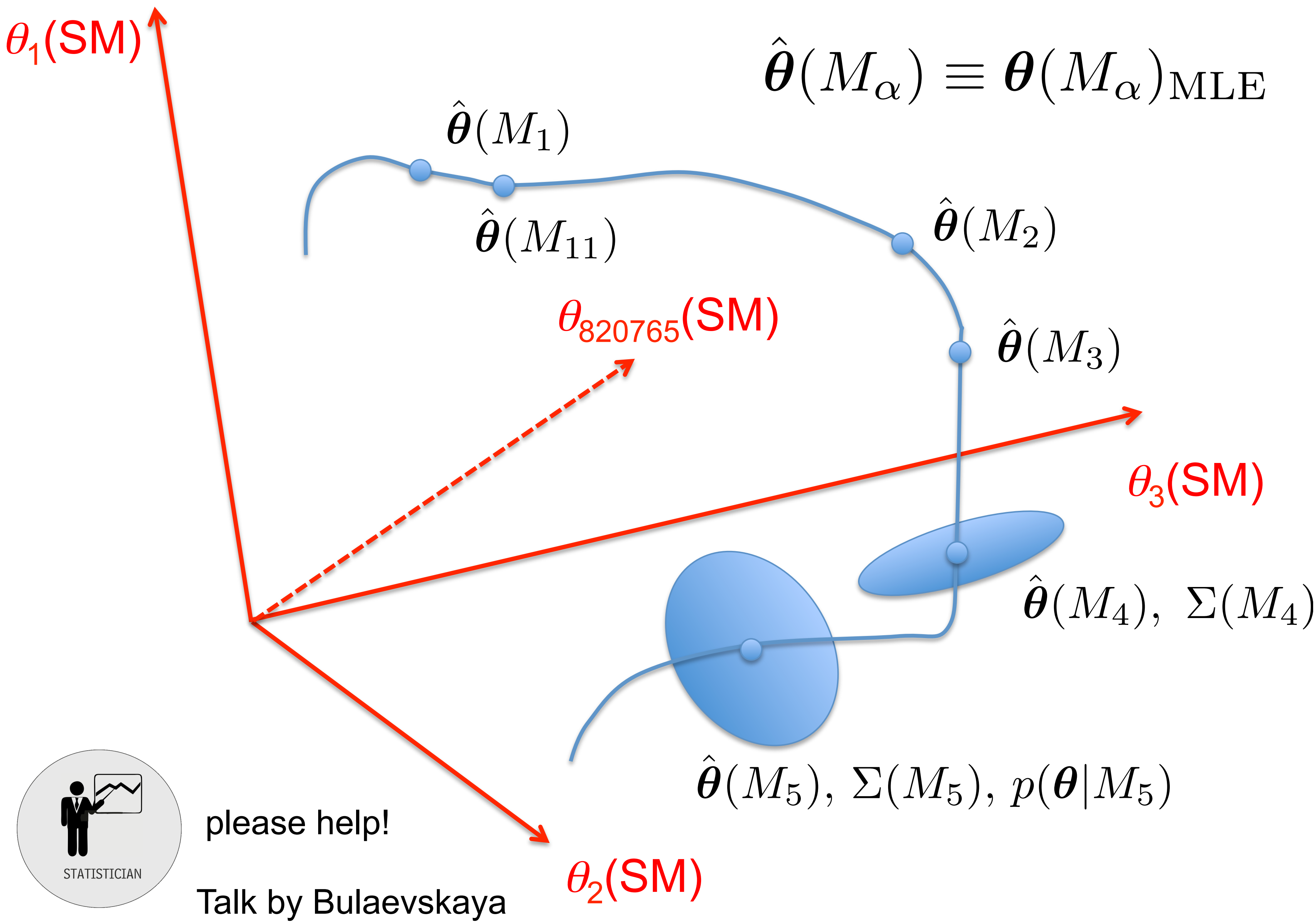
- Determine the new global relation/law
- Determine *unknown* y_2 given measured y_1
- Learn about constraints on models

Example of inter-model correlation analysis (2)

G. Hagen et al., *Nature Physics* **12**, 186 (2016)



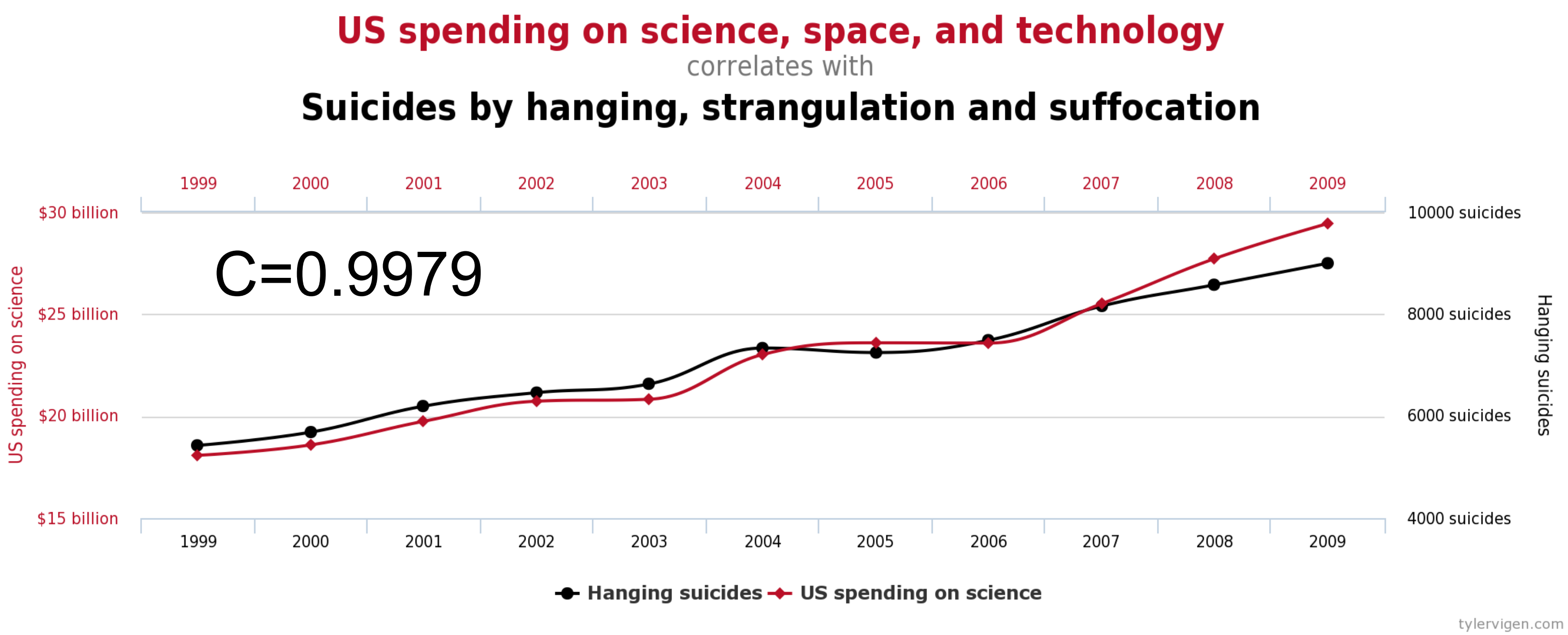
$$y_i[\hat{\boldsymbol{\theta}}(M_\alpha)]$$

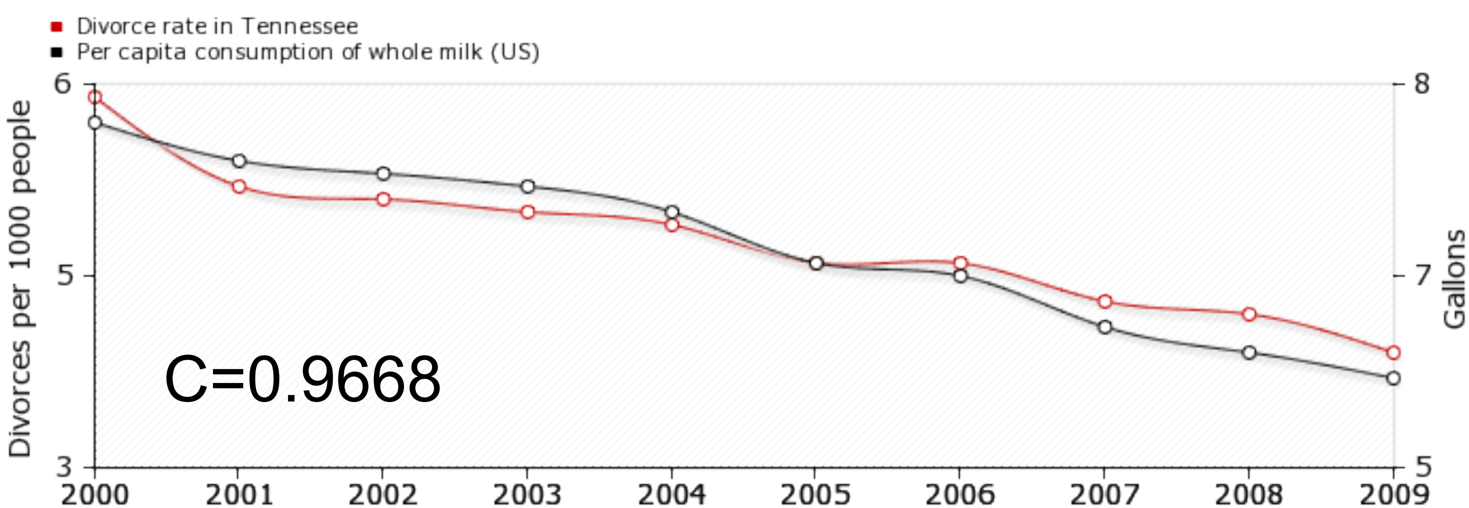


θ_1(SM)
$\hat{\boldsymbol{\theta}}(M_\alpha) \equiv \boldsymbol{\theta}(M_\alpha)_{\mathrm{MLE}}$
$\hat{\boldsymbol{\theta}}(M_1)$
$\hat{\boldsymbol{\theta}}(M_{11})$
$\hat{\boldsymbol{\theta}}(M_2)$
θ_{820765}(SM)
$\hat{\boldsymbol{\theta}}(M_3)$
θ_3(SM)
$\hat{\boldsymbol{\theta}}(M_4),\ \Sigma(M_4)$
$\hat{\boldsymbol{\theta}}(M_5),\ \Sigma(M_5),\ p(\boldsymbol{\theta}|M_5)$
STATISTICIAN
please help!
Talk by Bulaevskaya
θ_2(SM)

Beware of spurious correlations!

http://www.tylervigen.com/spurious-correlations





Naïve nuclear theorist's approach to a systematic (model) error estimate:

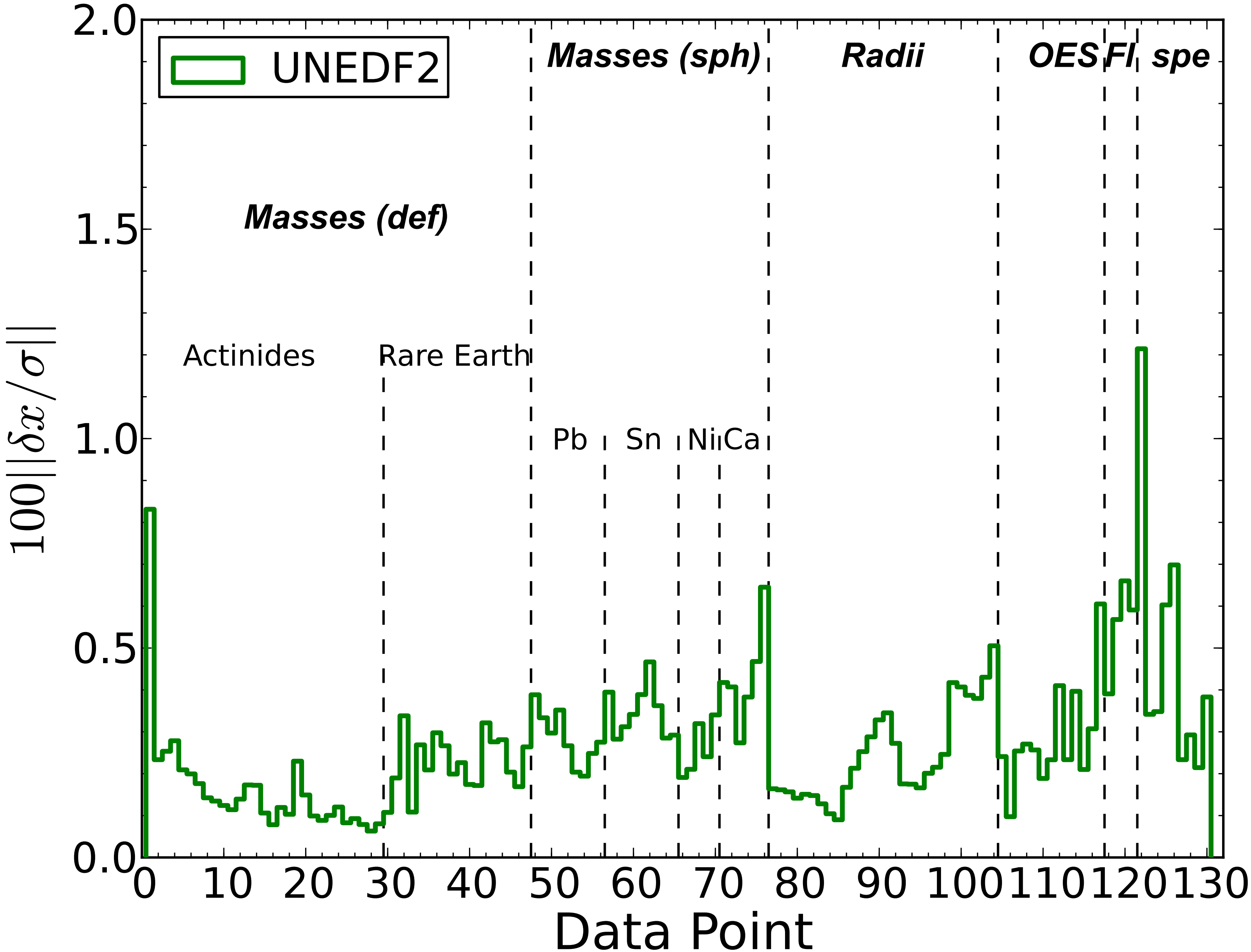
- Take a set of *reasonable* models M_i
- Make a prediction $E(y;M_i)$
- Compute average and variation within this set

- Compute rms deviation from existing experimental data. If the number of fit-observables is large, statistical error is small and the error is predominantly systematic.

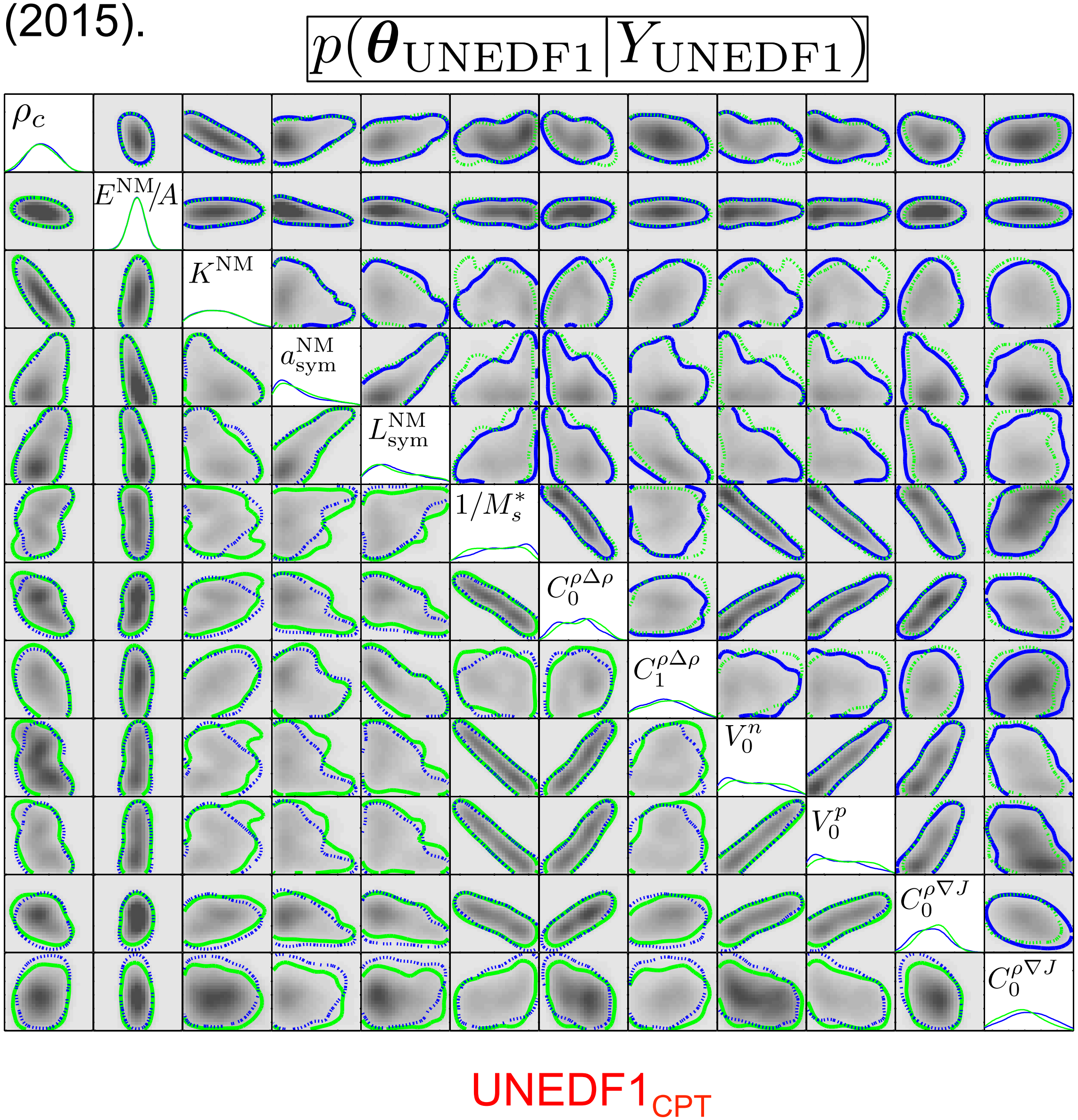
UNEDF2 functional

12 parameters

Phys. Rev. C 89, 054314 (2014)



Uncertainty Quantification for Nuclear Density Functional Theory and Information Content of New Measurements, J. McDonnell et al., Phys. Rev. Lett. 114, 122501 (2015).



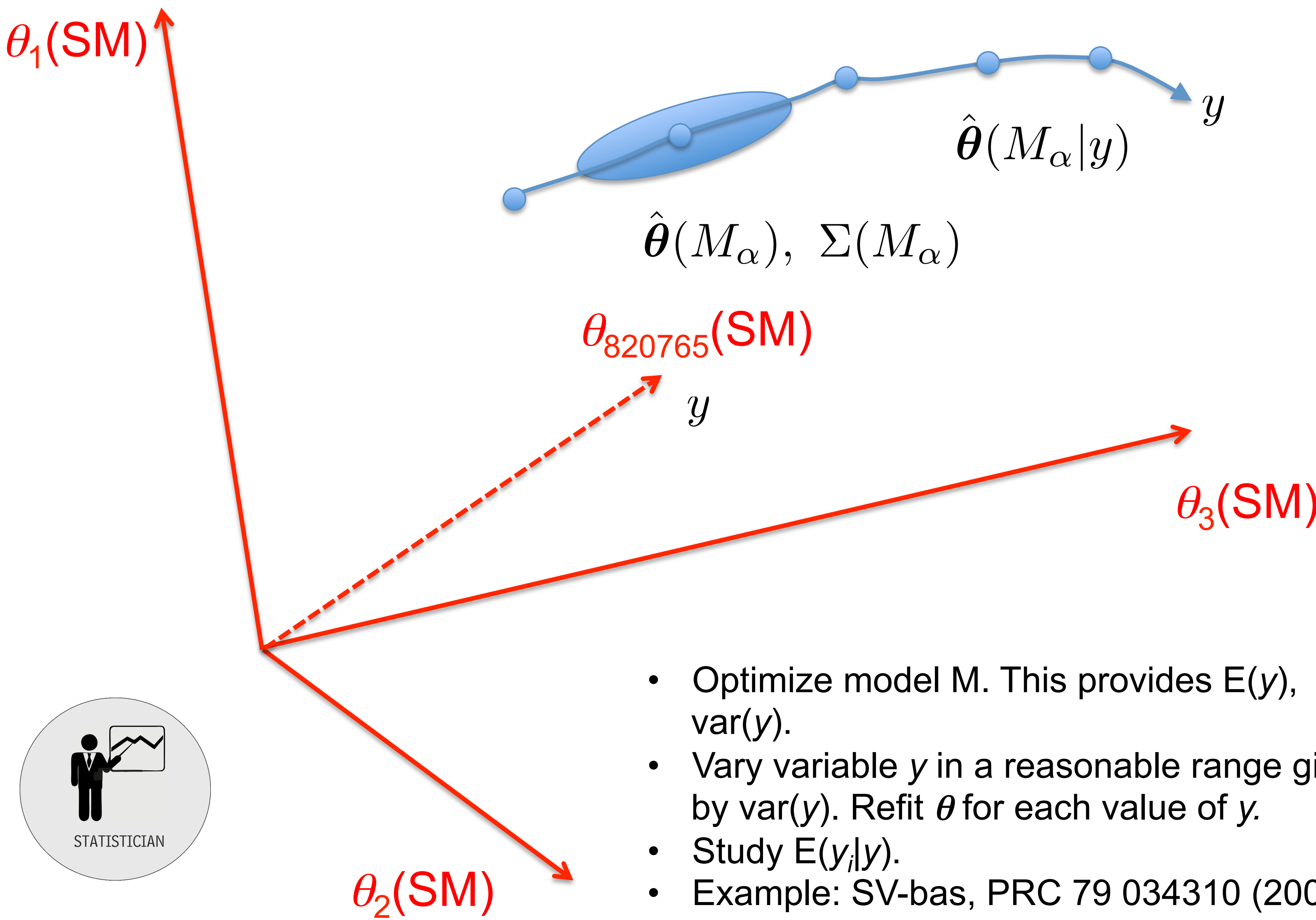
UNEDF1

Pilot Study Applied to UNEDF1

- Massively Parallel Approach
- 130 data points (including deformed nuclei)
- Gaussian process response surface
- 200 Test Parameter Sets
- Latin hyper-rectangle

No improvement on model's predictibility except for postdictions on additional data

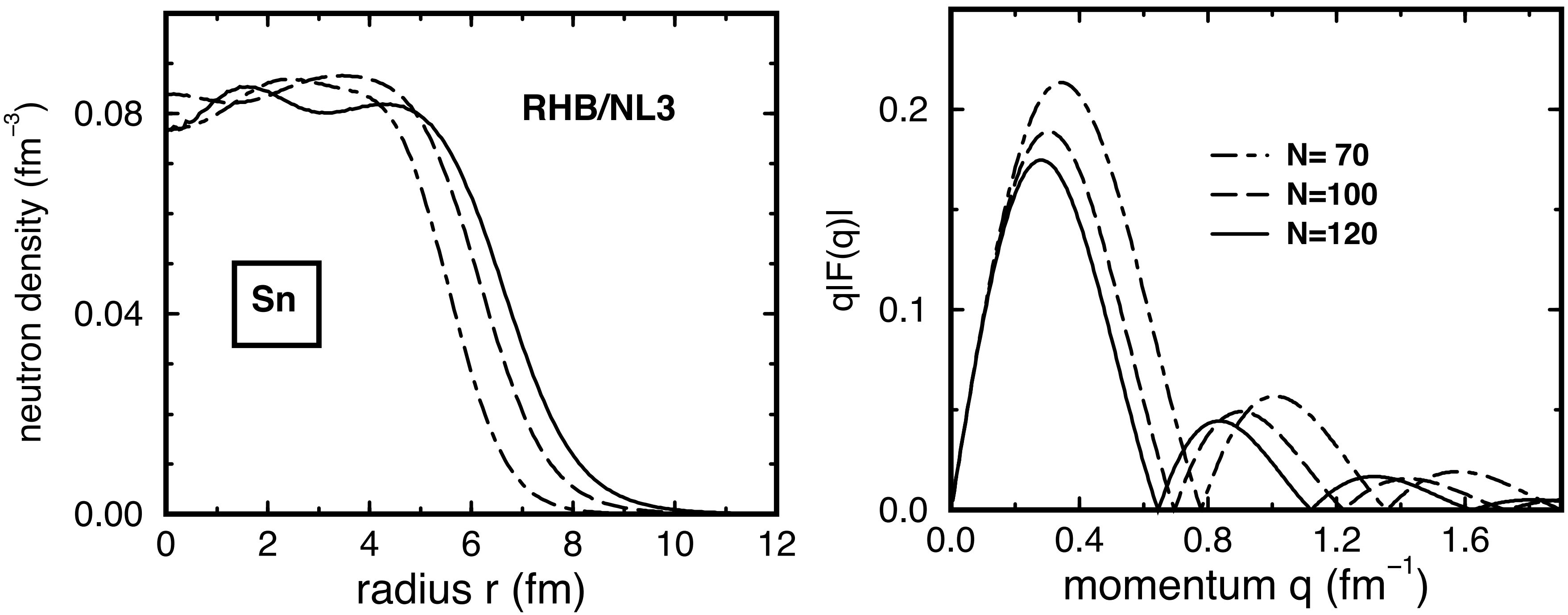
How to assess systematic trends?



- Optimize model M. This provides E(y), var(y).
- Vary variable y in a reasonable range given by var(y). Refit $\boldsymbol{\theta}$ for each value of y.
- Study E($y_i|y$).
- Example: SV-bas, PRC 79 034310 (2009)

Radii in nuclear DFT

S. Mizutori et al., *Phys. Rev. C* **61**, 044326 (2000)

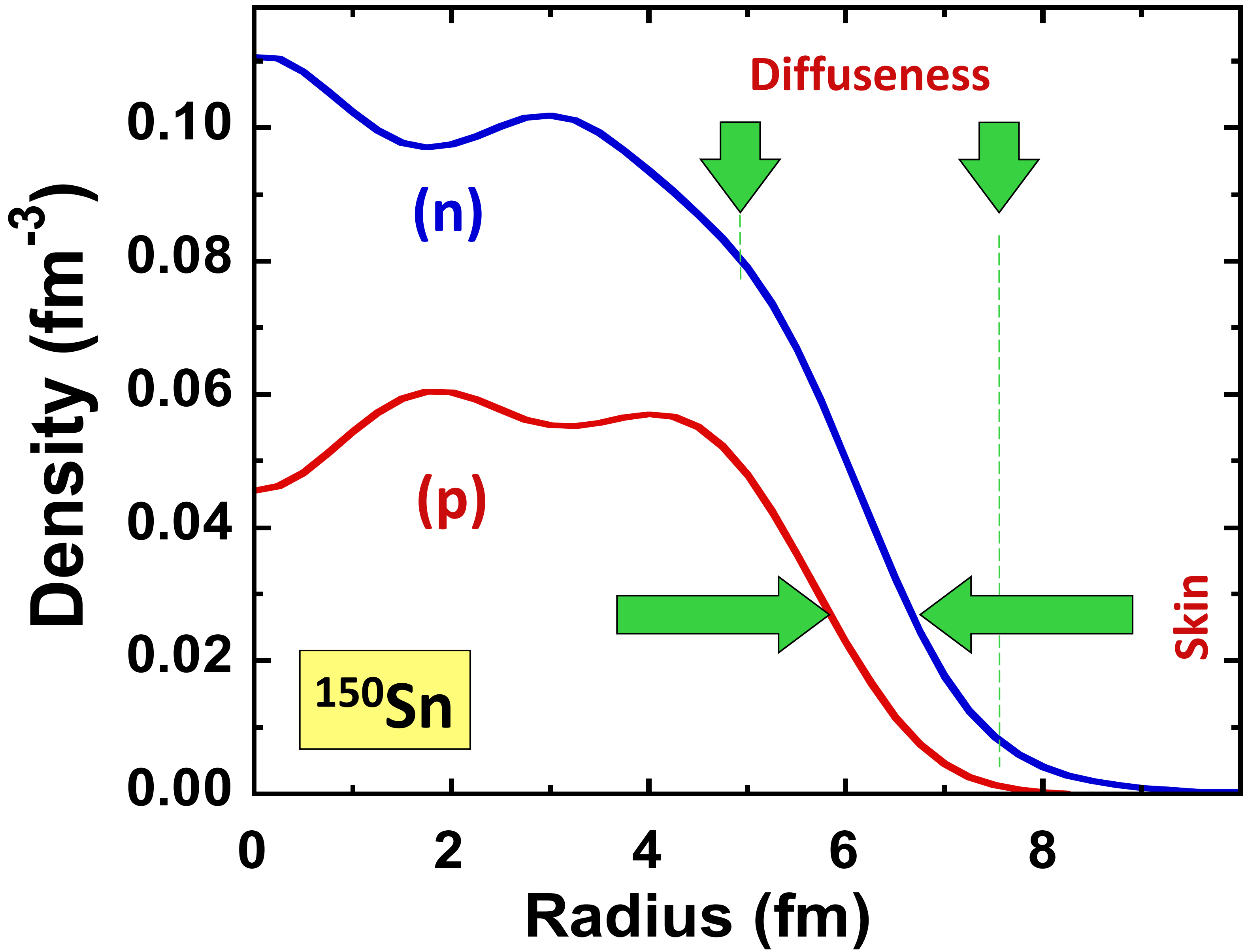


$$R_{\mathrm{diff}} = 4.49341/q_1$$

first zero of F(q)

$$R_{\mathrm{diff}} \approx r_0 A^{1/3}$$

Neutron & proton density distributions

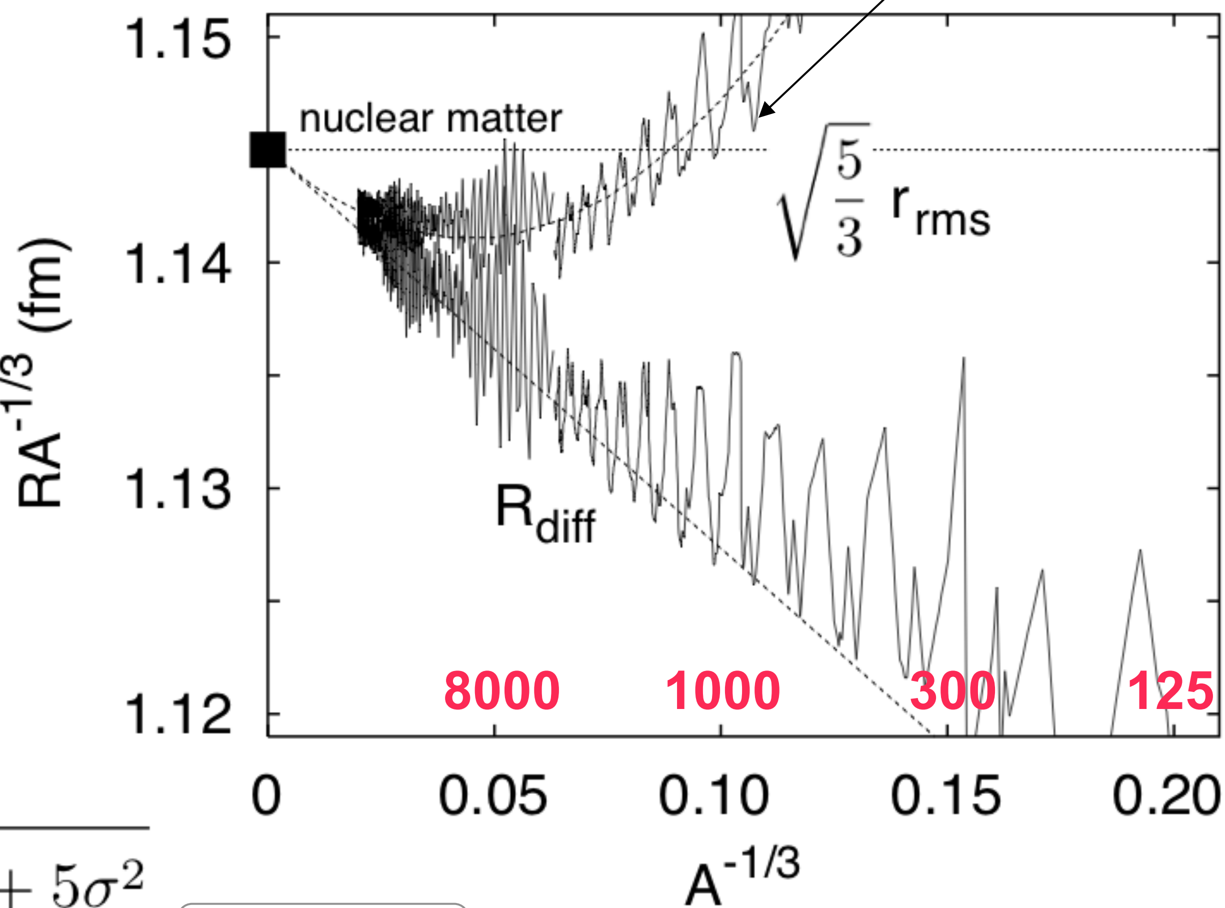


Finite size effects and leptodermous expansion

Phys. Rev. C **73**, 014309 (2006)

$$r_s = \left(\frac{3}{4\pi\rho_0}\right)^{1/3}$$

Wigner-Seitz radius



$$r_{\rm rms} = \sqrt{\frac{3}{5}}\sqrt{R^2_{\rm diff} + 5\sigma^2}$$

around 1fm

Neutron-skin uncertainties of Skyrme EDF

M. Kortelainen et al., Phys. Rev. C 88, 031305 (2013)

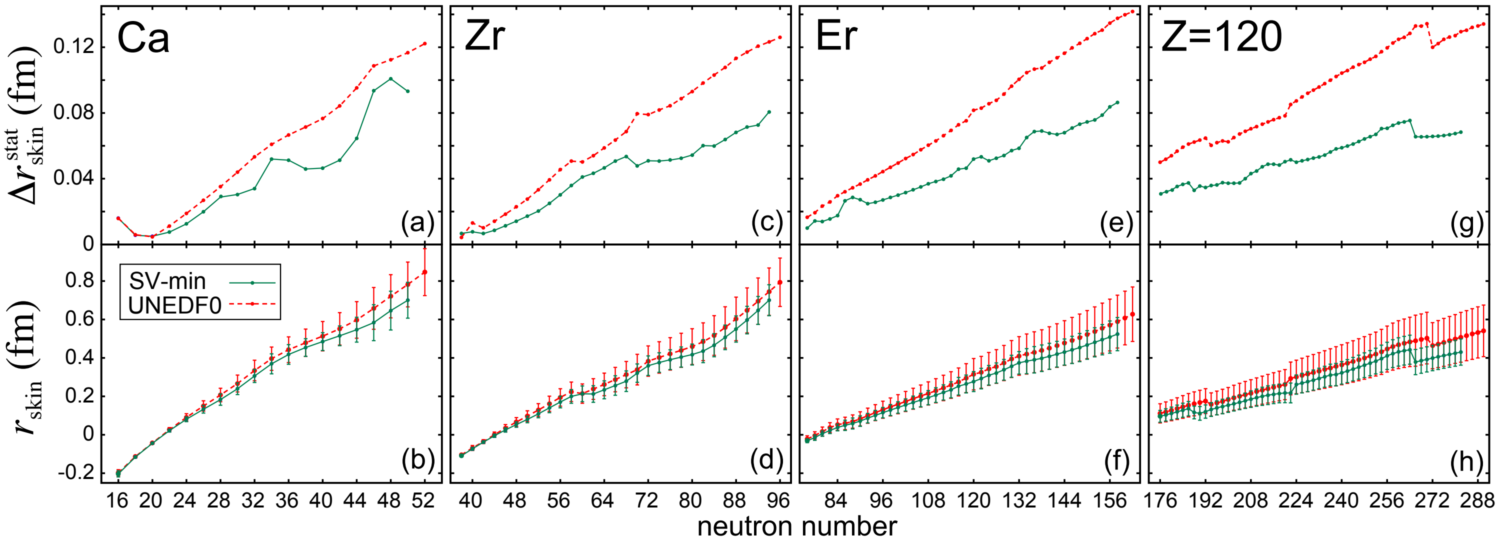
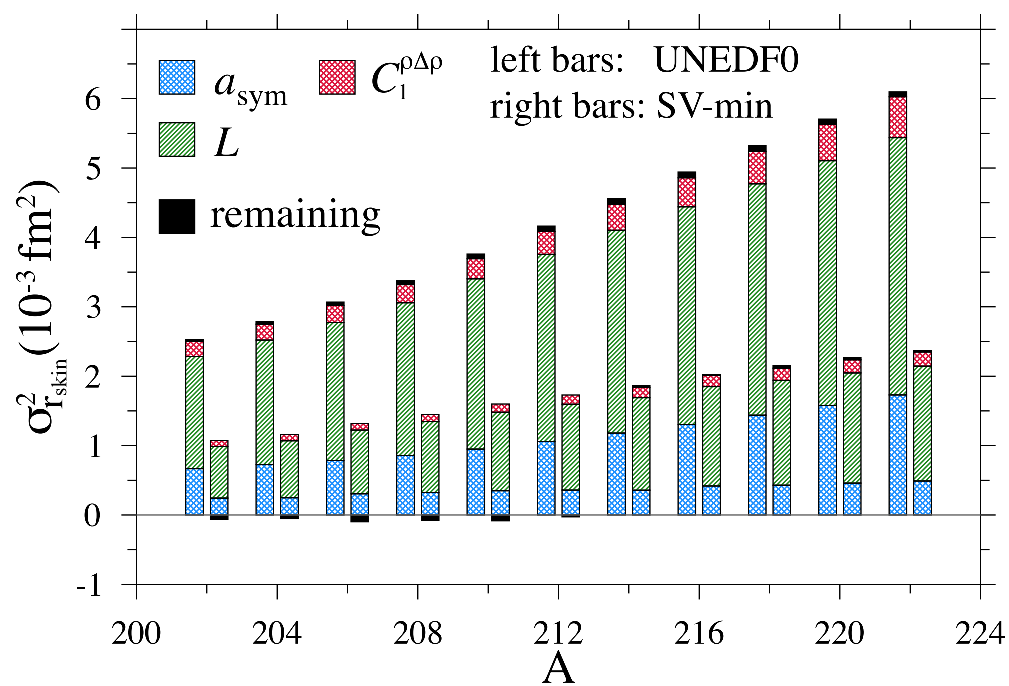


TABLE I. Theoretical uncertainties on $r_{\rm skin}$ in ^{208}Pb and ^{48}Ca (in fm). Shown are statistical errors of UNEDF0 and SV-min, systematic error $\Delta r_{\rm skin}^{\rm syst}$, the model-averaged deviation of Ref. [9], and errors of PREX [25] and planned PREX-II [29] and CREX [30] experiments.

nucleus	$\Delta r_{\rm skin}^{\rm stat}$ UNEDF0	$\Delta r_{\rm skin}^{\rm stat}$ SV-min	$\Delta r_{\rm skin}^{\rm syst}$	Ref. [9]	Experiment
^{208}Pb	0.058	0.037	0.013	0.022	0.18 [25], 0.06[29]
^{48}Ca	0.035	0.026	0.019	0.018	0.02 [30]



Nuclear charge and neutron radii and nuclear matter: trend analysis in Skyrme-DFT approach

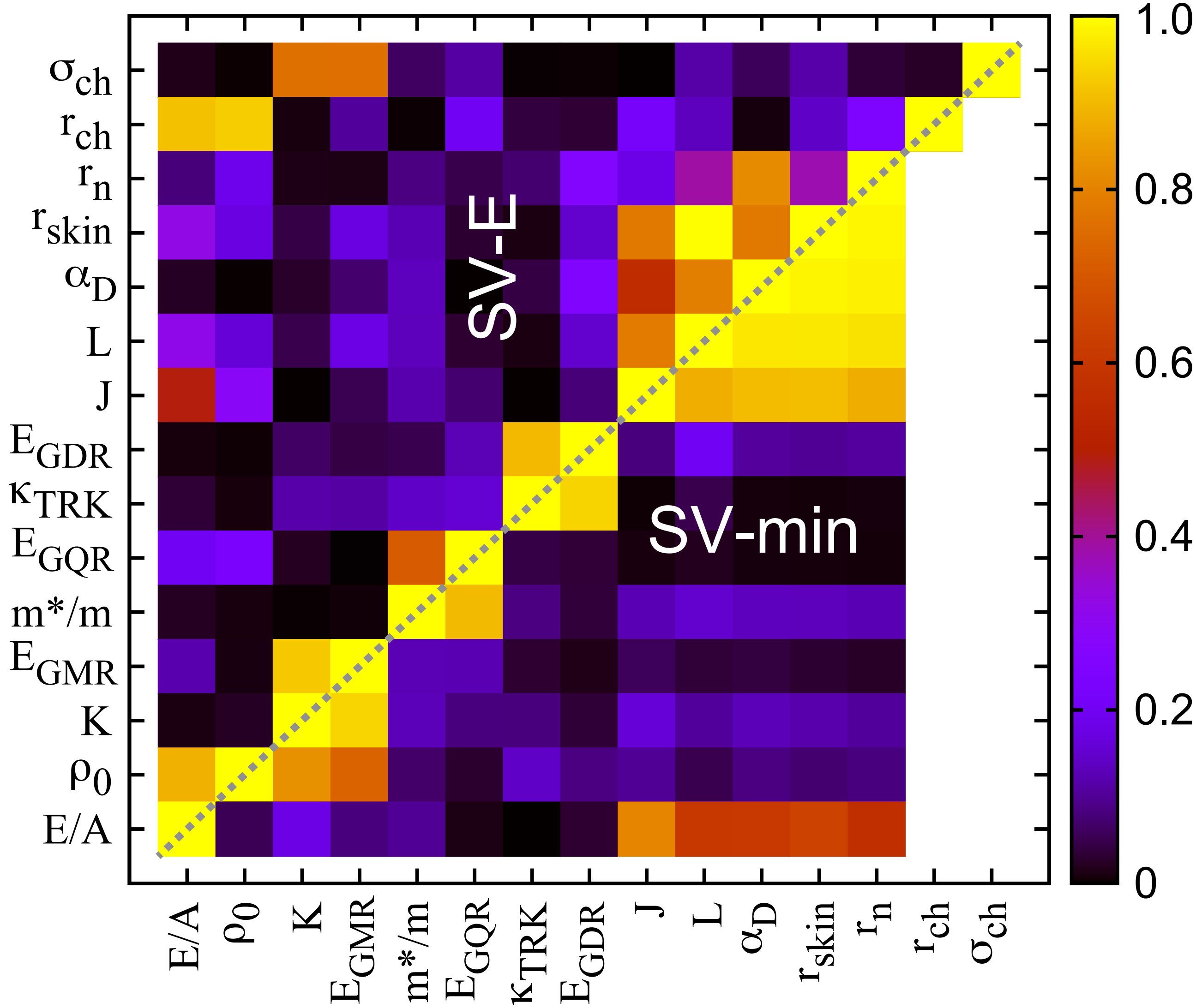
P.-G. Reinhard and WN, PRC 93, 051303 (R) (2016)

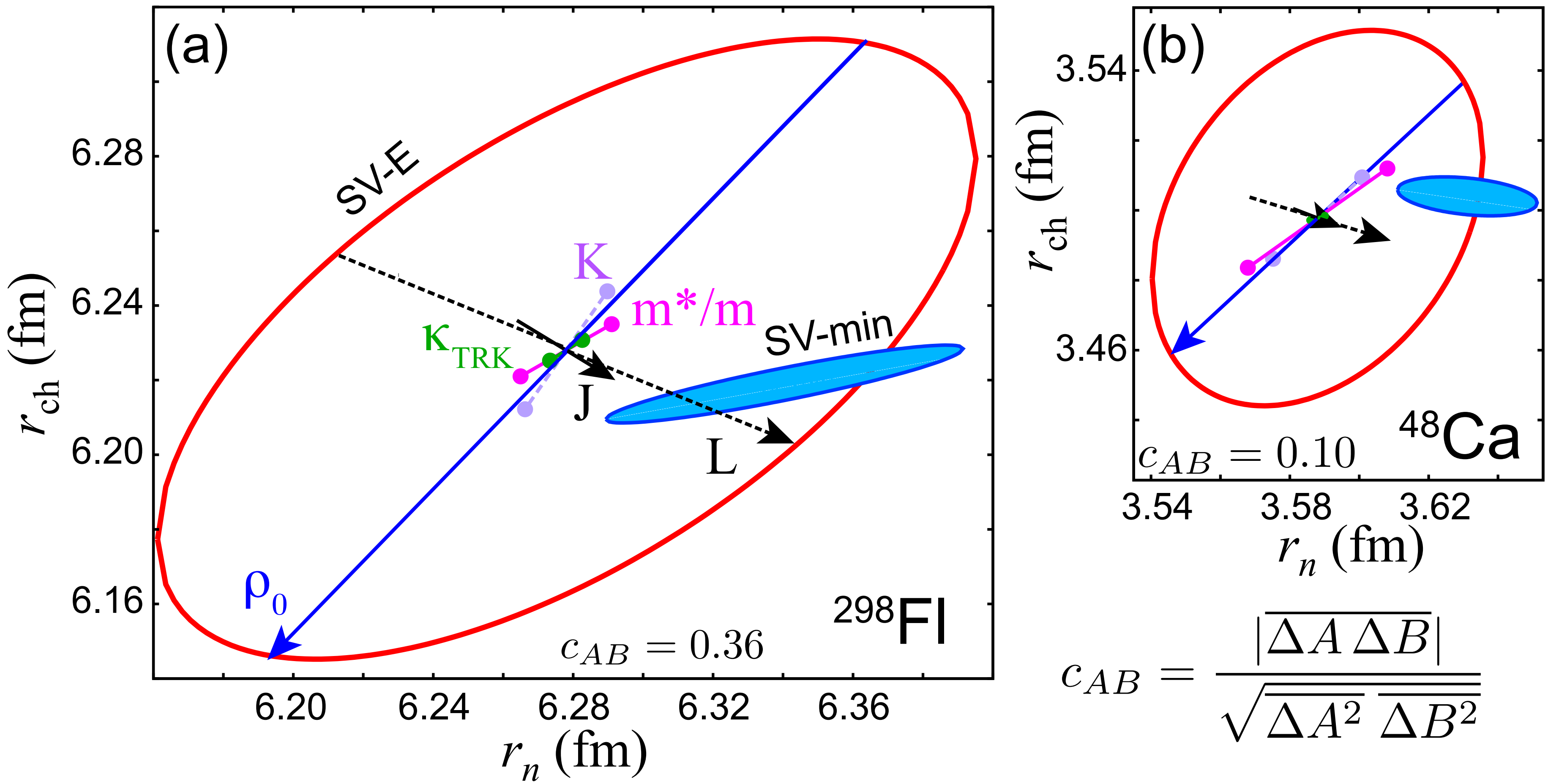
14-parameter model, optimized to 2 different sets of fit-observables

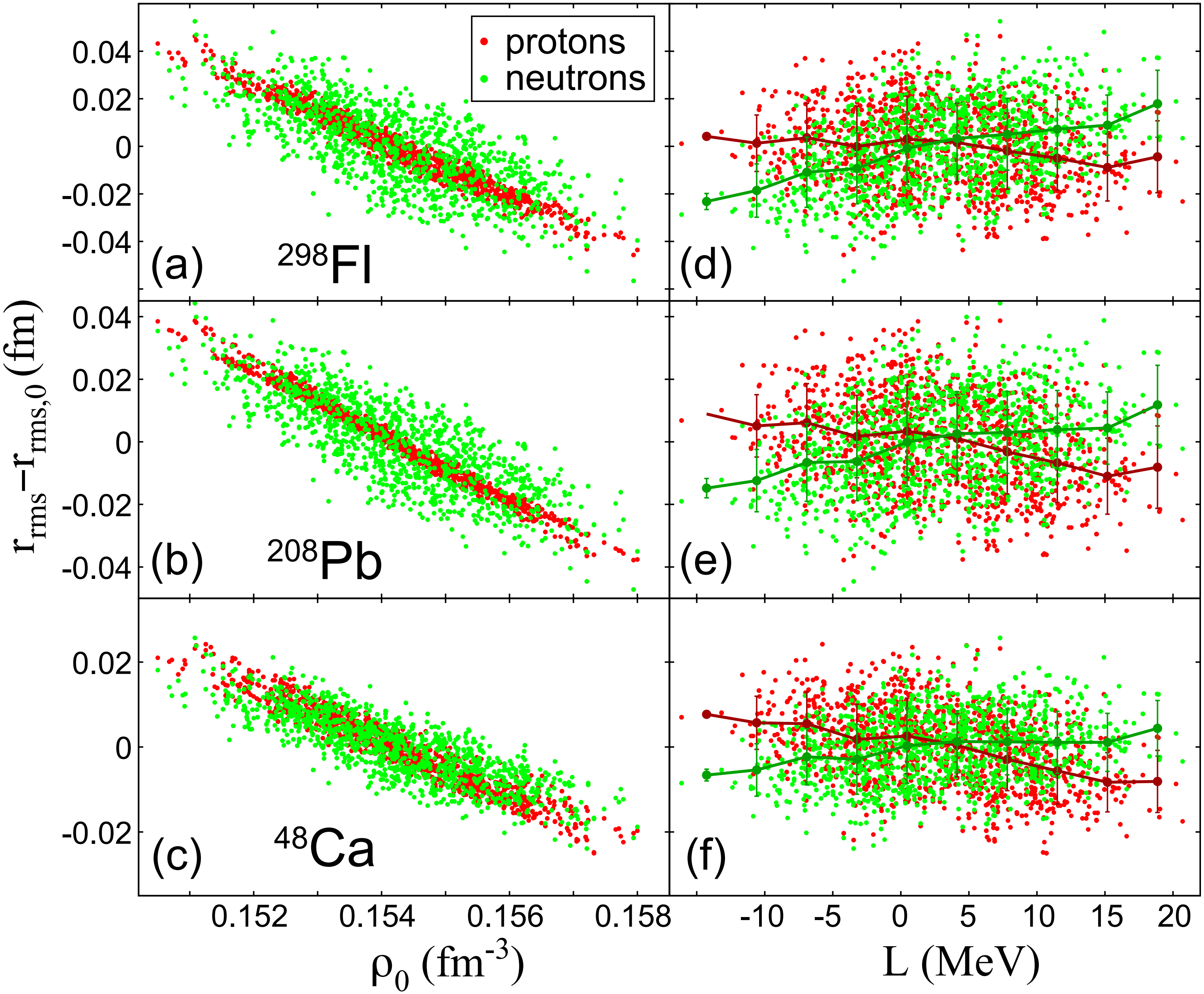
	SV-min	*(Y=E, R)*	SV-E	*(Y=E)*	
ρ_0 (MeV)	0.161085	$\pm$ 0.0011	0.154181	$\pm$ 0.0076	stiff
E/A (MeV)	-15.9099	$\pm$ 0.04	-15.8120	$\pm$ 0.17	stiff
K (MeV)	221.752	$\pm$ 8.1	273.733	$\pm$ 31.3	
m^*/m	0.951806	$\pm$ 0.067	1.07038	$\pm$ 0.103	
J (MeV)	30.6570	$\pm$ 1.9	27.2333	$\pm$ 2.4	
L (MeV)	44.8138	$\pm$ 25.7	2.92329	$\pm$ 62.9	sloppy
κ_{TRK}	0.076522	$\pm$ 0.1919	0.192	$\pm$ 0.349	
$C_0^{\Delta\rho}$ (MeV fm^5)	107.657	$\pm$ 6.6	85.39992	$\pm$ 10.7	
$C_1^{\Delta\rho}$ (MeV fm^5)	-141.506	$\pm$ 162	-80.90533	$\pm$ 391	sloppy
$C_0^{\nabla\mathbf{J}}$ (MeV fm^4)	-101.582	$\pm$ 5.5	-96.3170	$\pm$ 11.7	
$C_1^{\nabla\mathbf{J}}$ (MeV fm^4)	-22.9681	$\pm$ 16.2	-21.5881	$\pm$ 18.2	sloppy
$V_{\mathrm{pair,p}}$ (MeV fm^3)	601.160	$\pm$ 190	613.231	$\pm$ 209	
$V_{\mathrm{pair,n}}$ (MeV fm^3)	567.190	$\pm$ 154	568.739	$\pm$ 173	
$\rho_{0,\mathrm{pair}}$ (fm^{-3})	0.211591	$\pm$ 0.052	0.202513	$\pm$ 0.046	

Nuclear charge and neutron radii, and nuclear matter: intra-model trend analysis

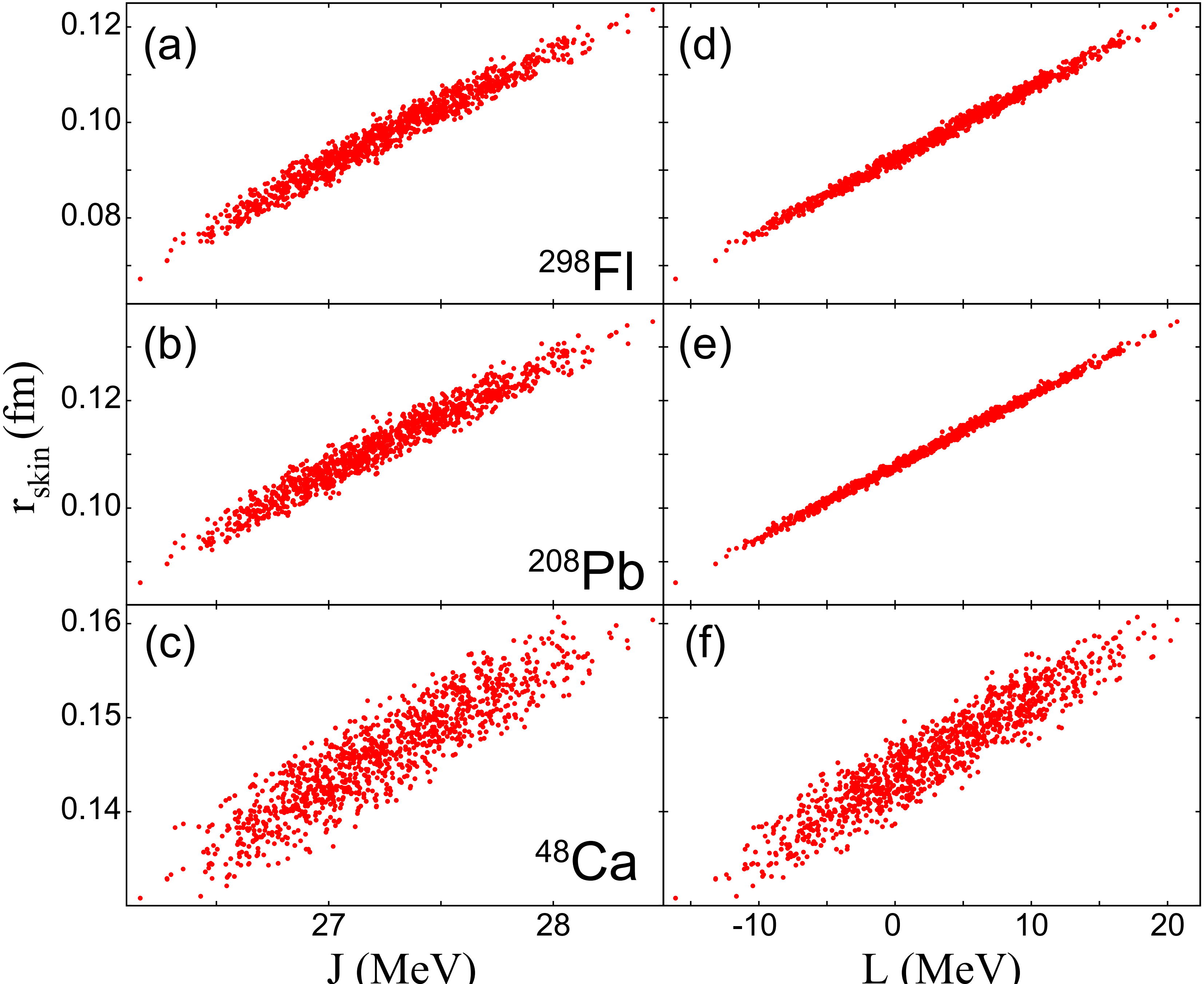
P.-G. Reinhard and WN, PRC (R) (2016)



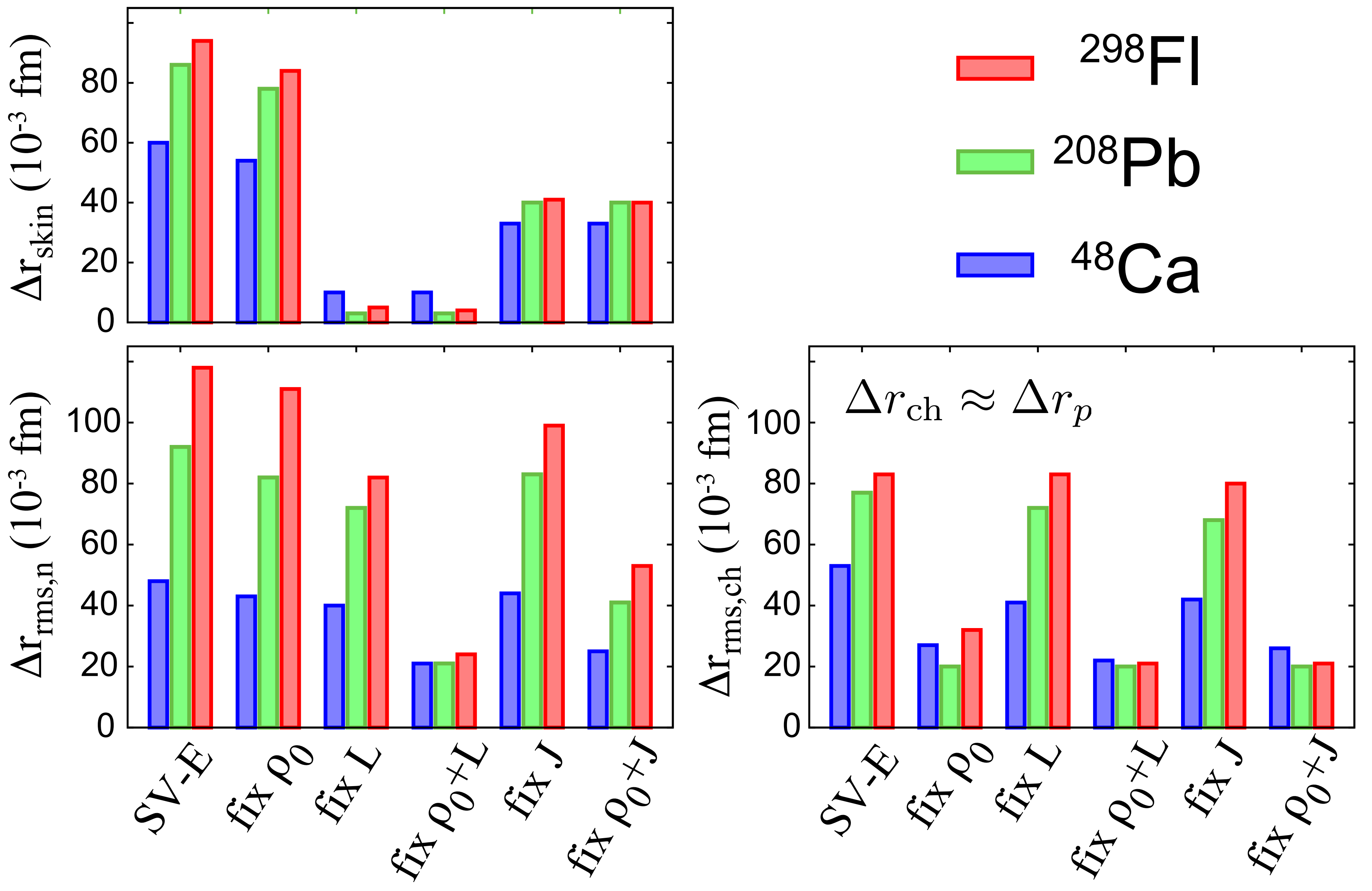

(a)
SV-E
K
m*/m
κ_{TRK}
SV-min
J
L
ρ_0
^{298}Fl
$c_{AB} = 0.36$
r_{ch} (fm)
6.28
6.24
6.20
6.16
6.20
6.24
6.28
6.32
6.36
r_n (fm)
(b)
^{48}Ca
$c_{AB} = 0.10$
3.54
3.46
3.54
3.58
3.62
$$c_{AB} = \frac{|\overline{\Delta A\,\Delta B}|}{\sqrt{\overline{\Delta A^2}\;\overline{\Delta B^2}}}$$



2000 Gaussian samples of $L(\theta)$



(a)
(b)
(c)
(d)
(e)
(f)
298Fl
208Pb
48Ca
r_skin (fm)
0.12
0.10
0.08
0.16
0.15
0.14
27
28
-10
0
10
20
J (MeV)
L (MeV)



$$\Delta r_n = \Delta r_p + \Delta r_{\text{skin}}$$

- We explored various trends of charge and neutron radii with nuclear matter properties.
- There exist, at least within the Skyrme-DFT theory, only two strong correlations:
  - one-to-one relation between charge radii in finite nuclei and ρ_0: $r_p \leftrightarrow \rho_0$
  - one-to-one relation between neutron skins in finite nuclei and L: $r_{skin} \leftrightarrow L$
- By including charge radii in a set of fit-observables, as done for the majority of realistic Skyrme EDFs, one practically fixes the saturation density.
- The relation $r_n \leftrightarrow \rho_0$ is much weaker than that for r_p, so by constraining the saturation density alone does not help significantly reducing the uncertainty on neutron (and mass) radii. However:

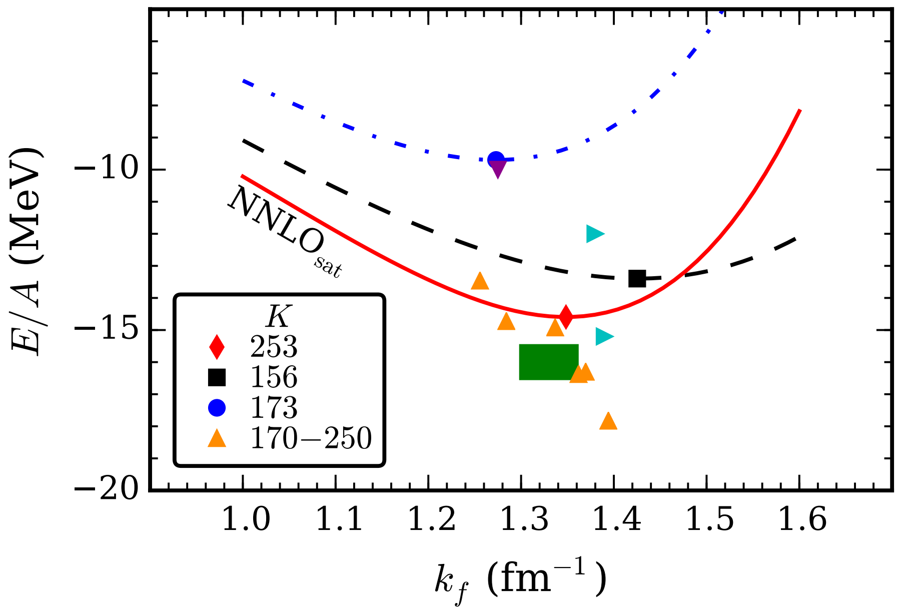
$$r_n = r_p + r_{skin}$$

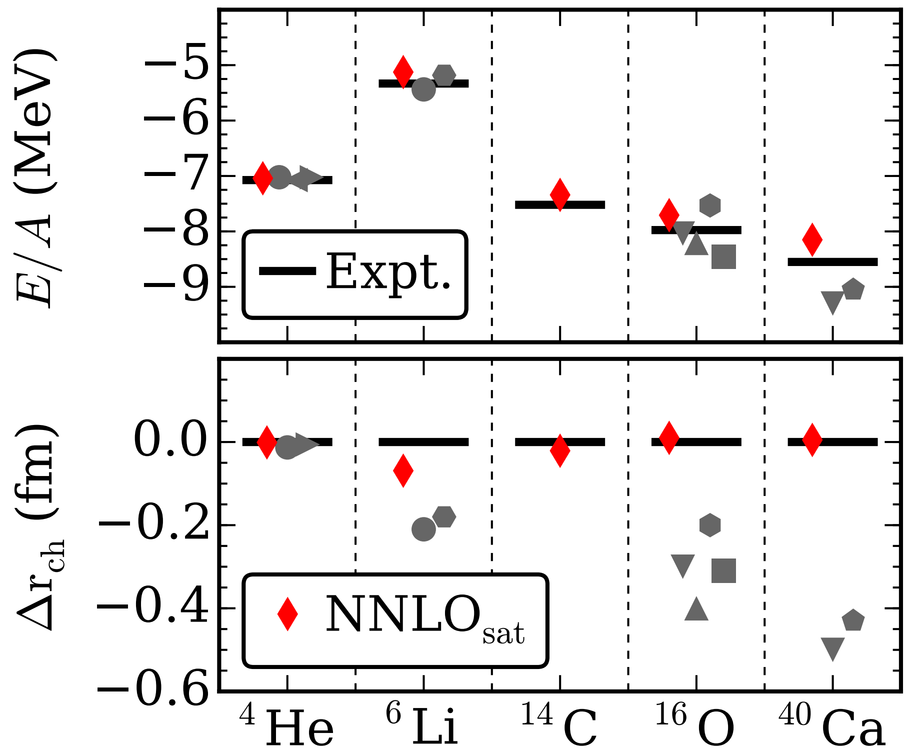
- The $r_n \leftrightarrow r_p$ relation is fairly complex: various trends are possible when moving along *a* trajectory in a parameter space.

N2LO$_{sat}$ describes low-energy NN and Nuclei

A. Ekström et al. Phys. Rev. C 91, 051301(R) (2015)

- Order-by-order optimization
- Constrained by data on few-body systems and light nuclei





Coupled Cluster informing DFT

and

DFT informing Coupled Cluster