Nuclear charge and neutron radii and nuclear matter: correlation analysis

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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.
Today's posterior is tomorrow's prior
Consider a model described by coupling constants $\theta_1, \theta_2...\theta_\kappa$. 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.

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

- Objective function
- Model predictions
- Expected uncertainties
- fit-observables (may include pseudo-data)
How to quantify inter-model correlations?

Parameter estimation. The set of fit-observables.
Example of inter-model correlation analysis


<table>
<thead>
<tr>
<th>Model</th>
<th>$C_{AB}^{\text{model}}$</th>
<th>Slope</th>
<th>Intercept</th>
</tr>
</thead>
<tbody>
<tr>
<td>Skyrme</td>
<td>0.9959</td>
<td>29.0847</td>
<td>15.5290</td>
</tr>
<tr>
<td>DD-ME</td>
<td>0.9939</td>
<td>31.9907</td>
<td>14.5206</td>
</tr>
<tr>
<td>NL3/FSU</td>
<td>0.9941</td>
<td>29.8864</td>
<td>13.9692</td>
</tr>
</tbody>
</table>

$\alpha_D^{[208\text{Pb}]}$

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

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

### Purpose:
- Determine the new global relation/law
- Determine unknown $y_2$ given measured $y_1$
- Learn about constraints on models

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

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

C_{AB}^{\text{models}} = 0.769
Example of inter-model correlation analysis (2)


\[ R_p \text{ (fm)} = y_1 \]

\[ R_{\text{skin}} \text{ (fm)} = y_2 \]

\[ R_n \text{ (fm)} = y_3 \]

\[ \alpha_D \text{ (fm}^3) = y_4 \]

\[ y_i [\hat{\theta}(M\alpha)] \]
\[ \hat{\theta}(M_\alpha) \equiv \theta(M_\alpha)_{\text{MLE}} \]

Talk by Bulaevskaya

please help!
Beware of spurious correlations!

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

US spending on science, space, and technology correlates with Suicides by hanging, strangulation and suffocation

C=0.9979

C=0.9668
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
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 $E(y)$, $\text{var}(y)$.
- Vary variable $y$ in a reasonable range given by $\text{var}(y)$. Refit $\theta$ for each value of $y$.
- Study $E(y|y)$.
- Example: SV-bas, PRC 79 034310 (2009)
Radii in nuclear DFT

\[ R_{\text{diff}} = \frac{4.49341}{q_1} \]

\[ R_{\text{diff}} \approx r_0 A^{1/3} \]
Neutron & proton density distributions

Density (fm$^{-3}$)

Radius (fm)

$^{150}\text{Sn}$

Diffuseness

Skin
Finite size effects and leptodermous expansion


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

Wigner-Seitz radius

\[ r_{\text{rms}} = \sqrt{\frac{3}{5}} \sqrt{R_{\text{diff}}^2 + 5q^2} \]

around 1fm
Neutron-skin uncertainties of Skyrme EDF

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

<table>
<thead>
<tr>
<th>nucleus</th>
<th>$\Delta r_{\text{skin}}^{\text{stat}}$</th>
<th>$\Delta r_{\text{skin}}^{\text{stat, UNEDF0}}$</th>
<th>$\Delta r_{\text{skin}}^{\text{stat, SV-min}}$</th>
<th>$\Delta r_{\text{skin}}^{\text{syst}}$</th>
<th>Ref. [9]</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{208}$Pb</td>
<td>0.058</td>
<td>0.037</td>
<td>0.013</td>
<td>0.022</td>
<td>0.18 [25], 0.06 [29]</td>
<td></td>
</tr>
<tr>
<td>$^{48}$Ca</td>
<td>0.035</td>
<td>0.026</td>
<td>0.019</td>
<td>0.018</td>
<td>0.02 [30]</td>
<td></td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>SV-min</th>
<th>(Y=E, R)</th>
<th>SV-E</th>
<th>(Y=E)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_0$ (MeV)</td>
<td>0.161085 ± 0.0011</td>
<td>0.154181 ± 0.0076</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$E/A$ (MeV)</td>
<td>−15.9099 ± 0.04</td>
<td>−15.8120 ± 0.17</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$K$ (MeV)</td>
<td>221.752 ± 8.1</td>
<td>273.733 ± 31.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$m^*/m$</td>
<td>0.951806 ± 0.067</td>
<td>1.07038 ± 0.103</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$J$ (MeV)</td>
<td>30.6570 ± 1.9</td>
<td>27.2333 ± 2.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$L$ (MeV)</td>
<td>44.8138 ± 25.7</td>
<td>2.92329 ± 62.9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\kappa_{TRK}$</td>
<td>0.076522 ± 0.1919</td>
<td>0.192 ± 0.349</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_0^\Delta\rho$ (MeV fm$^5$)</td>
<td>107.657 ± 6.6</td>
<td>85.39992 ± 10.7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_1^\Delta\rho$ (MeV fm$^5$)</td>
<td>−141.506 ± 162</td>
<td>−80.90533 ± 391</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_0^{\nabla J}$ (MeV fm$^4$)</td>
<td>−101.582 ± 5.5</td>
<td>−96.3170 ± 11.7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_1^{\nabla J}$ (MeV fm$^4$)</td>
<td>−22.9681 ± 16.2</td>
<td>−21.5881 ± 18.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$V_{\text{pair},p}$ (MeV fm$^3$)</td>
<td>601.160 ± 190</td>
<td>613.231 ± 209</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$V_{\text{pair},n}$ (MeV fm$^3$)</td>
<td>567.190 ± 154</td>
<td>568.739 ± 173</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\rho_0,\text{pair}$ (fm$^{-3}$)</td>
<td>0.211591 ± 0.052</td>
<td>0.202513 ± 0.046</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Nuclear charge and neutron radii, and nuclear matter: intra-model trend analysis

P.-G. Reinhard and WN, PRC (R) (2016)
$r_{ch}$ (fm)

$48$ Ca

$|\Delta A\Delta B|$

$\sqrt{\Delta A^2 \Delta B^2}$

$c_{AB} = 0.10$

$c_{AB} = 0.36$

$298$ Fl
2000 Gaussian samples of $L(\theta)$
\[ \Delta r_n = \Delta r_p + \Delta r_{\text{skin}} \]
• 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:
  o one-to-one relation between charge radii in finite nuclei and \( \rho_0 \): \( r_p \leftrightarrow \rho_0 \)
  o 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.
\( \text{N2LO}_{\text{sat}} \) describes low-energy NN and Nuclei


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

Coupled Cluster informing DFT
and
DFT informing Coupled Cluster