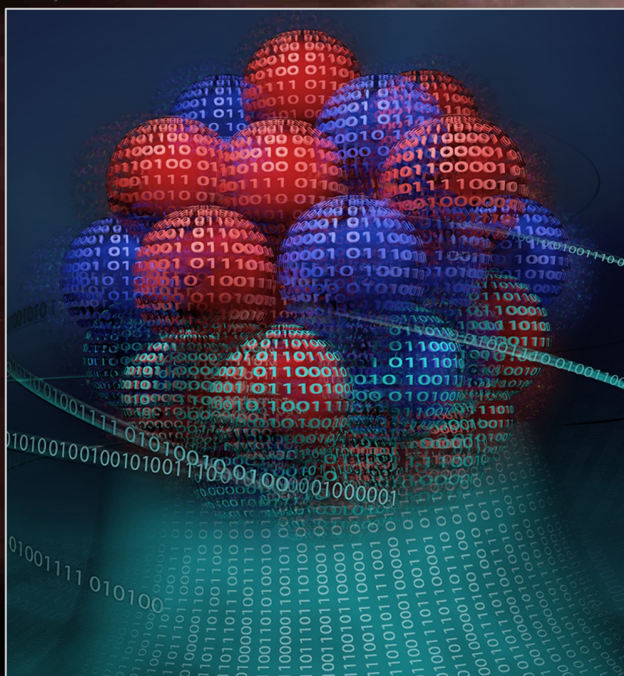
Nuclear radii in density functional theory

Witold Nazarewicz (FRIB/MSU)

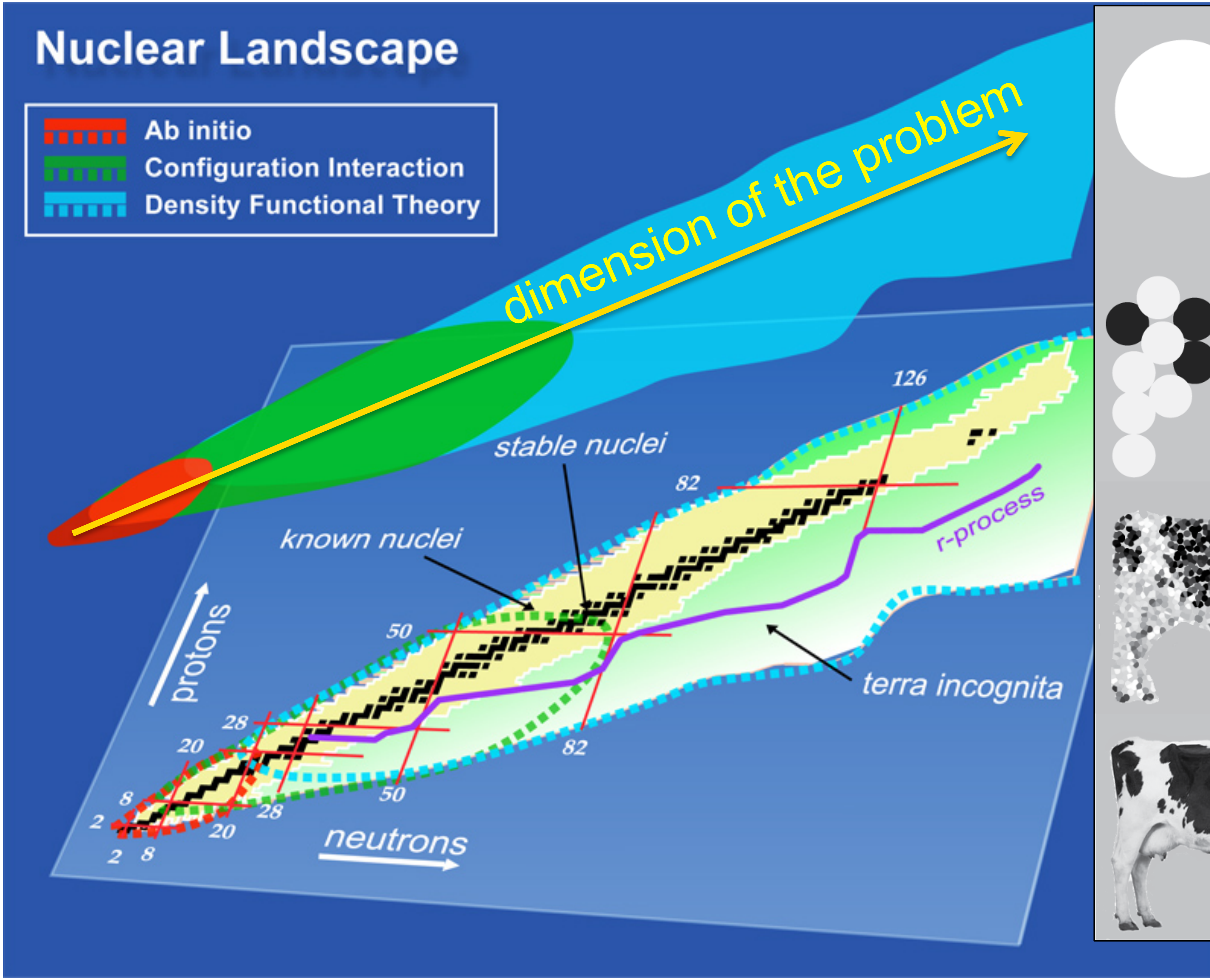
Neutron Skins in Nuclei

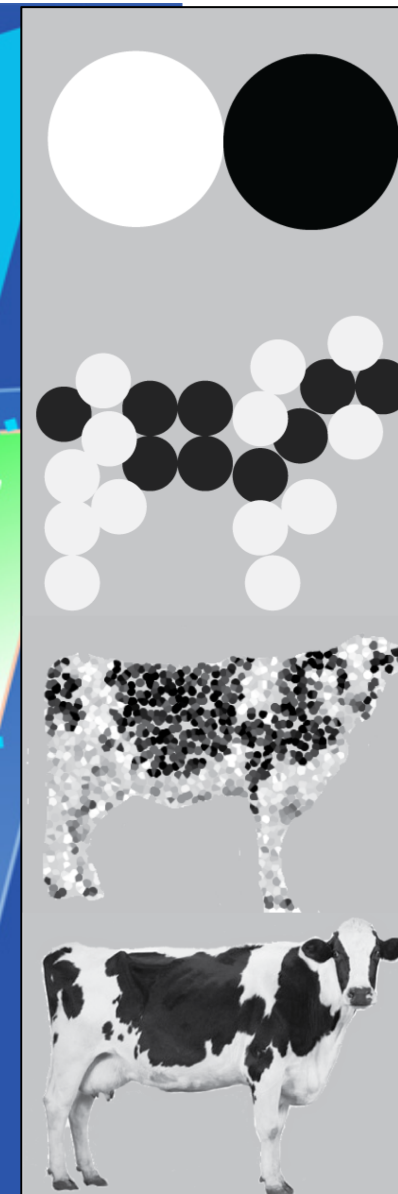
MITP, Mainz,, May 17-27, 2016



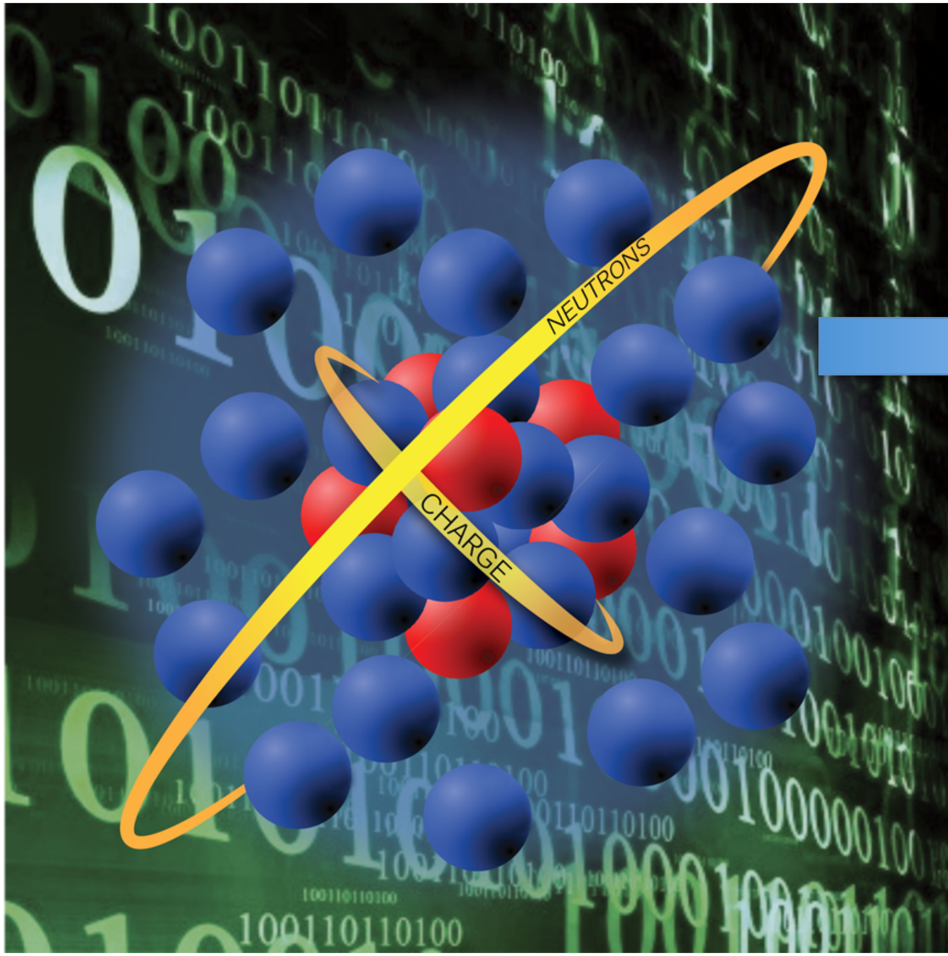
- Perspective
- Theoretical strategies
- Nuclear DFT
- Radii, skins, and halos
- Uncertainty quantification and correlation analysis
- Proton-, neutron radii, skins, and nuclear matter properties
- Conclusions

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





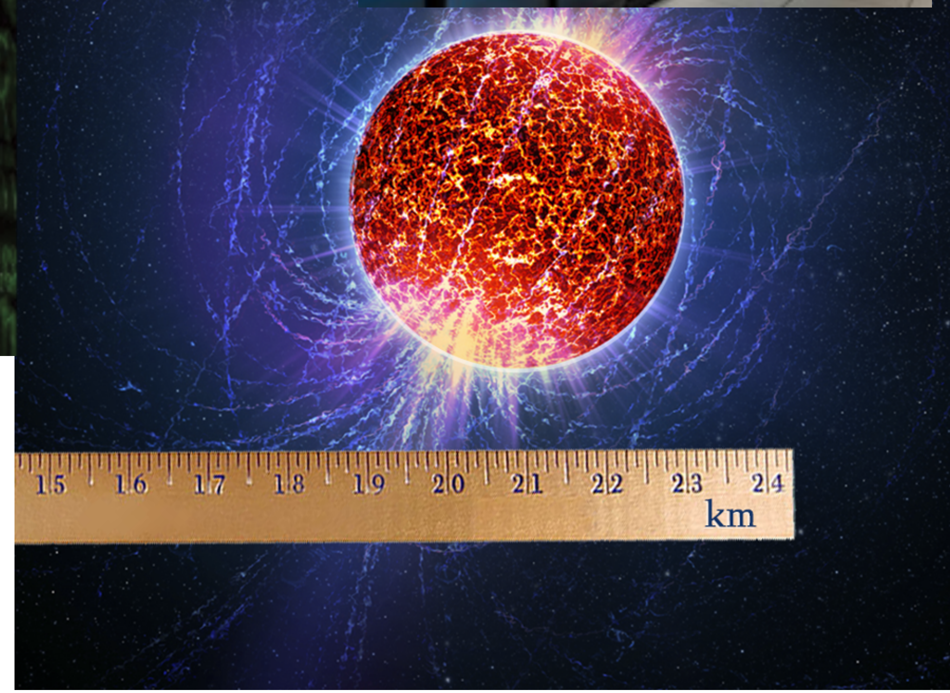
J. Phys. G 43, 044002 (2016)
http://iopscience.iop.org/article/10.1088/0954-3899/43/4/044002



nature physics
ARTICLES
PUBLISHED ONLINE: 2 NOVEMBER 2015 | DOI: 10.1038/NPHYS3529

Neutron and weak-charge distributions of the ^{48}Ca nucleus

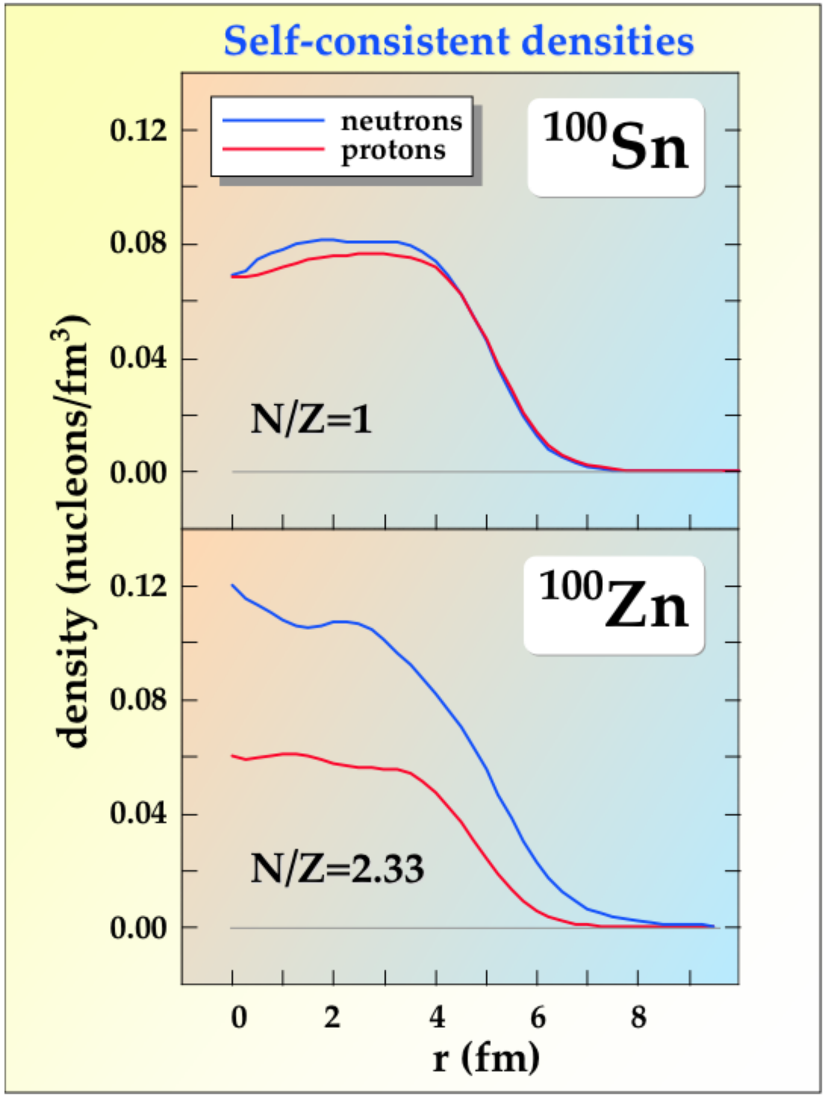
G. Hagen[1,2*], A. Ekström[1,2], C. Forssén[1,2,3], G. R. Jansen[1,2], W. Nazarewicz[1,4,5], T. Papenbrock[1,2], K. A. Wendt[1,2], S. Bacca[6,7], N. Barnea[8], B. Carlsson[3], C. Drischler[9,10], K. Hebeler[9,10], M. Hjorth-Jensen[4,11], M. Miorelli[6,12], G. Orlandini[13,14], A. Schwenk[9,10] and J. Simonis[9,10]



Hagen's talk

Mean-Field Theory ⇒ Density Functional Theory

Degrees of freedom: nucleonic densities



Nuclear DFT

- two fermi liquids
- self-bound
- superfluid

- mean-field ⇒ one-body densities
- zero-range ⇒ local densities
- finite-range ⇒ gradient terms
- particle-hole and pairing channels
- Has been extremely successful. A broken-symmetry generalized product state does surprisingly good job for nuclei.

Nuclear Energy Density Functional

isoscalar (T=0) density $\left(\rho_0 = \rho_n + \rho_p\right)$

isovector (T=1) density $\left(\rho_1 = \rho_n - \rho_p\right)$

+isoscalar and isovector densities:
spin, current, spin-current tensor,
kinetic, and kinetic-spin
+ pairing densities

$$E = \int \mathcal{H}(r) d^3 r$$

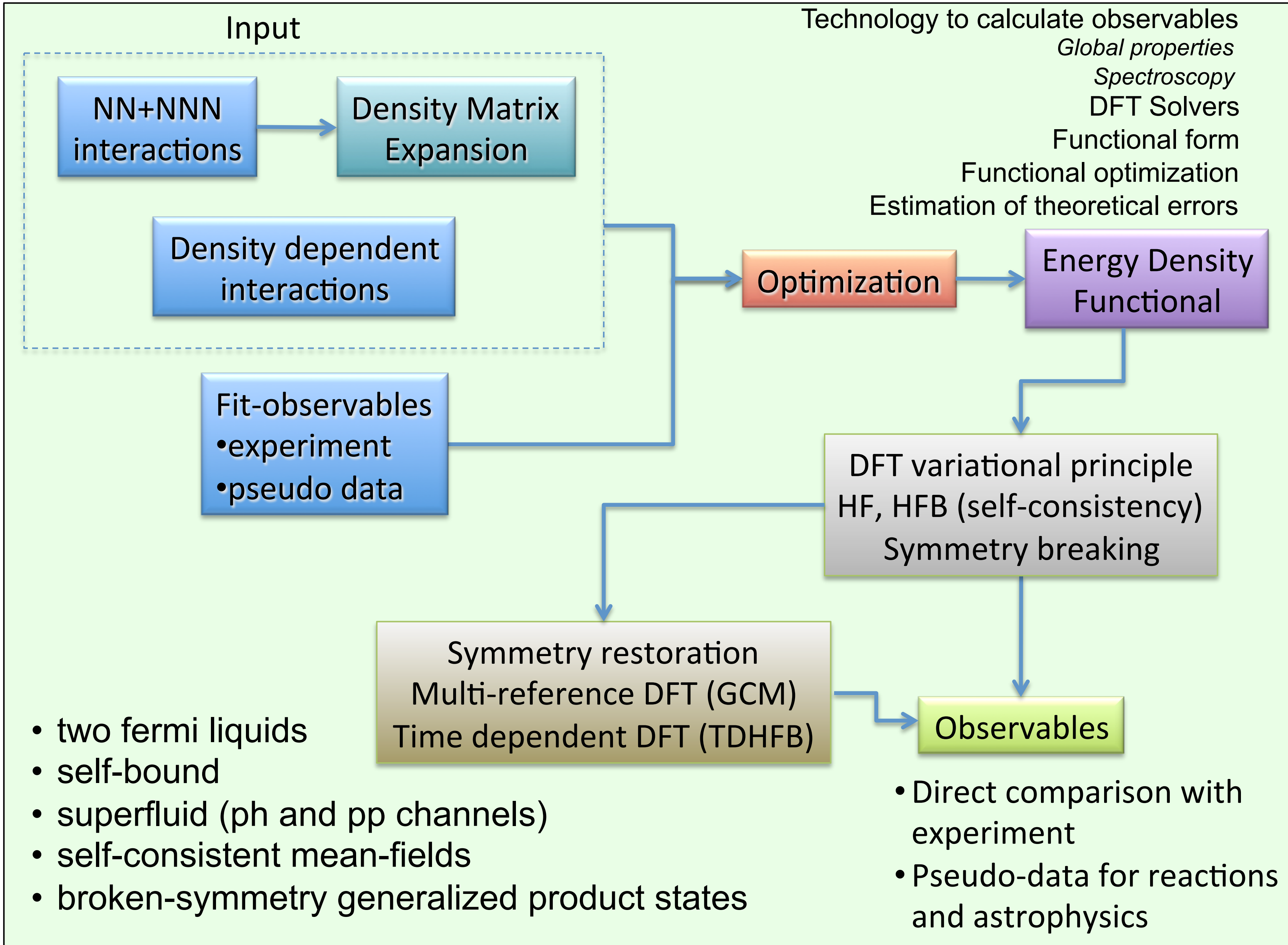
p-h density p-p density (pairing functional)

$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0(r) + \sum_{t=0,1}\left(\chi_t(r) + \breve{\chi}_t(r)\right)$$

Expansion in densities and their derivatives

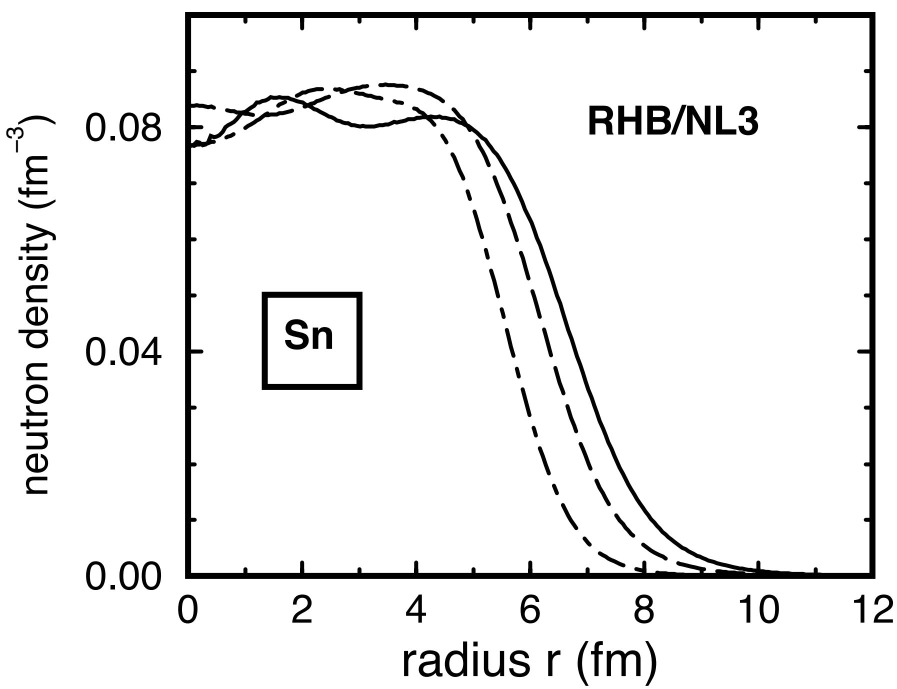
- Constrained by microscopic theory: ab-initio functionals provide quasi-data!
- Not all terms are equally important. Usually ~12 terms considered
- Some terms probe specific experimental data
- Pairing functional poorly determined. Usually 1-2 terms active.
- Becomes very simple in limiting cases (e.g., unitary limit)
- Can be extended into multi-reference DFT (GCM) and projected DFT

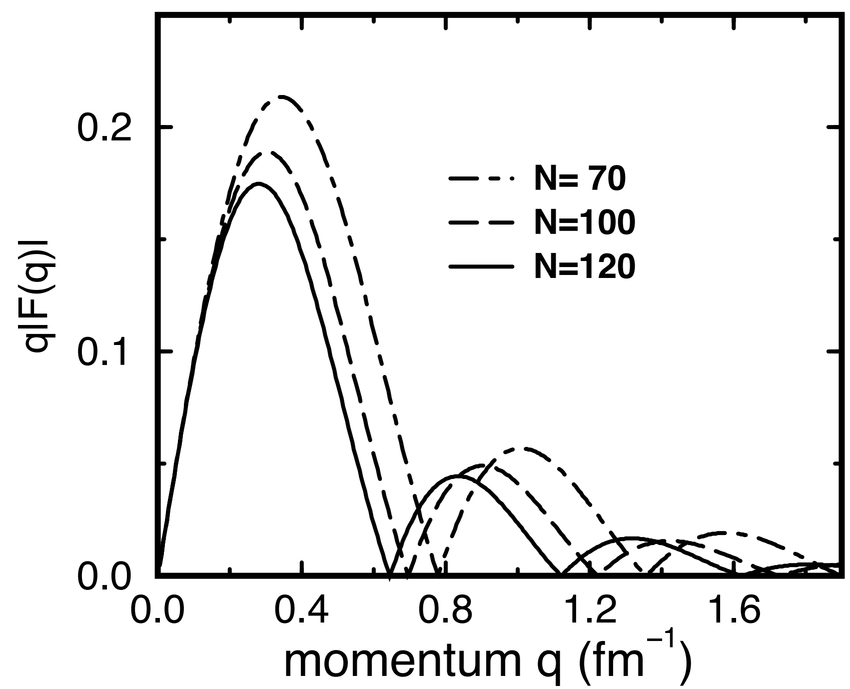
Nuclear Density Functional Theory and Extensions



Neutron skins and halos in nuclear DFT

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



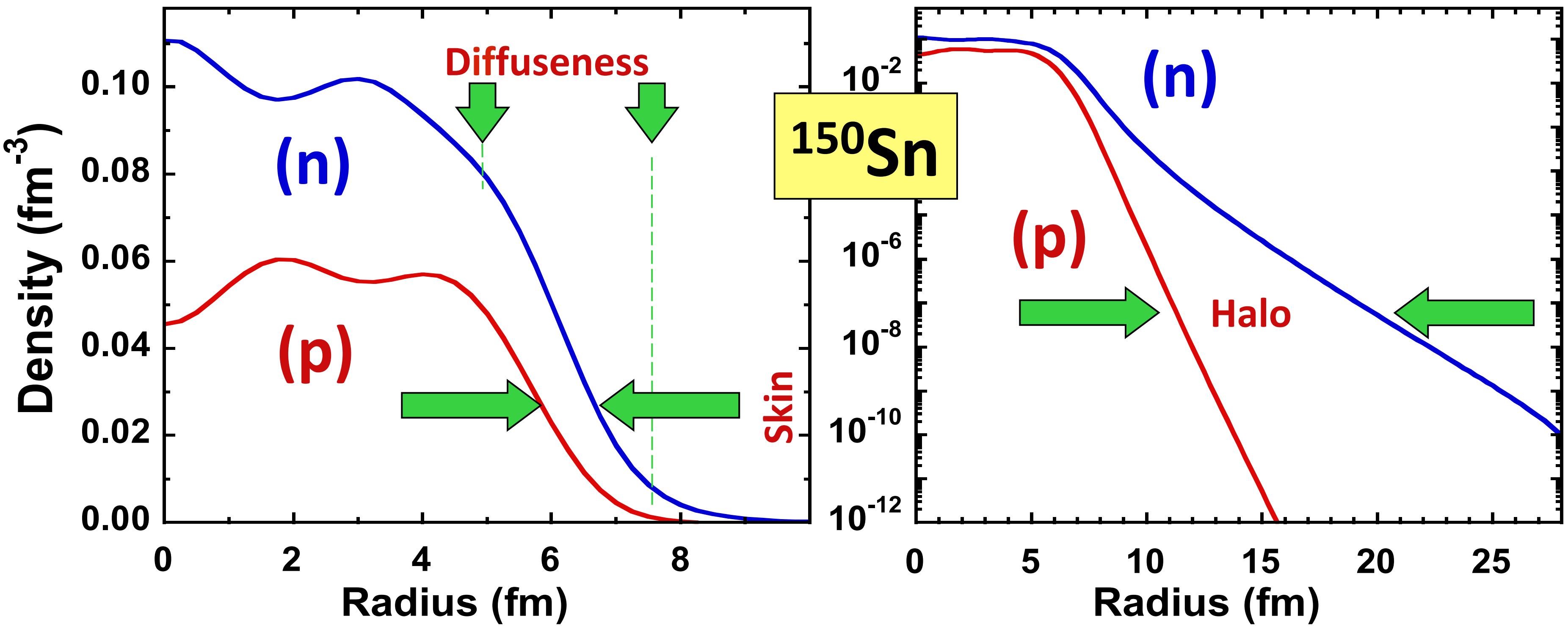


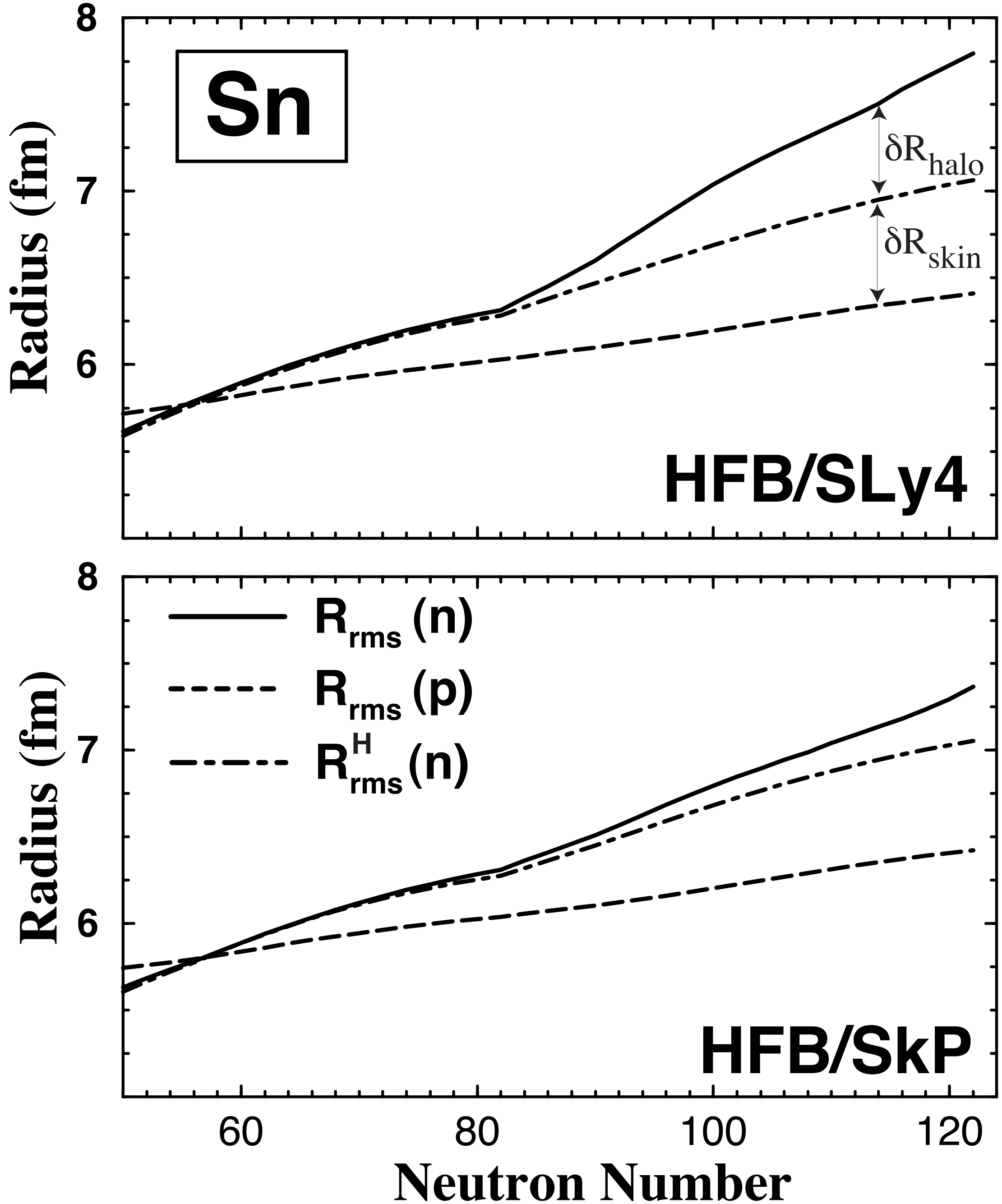
$$R_0 = 4.49341/q_1$$

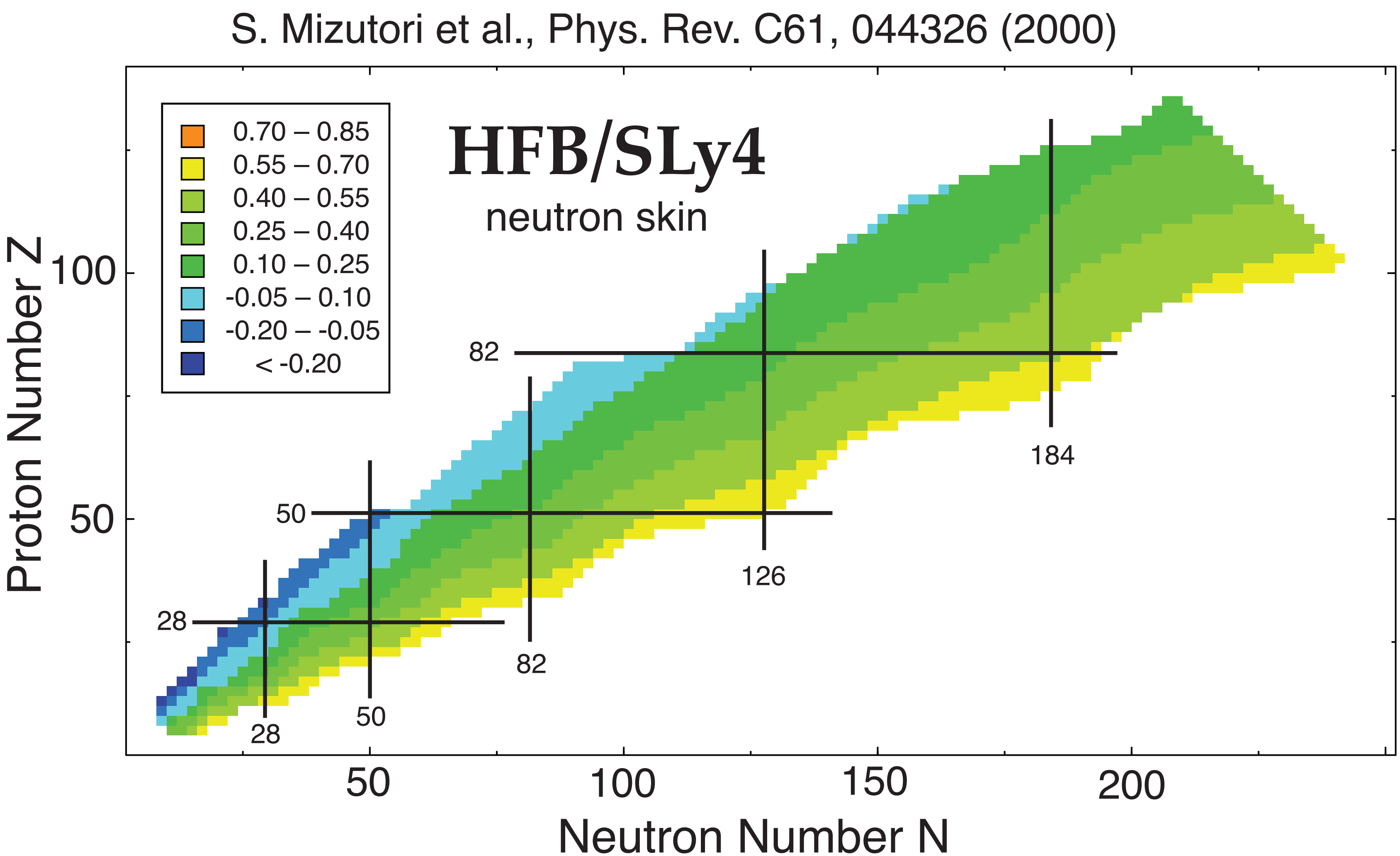
first zero of F(q)

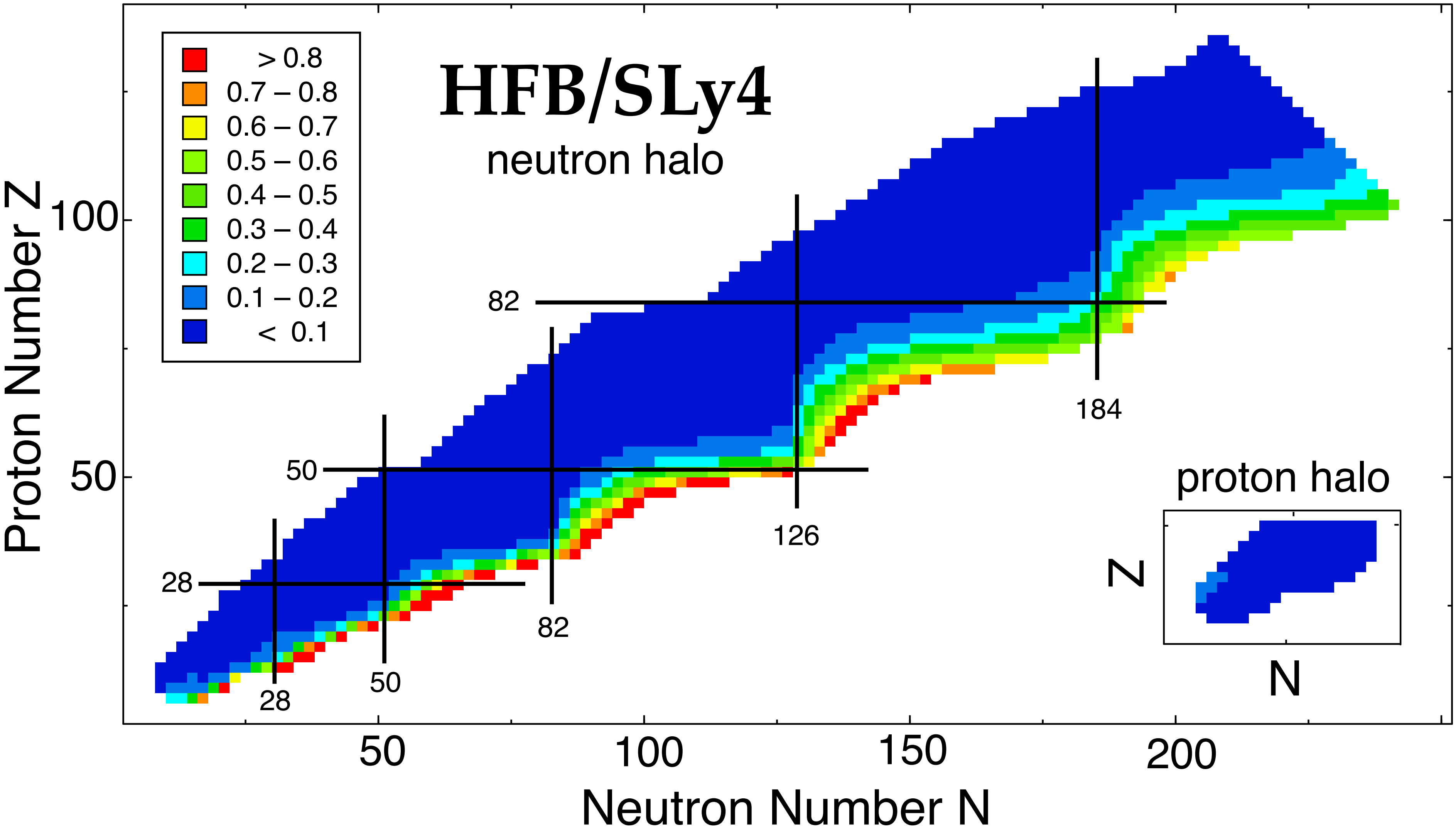
Horowitz's talk

Neutron & proton density distributions




Sn
δR_halo
δR_skin
HFB/SLy4
Radius (fm)
8
7
6
R_rms (n)
R_rms (p)
R^H_rms(n)
HFB/SkP
Radius (fm)
60
80
100
120
Neutron Number

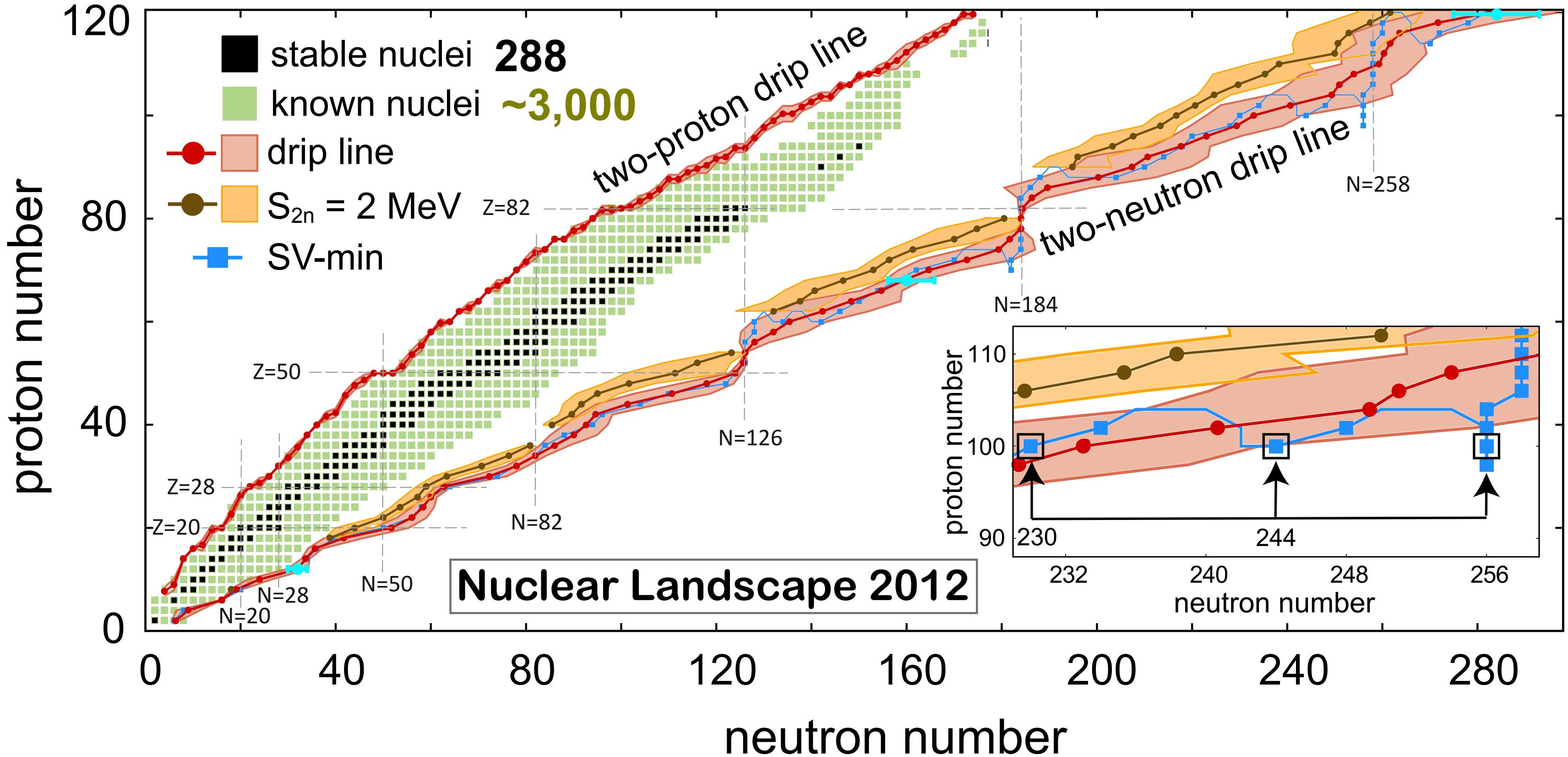

S. Mizutori et al., Phys. Rev. C61, 044326 (2000)
HFB/SLy4
neutron skin
0.70 – 0.85
0.55 – 0.70
0.40 – 0.55
0.25 – 0.40
0.10 – 0.25
-0.05 – 0.10
-0.20 – -0.05
< -0.20
Proton Number Z
Neutron Number N
100
50
150
200
28
82
126
184

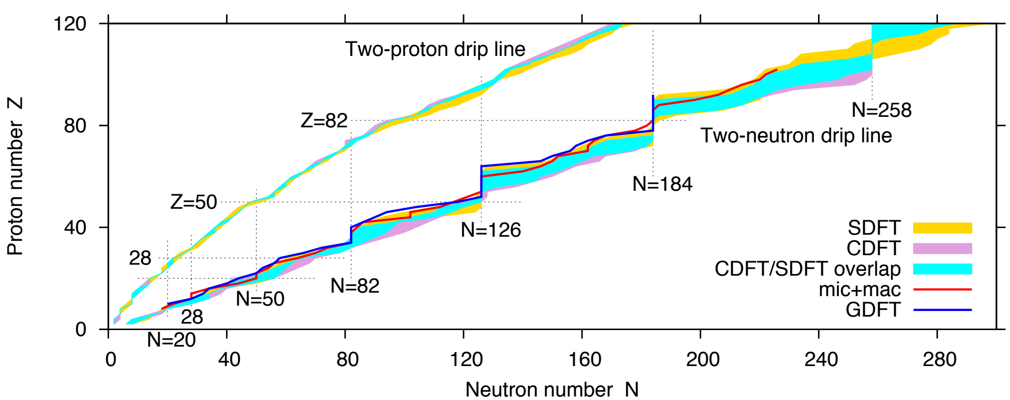


HFB/SLy4
neutron halo
> 0.8
0.7 – 0.8
0.6 – 0.7
0.5 – 0.6
0.4 – 0.5
0.3 – 0.4
0.2 – 0.3
0.1 – 0.2
< 0.1
proton halo
N
N
Proton Number Z
Neutron Number N
28
50
82
126
184
50
100
150
200

The limits: Skyrme-DFT Benchmark 2012

Erler et al, Nature 486, 509 (2012)





A.V. Afanasjev, et al. Phys. Lett. B (2013)

FRIB

Mass eXplorer

AJAX POWERED

Contact

DFT Mass Tables

People

Plotting Tools

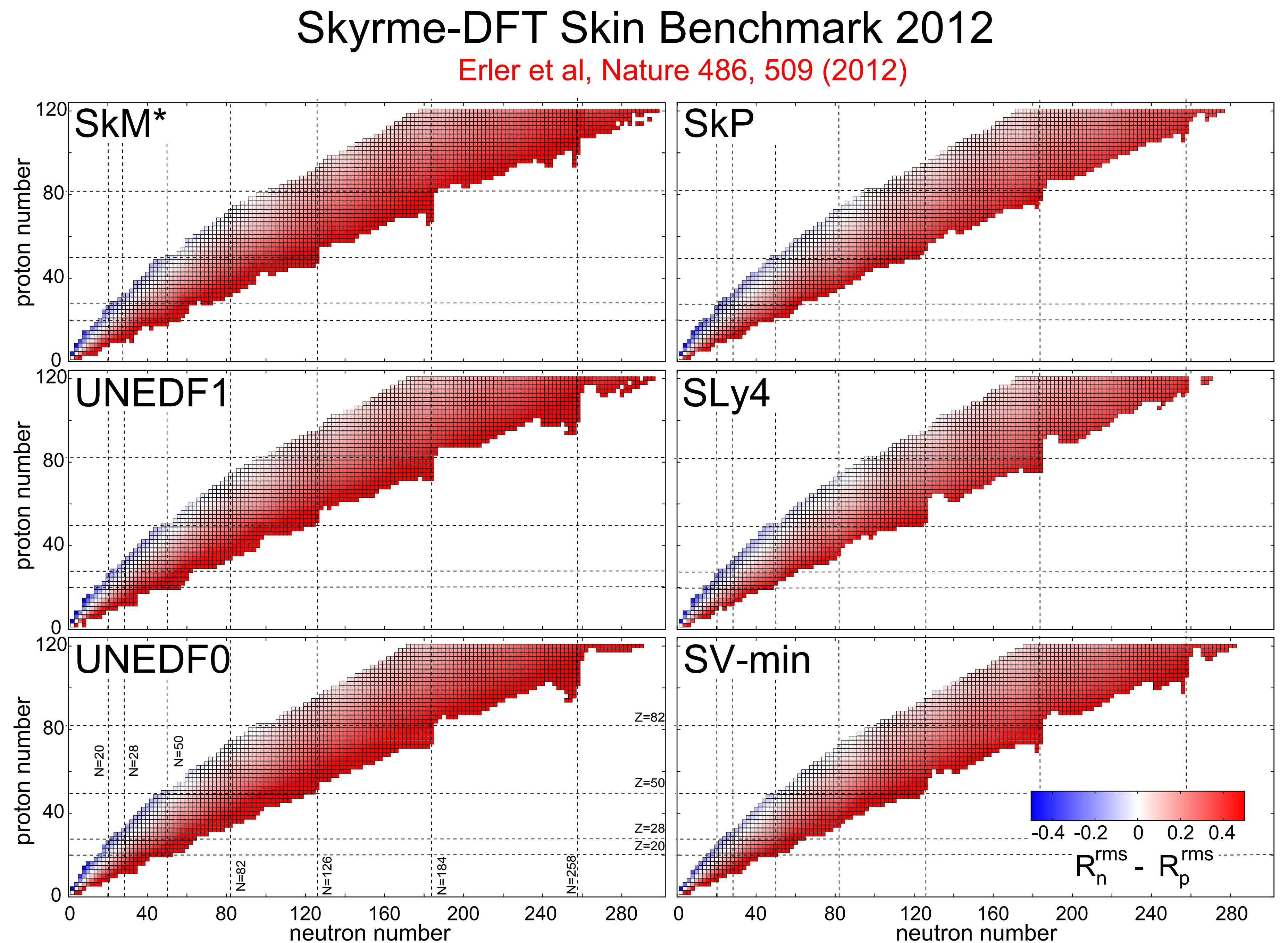
Useful Links

Plotting Tools

Features:

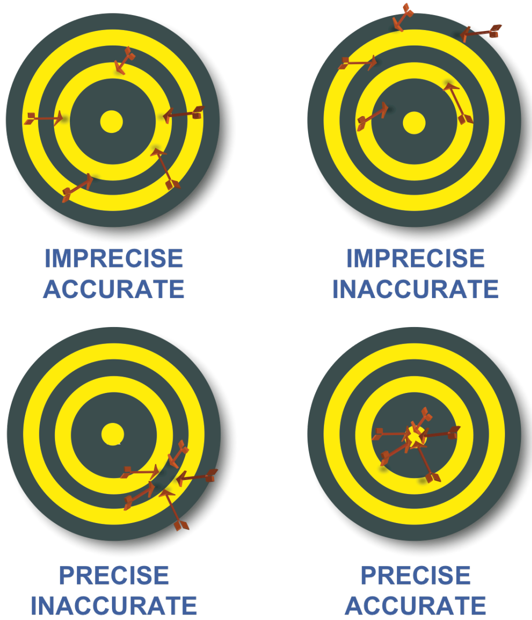
1. Nucleus Data Search
2. Isotope/Isotone/Isobar Chain Plot
3. Separation Energy Plot
4. 3D Quadrupole Deformation Plot

http://massexplorer.frib.msu.edu



Skyrme-DFT Skin Benchmark 2012
Erler et al, Nature 486, 509 (2012)
SkM*
SkP
UNEDF1
SLy4
UNEDF0
SV-min
proton number
neutron number
N=20
N=28
N=50
N=82
N=126
N=184
N=258
Z=82
Z=50
Z=28
Z=20
-0.4 -0.2 0 0.2 0.4
$R_n^{rms} - R_p^{rms}$

"Remember that all models are wrong; the practical question is *how wrong do they have to be to not be useful"* (E.P. Box)



ISNET: Enhancing the interaction between nuclear experiment and theory through information and statistics

JPG Focus Issue: http://iopscience.iop.org/0954-3899/page/ISNET

EXTRAPOLATIONS!

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

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)

Statistical uncertainty in variable A:

$$\overline{\Delta A^2} = \sum_{ij} \partial_{p_i} A (\hat{M}^{-1})_{ij} \partial_{p_j} A, \quad \partial_{p_i} A = \partial_{p_i} A \Big|_{\mathbf{p}_0}$$

covariance matrix

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

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

$$A = \bar{A} \pm (\Delta A)_{\rm stat} \pm (\Delta A)_{\rm syst}$$

Neutron-skin uncertainties of Skyrme EDF

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

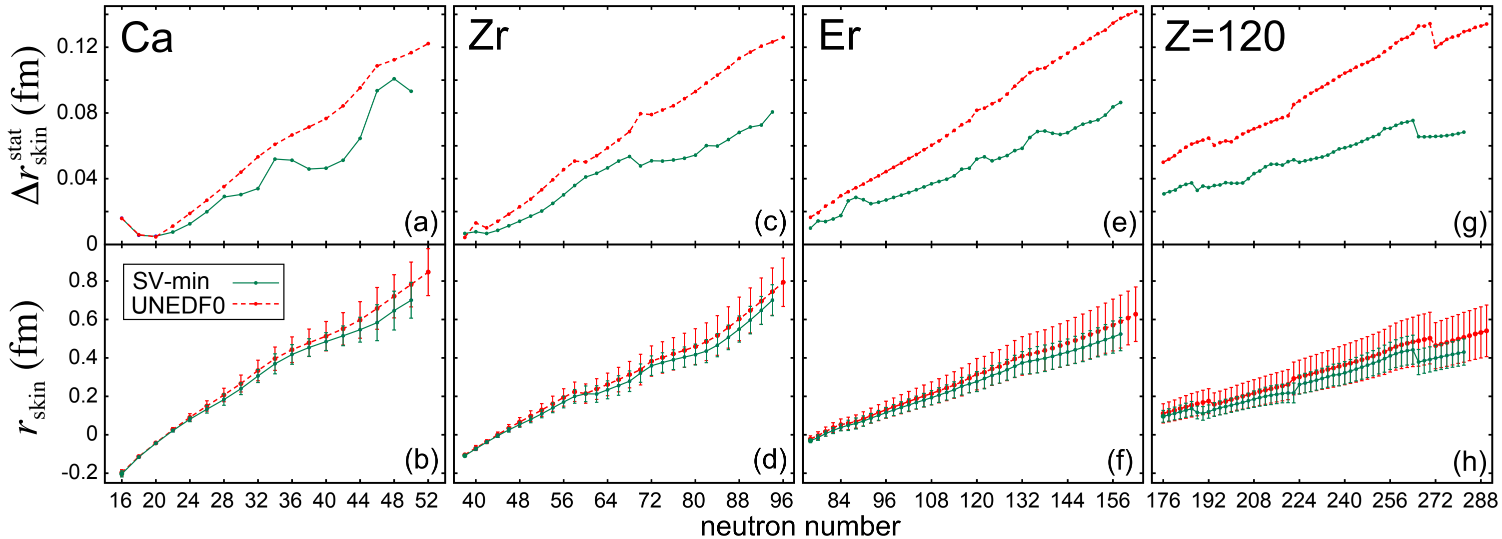
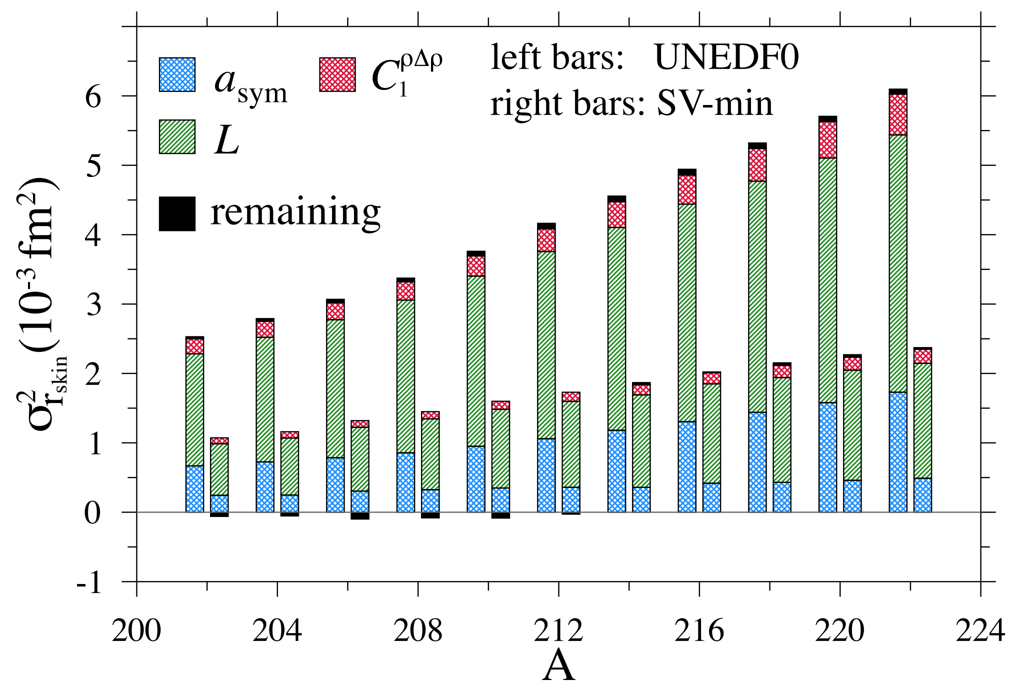


TABLE I. Theoretical uncertainties on r_{skin} in ^{208}Pb and ^{48}Ca (in fm). Shown are statistical errors of UNEDF0 and SV-min, systematic error Δr_{skin}^{syst}, the model-averaged deviation of Ref. [9], and errors of PREX [25] and planned PREX-II [29] and CREX [30] experiments.

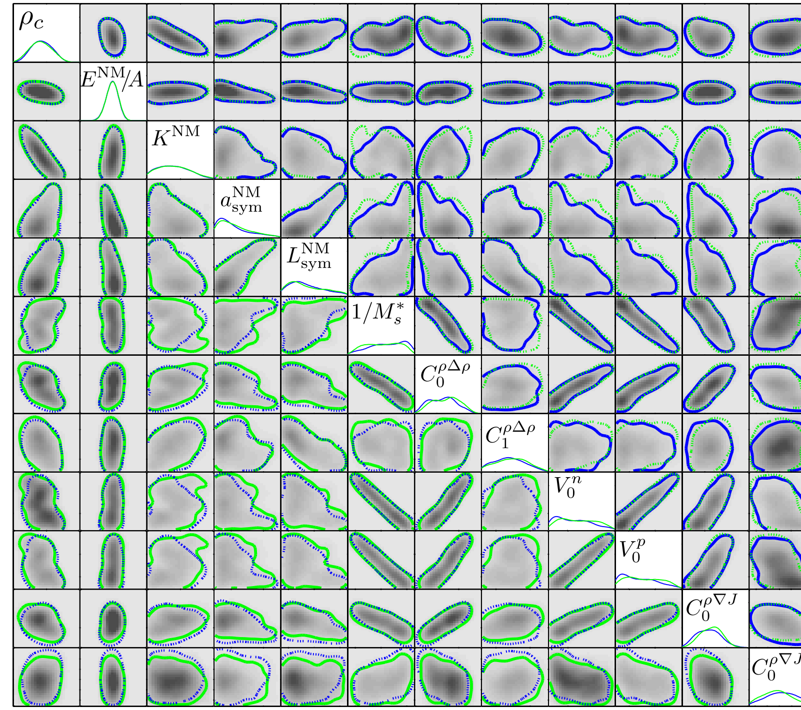
nucleus	Δr_{skin}^{stat} UNEDF0	Δr_{skin}^{stat} SV-min	Δr_{skin}^{syst}	Ref. [9]	Experiment
^{208}Pb	0.058	0.037	0.013	0.022	0.18 [25], 0.06[29]
^{48}Ca	0.035	0.026	0.019	0.018	0.02 [30]

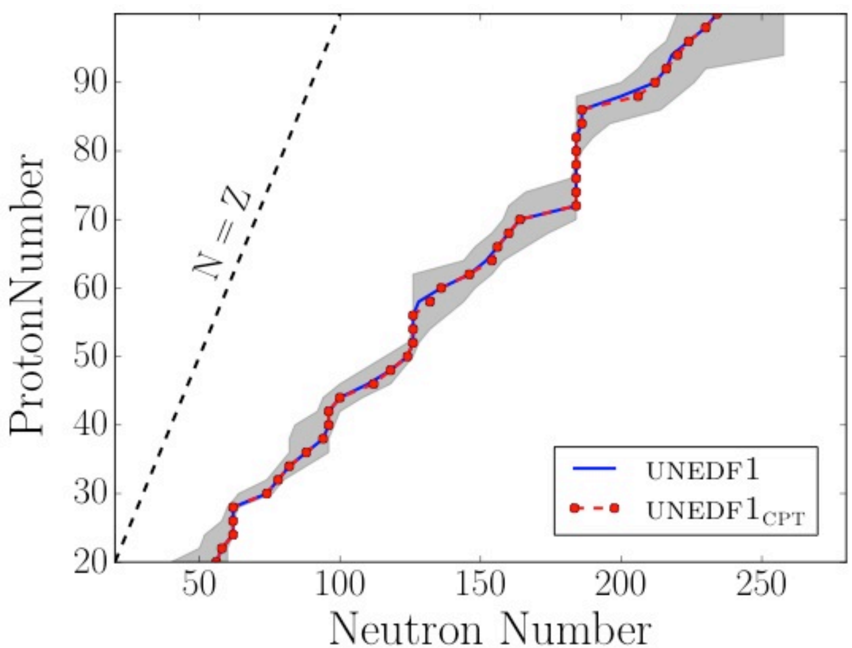


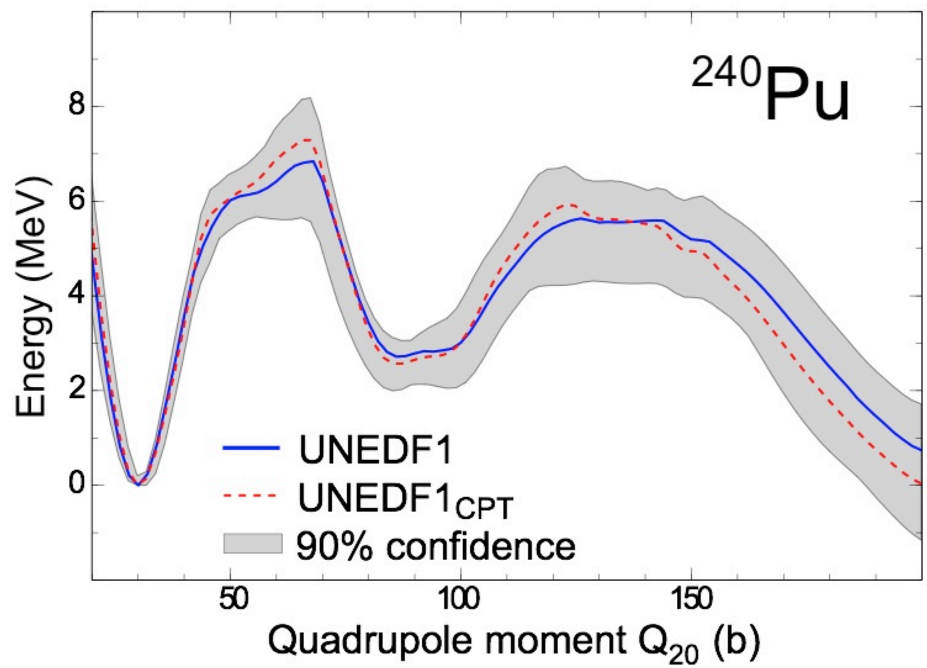
Bayesian inference methods

Uncertainty Quantification for Nuclear Density Functional Theory and Information Content of New Measurements

J. McDonnell et al. Phys. Rev. Lett 114, 122501 (2015).



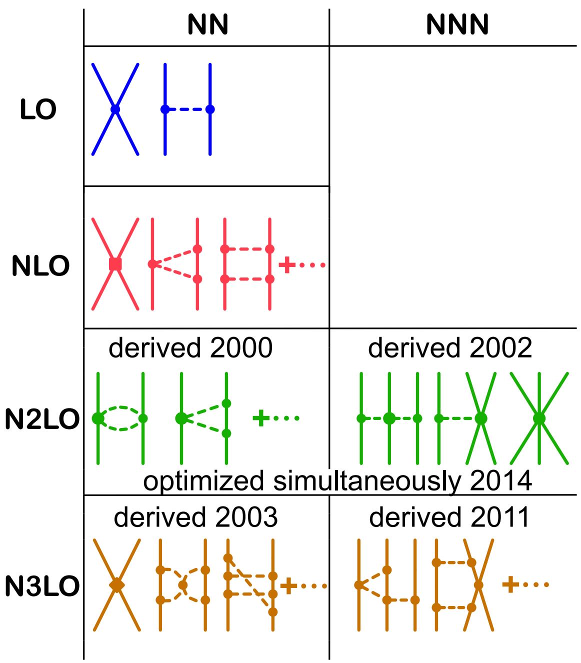


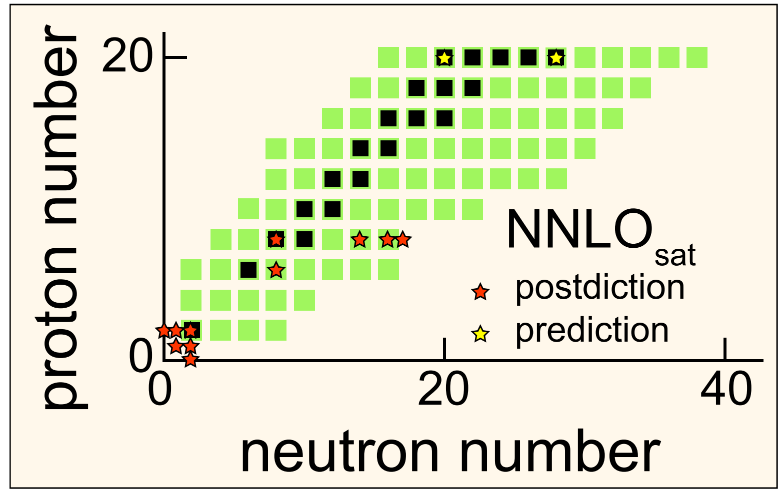


The frontier: calcium isotopes

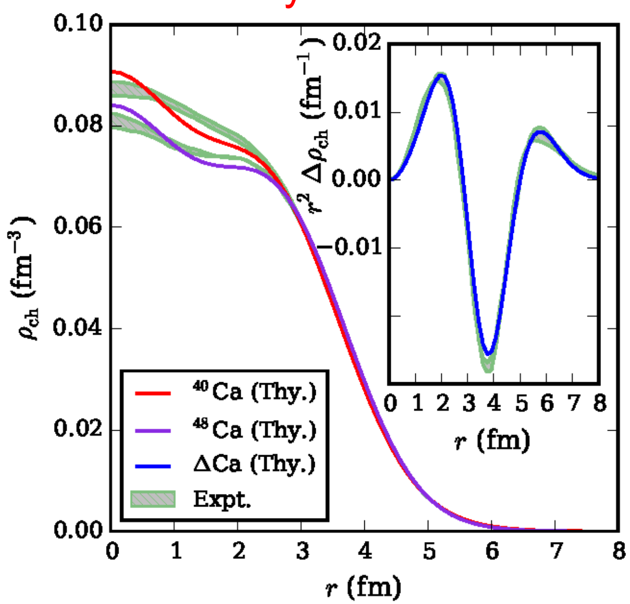
Quantified input

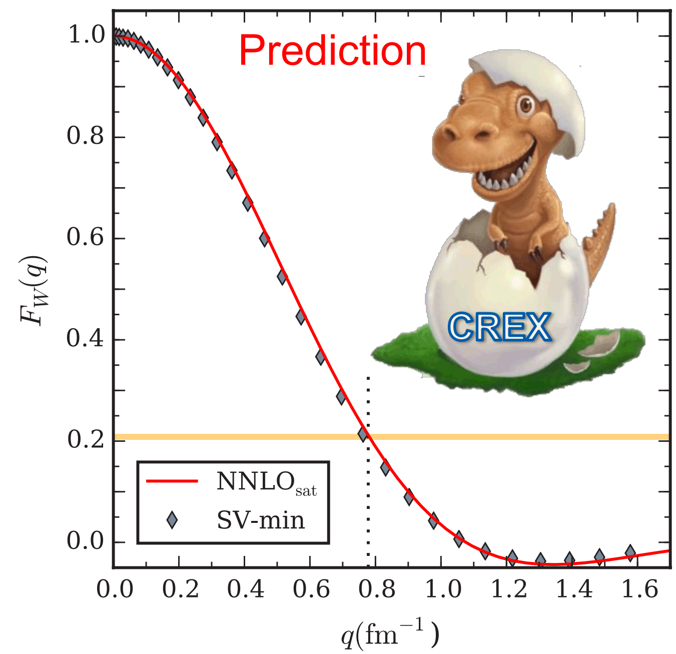
Nuclear Forces from χEFT





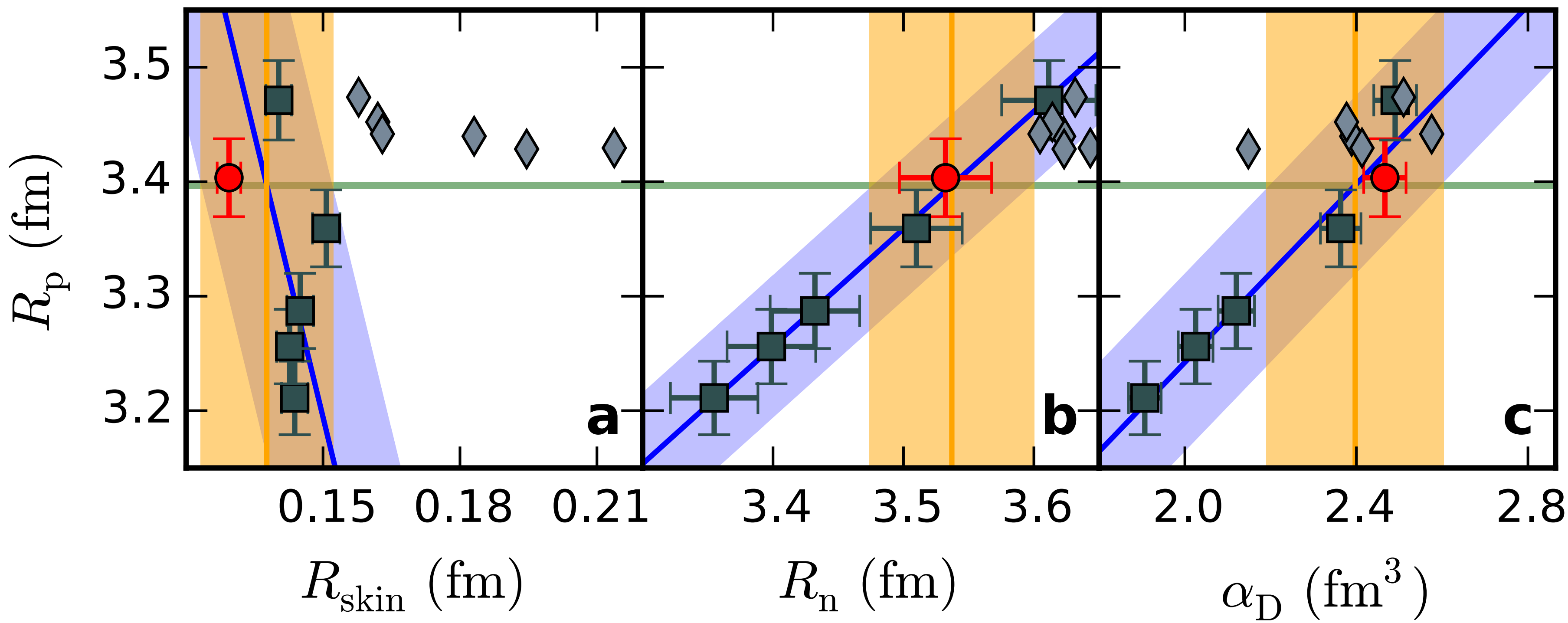
Consistency with known data





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

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



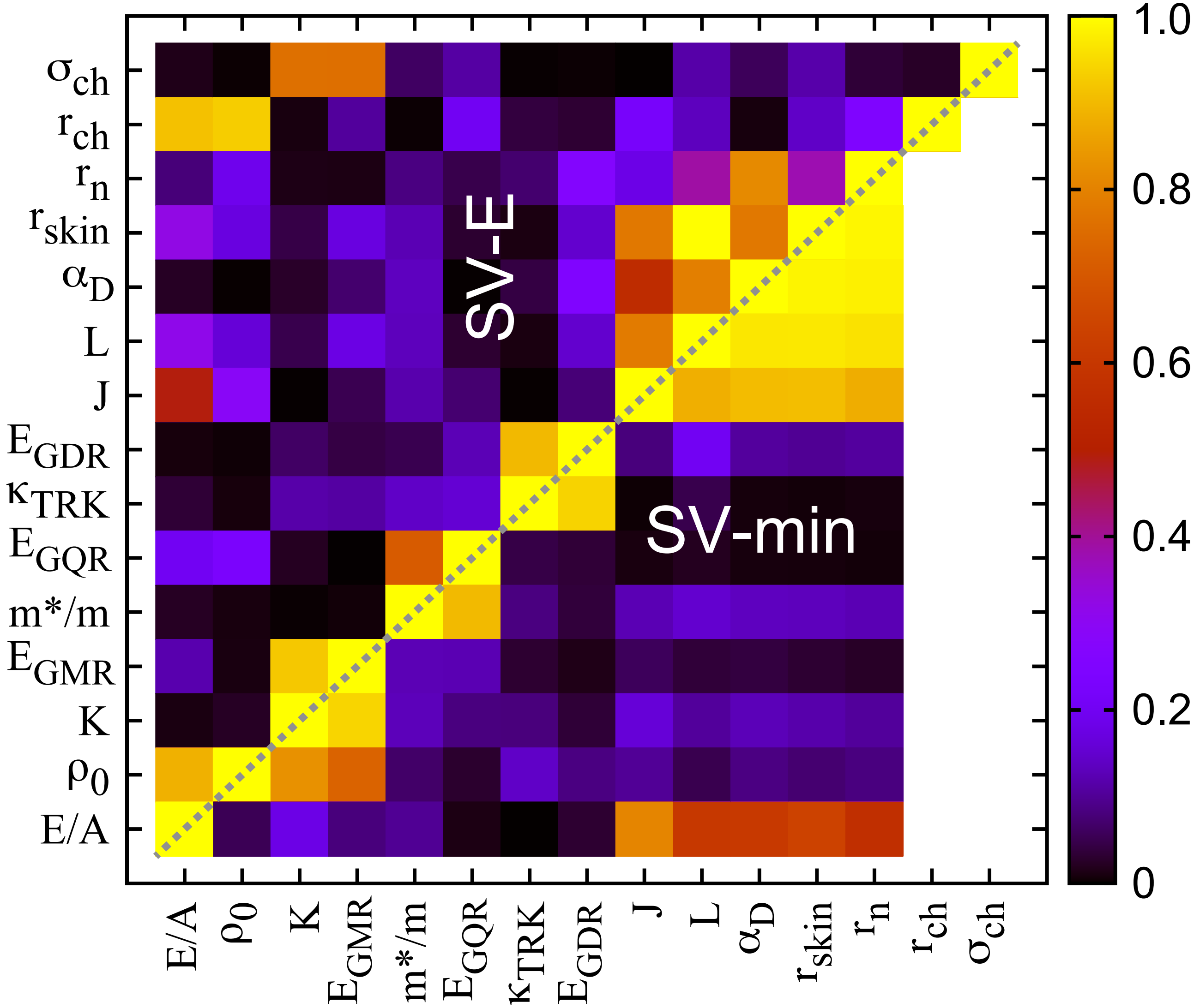
Nuclear charge and neutron radii and nuclear matter: trend analysis in Skyrme-DFT approach

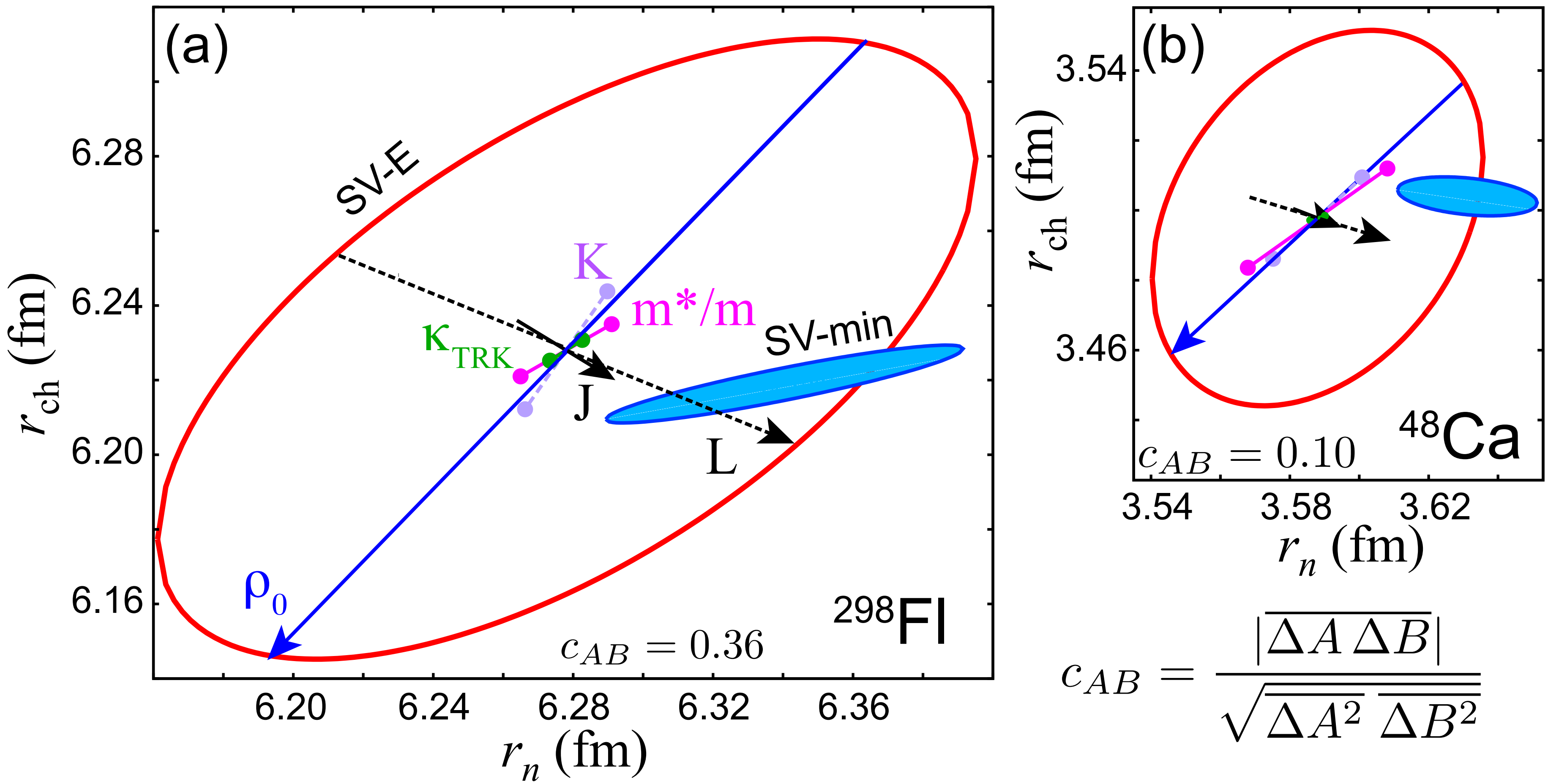
P.-G. Reinhard and WN, PRC 93, 051303 (R) (2016)

	SV-min	(E, R)	SV-E	(E)
ρ_0 (MeV)	0.161085	$\pm$ 0.0011	0.154181	$\pm$ 0.0076
E/A (MeV)	-15.9099	$\pm$ 0.04	-15.8120	$\pm$ 0.17
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
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
$C_0^{\nabla \mathbf{J}}$ (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
$V_{\mathrm{pair,p}}$ (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

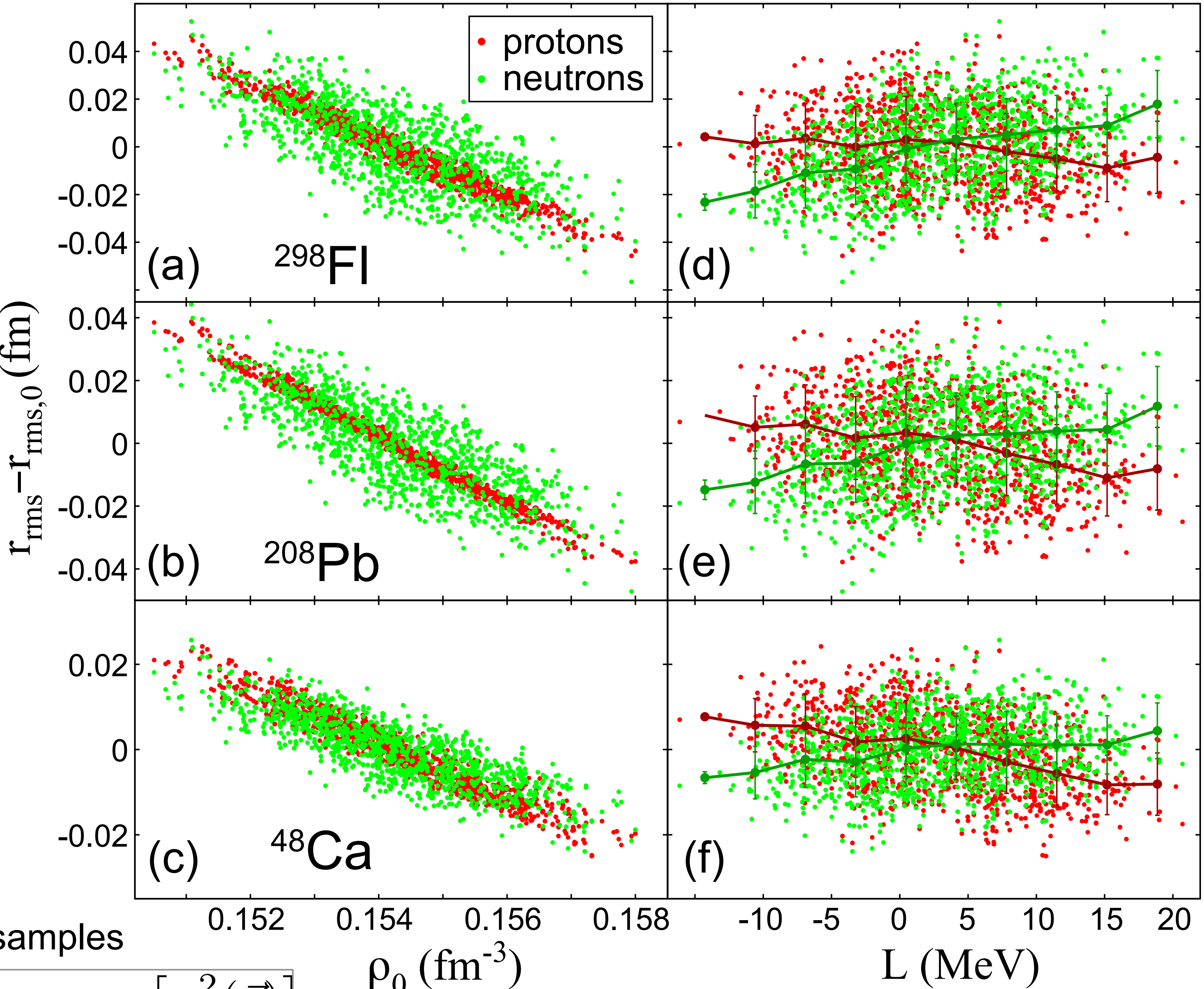
Nuclear charge and neutron radii and nuclear matter: trend analysis in Skyrme-DFT approach

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



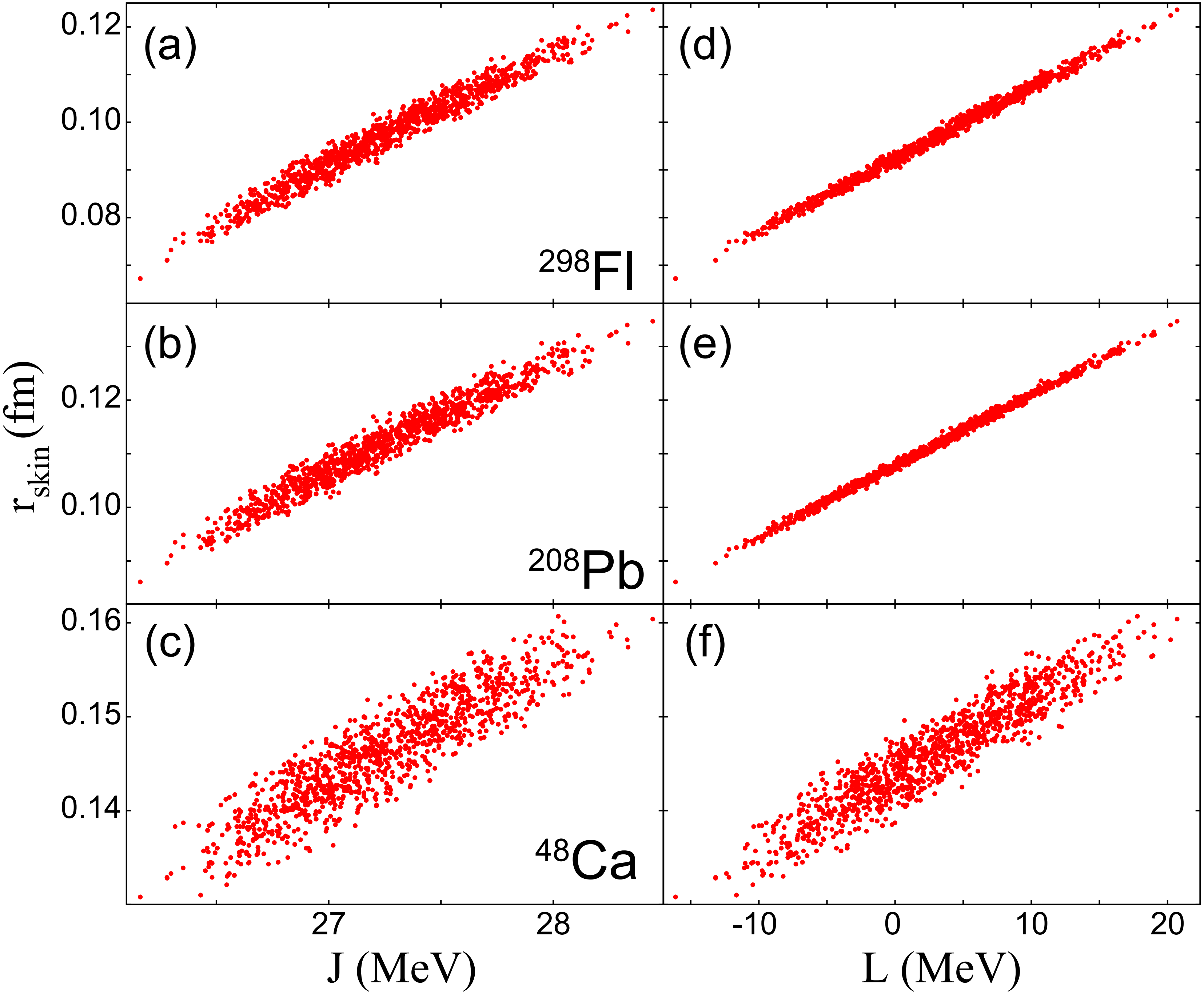


$$c_{AB} = \frac{|\overline{\Delta A\, \Delta B}|}{\sqrt{\overline{\Delta A^2}\ \overline{\Delta B^2}}}$$

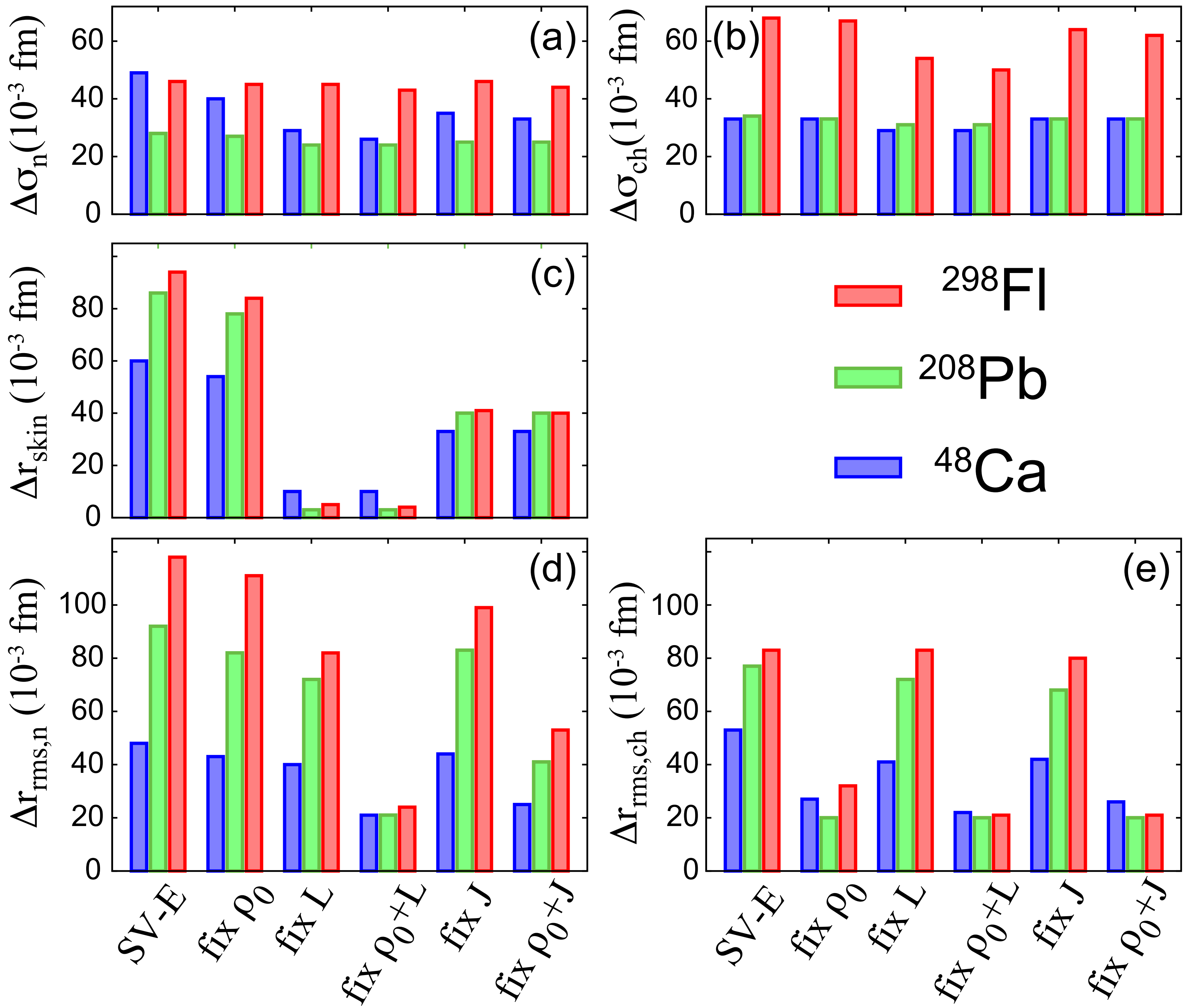


2000 samples

$$W(\vec{p}) \propto \exp\left[\chi^2(\vec{p})\right]$$



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



(a)
(b)
(c)
(d)
(e)
$\Delta\sigma_n (10^{-3}$ fm)
$\Delta\sigma_{ch} (10^{-3}$ fm)
Δr_{skin} (10^{-3} fm)
$\Delta r_{rms,n}$ (10^{-3} fm)
$\Delta r_{rms,ch}$ (10^{-3} fm)
^{298}Fl
^{208}Pb
^{48}Ca
SV-E
fix ρ_0
fix L
fix ρ_0+L
fix J
fix ρ_0+J

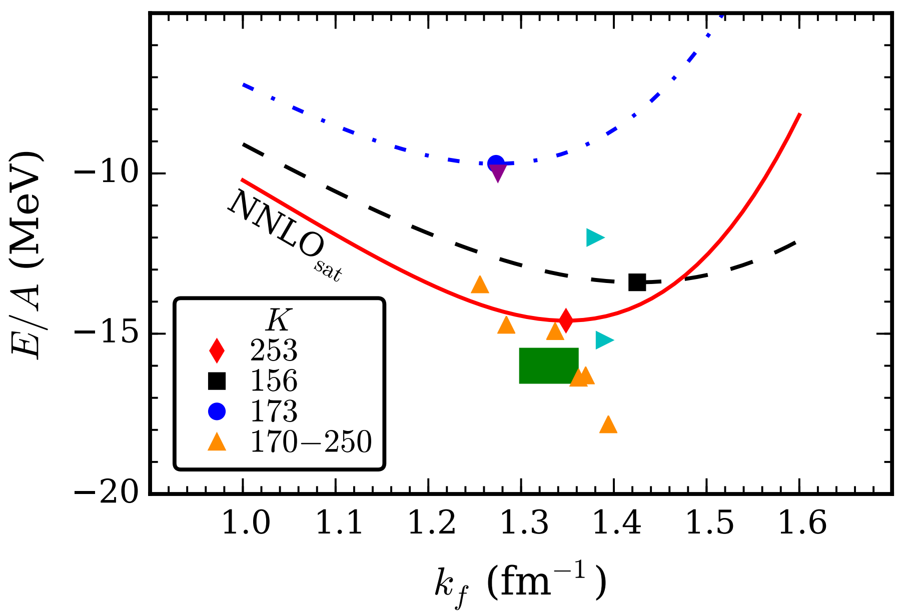
- We explored various trends of charge and neutron radii with nuclear matter properties.
- There exist, at least within the Skyrme-DFT theory, only two strong correlations:
  - one-to-one relation between charge radii in finite nuclei and ρ_0: $R_{ch} \leftrightarrow \rho_0$
  - one-to-one relation between 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_{ch}, so by constraining the saturation density alone does not help significantly reducing the uncertainty on neutron (and mass) radii.
- The $R_n \leftrightarrow R_p$ relation is fairly complex: various trends are possible when moving along *a* trajectory in a parameter space.

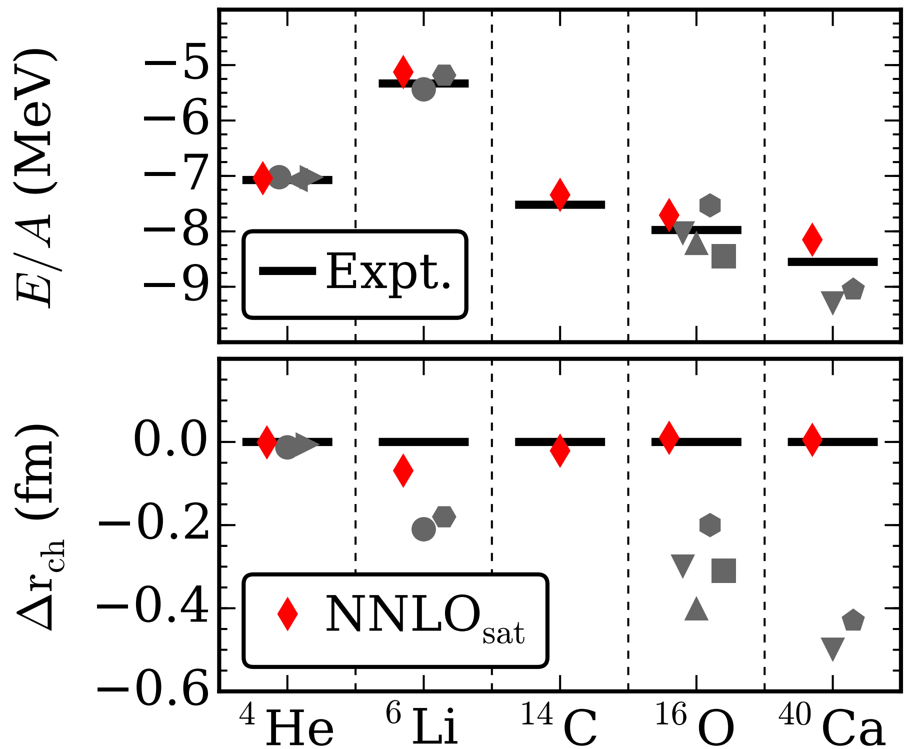
Coupled Cluster informing DFT
and
DFT informing Coupled Cluster

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

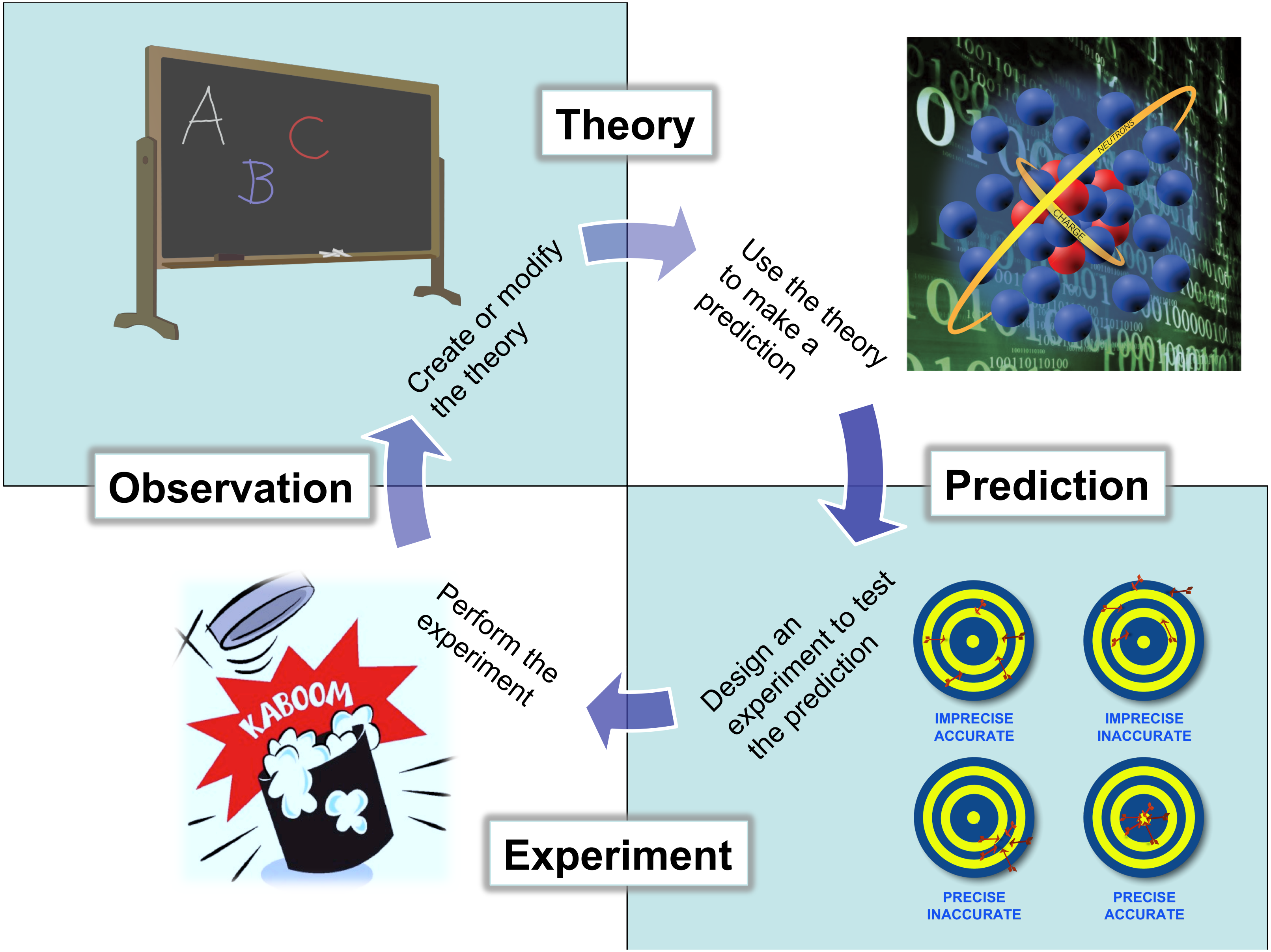
A. Ekström et al. Phys. Rev. C 91, 051301(R) (2015)

- Order-by-order optimization (here: NN and NNN in N2LO)
- Constrained by data on few-body systems and light nuclei
- Focus on low-momentum physics





Instead of conclusions…



WN, J. Phys. G 43, 044002 (2016)
http://iopscience.iop.org/article/10.1088/0954-3899/43/4/044002

BACKUP

"It is exceedingly difficult to make predictions, particularly about the future" (Niels Bohr)

Outlook: Looking into the crystal ball
10 nuclear structure theory greatest hits for the next 10–15 years

J. Phys. G 43, 044002 (2016) http://iopscience.iop.org/article/10.1088/0954-3899/43/4/044002

1. We will describe the lightest nuclei in terms of lattice QCD and understand the QCD origin of nuclear forces.
2. We will develop a predictive framework for light, medium-mass nuclei, and nuclear matter from 0.1 to twice the saturation density. *Ab initio* methods will reach heavy nuclei in the next decade.
3. We will develop predictive and quantified nuclear energy density functional rooted in *ab initio* theory. This spectroscopic-quality functional will properly extrapolate in mass, isospin, and angular momentum to provide predictions in the regions where data are not available.
4. We will provide the microscopic underpinning of collective models that explain dynamical symmetries and simple patterns seen in nuclei. In this way, we will link fundamental and emergent aspects of nuclear structure.
5. By developing many-body approaches to light-ion reactions and large-amplitude collective motion, we will have at our disposal predictive models of fusion and fission.
6. By exploring quantum many-body approaches to open systems, we will understand the mechanism of clustering and explain properties of key cluster states and cluster decays.
7. By taking advantage of realistic many-body theory, we will unify the fields of nuclear structure and reactions.
8. We will achieve a comprehensive description, based on realistic structural input, of nuclear reactions with complex projectiles and targets, involving direct, semi-direct, pre-equilibrium, and compound processes.
9. We will carry out predictive and quantified calculations of nuclear matrix elements for fundamental symmetry tests in nuclei and for neutrino physics.
10. By taking the full advantage of extreme-scale computers, we will master the tools of uncertainty quantification. This will be essential for enhancing the coupling between theory and experiment —to provide predictions that can be trusted.