Sloppiness of nuclear structure models

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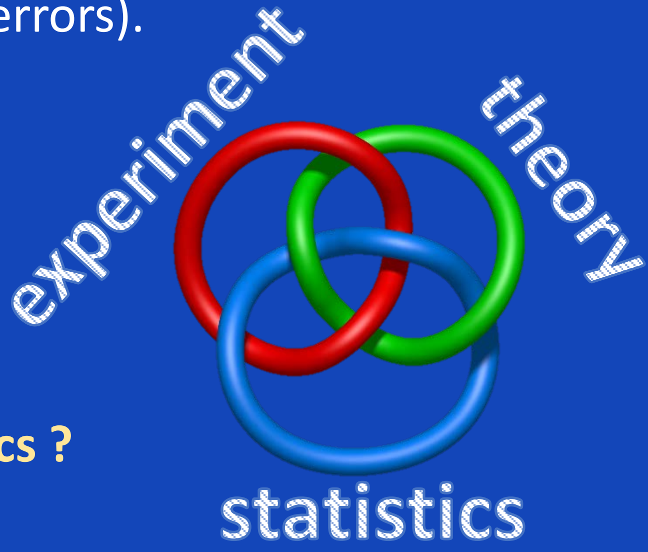
Bayesian Methods in Nuclear Physics, INT Seattle

Research aim:

understand how statistics can be merged with physics to construct <u>better</u> theoretical models and drive the experimental effort.

<u>Better:</u>

- Experimental data - theoretical model adequacy,
- Quantified predictive power,
- Quantified information contents of (missing) observables, what will be the impact of new data on theory (experiment design) ?
- Bias under control (priors, role of systematic errors).



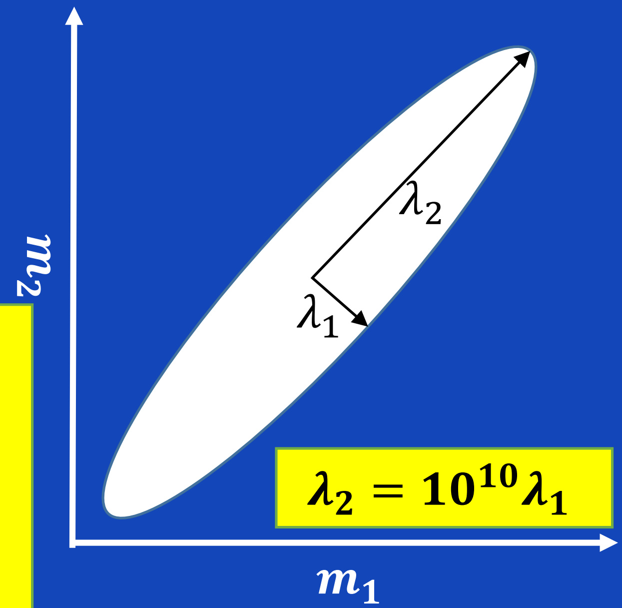
A paradigm shift in (theoretical) nuclear physics ?

Sloppiness in nuclear physics, why we should care ?

$$d^{th} = Gm$$
$$m^{L2} = (\mathbf{G}^T\mathbf{G})^{-1}G^T d^{exp}$$
$$cov(m^{L2}) = \sigma^2(\mathbf{G}^T\mathbf{G})^{-1}$$

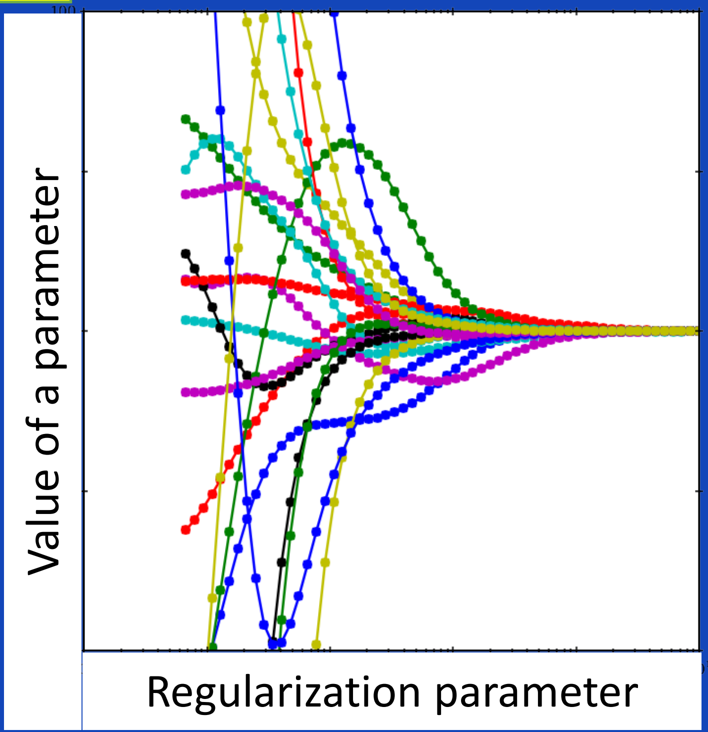
$$H_{ij} = \frac{C^2}{\partial m_i \partial m_j} \approx J^T J$$

Condition number of G ($\sigma_{max}/\sigma_{min}$) very large!
Minor changes in G cause great changes in G^{-1} (noise amplification)



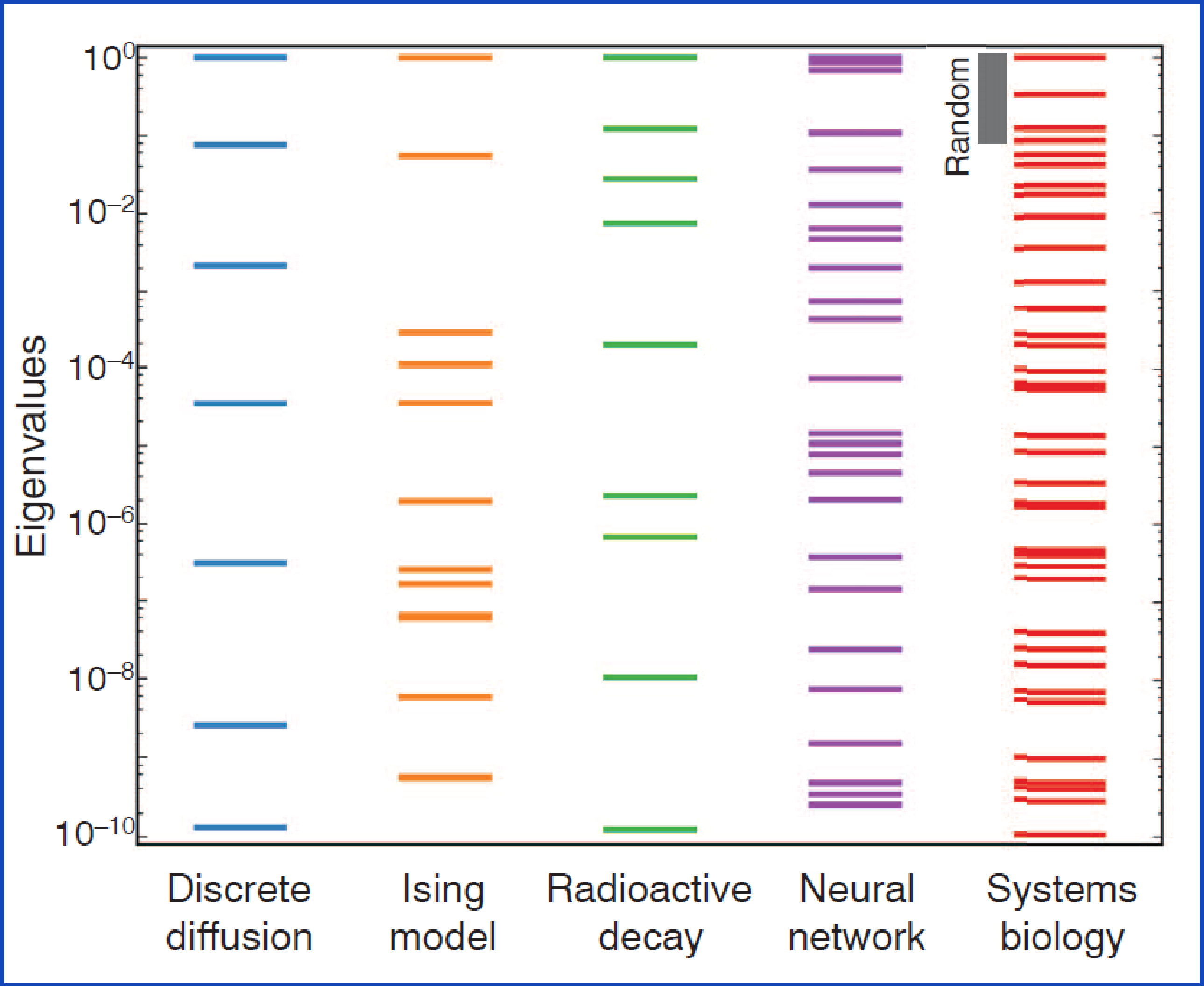
In statistics known as a collinearity.
“Rediscovered” and extended in the field of system biology.
Differential geometry interpretation – D. Vretenar will show the first applications in nuclear physics!

M. K. Transtrum et.al., PRL 104, 060201 (2010)
B. B. Machta et al., Science, 342 (2013)
M. K. Transtrum et.al., PRE 83, 036701 (2011)



Parameters fluctuate but model remains predictive.
Model calibration can become challenging.

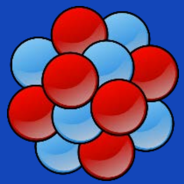
Eigenvalues of the Fisher Information Matrix



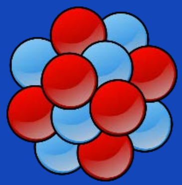
Parameter Space Compression Underlines Emergent Theories and Predictive Models

Benjamin B. Machta, Ricky Chachra, Mark K. Transtrum, James P. Sethna

Science vol. 342, nov. 2013



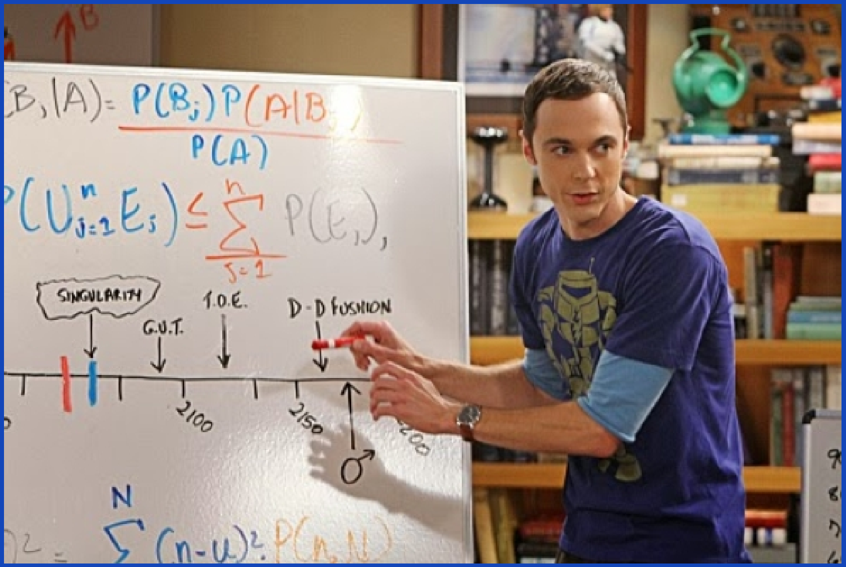
Low-energy nuclear physics models are different.
Most of them are inexact.
Most of them are sloppy.



Nuclear data is different.
Similar information content, redundancy.

How to deal with these ?

Add *a priori expectations*, physical constraints and use Bayesian methods to reduce the sloppiness of models.



Learn from inverse problems field.

Toys

- Nuclear shell model
- Energy Density Functionals

Tools

- Nonlinear least-squares (sorry!)
- Regularization methods

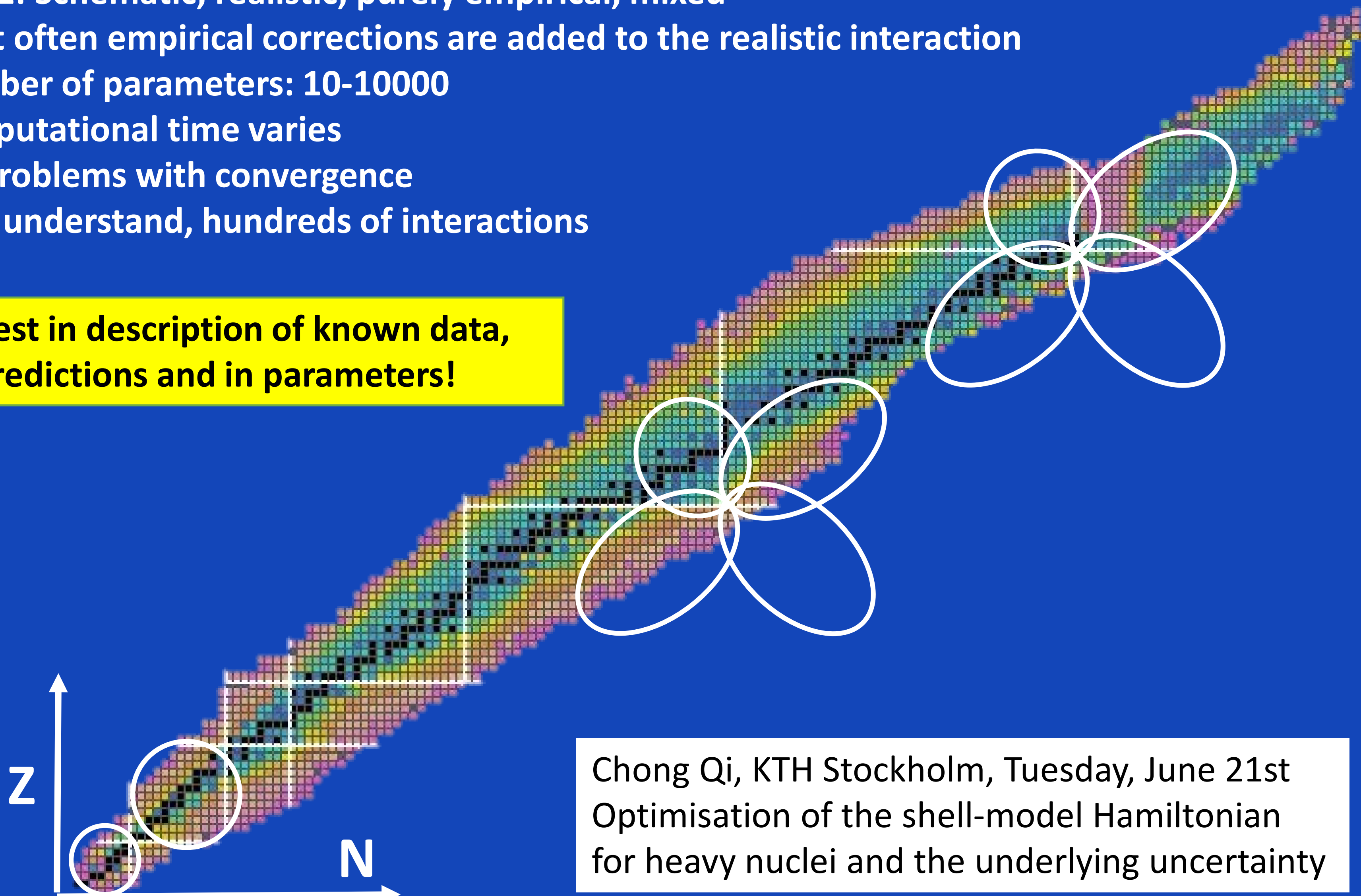
Illustrations

Nuclear structure models (part 1/5)

Shell model

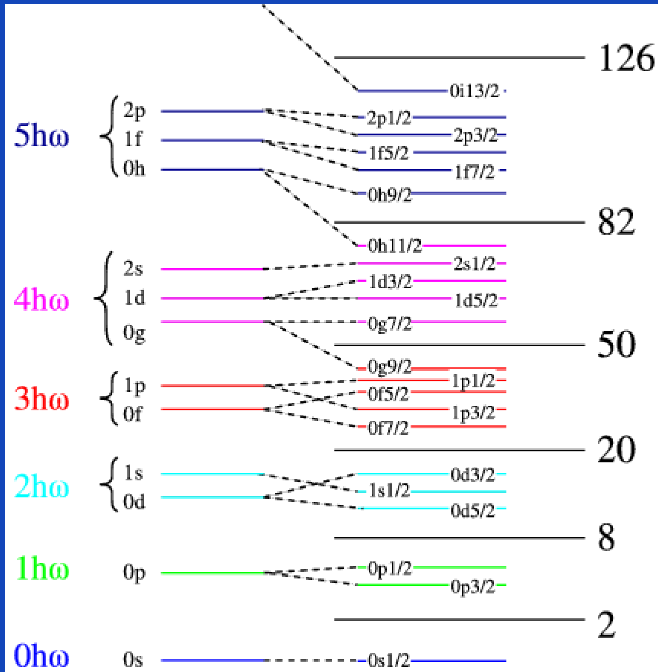
- Local: defined valence space, two-body matrix elements and single particle energies
- TBME: Schematic, realistic, purely empirical, mixed
- Most often empirical corrections are added to the realistic interaction
- Number of parameters: 10-10000
- Computational time varies
- No problems with convergence
- Well understand, hundreds of interactions

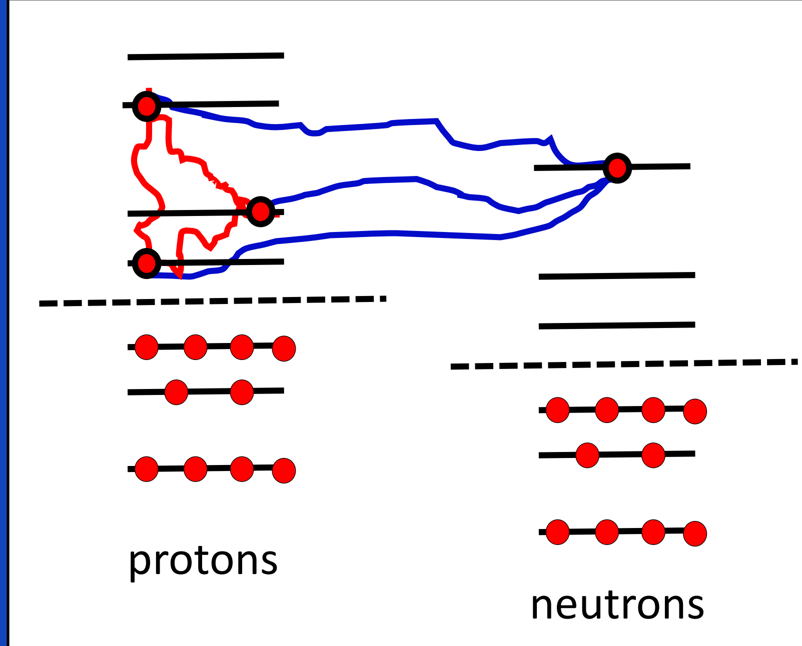
Interest in description of known data, predictions and in parameters!



Chong Qi, KTH Stockholm, Tuesday, June 21st
Optimisation of the shell-model Hamiltonian for heavy nuclei and the underlying uncertainty

Nuclear structure models (part 2/5)





(shell gaps not in scale)

$$H = \sum_a \epsilon_a \hat{n}_n + \sum_{a \leqslant b, c \leqslant d} \sum_{JT} V_{JT}(ab;cd)\hat{T}_{JT}(ab;cd)$$

$$\hat{T}_{JT}(ab;cd) = \sum_{MT_z} A^{\dagger}_{JMTT_z}(ab) A_{JMTT_z}(cd)$$

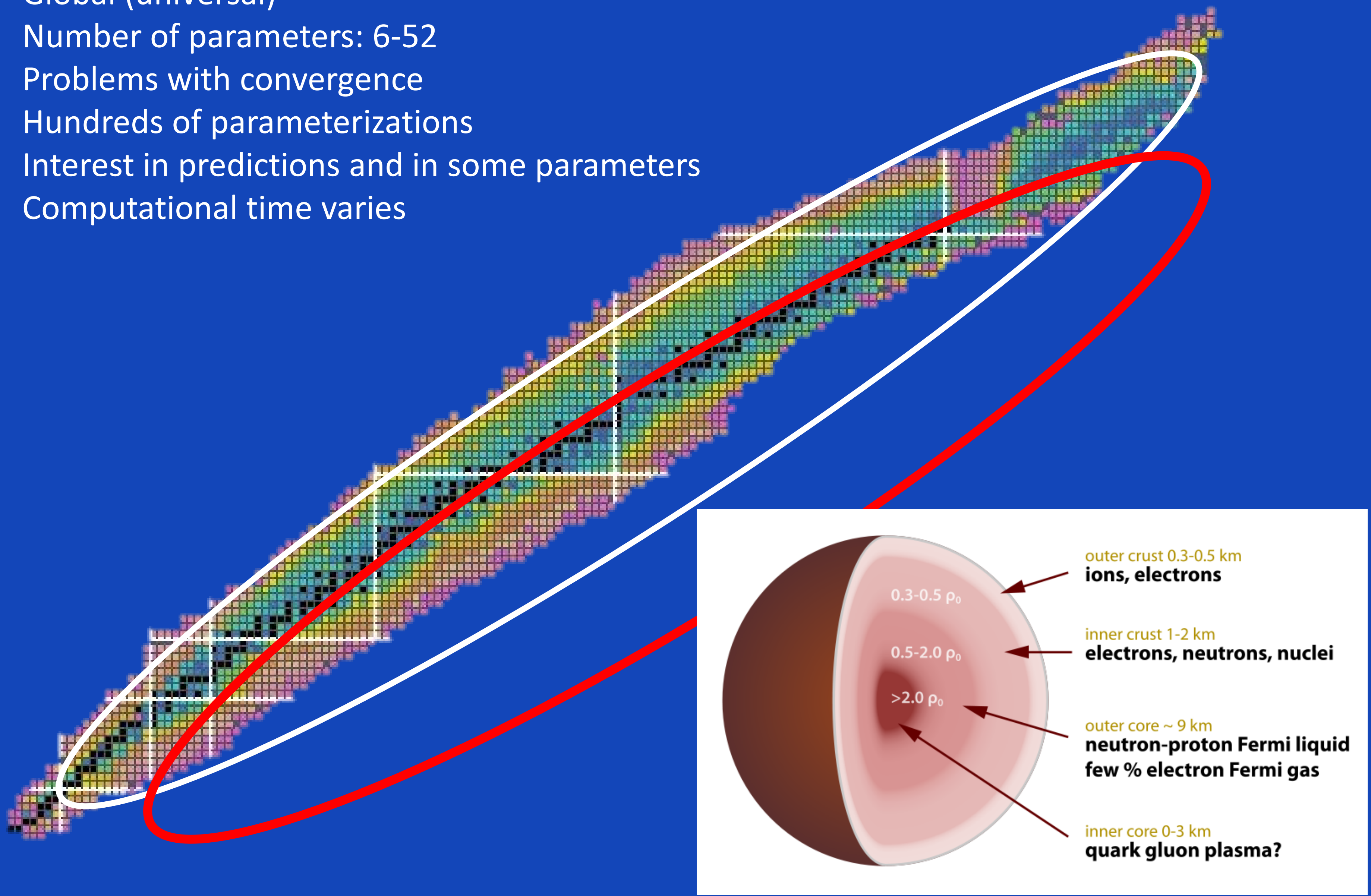
$$H = \sum_{i=1}^{p} x_i O_i$$

$$\lambda_k = \langle \phi_k | H | \phi_k \rangle = \sum_{i=1}^{p} x_i \langle \phi_k | O_i | \phi_k \rangle$$

No experimental paper about the structure of nuclei around doubly-magic core without shell model calculations for comparison.

Energy Density Functionals

- Global (universal)
- Number of parameters: 6-52
- Problems with convergence
- Hundreds of parameterizations
- Interest in predictions and in some parameters
- Computational time varies

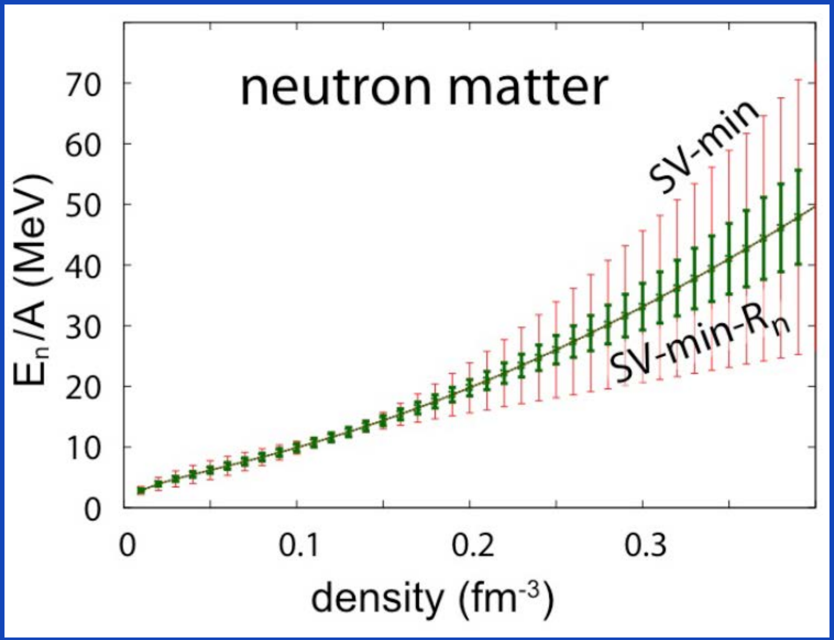


Nuclear structure models (part 4/5)

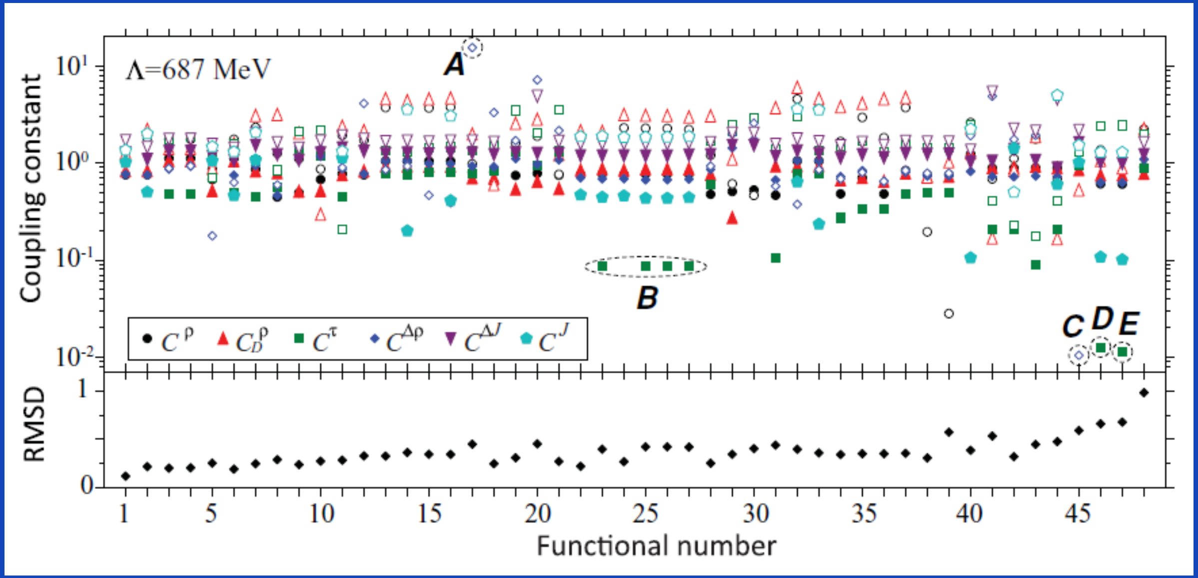
$$E = E_{kin} + \int d^3 r E_{sk} + E_{coul} + E_{pair} - E_{corr}$$

$$\rho_{T=0} = \rho_p + \rho_n \qquad \rho_{T=1} = \rho_p - \rho_n$$

$$E_{sk} = \sum_{T=0,1} C_T^i \mathrm{O}_T^i$$



P. G. Reinhard & W. Nazarewicz, PRC 81, 051303 (R) (2010)



$$S = f_\pi^{2(l-1)} \Lambda^{n+l-2}$$

l – power of densities,

n – numer of deriviatives

M. Kortelainen, R.J. Furnstahl, W. Nazarewicz, M. V. Stoistov, PRC 82, 011304(R) (2010)

N3LO Energy Density Functional (part 5/5)

Nuclear energy density functionals constructed in terms of derivatives of densities up to sixth, next-to-next-to-next-to-leading order (N3LO).

It builds on the standard functionals related to the contact and Skyrme forces, which constitute the zero-order (LO) and second-order (NLO) expansions, respectively.

Number of independent parameters assuming **galilean**, spherical, space-inversion and time-reversal symmetries:

Order	Number of terms
0	1
2	4
4	8
6	15
N3LO	**25**

Full functional 25x2 + 2 giving 52 coupling constants.

Introduced in:

PHYSICAL REVIEW C **78**, 044326 (2008)

Local nuclear energy density functional at next-to-next-to-next-to-leading order

B. G. Carlsson,[1] J. Dobaczewski,[1,2] and M. Kortelainen[1]
[1]*Department of Physics, Post Office Box 35 (YFL), FI-40014 University of Jyväskylä, Finland*
[2]*Institute of Theoretical Physics, University of Warsaw, ul. Hoża 69, PL-00-681 Warsaw, Poland*
(Received 31 July 2008; published 27 October 2008)

Spherical solver available:

Computer Physics Communications 181 (2010) 1641–1657

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Solution of self-consistent equations for the N^3LO nuclear energy density functional in spherical symmetry. The program HOSPHE (v1.02) ☆

B.G. Carlsson [a], J. Dobaczewski [a,b,*], J. Toivanen [a], P. Veselý [a]
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Toys

- Nuclear shell model
- Energy Density Functionals

Tools

- Nonlinear least-squares
- Regularization methods

Illustrations

Regularization of least-square problems

REGULARIZATION FACTOR

$$\min\{\|\boldsymbol{Gm}-\boldsymbol{d}\|_2^2+\boldsymbol{\lambda}^2\|\boldsymbol{L}(\boldsymbol{m}-\boldsymbol{m}^{prior})\|_2^2\}$$

LEAST-SQUARE TERM

DISTANCE FROM THE EXPECTED POINT

As the considered problem is nonlinear we use the dumped Gauss-Newton iteration scheme.
Need to approximate Jacobian.

Regularization factor is kept constant during iterations.

$$\boldsymbol{T}=\lambda^2\boldsymbol{I}$$
$$\boldsymbol{x}=\lambda^2\left(m-m^{prior}\right)$$
$$\boldsymbol{S}=(\boldsymbol{J}^T\boldsymbol{J}+\boldsymbol{T})^{-1}$$
$$p1=\boldsymbol{SJ}^T\boldsymbol{y}$$
$$p2=-\boldsymbol{Sx}^T$$
$$\Delta m=p1+p2$$

$$d^{th}=Gm$$
$$m^{L2}=G^{+}d$$
$$m^{\#}=G^{\#}d$$

$$G^{+}=(G^TG)^{-1}G^T$$
$$G^{\#}=(G^TG+\lambda^2L^TL)^{-1}G^T$$
$$cov\left(m^{\#}\right)=\sigma^2G^{\#}G^{\#^T}$$

$$R_m=G^{(+,\#)}G$$
$$m_{est}=R_m m_{true}$$

Shell model: TBME and SPE are in the same units and of the same order of magnitude.
EDF: We work in natural units.

The distance from the prior point is meaningful.

The approach can be interpreted within the Bayesian framework.

Major problems:

- choice and interpretation of the regularization parameter, its influence on uncertainty estimation,
- **validity of approach for nonlinear problems**

Toys

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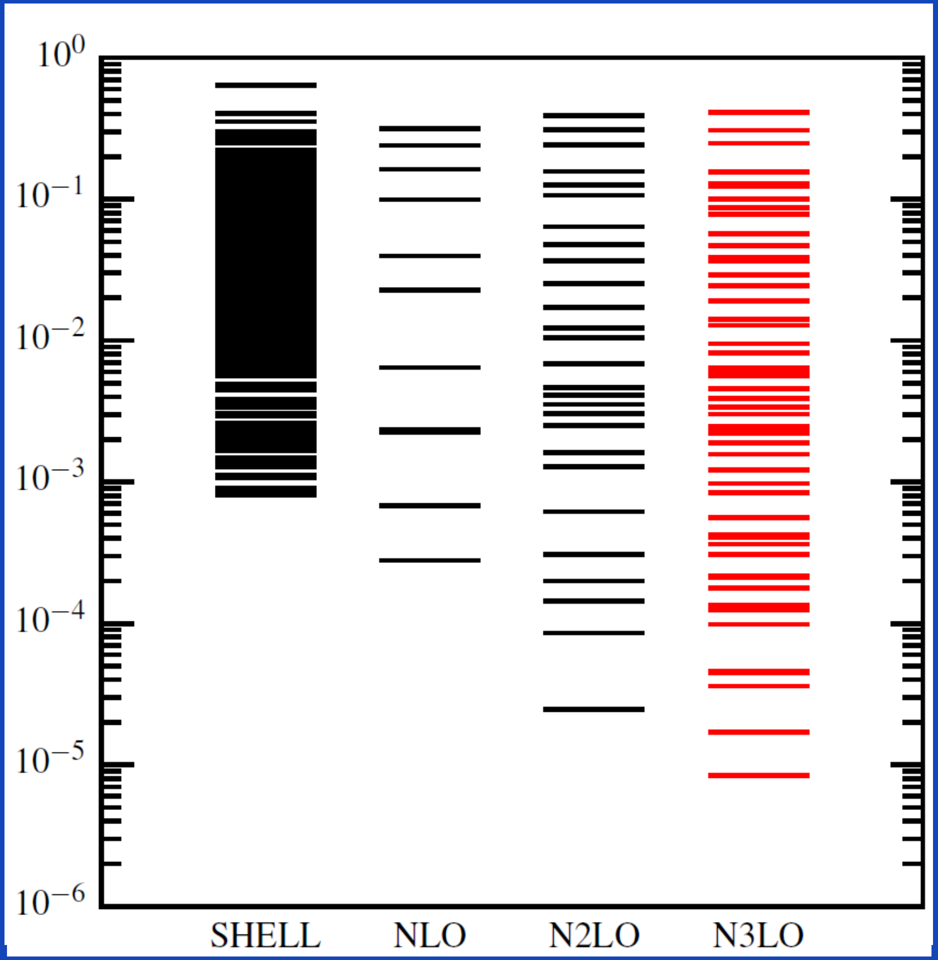
Illustrations

Which problem would you prefer to solve ?

Option 1
Estimate parameters of the nuclear shell model for the *sd* shell nuclei: approx. **160 parameters**, **400 data points** (binding and excitation energies)

Option 2
Estimate parameters of the of the Skyrme like EDF:
12 parameters, 150 data points
(binding energies, single particle energies, charge radii)

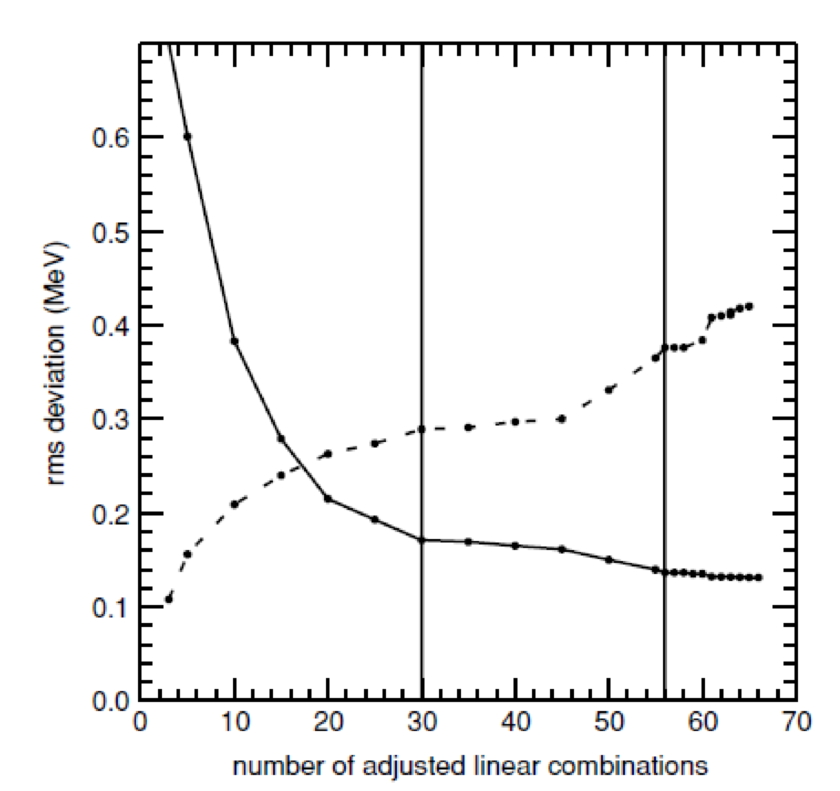
Normalized spectrum of singular values



2.2. Linear Combination (LC) method

In the above fitting procedure, not all matrix elements are well determined, and some of them can be determined only with certain ambiguities, because available data are limited. In order to resolve this problem, the Linear Combination (LC) method [11] was proposed, which enables us to separate well-determined parameters from such poorly determined ones.

M. Honma, B. A. Brown, T. Mizusaki, T. Otsuka, NPA 704 (2002)



No single paper analyzing the uncertainties of model parameters and predictions from statistical perspective.

Parameters are re-adjusted, often no details published.

Data explained a posteriori.

B. A. Brown, W. A. Richter, PRC 74, 034315 (2006)

Nuclear Shell Model

Nuclear shell model for sd shell nuclei: ^{16}O-^{40}Ca

Parameters:

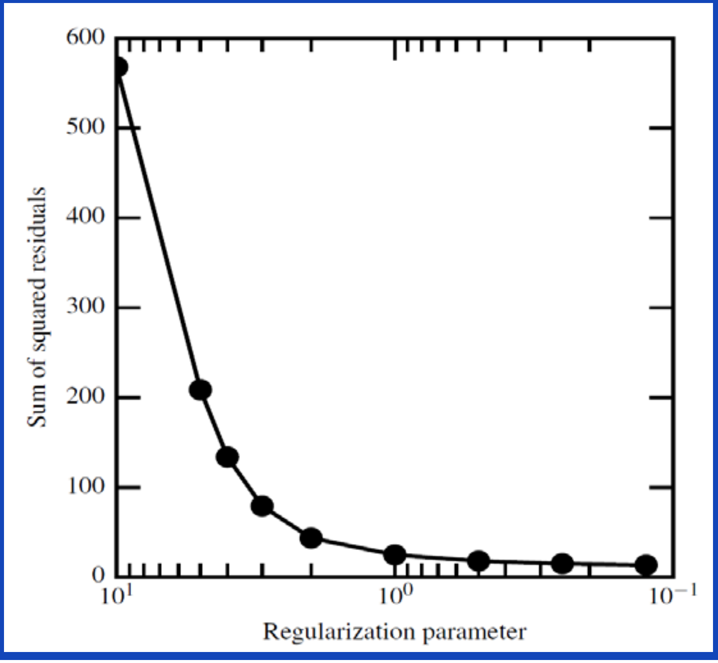
158 TBME and 6 SPE (no isospin symmetry)

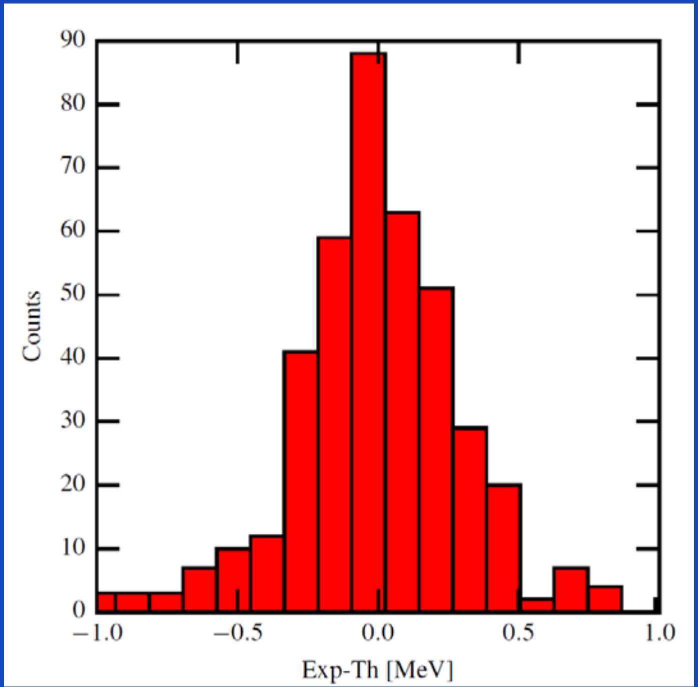
Experimental data:

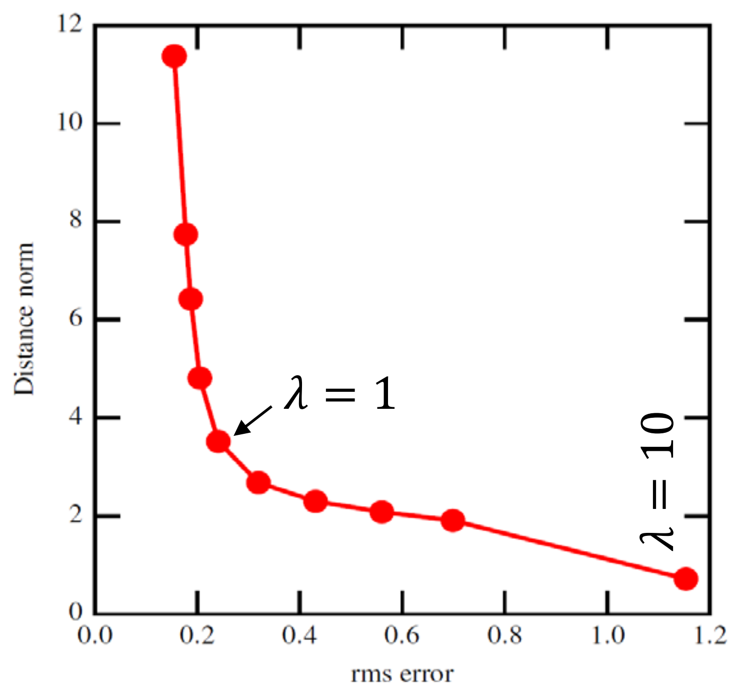
binding energies, excitation energies (427 points)

Prior information:

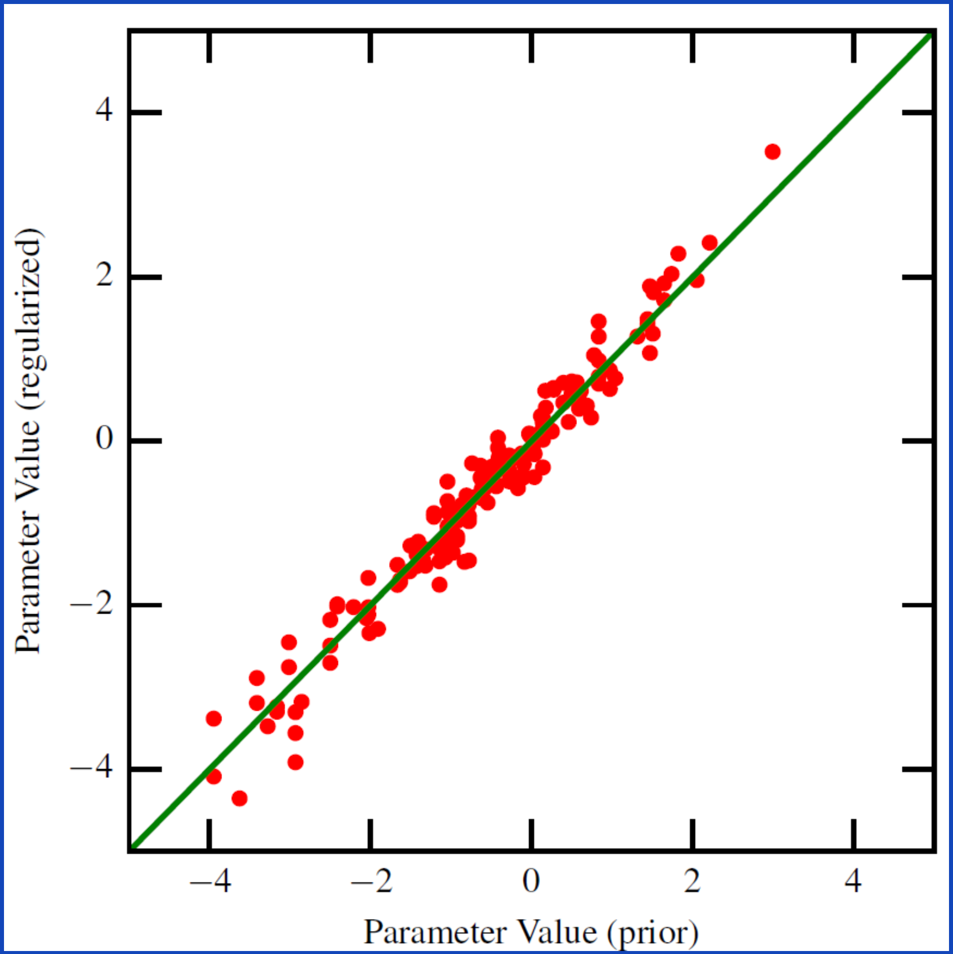
realistic interaction (how to quantify uncertainty ?)

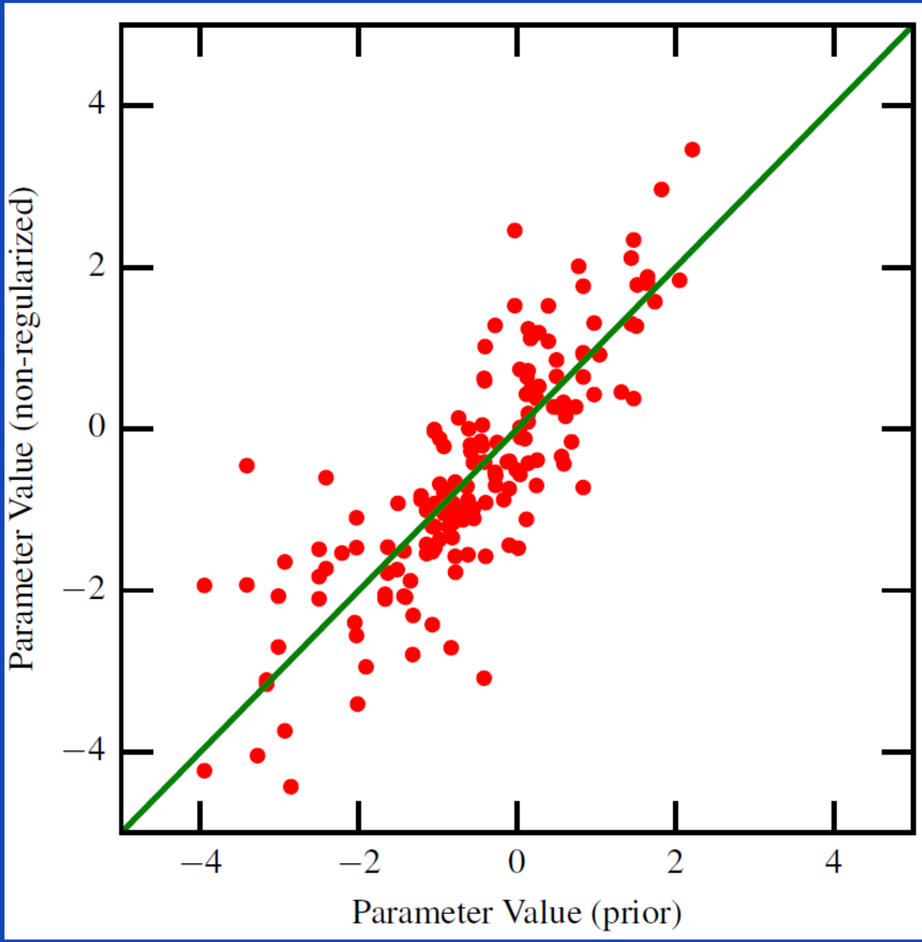




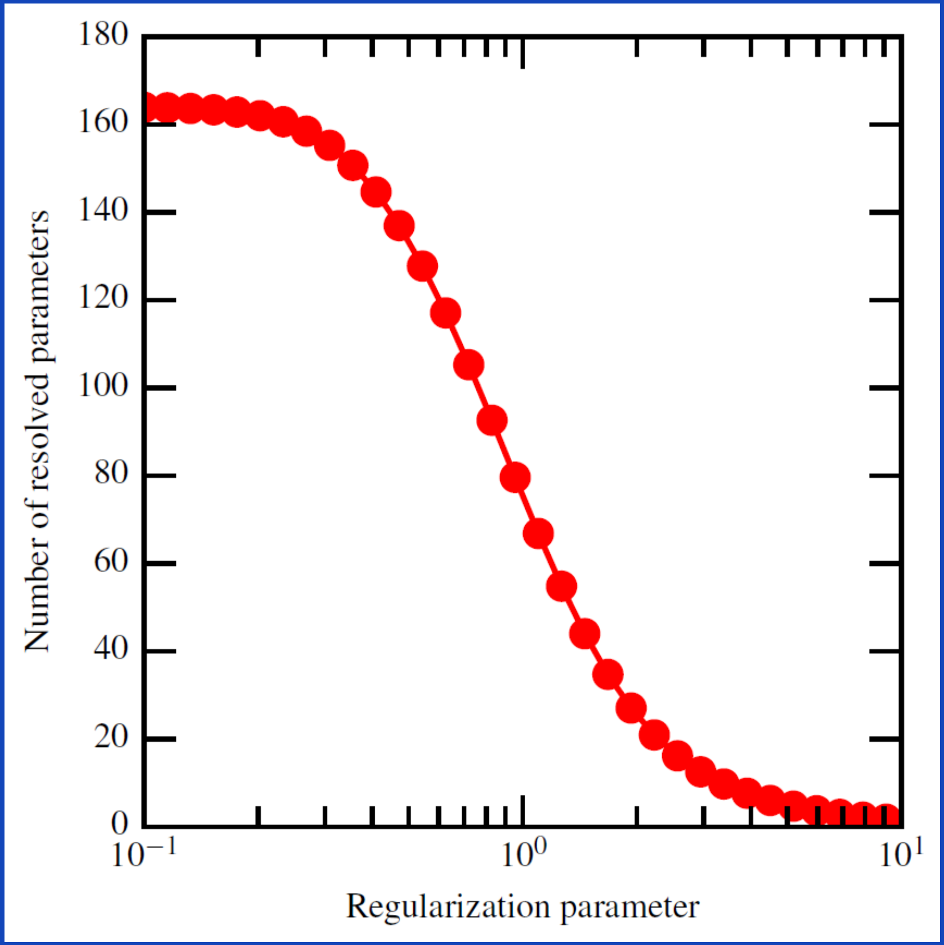


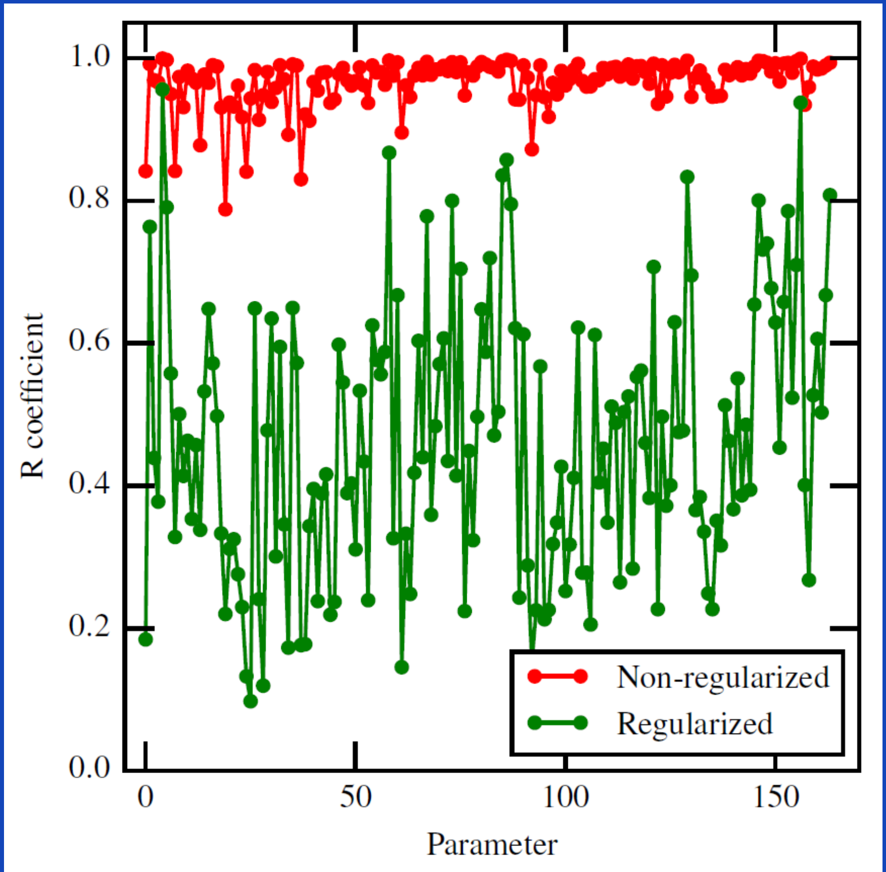
Nuclear Shell Model



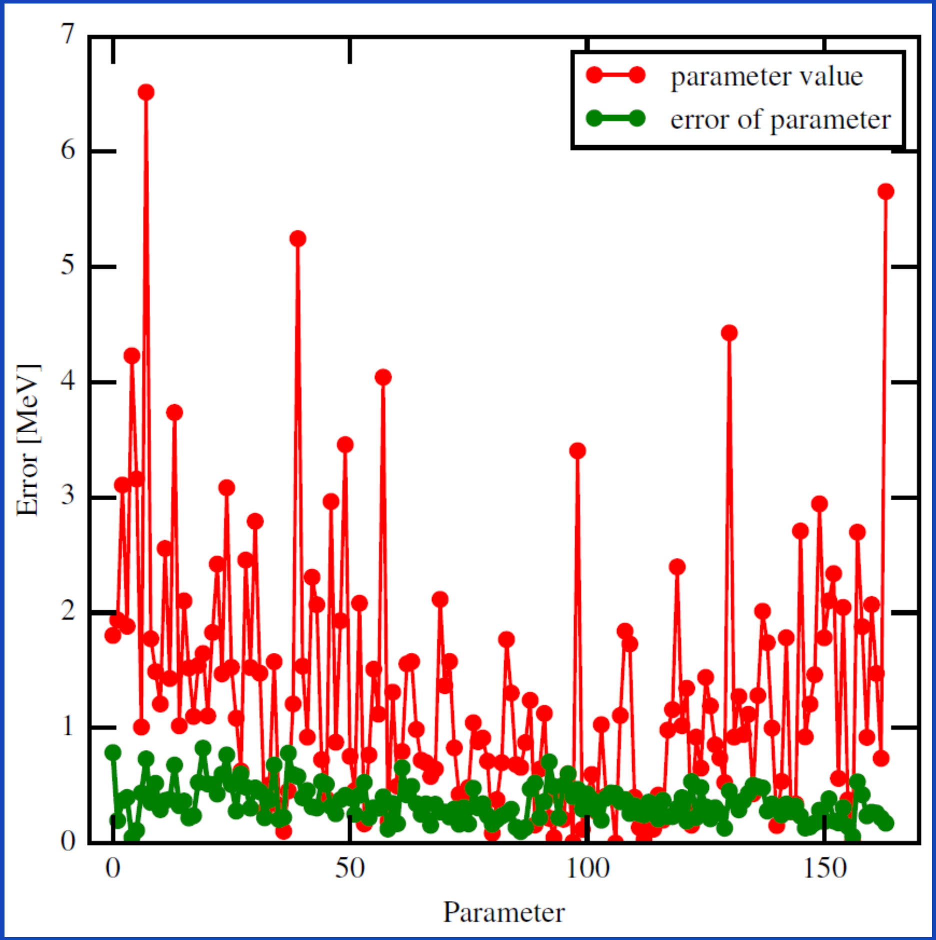


Nuclear Shell Model



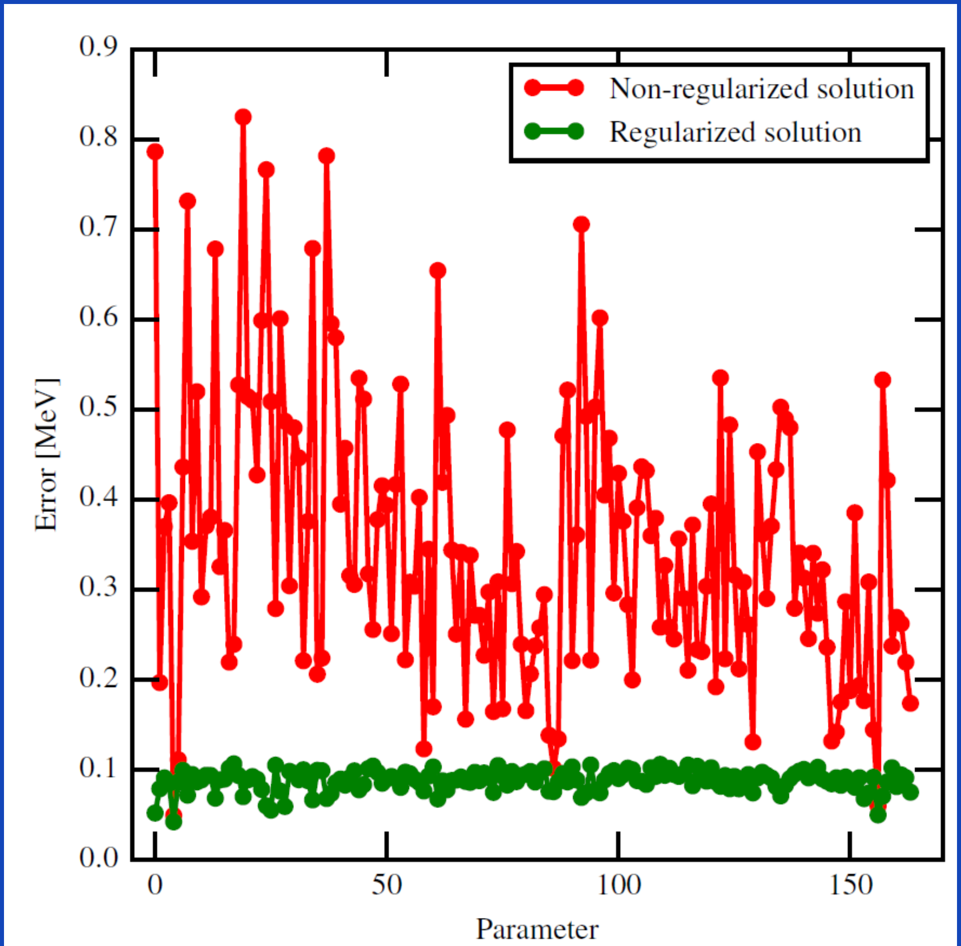


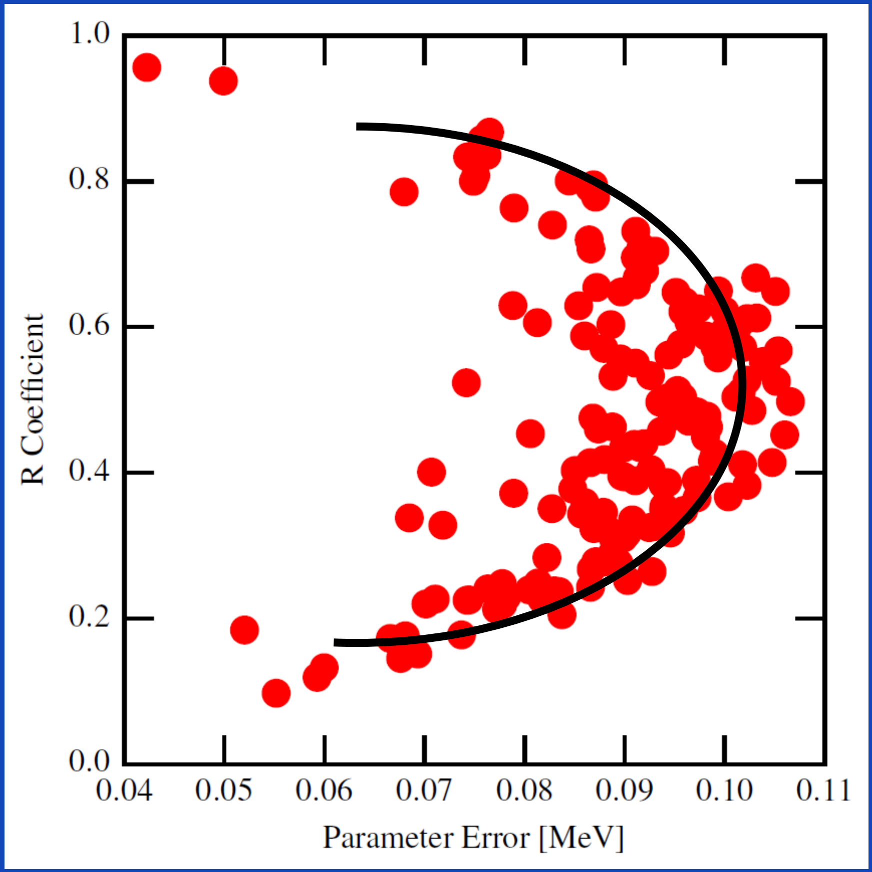
Nuclear Shell Model



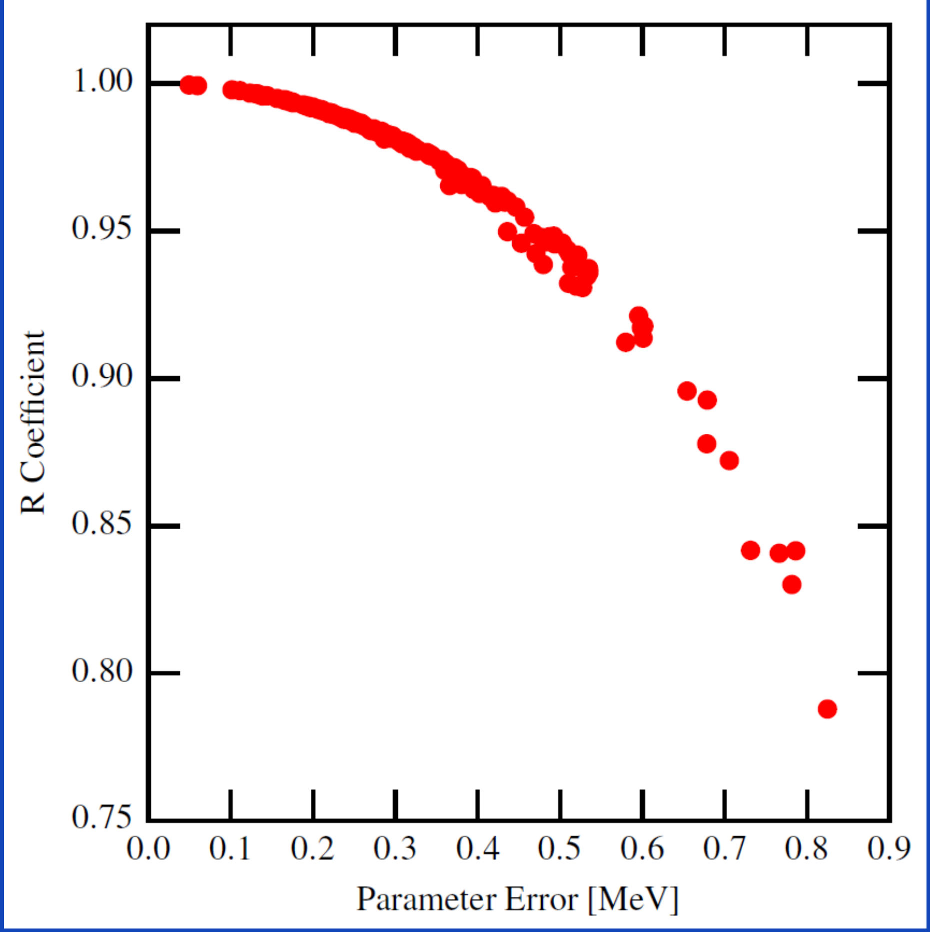
Parameter values and their errors, for non-regularized solution.

Comparison of error estimates for regularized and non-regularized solutions.



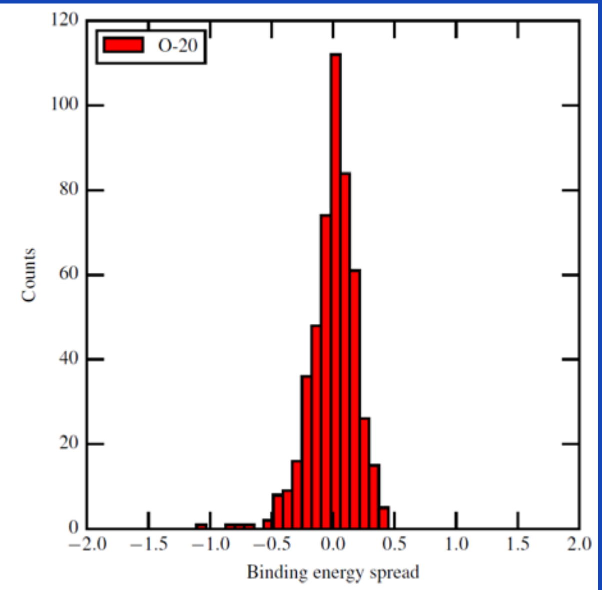


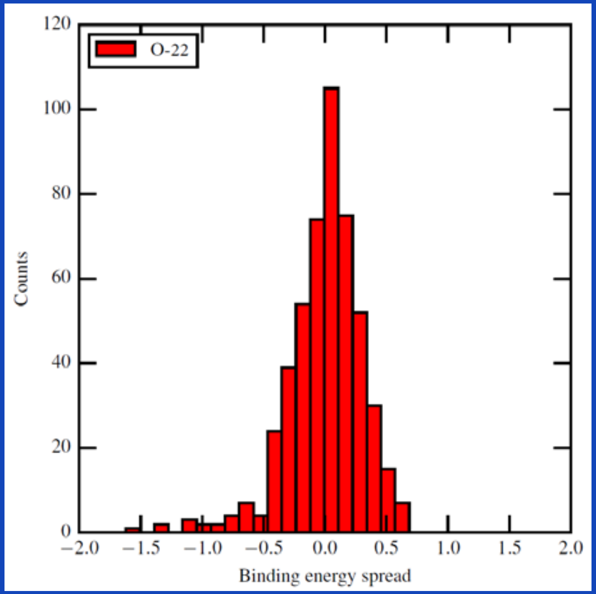
Correlation between error estimate and R coeff. for regularized solution.

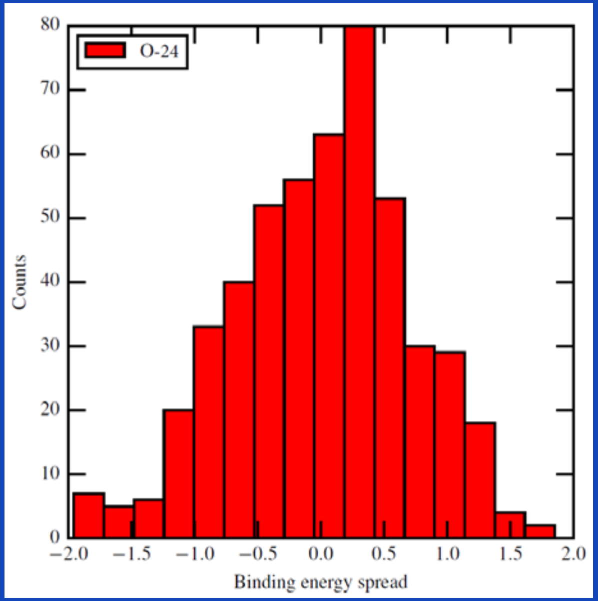


Correlation between error estimate and R coeff. for non-regularized solution.

Nuclear Shell Model

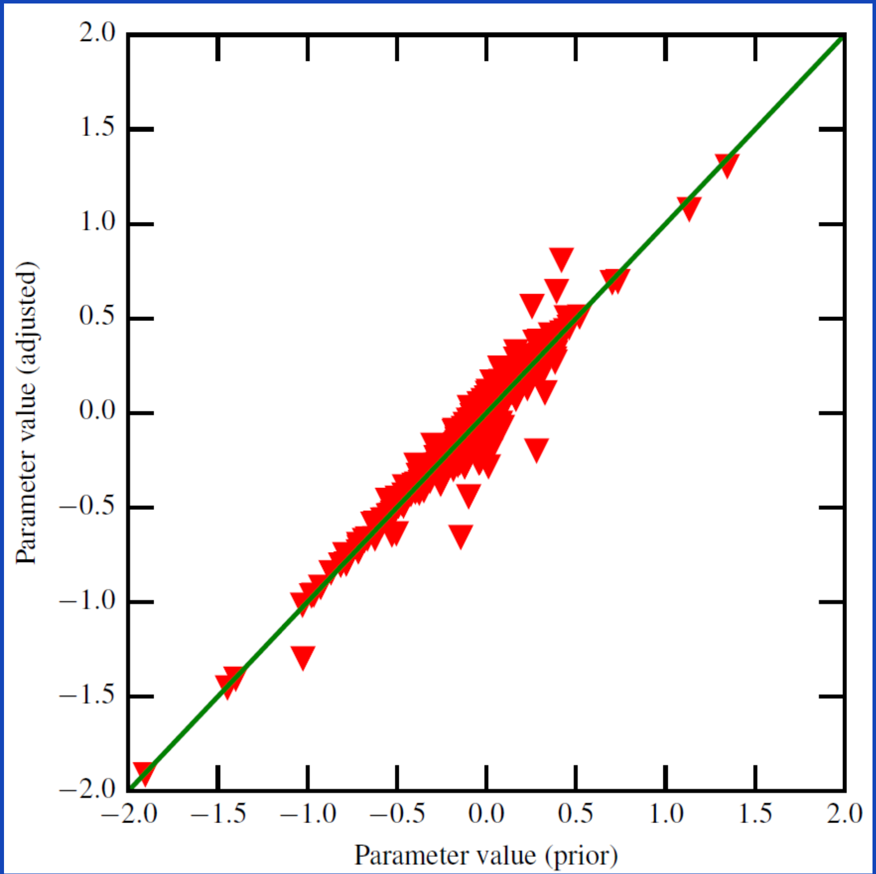


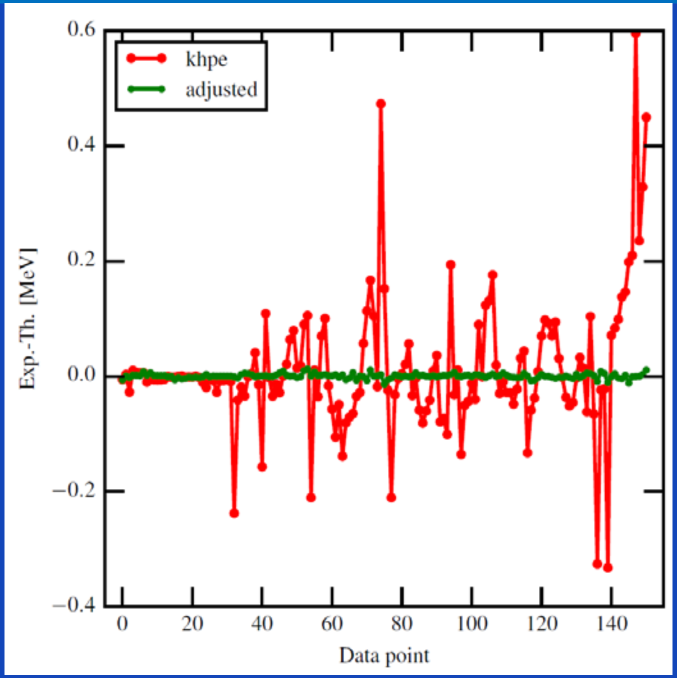


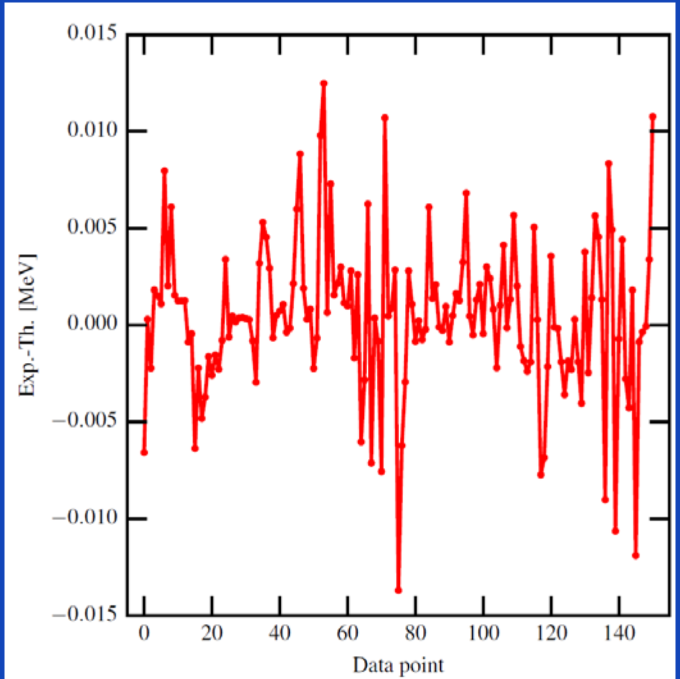


Shell model above ^{208}Pb:

- **2838 parameters**
- **151 data points**







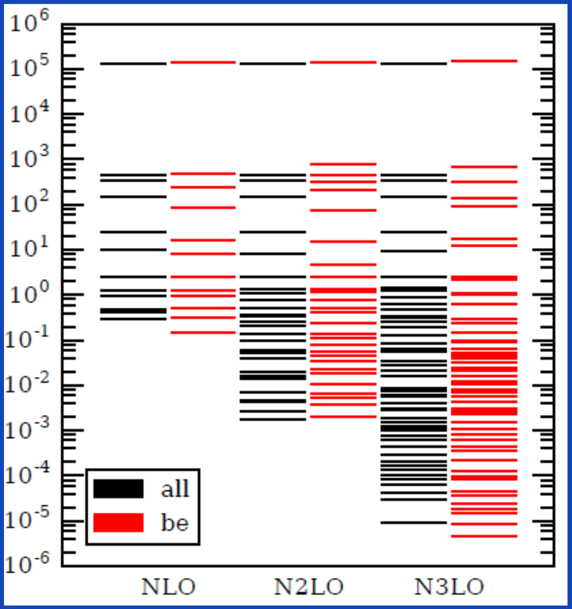
Energy Density Functionals: novel forms

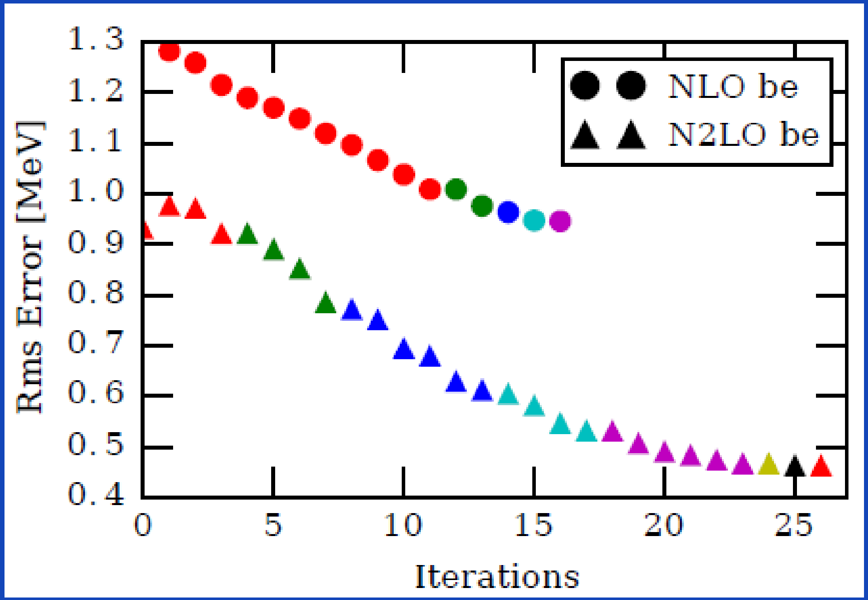
Work done in collaboration with Jacek Dobaczewski and his groups at York and Jyvaskyla.
Work performed during my employment at the University of Warsaw in 2014-2015.

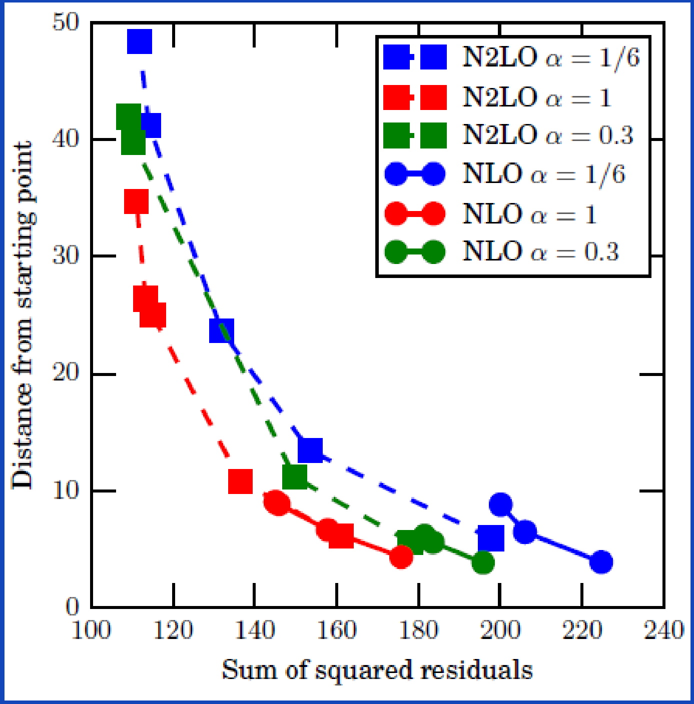
The experimental data set consist of:

- **Single particle energies (48 points)**
- **Binding energies (71 nuclei)**
- **Charge radii (48 points)**

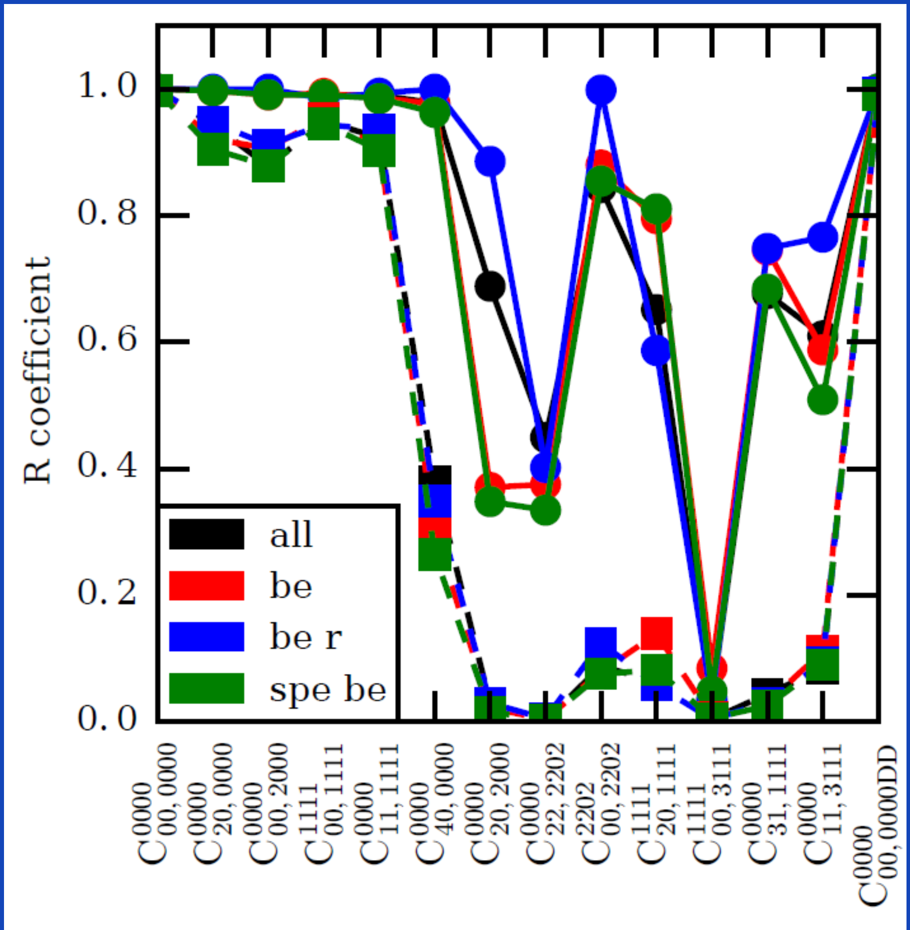
of spherical even-even nuclei.

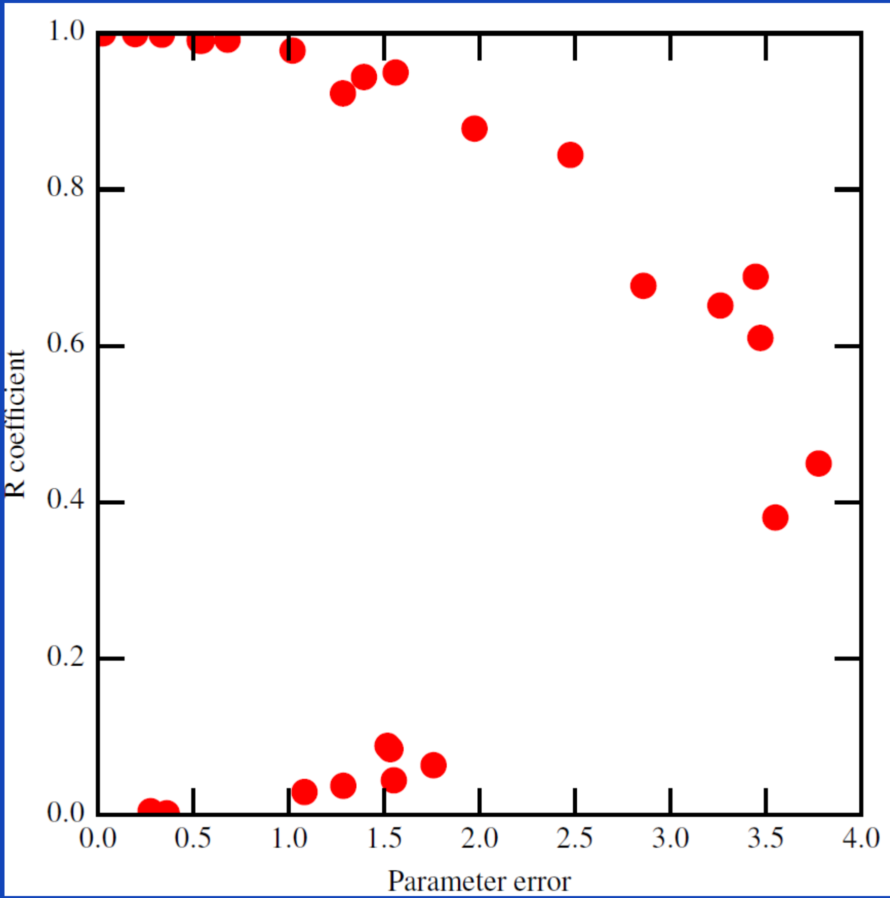




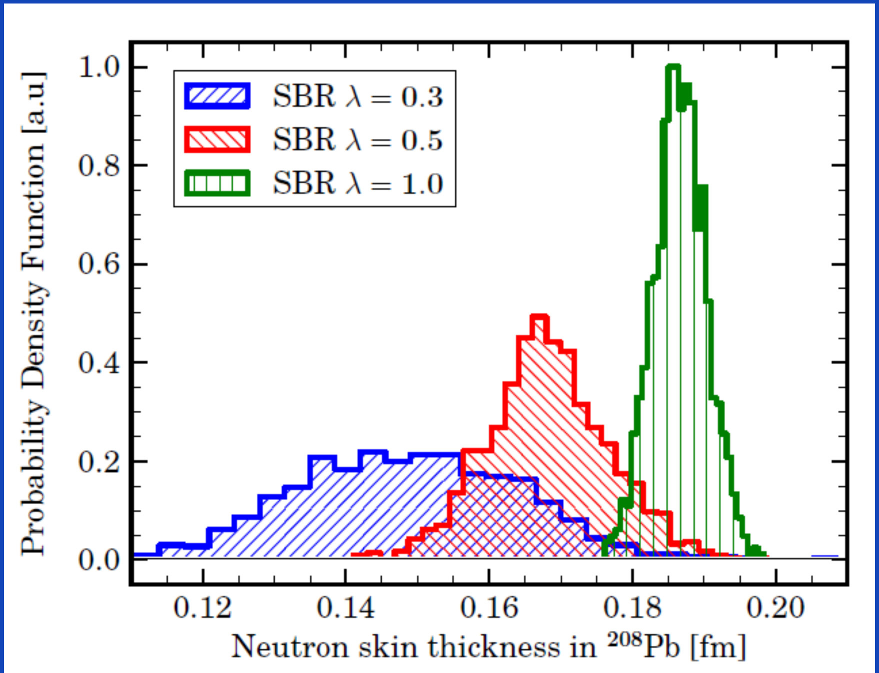


Energy Density Functionals: novel forms





Conclusions & Perspectives



A priori information play a role!
This role can be positive or destructive.
How to quantify its uncertainty ?

Some nuclear structure models are easier to work with than the others.

Single criterium for sloppiness is still missing.
You will not know before you try.

Information content of nuclear observables can be very different.

Application of variable selection/model reduction methods remains unexplored.