

Sensitivity of nuclear pairing properties to chiral EFT interaction contributions

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Overview

- Our interpretation of *ab initio* in nuclear theory
- Bayesian inference and χ EFT
- Global sensitivity analysis
- Emulating nuclear observables
- Sensitivity of nuclear deformation, pairing, and radii to χ EFT parameters?

Our interpretation of nuclear *ab initio*

Nuclear *ab initio*: a *systematically improvable* approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities.

we therefore let nucleons define the beginning

χ EFT to approximate
low-energy QCD

$$H(\vec{\alpha}) |\Psi\rangle = E |\Psi\rangle$$

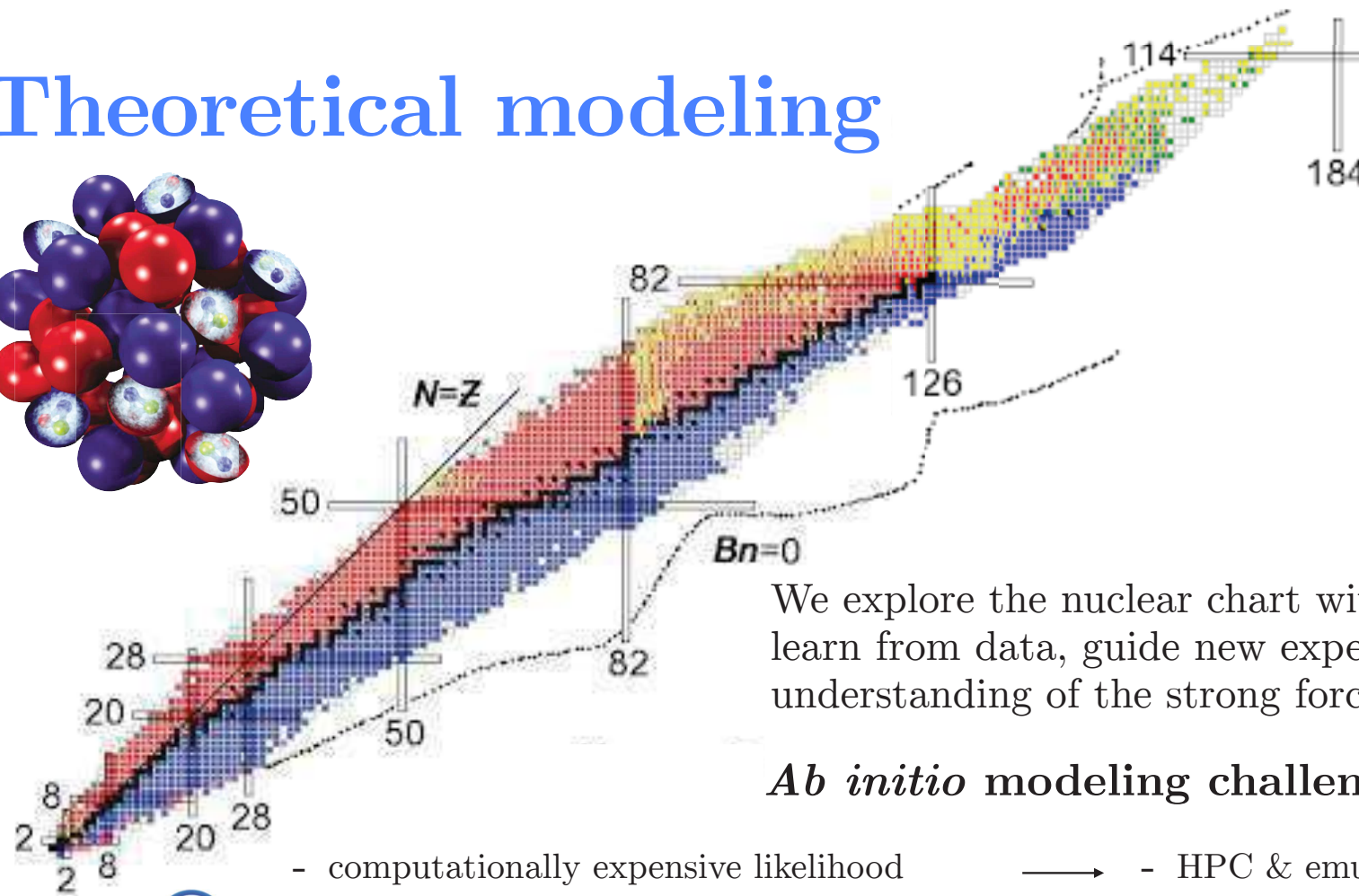
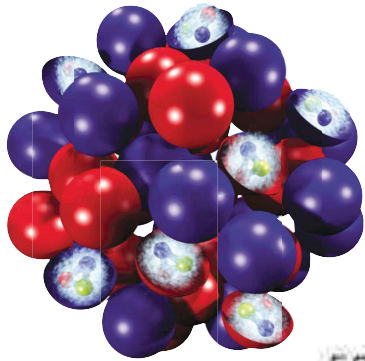
A-body methods with
controllable approximation

$$H(\vec{\alpha}) = T + V^{(0)}(\vec{\alpha}_{(0)}) + V^{(1)}(\vec{\alpha}_{(1)}) + V^{(2)}(\vec{\alpha}_{(2)}) + \dots \quad |\Psi\rangle = |\Phi^{(0)}\rangle + |\Phi^{(1)}\rangle + |\Phi^{(2)}\rangle + \dots$$

This systematicity creates an *inferential advantage*. We can test our assumptions about the model and the model discrepancy as we increase the model fidelity.

$$y_{\text{exp}}(\vec{x}) = \underbrace{y_{\text{th}}(\vec{\alpha}; \vec{x}) + \delta y_{\text{th}}(\vec{\alpha}; \vec{x})}_{\text{'Model'}} + \delta y_{\text{exp}}(\vec{x})$$

Theoretical modeling



We explore the nuclear chart with theoretical models to learn from data, guide new experiments, and advance our understanding of the strong force and atomic nuclei.

Ab initio modeling challenges:



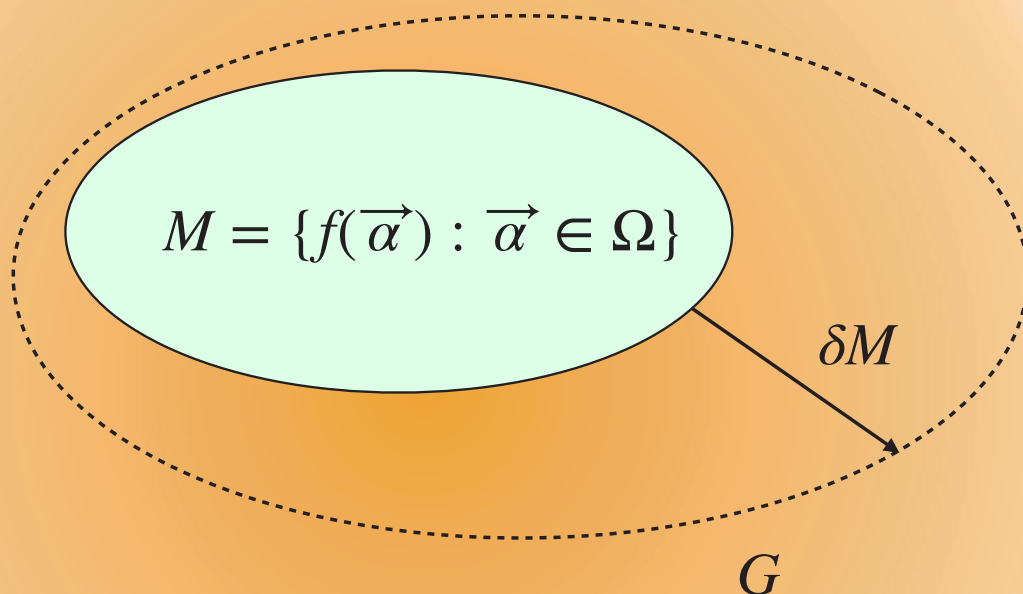
- | | | |
|--|---|------------------------------------|
| - computationally expensive likelihood | → | - HPC & emulators |
| - multimodal and high-D parameter space | → | - history matching / HMC |
| - <i>ab initio</i> method errors difficult to quantify | → | - systematics & method comparisons |
| - χ EFT in Weinberg PC not renormalizable | → | - RG-invariant proposals |



Remember: models are not reality

- we simplify and/or do not know the full story

We consider a **model** of some nuclear observable as a function $y = f(\vec{\alpha})$, $\vec{\alpha} \in \Omega \subset \mathbb{C}^d$, where Ω is some specified parameter space



“All models are wrong”
i.e., data $D \sim G$ where $G \notin M$

G. E. P. Box (1976)

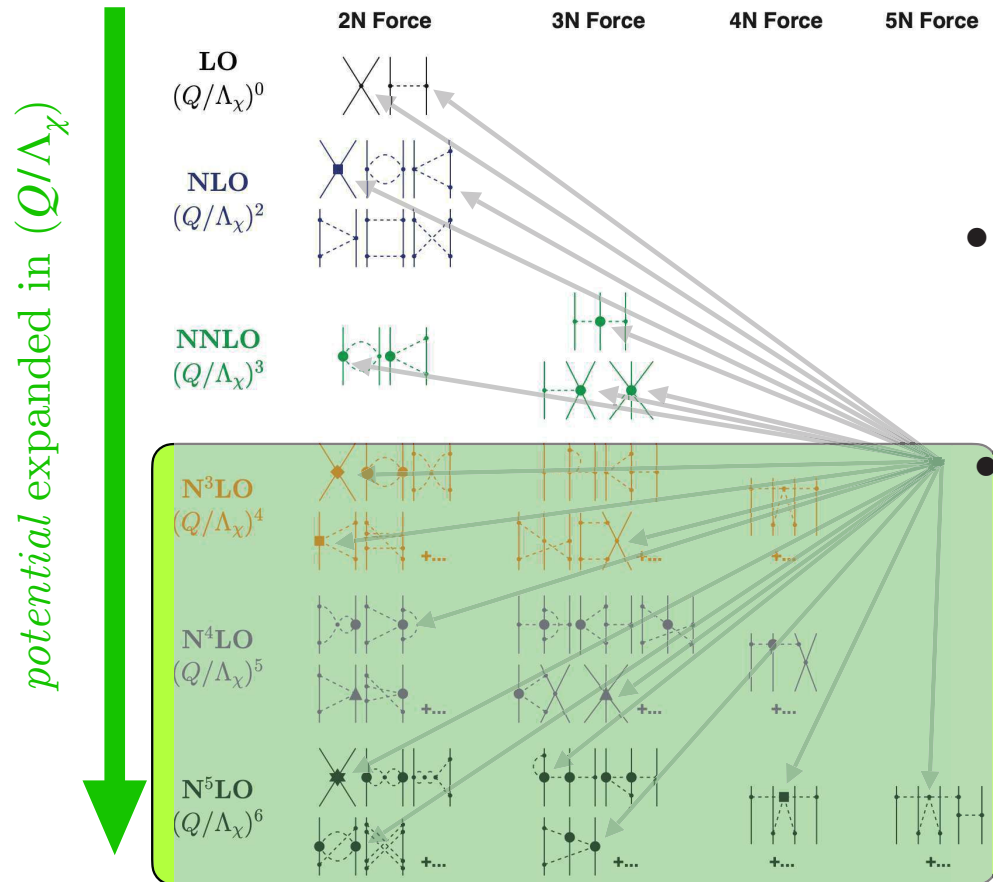
We should include an estimate of the model discrepancy δM to (hopefully) make more meaningful inferences and predictions.

Kennedy and O’Hagan (2001)

Brynjarsdóttir and O’Hagan (2014)

Chiral effective field theory (χ EFT)

- Weinberg power counting (WPC)



$$H(\vec{\alpha}) = T + V^{(0)}(\vec{\alpha}_{(0)}) + V^{(1)}(\vec{\alpha}_{(1)}) + V^{(2)}(\vec{\alpha}_{(2)}) + \dots$$

EFTs promise a very useful systematicity

- **Order-by-order expansion** in a dimensionless ratio (Q/Λ_χ) constructed from a separation of scales; A soft scale ($Q \sim m_\pi$) and a hard scale ($\Lambda_\chi \sim m_N$), separating the resolved and unresolved dynamics of the nuclear interaction.

• $\sim (15 - 30)$ **Low-energy** constants to be inferred from data

$$y_{\text{th}}^{(k)} = y_{\text{ref}} \sum_{\nu=0}^k c_\nu \left(\frac{Q}{\Lambda_\chi} \right)^\nu \text{ and}$$

EFT prediction

$$\delta y_{\text{th}}^{(k)} = y_{\text{ref}} \sum_{\nu=k+1}^{\infty} c_\nu \left(\frac{Q}{\Lambda_\chi} \right)^\nu$$

EFT truncation error

Why uncertainty quantification

- Predicting future data \tilde{y} from past data y is an uncertain
- Quantifying this uncertainty with probability:
 - enhances transparency and communication of results
 - informs decision-making and helps model assessment

Why Bayesian inference?

The probability for \tilde{y} given y is called the *posterior prediction*. This quantity is central to Bayesian inference.

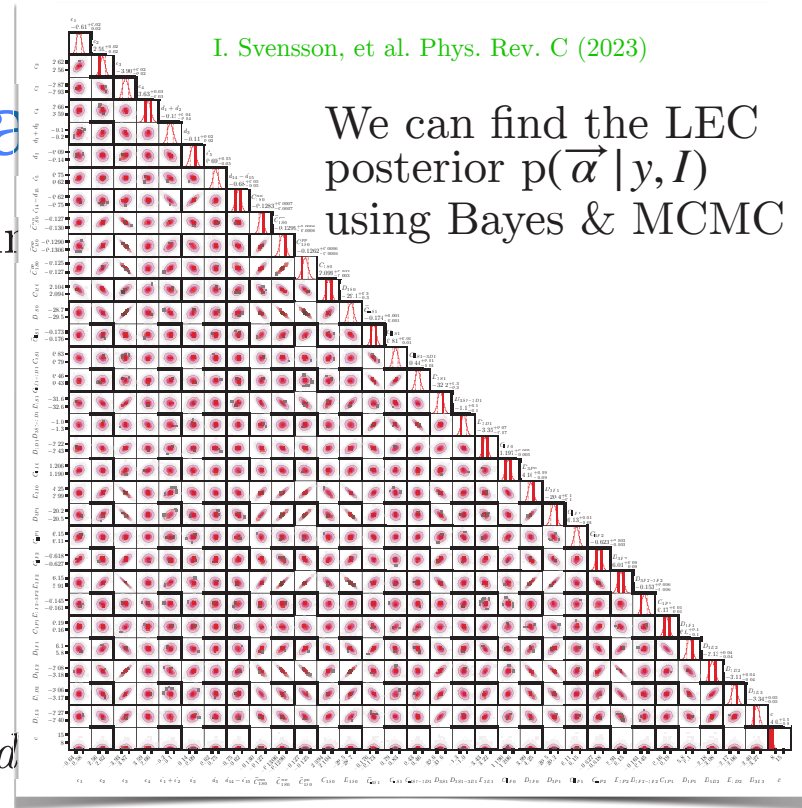
$$p(\tilde{y} | y, I)$$

Here, I denotes *your* background knowledge. To enable quantitative statements, we construct a *model* M . Any model comes with uncertain parameters $\vec{\alpha}$.

$$p(\tilde{y} | y, M, I) = \int p(\tilde{y} | \vec{\alpha}, M, I) p(\vec{\alpha} | y, M, I) d\vec{\alpha}$$

I. Svensson, et al. Phys. Rev. C (2023)

We can find the LEC posterior $p(\vec{\alpha} | y, I)$ using Bayes & MCMC



D. V. Lindley, The Statistician (2000)
Bernardo and Smith, Wiley (1994)

PPD for complex nuclei

^{28}O separation energies

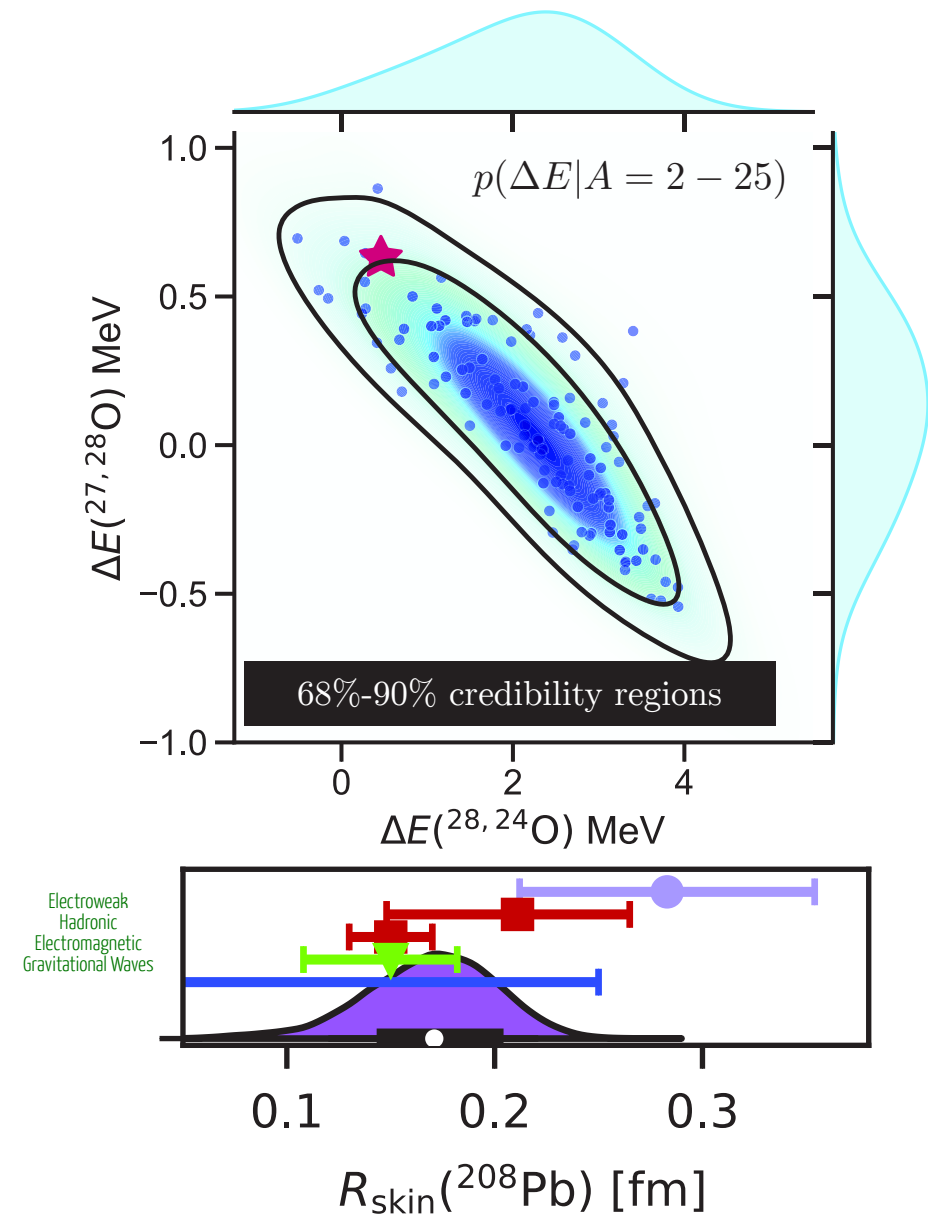
- We claim with 98% certainty that ^{28}O is unbound with respect to ^{24}O :
- The experimental data point (red star) is away from the posterior maximum. This suggests that only a few finely-tuned chiral interactions are able to reproduce low-energy and exotic oxygen structure Y. Kondo et al. Nature (2023)

^{208}Pb neutron skin-thickness

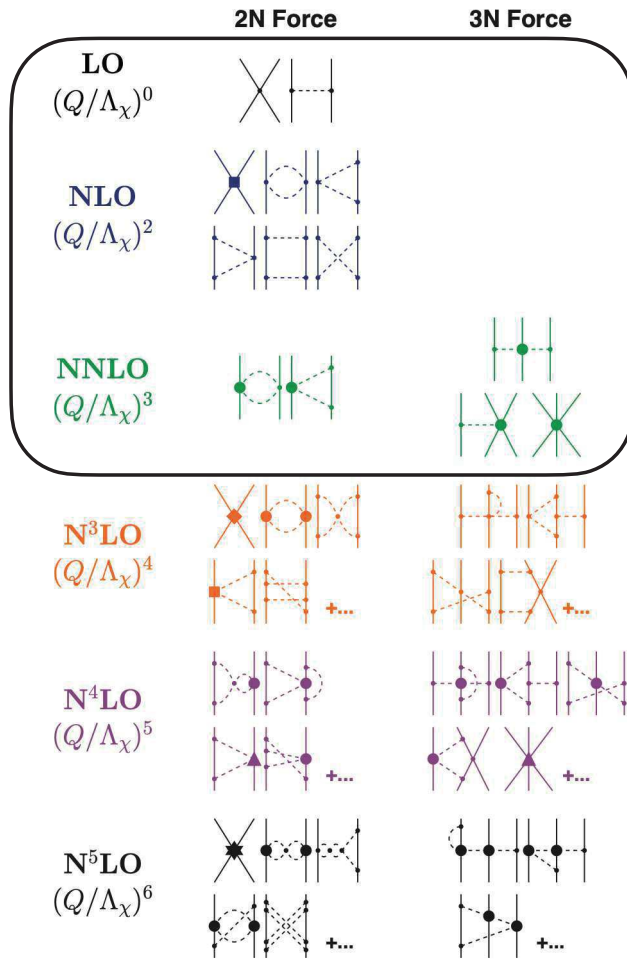
n.b. similarly curated history matching data

- We predict a small skin thickness 0.14-0.20 fm in mild (1.5σ) tension with electroweak (PREX) measurement.

B. Hu et al Nature Physics (2022)



Which parts of the nuclear interaction do what?



ab initio many-body

$$M(\vec{\alpha}) : V_\chi(\vec{\alpha}) \rightarrow y_{\text{th}}(\vec{\alpha}) + \delta y_{\text{th}}$$

“sensitivity analysis”

$$\begin{aligned}
 M(\vec{\alpha}) := V(\vec{p}', \vec{p}) = & -\frac{g_A^2}{4f_\pi^2} \tau_1 \cdot \tau_2 \frac{\vec{\sigma}_1 \cdot \vec{q} \vec{\sigma}_2 \cdot \vec{q}}{q^2 + m_\pi^2} + \tilde{C}_{1S0}^{(nn)} + \tilde{C}_{1S0}^{(pp)} + \tilde{C}_{1S0}^{(np)} + \tilde{C}_{3S1} \\
 & + [C_{3P0} + C_{3P1} + C_{3P2} + C_{1P1}] pp' + [C_{1S0} + C_{3S1} + C_{E1}] (p^2 + p'^2) \\
 & + \frac{L(\tilde{\Lambda}; q)}{384\pi^2 f_\pi^4} \left[4m_\pi^2 (1 + 4g_A^2 - 5g_A^4) + q^2 (1 + 10g_A^2 - 23g_A^4) - \frac{48g_A^4 m_\pi^4}{w^2} \right] \tau_1 \cdot \tau_2 \\
 & - \frac{3g_A^4}{64\pi^2 f_\pi^4} L(\tilde{\Lambda}; q) [\vec{\sigma}_1 \cdot \vec{q} \vec{\sigma}_2 \cdot \vec{q} - q^2 \vec{\sigma}_1 \cdot \vec{\sigma}_2] + \frac{3g_A^2}{16\pi f_\pi^4} [2m_\pi^2 (\tilde{c}_3 - 2\tilde{c}_1 + \tilde{c}_3 q^2) (2m_\pi^2 + q^2) A(\tilde{\Lambda}; q) \\
 & - \frac{g_A^2}{92\pi f_\pi^4} \tilde{c}_4 w^2 A(\tilde{\Lambda}; q) \tau_1 \cdot \tau_2 [\vec{\sigma}_1 \cdot \vec{q} \vec{\sigma}_2 \cdot \vec{q} - q^2 \vec{\sigma}_1 \cdot \vec{\sigma}_2] + \sum_{i \neq j \neq k} \frac{1}{2} \left(\frac{g_A}{2f_\pi} \right)^2 \frac{(\vec{\sigma}_i \cdot \vec{q}_i)(\vec{\sigma}_j \cdot \vec{q}_j)}{(\vec{q}_i^2 + M_\pi^2)(\vec{q}_j^2 + M_\pi^2)} \times \\
 & \times \left\{ \delta^{\alpha\beta} \left[-\frac{4\tilde{c}_1 M_\pi^2}{f_\pi^2} + \frac{2\tilde{c}_3}{f_\pi^2} \vec{q}_i \cdot \vec{q}_j \right] + \sum_\gamma \frac{\tilde{c}_4}{f_\pi^2} \epsilon^{\alpha\beta\gamma} \tau_k^\gamma \vec{\sigma}_k \cdot [\vec{q}_i \times \vec{q}_j] \right\} \tau_i^\alpha \tau_j^\beta \\
 & - \sum_{i \neq j \neq k} \frac{g_A}{8f_\pi^2} \frac{\tilde{c}_D}{f_\pi^2 \Lambda_\chi} \frac{\vec{\sigma}_j \cdot \vec{q}_j}{\vec{q}_j^2 + M_\pi^2} (r_i \cdot \tau_j) (\vec{\sigma}_i \cdot \vec{\sigma}_j) + \frac{1}{2} \sum_{j \neq k} \frac{\tilde{c}_E}{f_\pi^4 \Lambda_\chi} (\tau_j \cdot \tau_k)
 \end{aligned}$$

Global sensitivity analysis (GSA)

A sensitivity analysis addresses the question ‘*How much does each model parameter contribute to the variance in the prediction?*’

GSA decompose the variance of a certain model output in terms of each input and their combinations.

Global methods deal with the uncertainties of the outputs due to input variations over the whole domain.

Bottleneck: Converging the MC sampling of the variance integrals require approximately 10^6 samples



Global sensitivity analysis

- what is responsible for the variance in the output?

Consider a model $Y = f(\mathbf{X})$ where $\mathbf{X} = (X_1, X_2, \dots, X_n)$ follow some (iid) distribution.

- If we fix $X_i = x_i^\star$ (true), how much uncertainty / variance $\text{Var}(Y)$ remain?
- This is measured by the conditional variance $\text{Var}_{\mathbf{X}_{-i}}(Y | X_i = x_i^\star)$
- However, since we don't know x_i^\star , we average $\mathbb{E}_i[\text{Var}_{\mathbf{X}_{-i}}(Y | X_i)]$

By the law of total variance $\text{Var}(Y) = \text{Var}_i(\mathbb{E}_{\mathbf{X}_{-i}}[Y | X_i]) + \mathbb{E}_i[\text{Var}_{\mathbf{X}_{-i}}(Y | X_i)]$

$$\mathbb{E}_{\mathbf{X}_{-i}}[Y | X_i] = \int d\mathbf{X}_{-i} f(X_1, \dots, X_n) p(\mathbf{X}_{-i} | X_i)$$

large/small

small/large

From this we *define* the *main effect* $S_i = \frac{\text{Var}_i(\mathbb{E}_{\mathbf{X}_{-i}}[Y | X_i])}{\text{Var}(Y)} \in [0,1]$

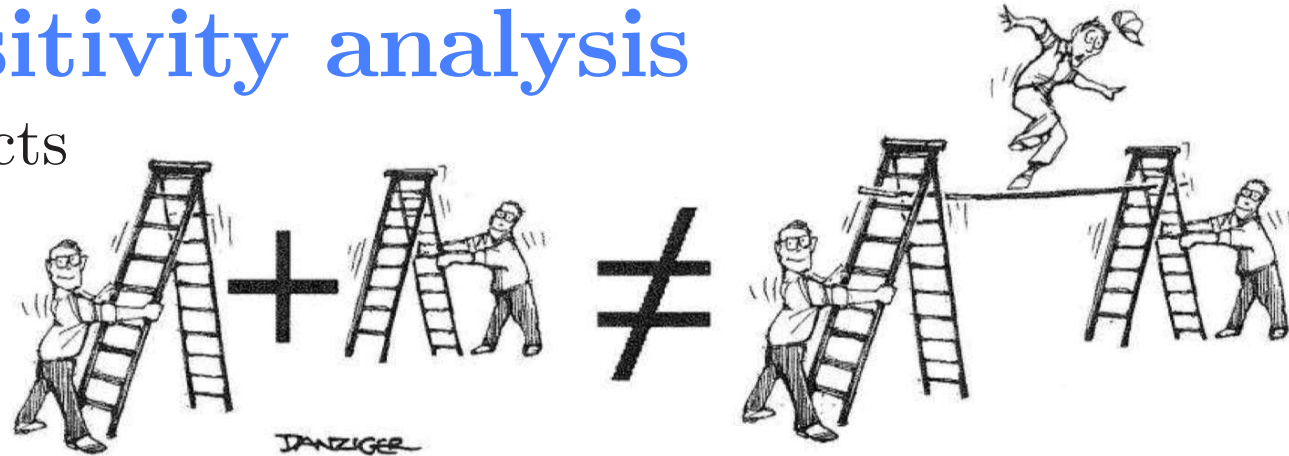
This is a very convenient scalar quantity to convey essential information about a model

A large value of S_i indicates large first-order sensitivity to X_i

A small value of S_i indicates small first-order sensitivity to X_i

Global sensitivity analysis

- higher-order effects



We can define high-order sensitivities $S_{ij} = \frac{\text{Var}_{ij}(\mathbb{E}_{X_{-ij}}[Y | X_i, X_j])}{\text{Var}(Y)} - S_i - S_j$ etc.

Computing S_{ijk} and even higher-order sensitivities quickly becomes a formidable task. Fortunately, it is possible to compute the total effect S_{Ti} of model parameter i , including its first order effect and sensitivities to all orders as

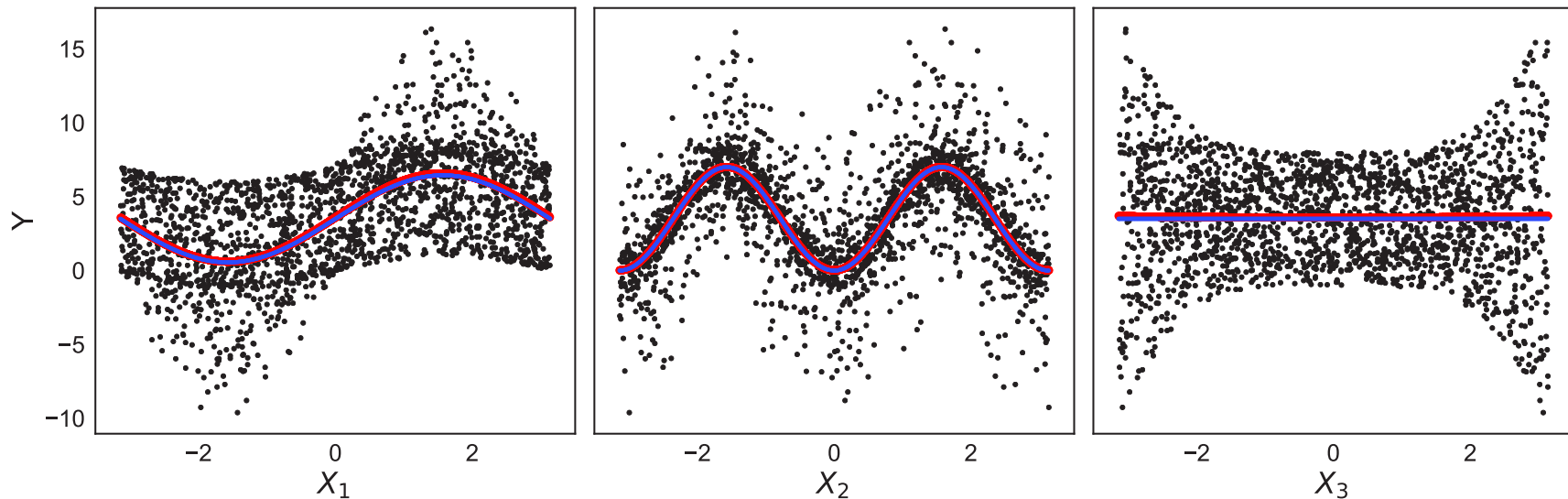
$$S_{Ti} = 1 - \frac{\text{Var}_{X_{-i}}(\mathbb{E}_i[Y | X_{-i}])}{\text{Var}(Y)} = S_i + S_{ij} + S_{ijk} + \dots \quad (S_{Ti} \geq S_i, \text{ equality for additive models})$$

The Ishigami function

a toy model: Non-linear, and not additive

$$S_i = \frac{\text{Var}_i(\mathbb{E}_{X_{-i}}[Y|X_i])}{\text{Var}(Y)} \in [0,1]$$

$$f(X_1, X_2, X_3) = \sin X_1 + A \sin^2 X_2 + B X_3^4 \sin X_1, \quad X_i \sim \mathcal{U}(-\pi, +\pi), \quad A = 7.0, \quad B = 0.1$$



$$S_1 = 0.31$$
$$ST_1 = 0.56$$

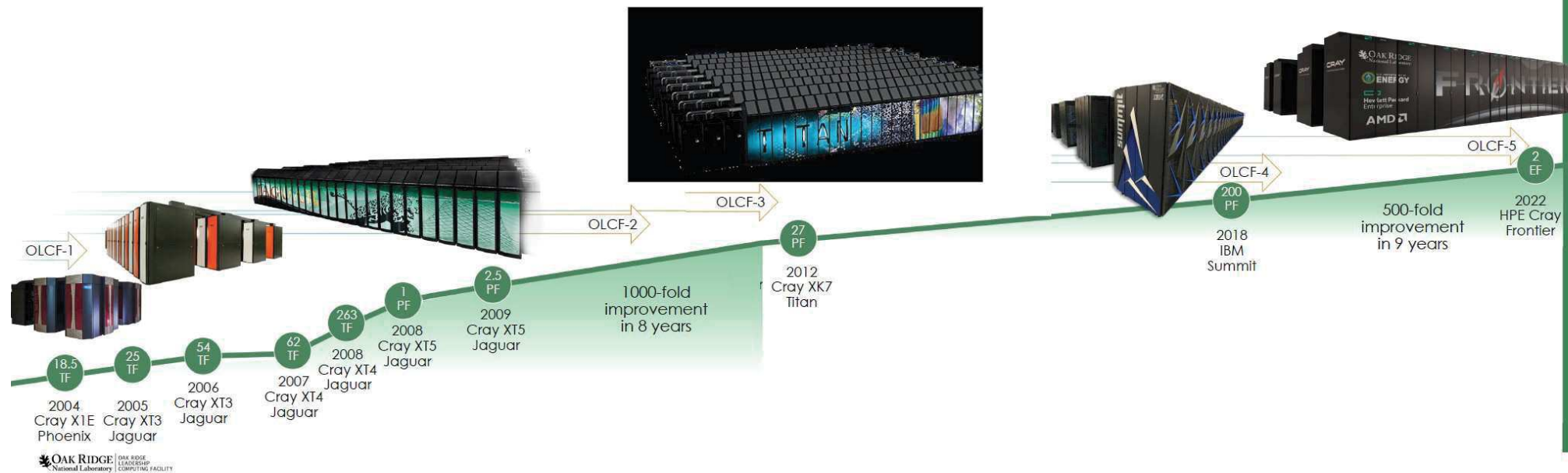
$$S_2 = 0.44$$
$$ST_2 = 0.44$$

$$S_3 = 0.00$$
$$ST_3 = 0.24$$
$$S_{13} = 0.24$$

X_3 has no additive effect on Y
interacts only via X_1

Computing nuclei: an HPC problem

Solving the Schrödinger equation for a large collection of strongly interacting nucleons typically requires substantial high-performance computing resources. Naively, the computational cost to solve the Schrödinger equation grows exponentially with nucleon number and basis size. Polynomially scaling methods exist but are still computationally expensive.

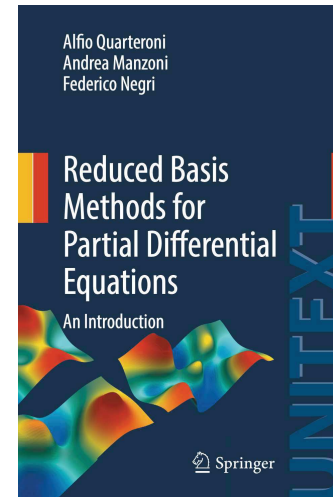


Eigenvector continuation

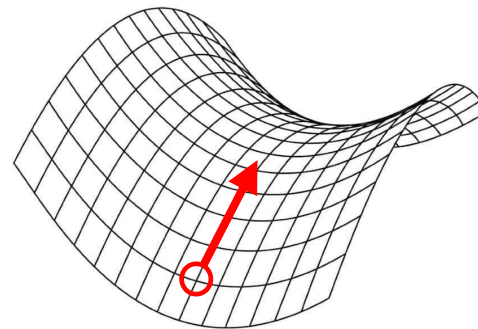
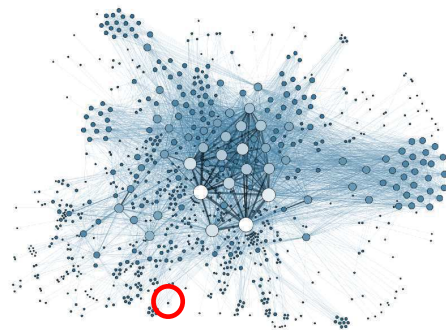
a reduced basis method

$$H(\alpha) = H_0 + \alpha H_1$$

continuous parameter

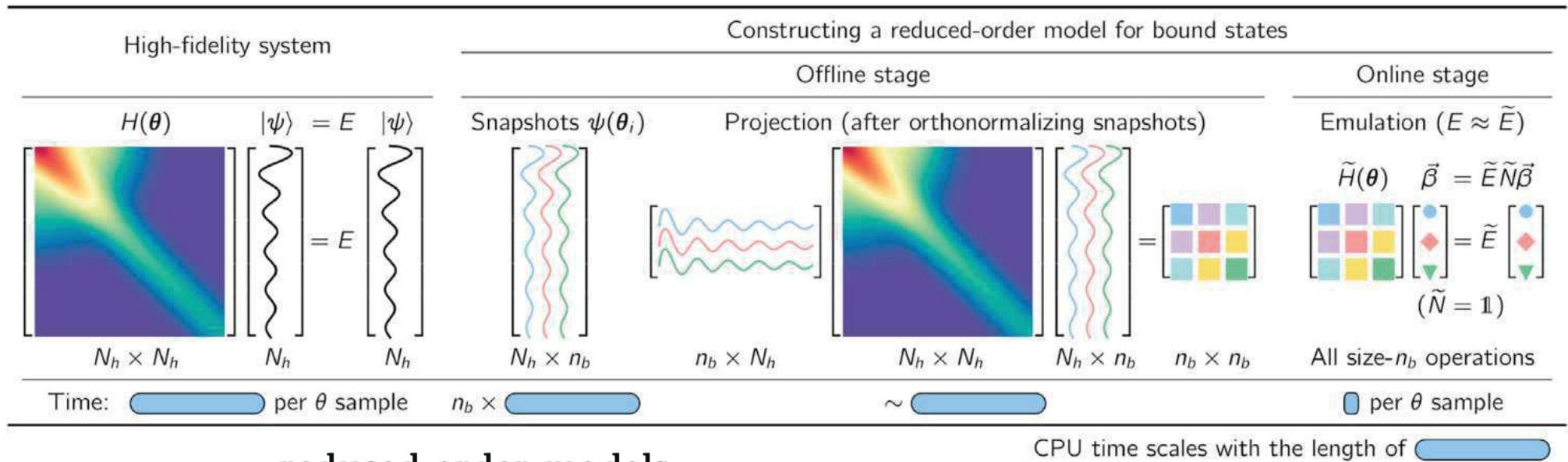


The key insight is that while an eigenvector resides in a linear space with enormous dimensions, the eigenvector trajectory generated by smooth changes of the Hamiltonian matrix is well approximated by a very low-dimensional manifold in many applications.

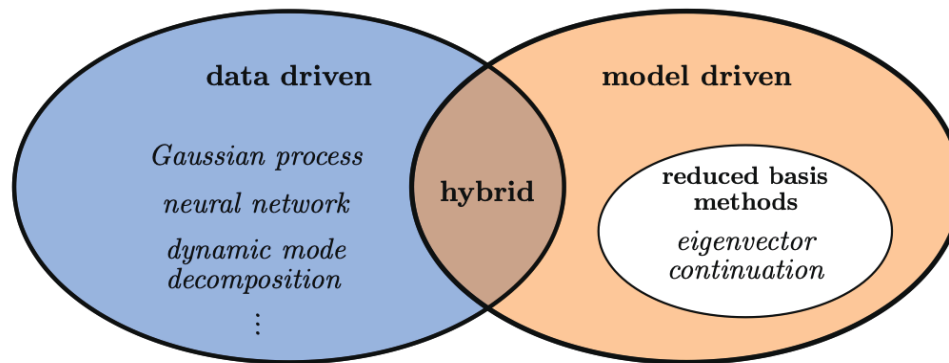


D. Frame, et al. Phys. Rev. Lett. **121**, 032501 (2018)

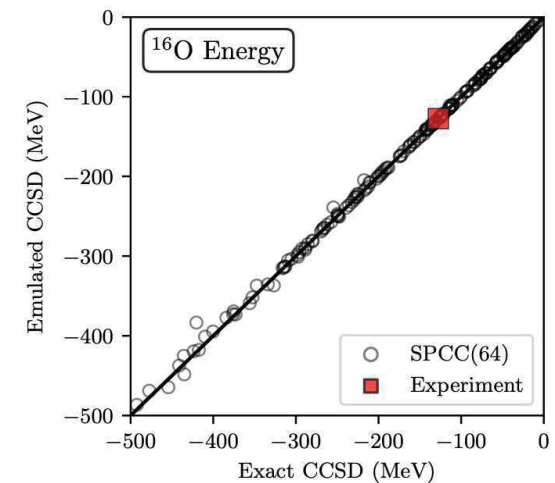
T. Duguet, A. Ekström, R. J. Furnstahl, S. König, D. Lee Rev. Mod. Phys **96**, 031002 (2024)



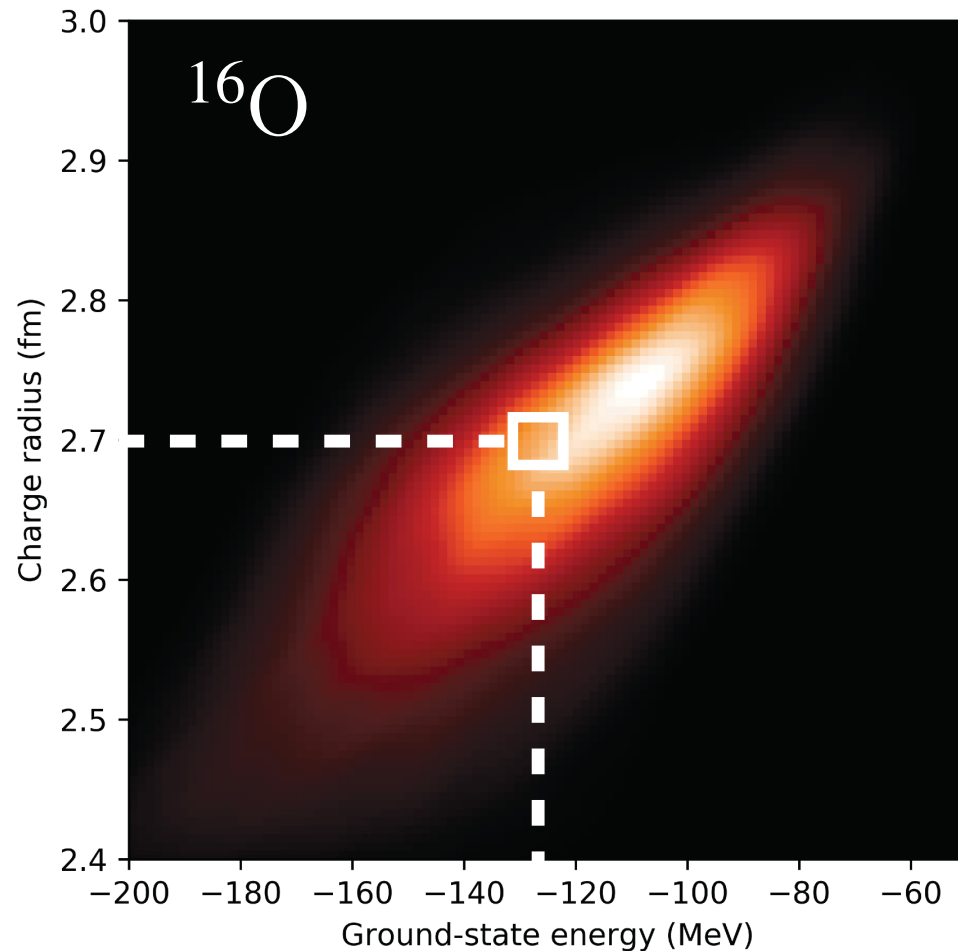
reduced order models



RBM emulators can be created for bound and scattering states!



Emulator speedup: 20 years vs 1 hour!

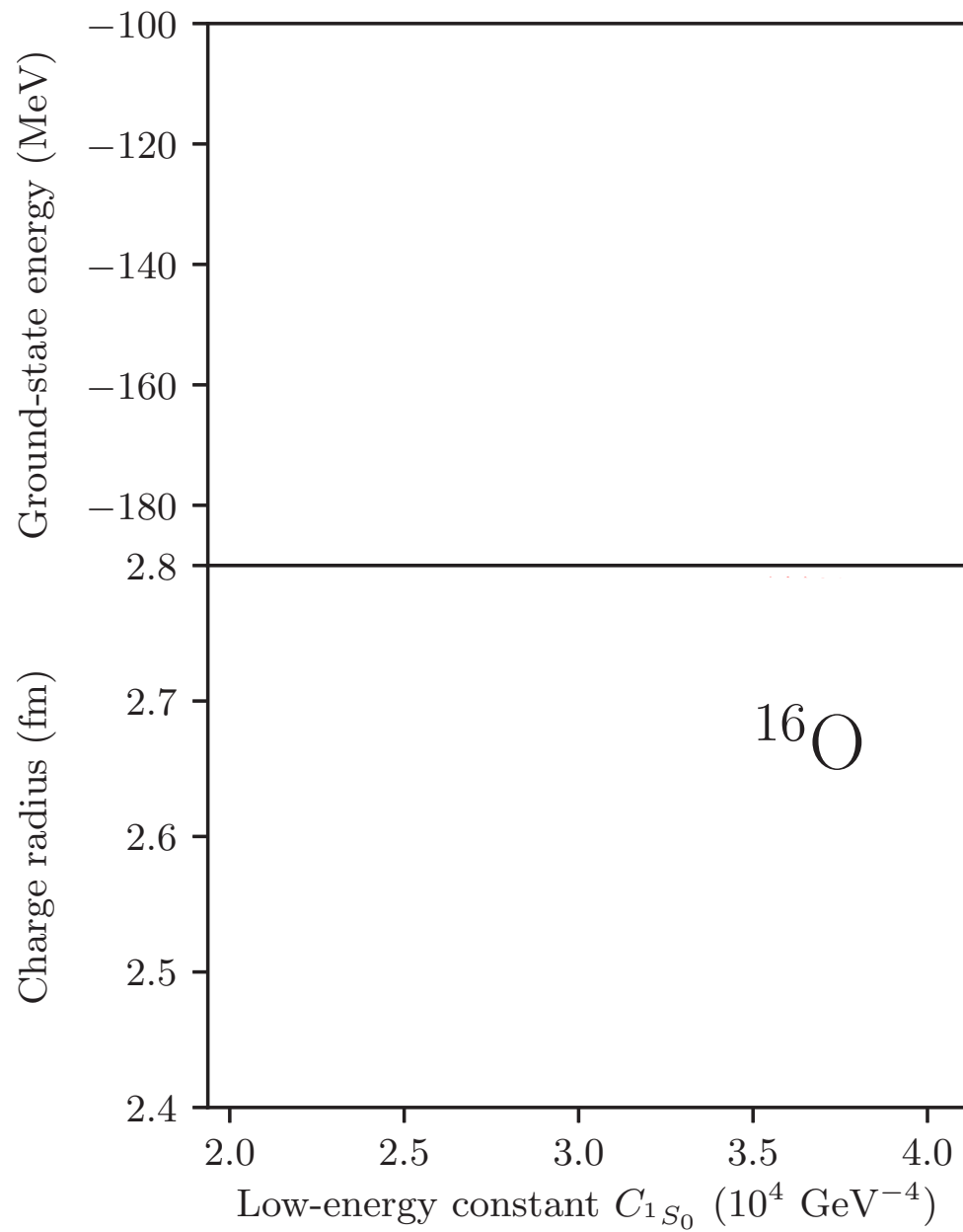


Plot of 100,000 predictions of the radius & energy of ^{16}O for different LEC values of a chiral NNLO interaction.

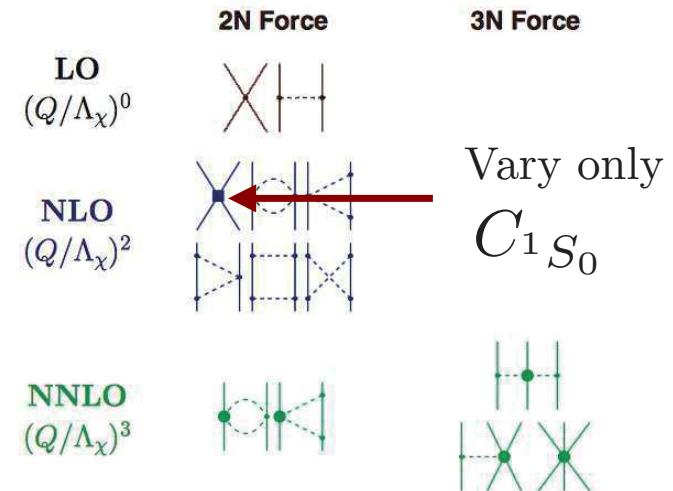
Using emulators, we generated the results on a laptop in just a few minutes.

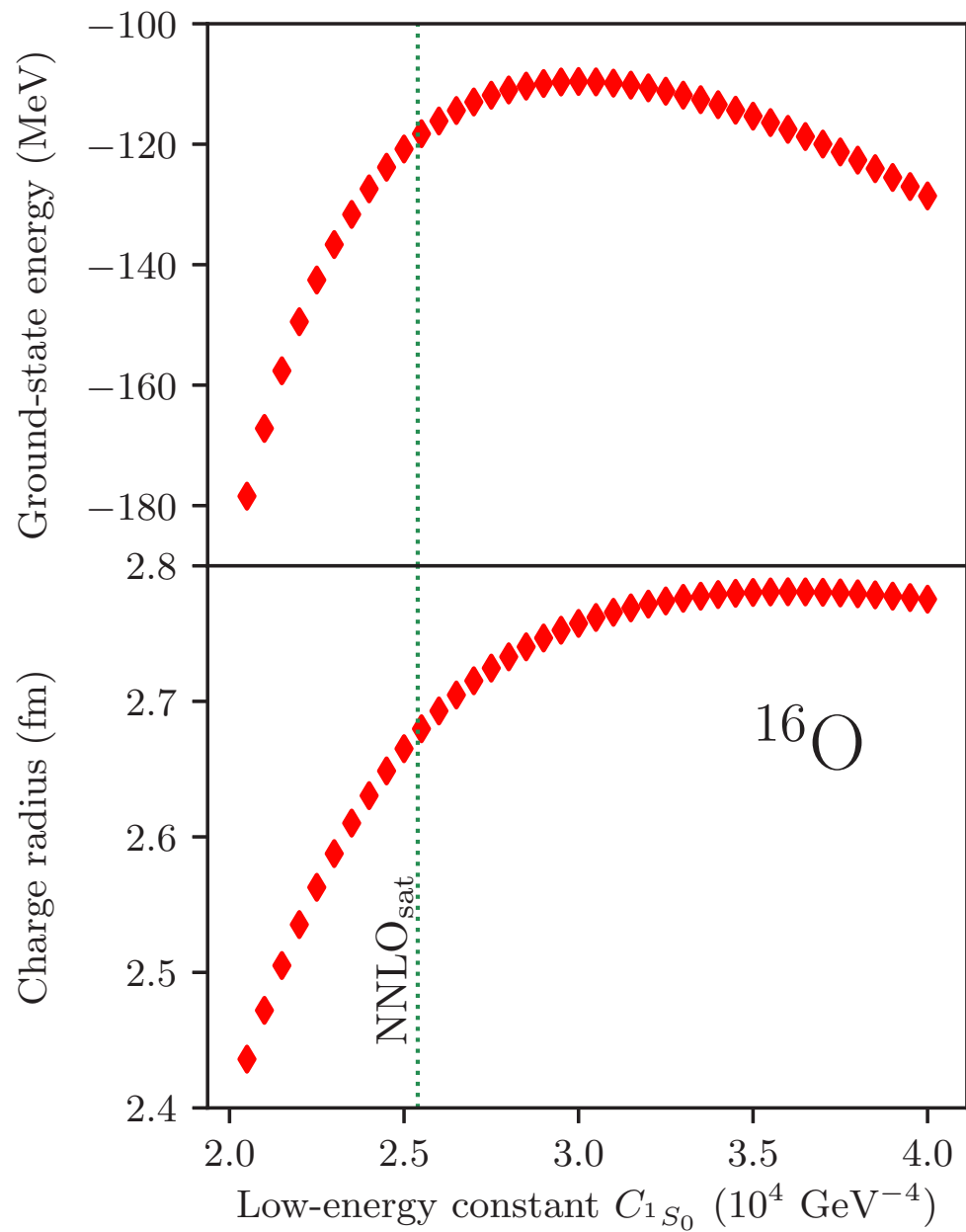
Dashed lines show experimental data.

Emulator error is 1%.

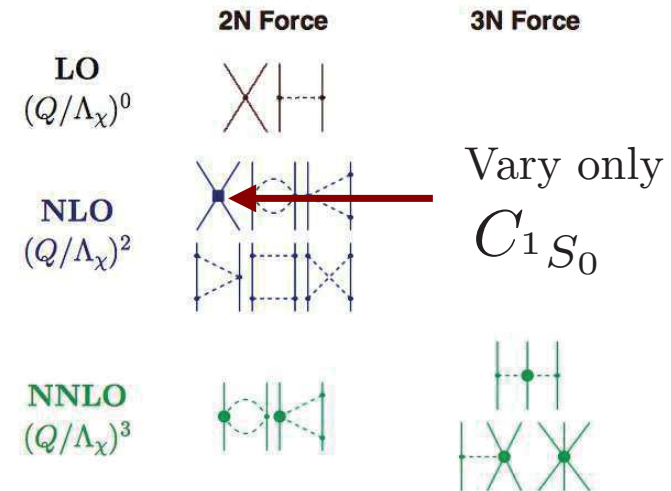


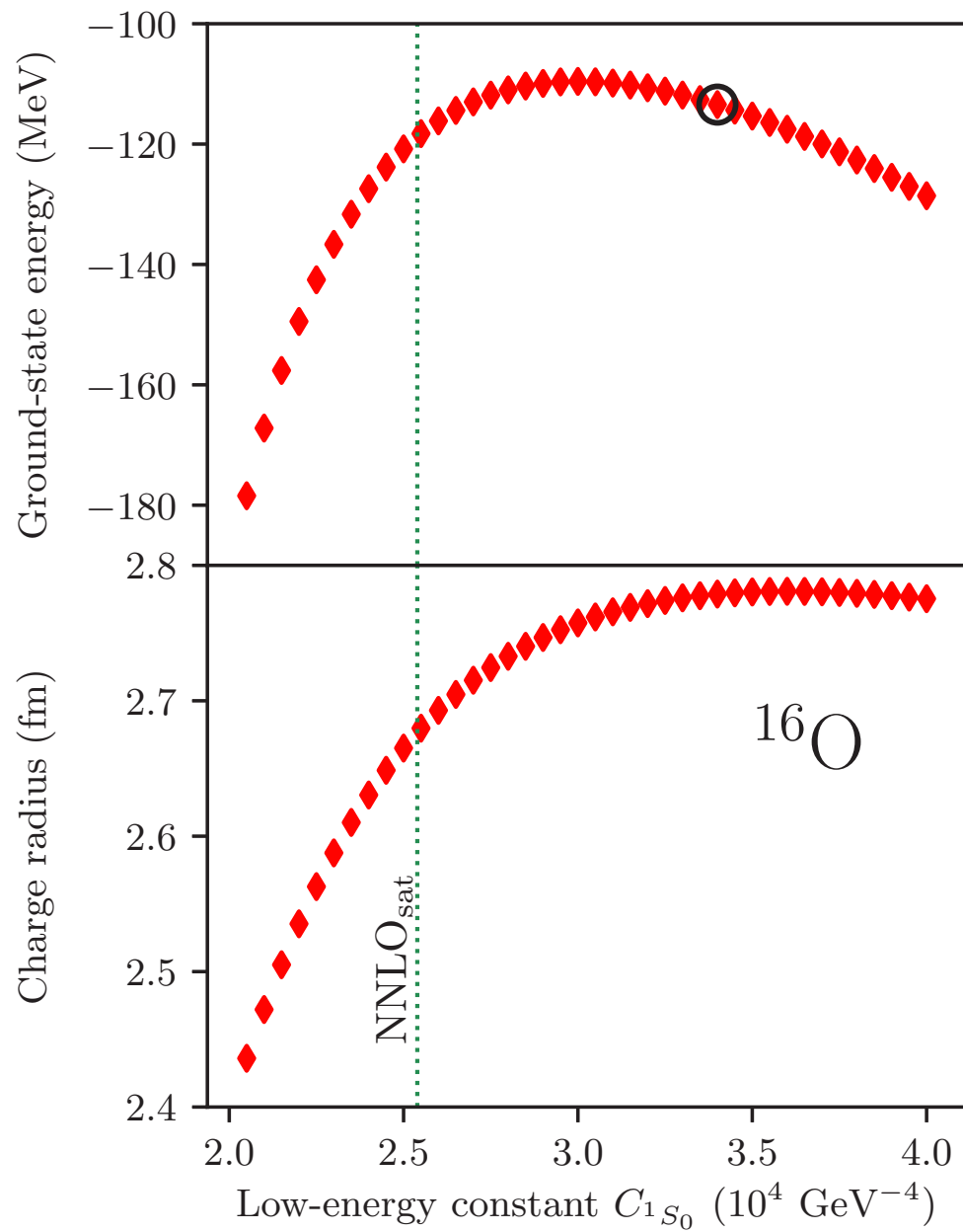
Exact coupled cluster calculations
at the singles and doubles level



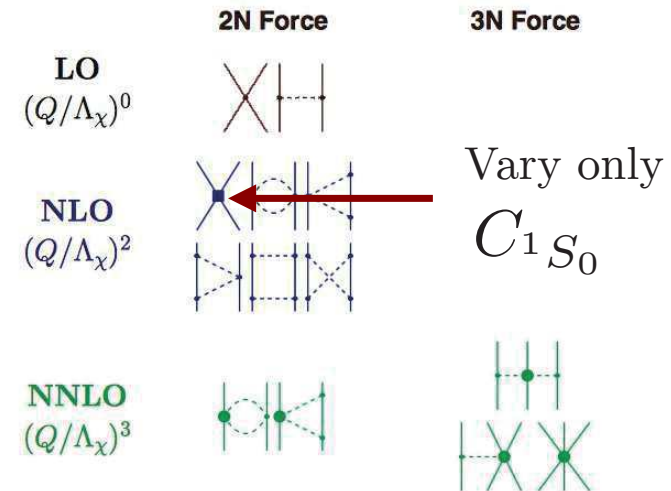


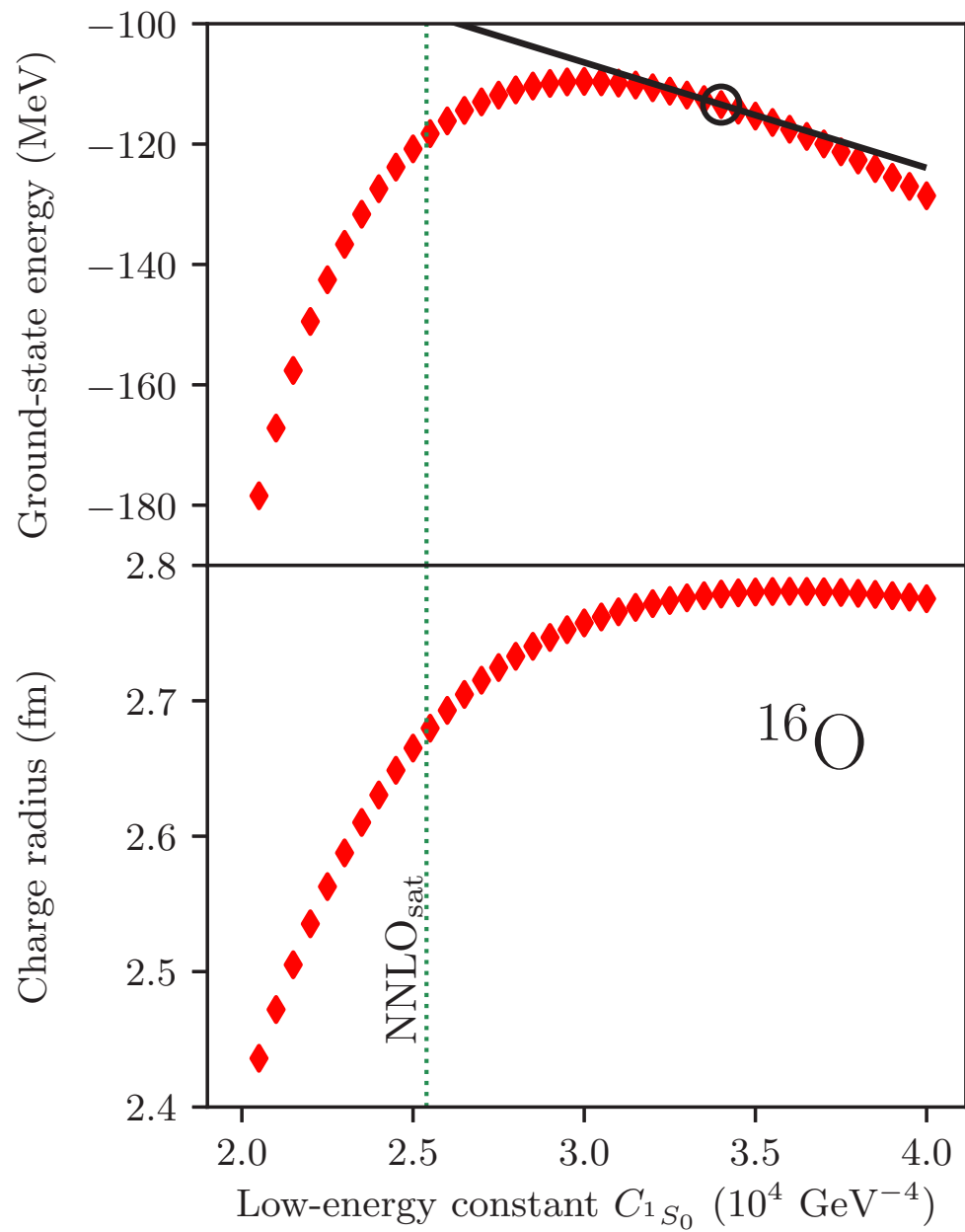
 Exact coupled cluster calculations at the singles and doubles level



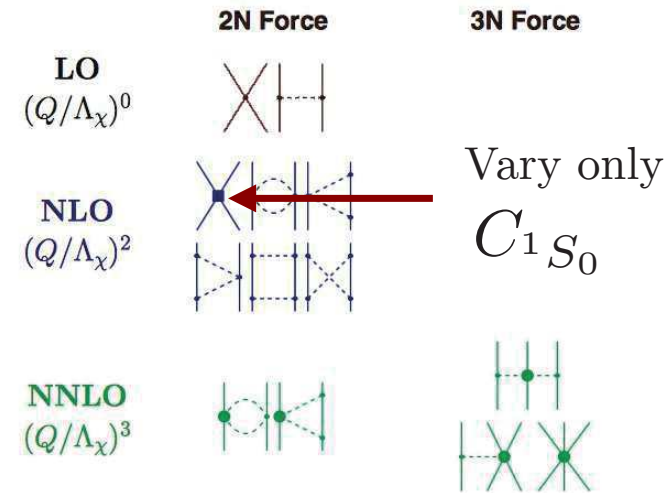


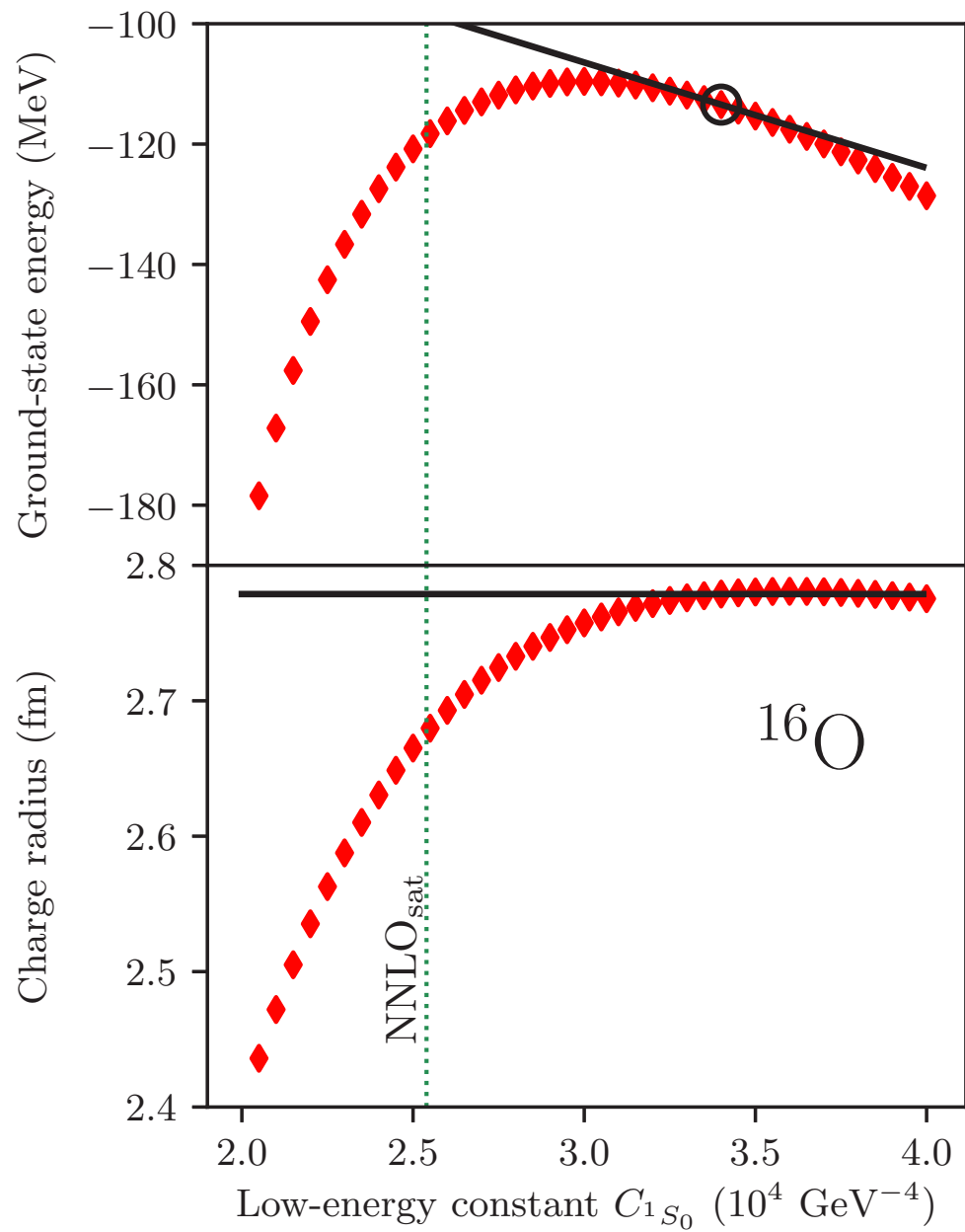
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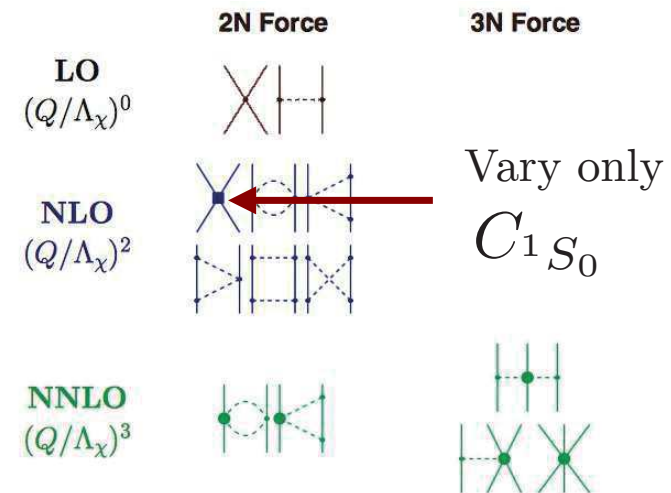


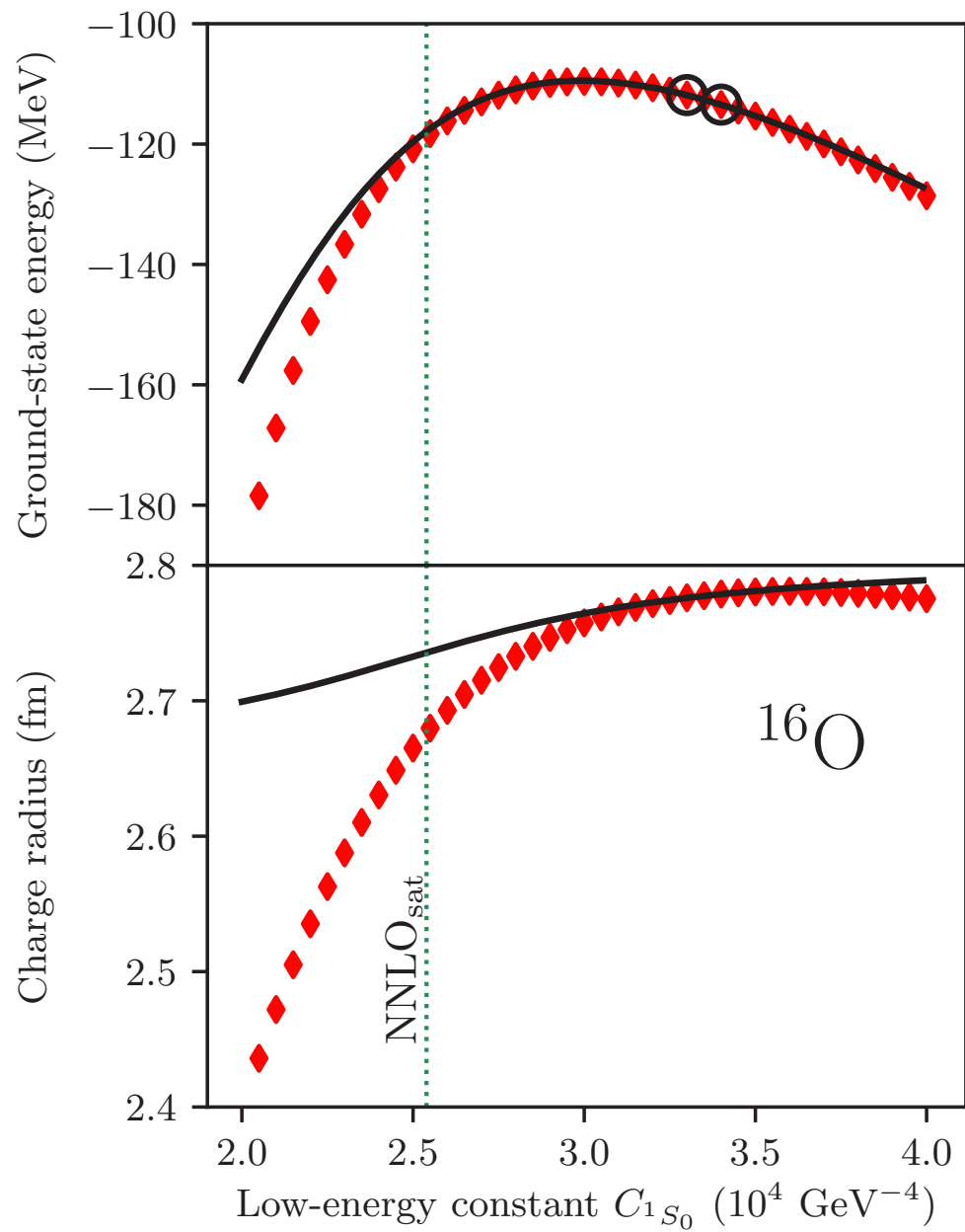
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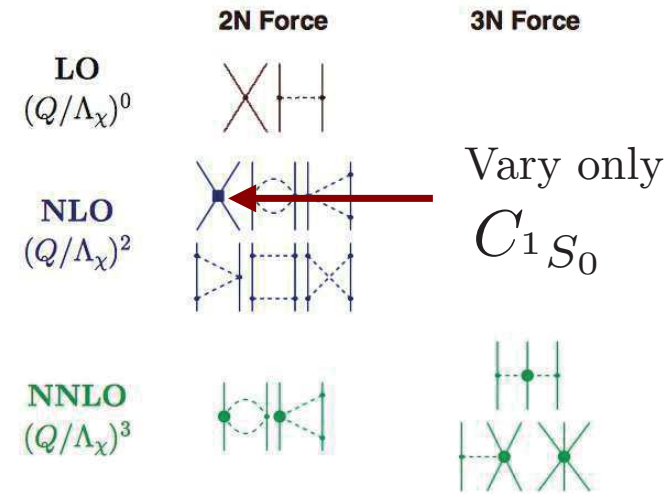


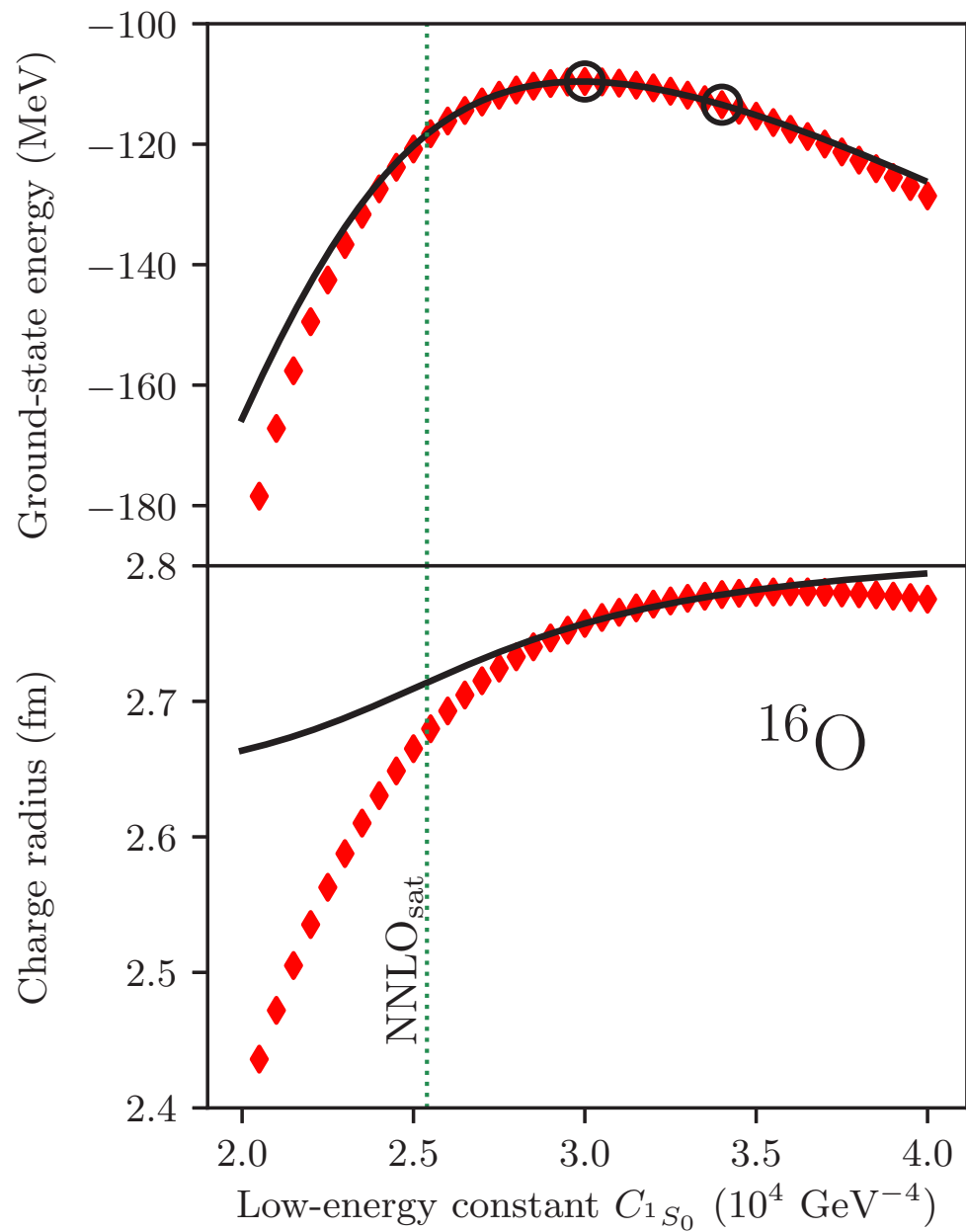
 Exact coupled cluster calculations at the singles and doubles level



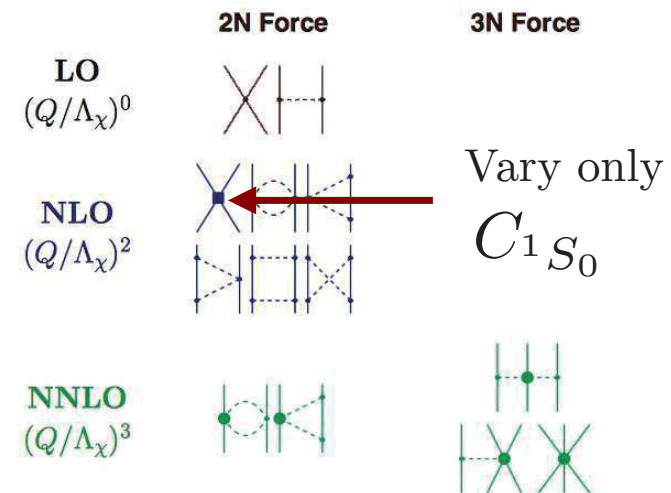


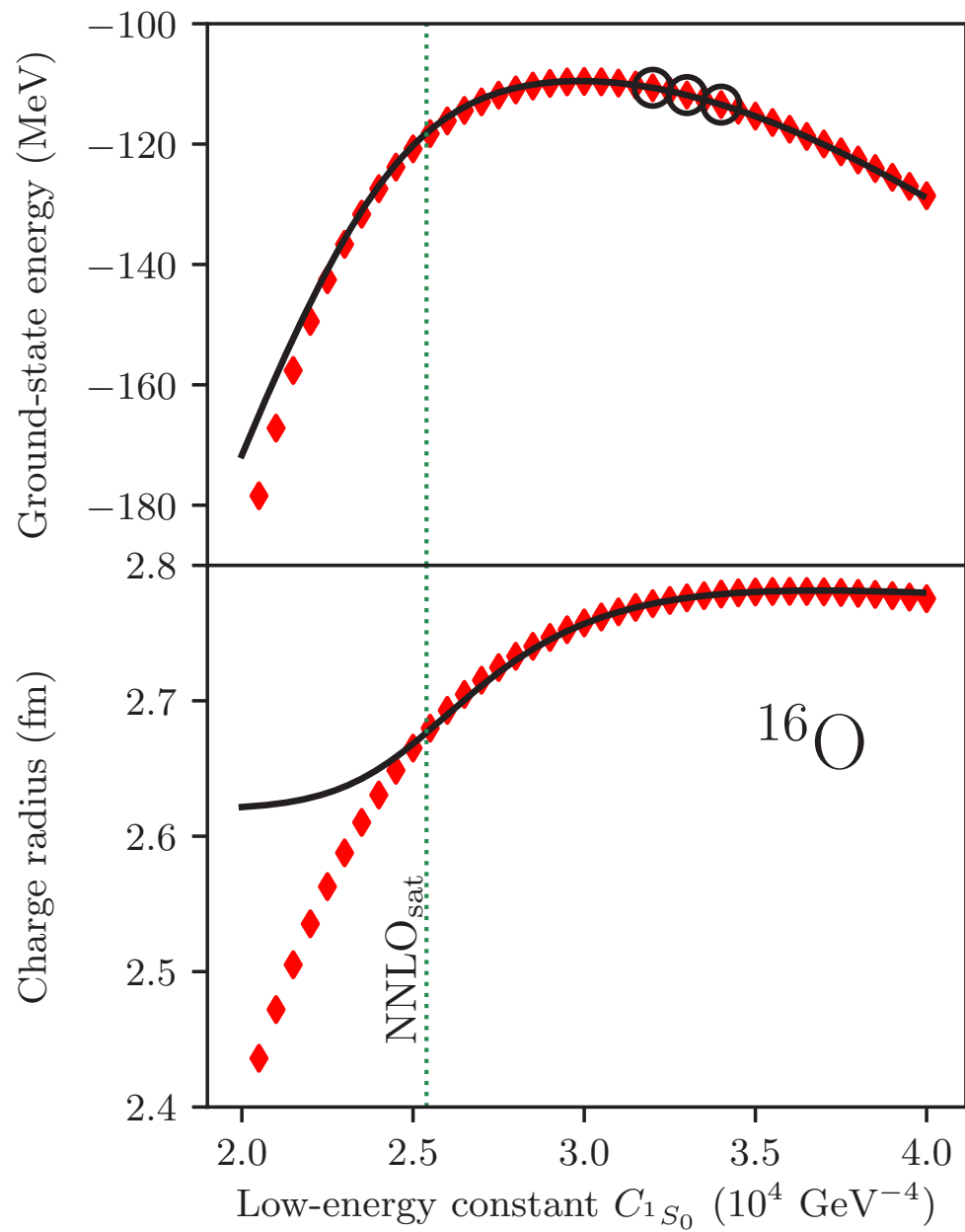
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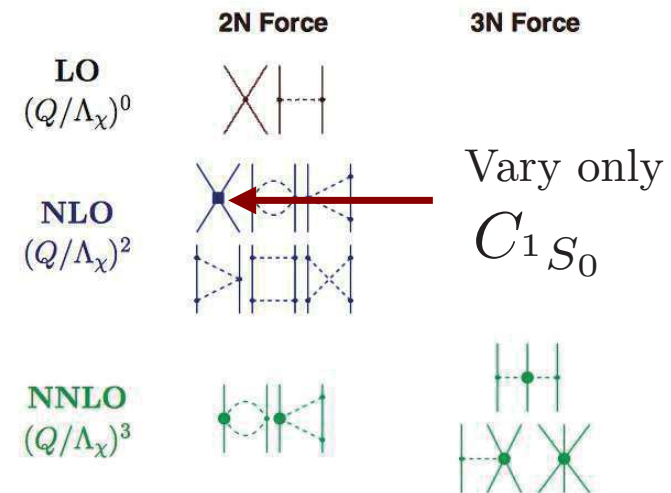


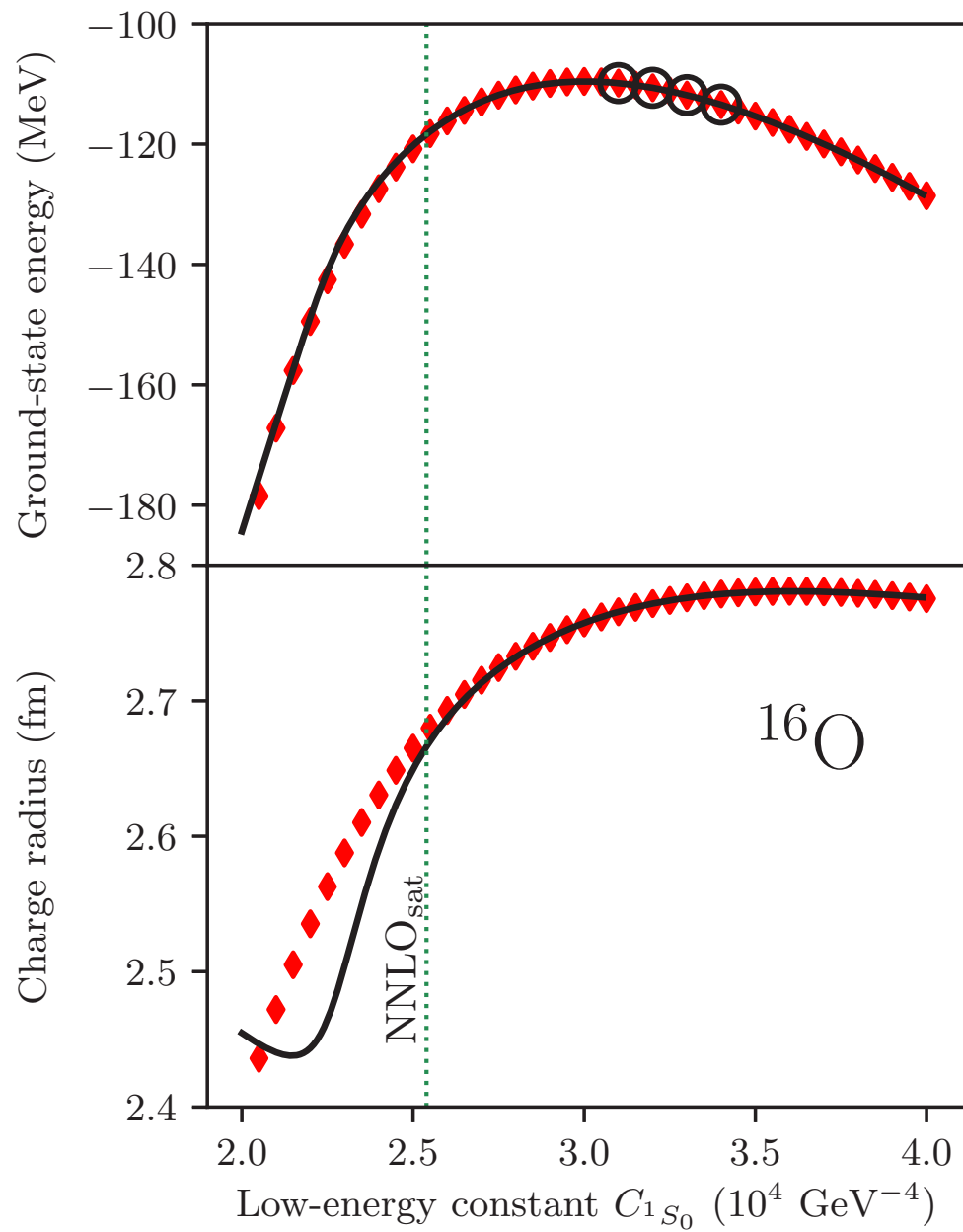
 Exact coupled cluster calculations at the singles and doubles level



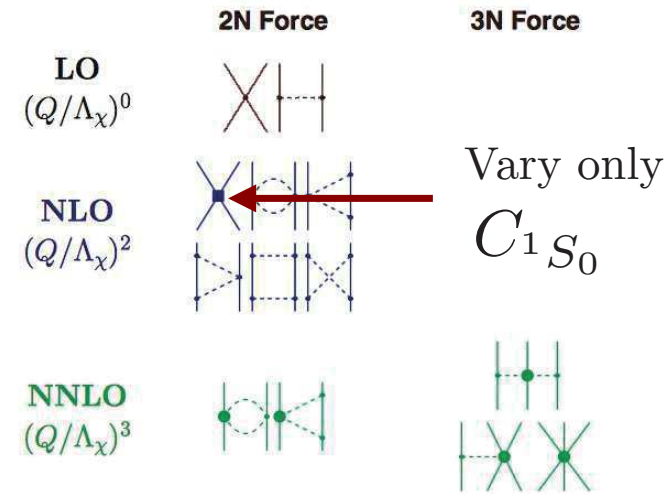


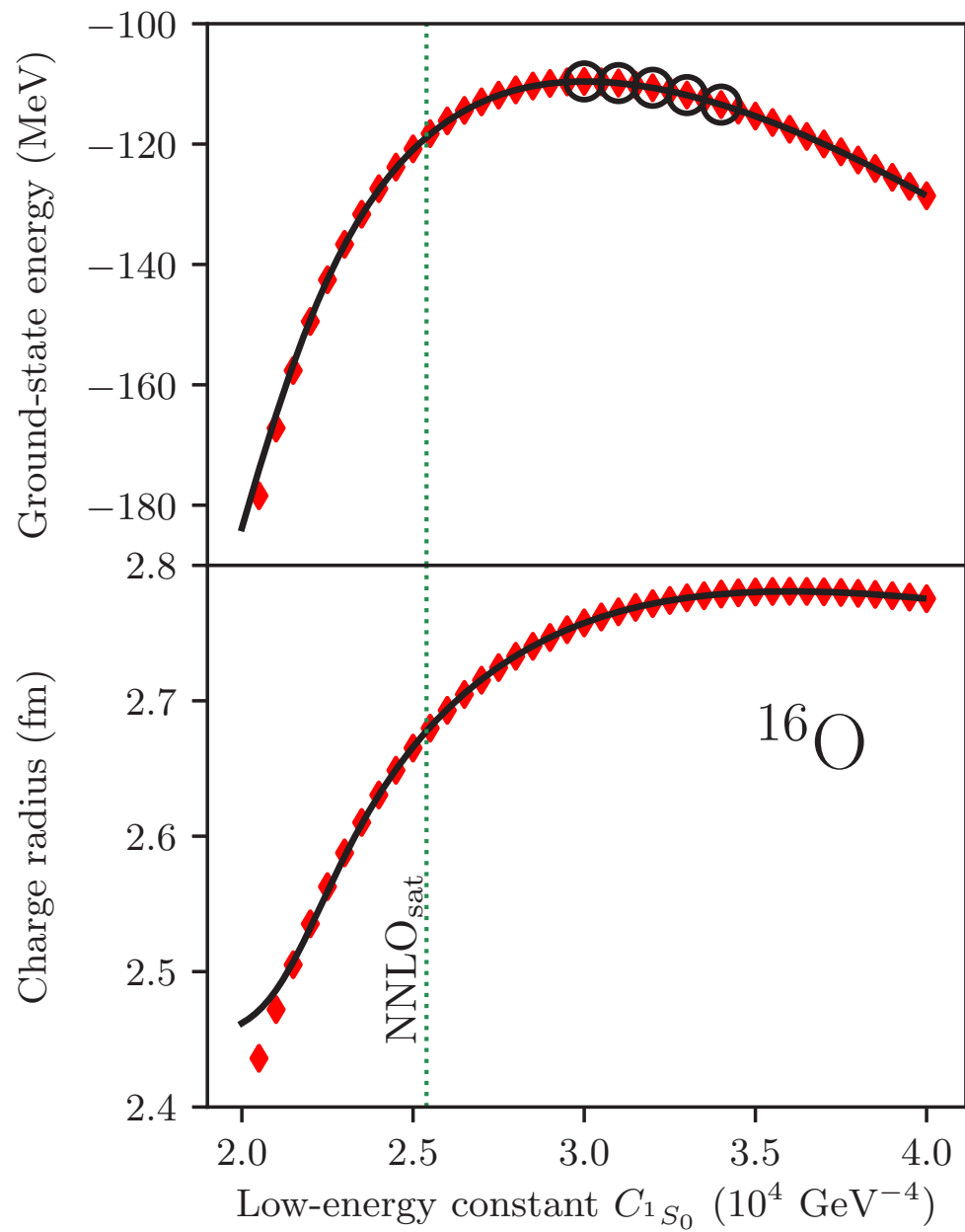
 Exact coupled cluster calculations at the singles and doubles level



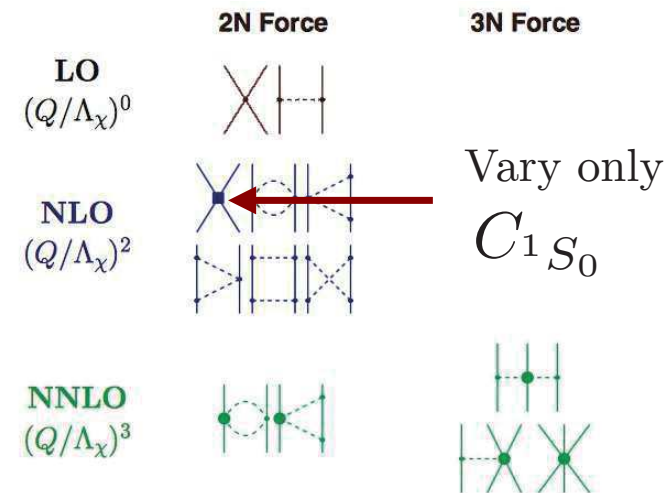


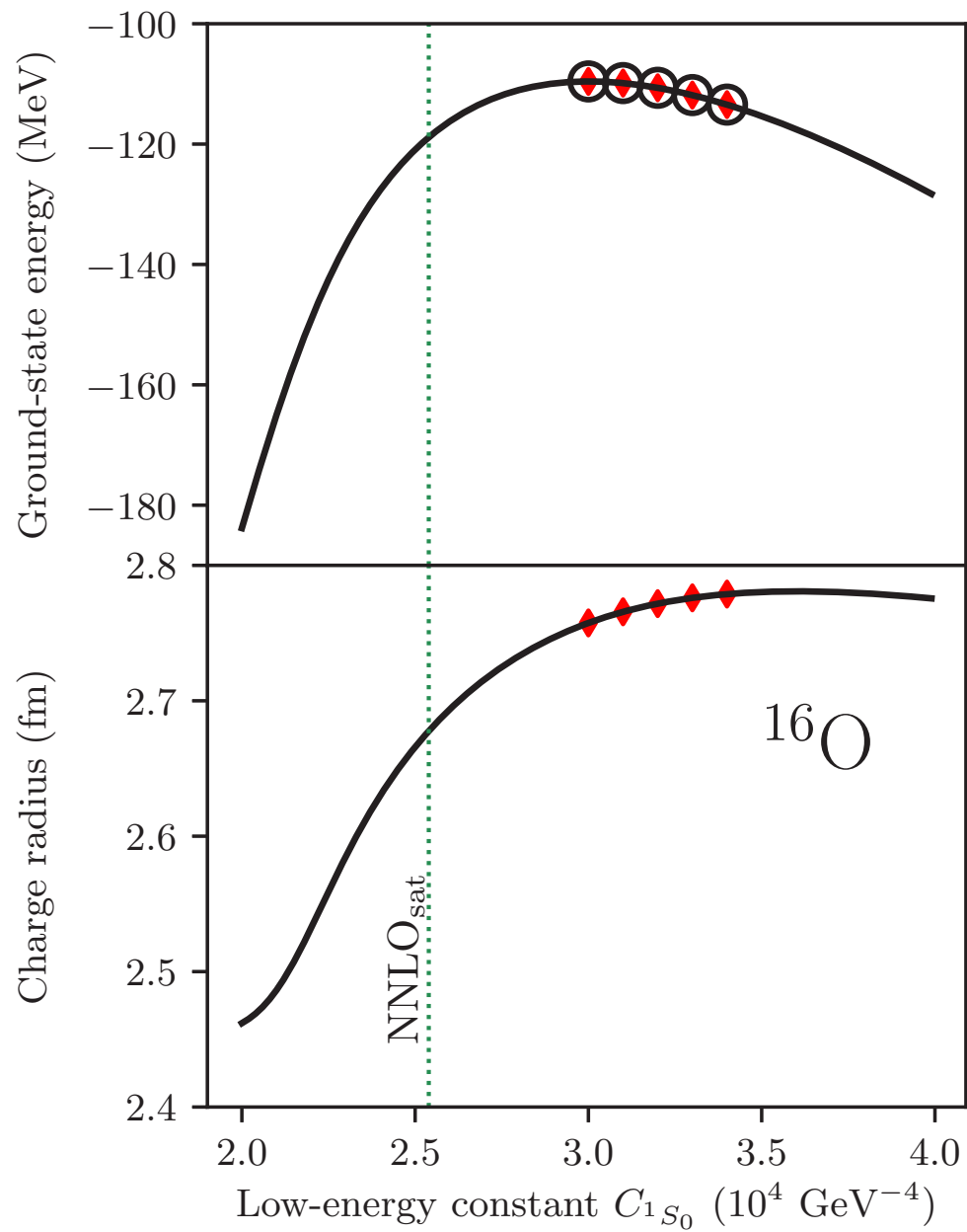
 Exact coupled cluster calculations at the singles and doubles level



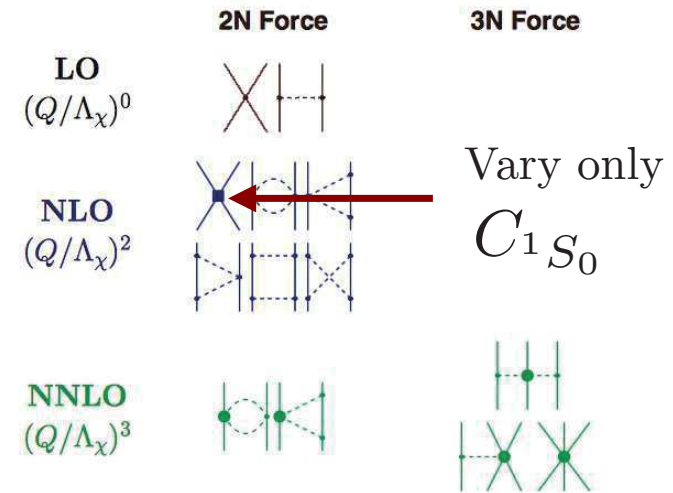


Exact coupled cluster calculations at the singles and doubles level



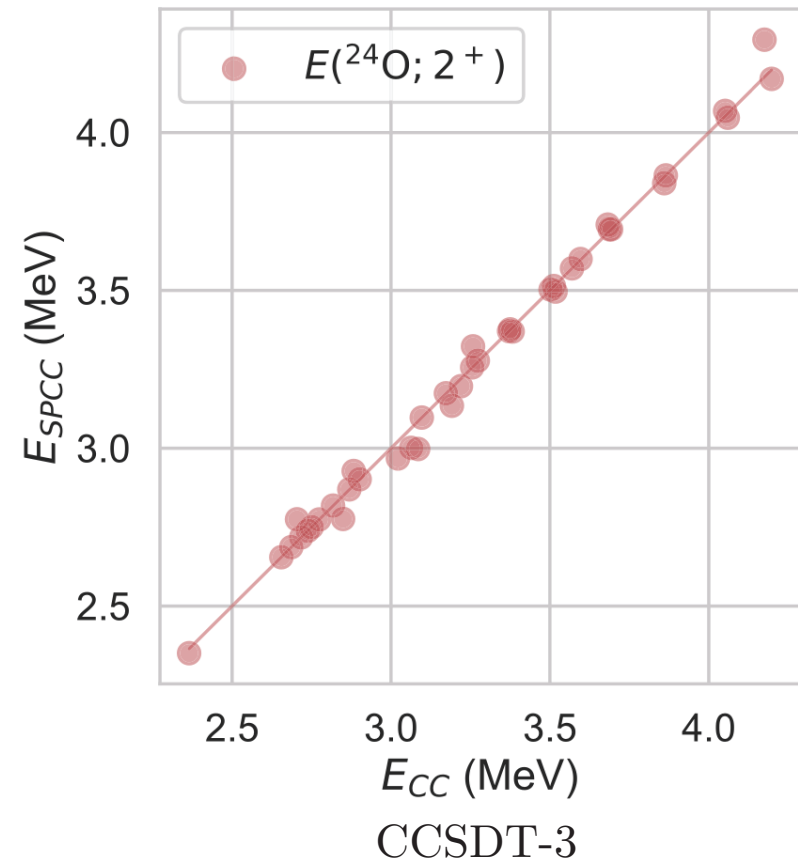


Exact coupled cluster calculations at the singles and doubles level



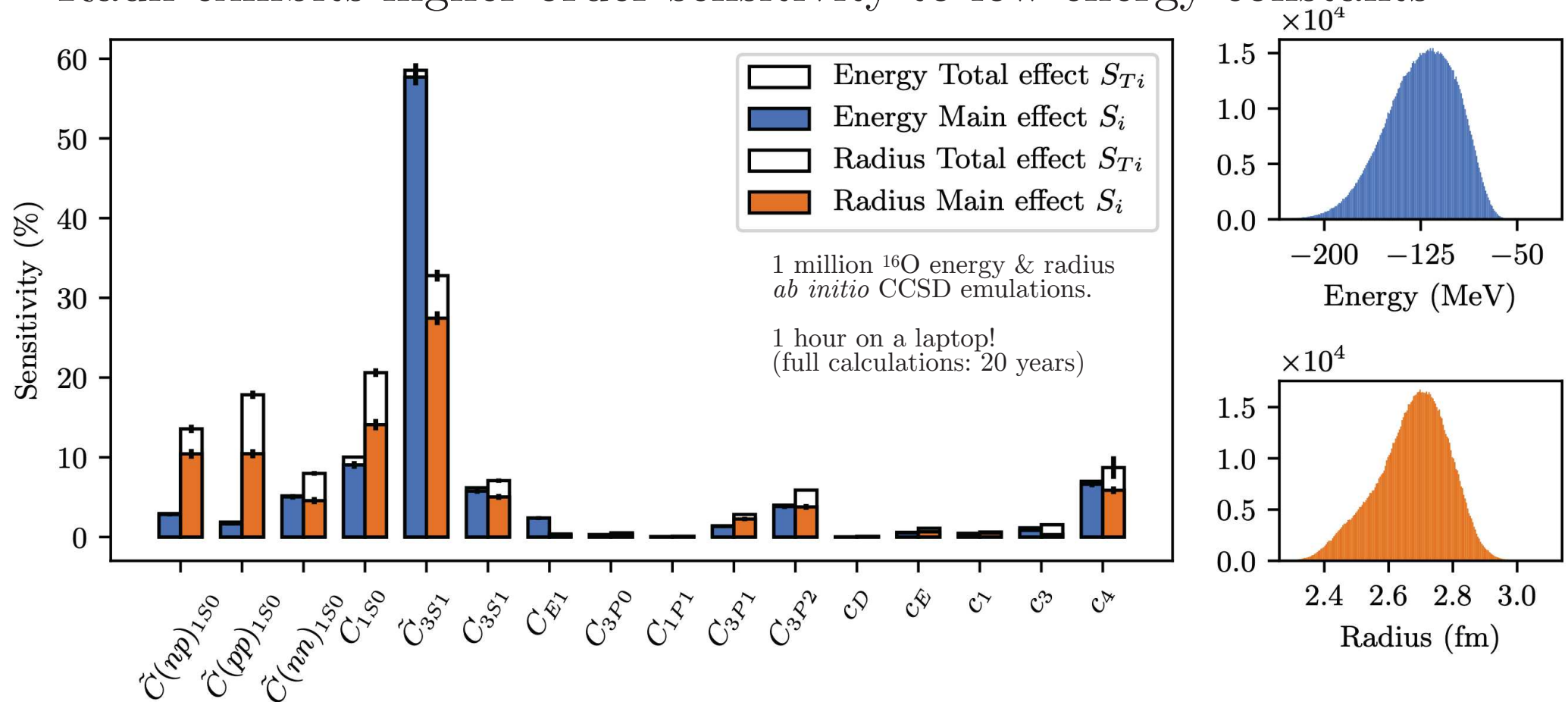
A computational statistics laboratory

- using fast and accurate emulators



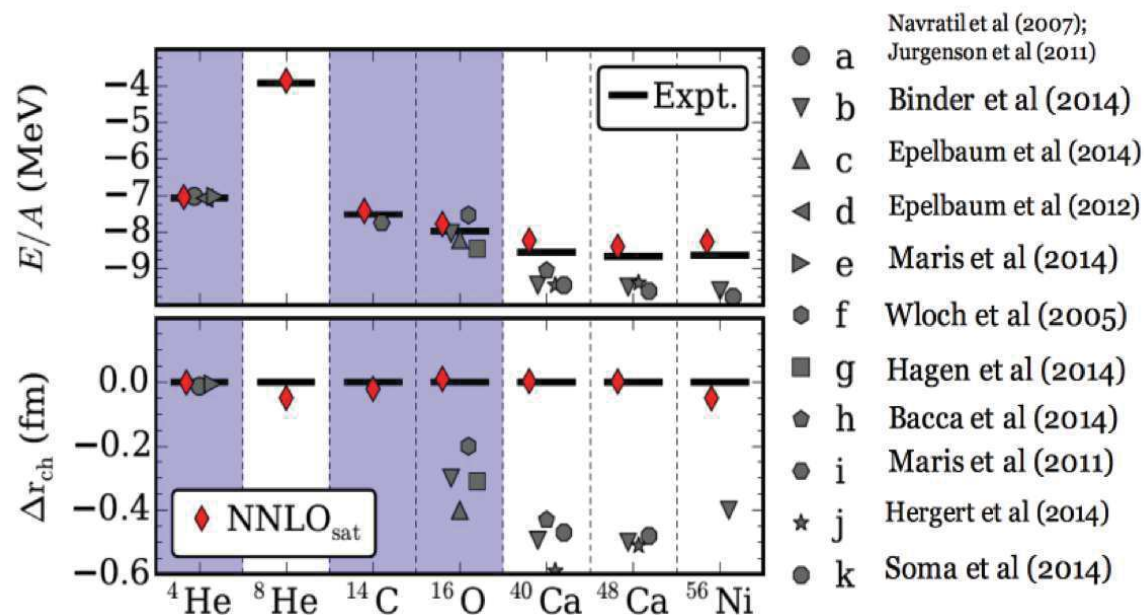
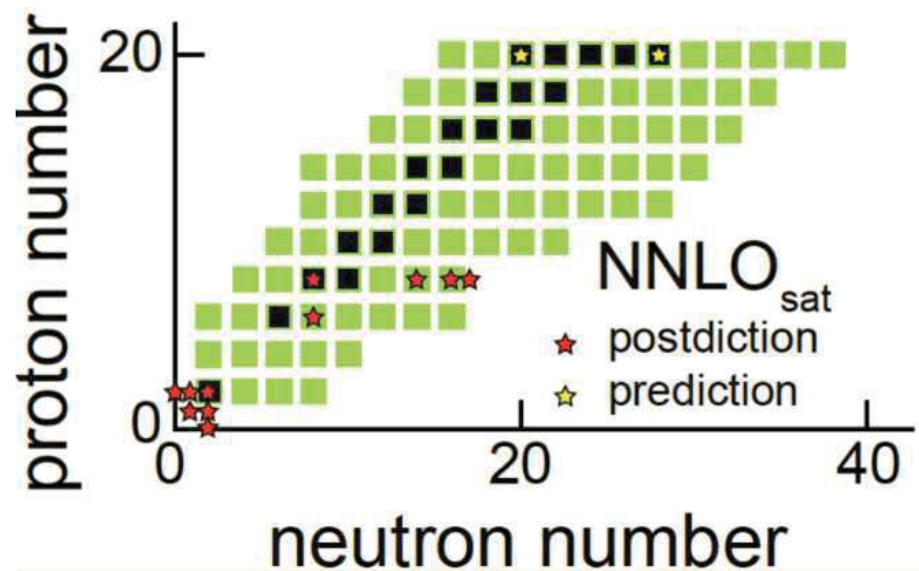
Global sensitivity analysis of an atomic nucleus (^{16}O)

- Radii exhibits higher-order sensitivity to low-energy constants

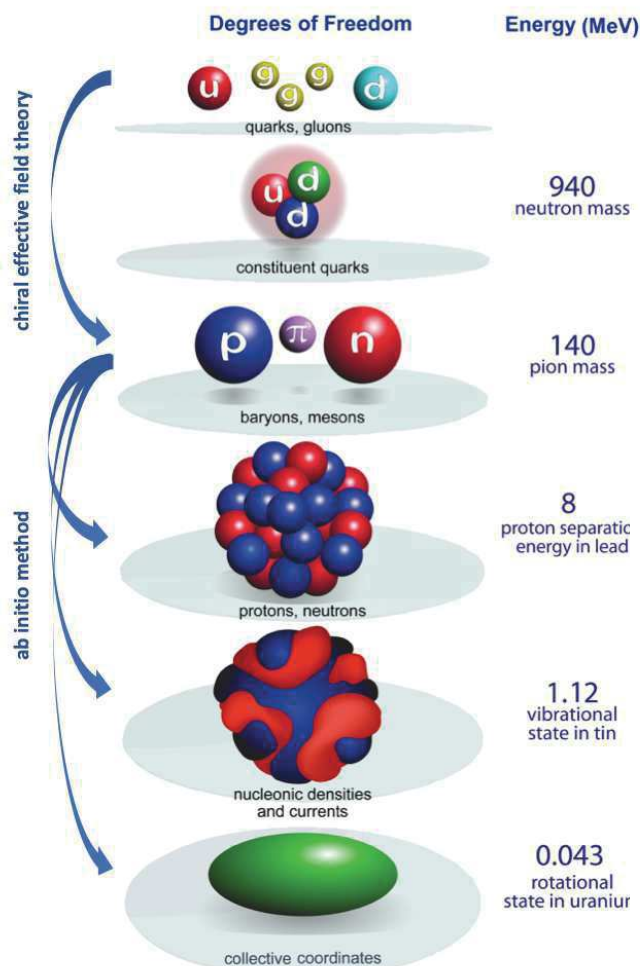


Understanding the challenge of computing radii

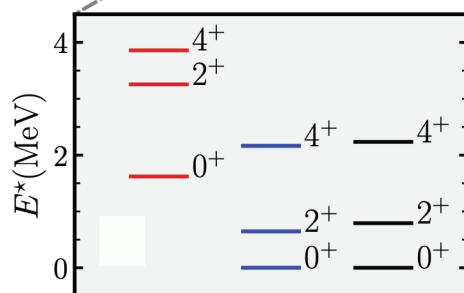
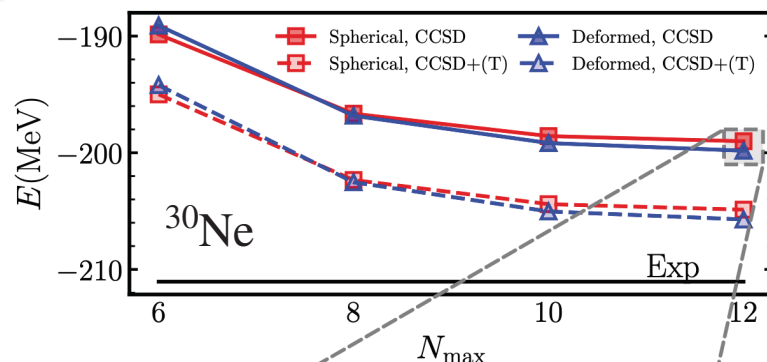
Heavy-mass data is important in nuclear physics calibration.



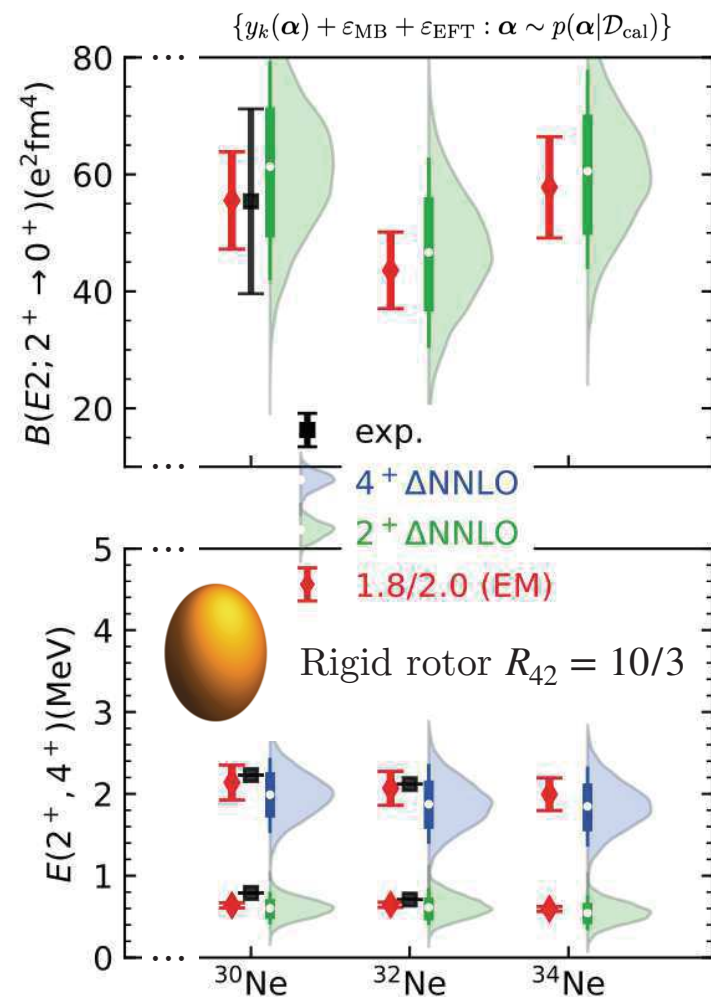
Multiscale physics of atomic nuclei in *ab initio*



PPDs sampled starting from LEC values obtained in the 28-O History Matching.



Spherical Deformed Exp

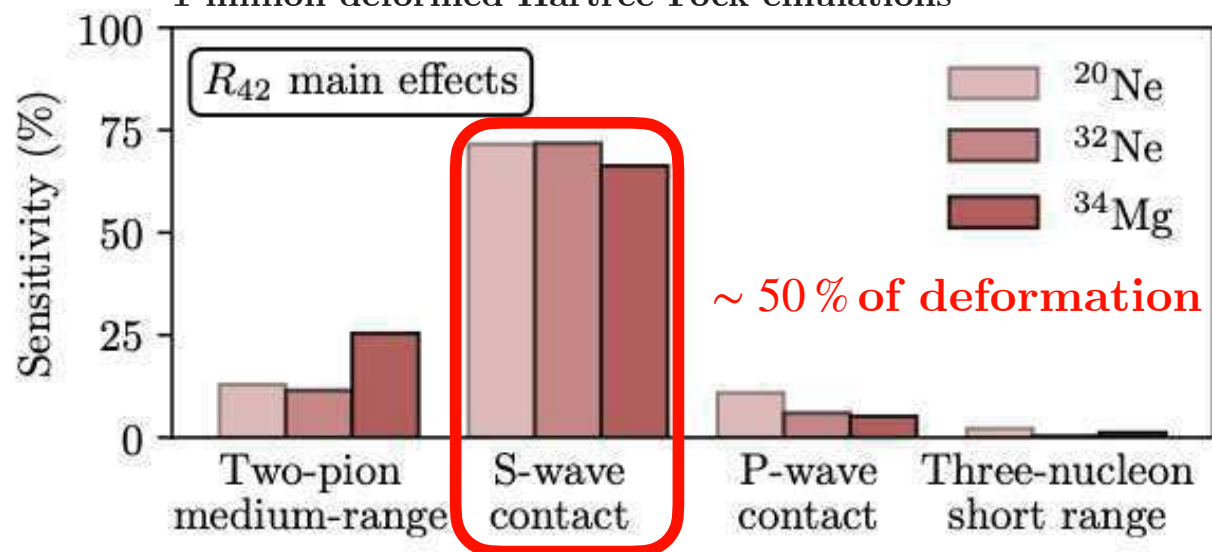


Z. H. Sun, et al. Phys. Rev. X 15, 011028 (2025)

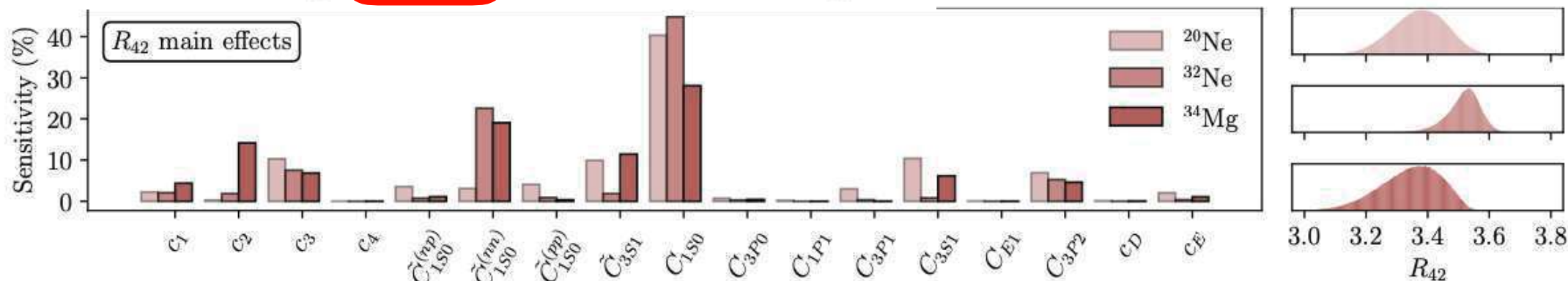
Adapted from NSAC LRP (2007)

Linking deformation and chiral nuclear forces

1 million deformed Hartree-Fock emulations

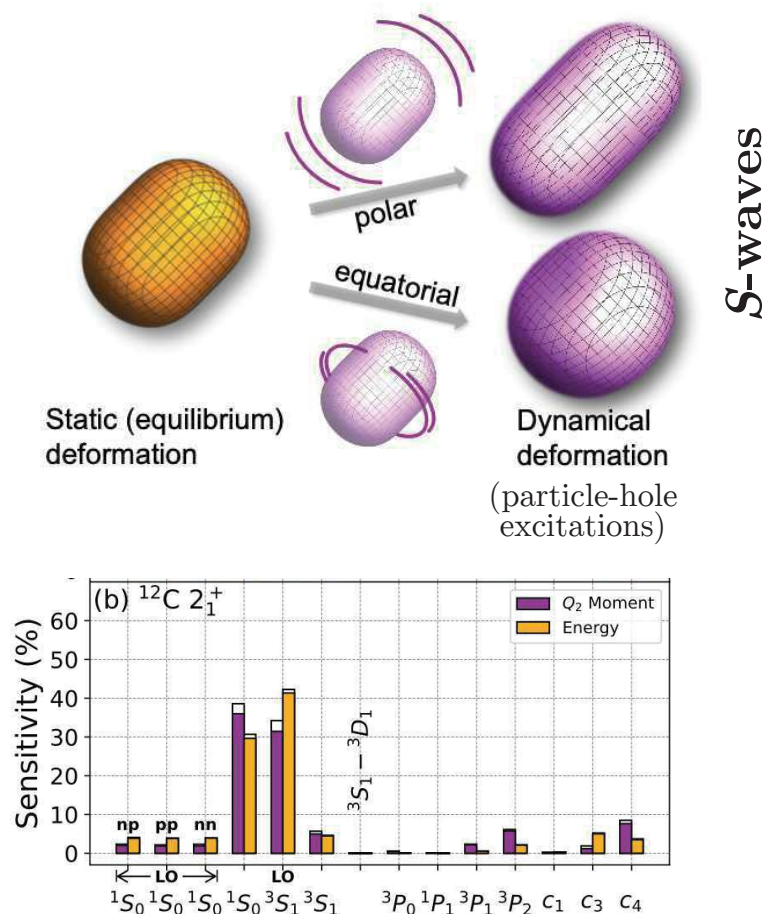


- Adding short-range repulsion appears to increase deformation, probably via reduced pairing.
- Increasing medium-range 2π -exchange increases deformation, presumably by adding attraction in higher partial waves



Linking deformation and chiral nuclear forces

Symmetry-adapted NCSM study of Q_2 in ${}^6\text{Li}$ and ${}^{12}\text{C}$



- We find that quadrupole collectivity in low-lying states of ${}^6\text{Li}$ and ${}^{12}\text{C}$ is mainly influenced by S -wave contacts that alter the (dynamical) surface oscillations of one largely (static) deformed nuclear shape, without changing that shape's overall contribution within the nucleus.
- Challenges the traditional understanding that nuclear collectivity is driven primarily by long-range correlations.
- Quadrupole moments are likely important observables for constraining realistic nuclear forces (10% variation in S LEC \rightarrow 40% variation in Q_2)

Pairing in the calcium isotopic chain

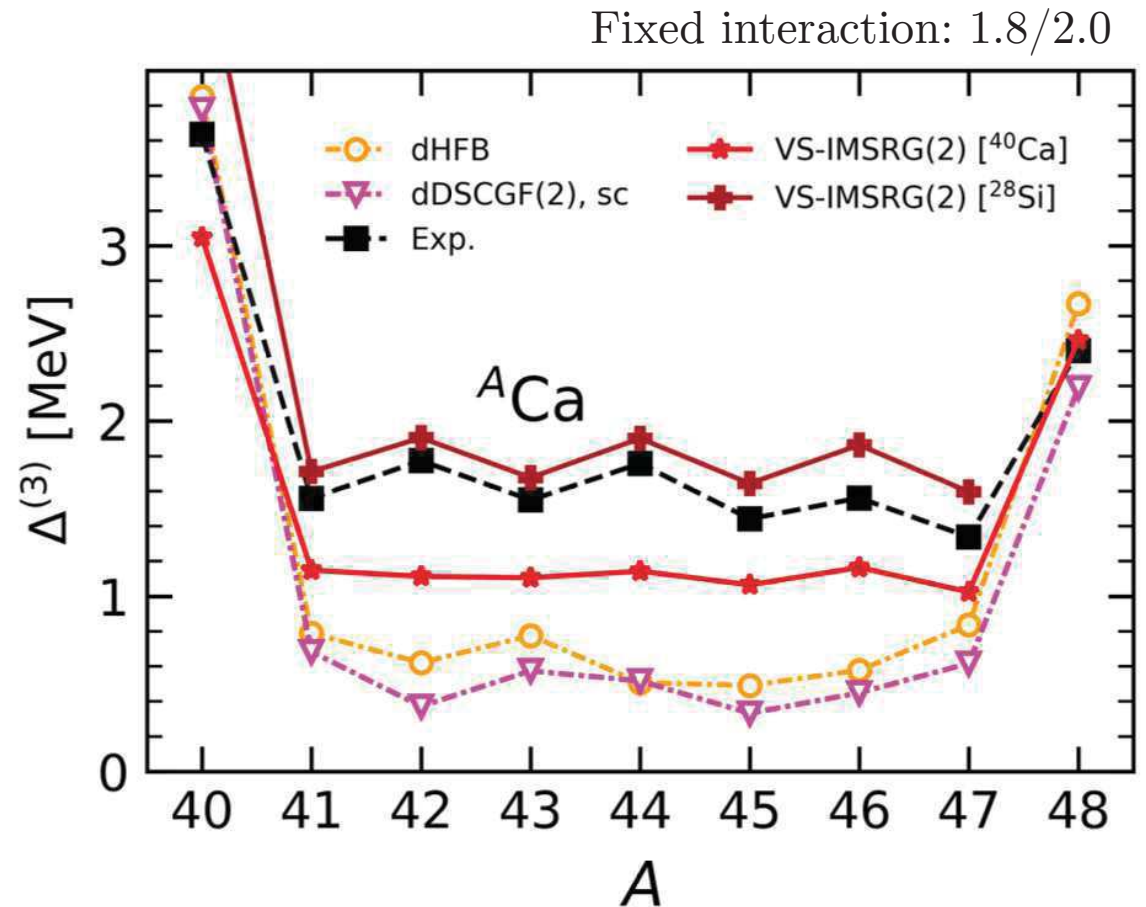
odd-even staggering of masses

$$\Delta^{(3)}(N) \equiv \frac{(-1)^N}{2} [E(N+1) - 2E(N) + E(N-1)].$$

Insufficient $\Delta^{(3)}$ at low-order polynomial cost

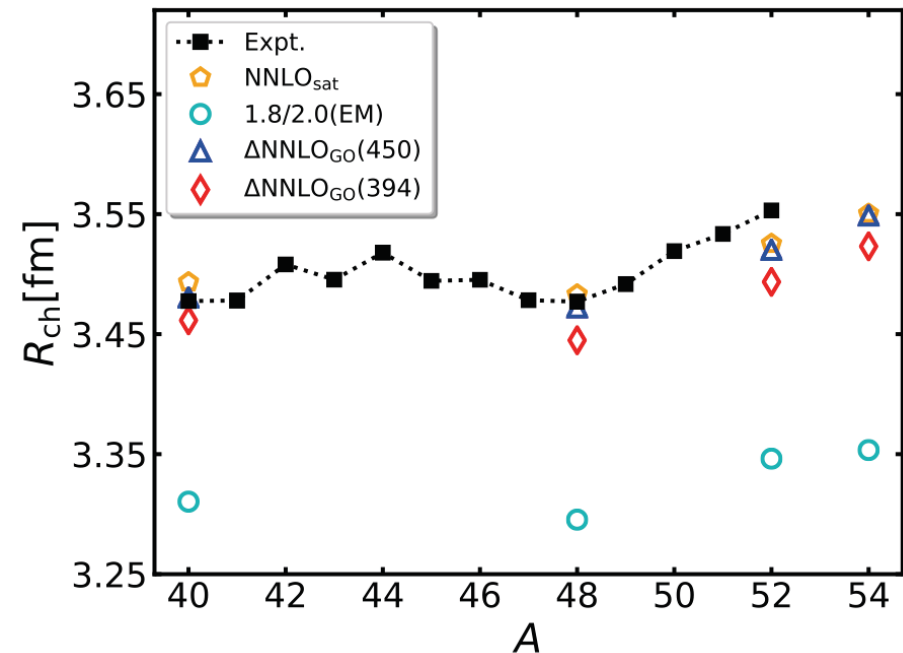
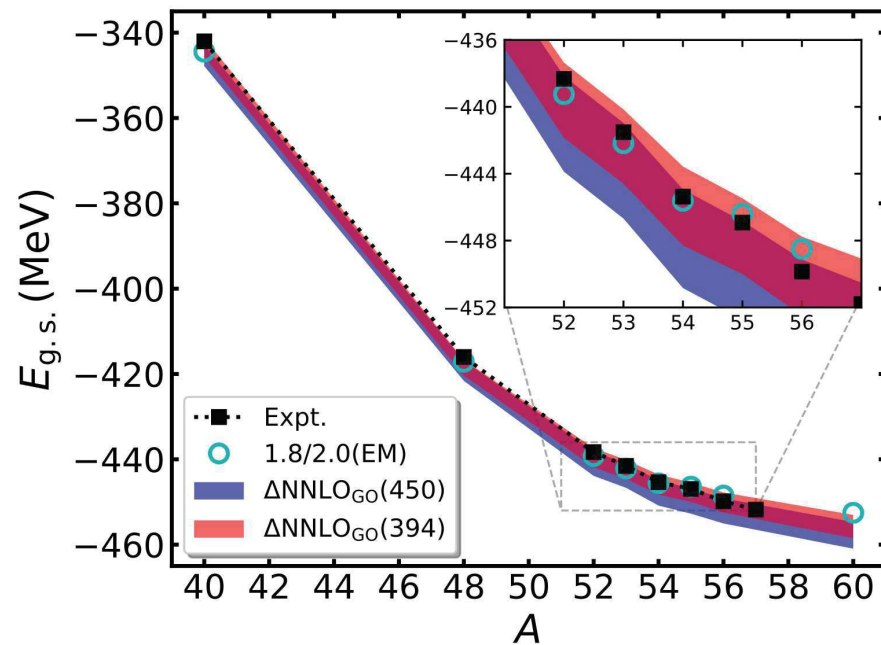
Improvement with VS-IMSRG(2) diagonalization in fp shell with ^{40}Ca core

Agreement with experiment when opening the ^{40}Ca core (^{28}Si) and using VS-IMSRG(2)



Pairing in the calcium isotopic chain

Let's use a different interaction: $\Delta\text{NNLO}_{\text{GO}}(394)$

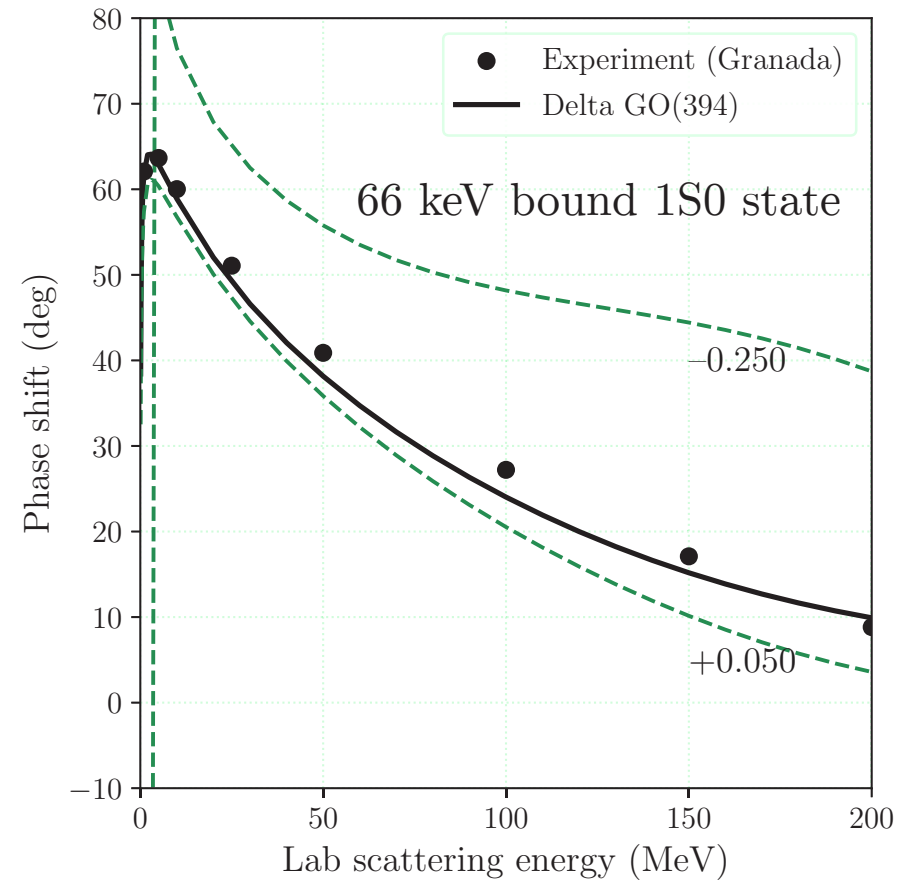
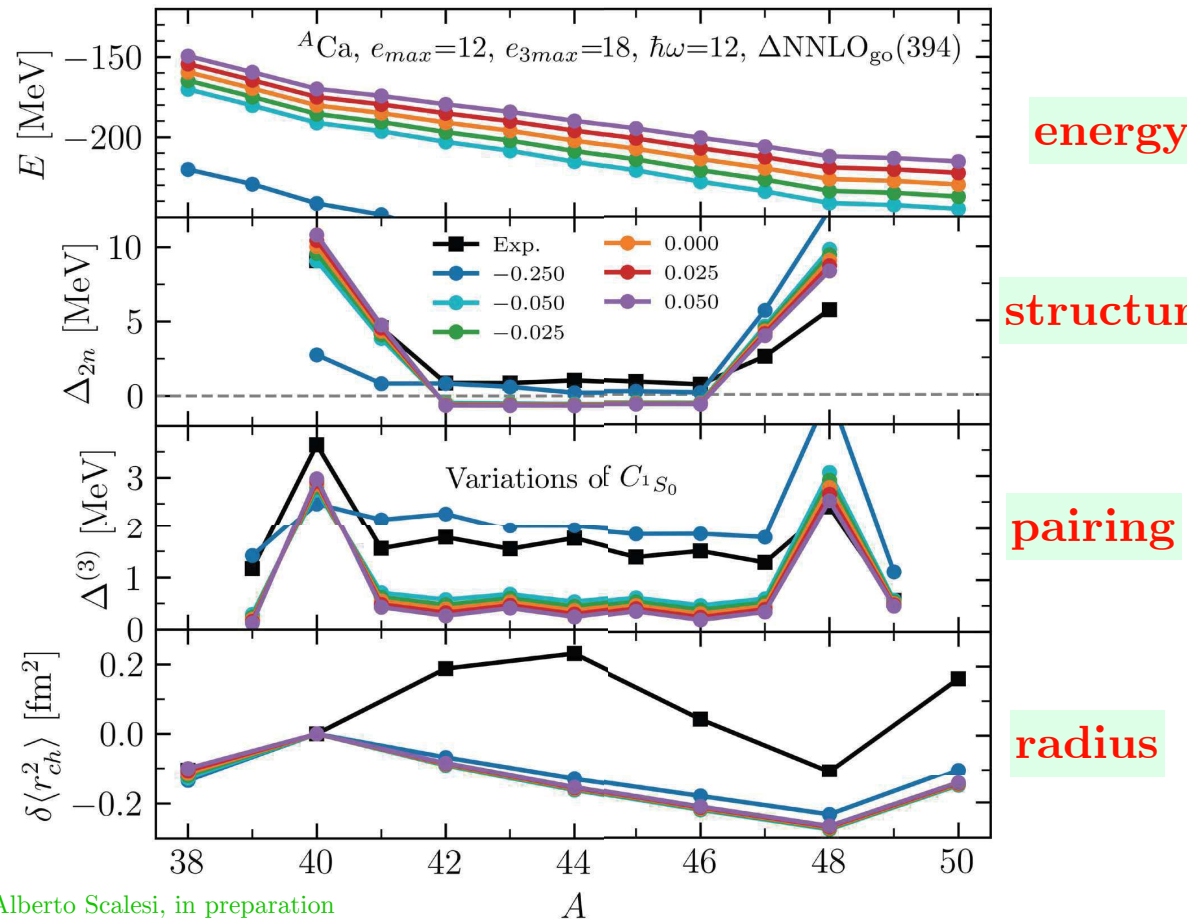


EFT truncation error in calcium $E_{\text{gs}} \approx 7$ MeV

$\Delta\text{NNLO}_{\text{GO}}(394)$ calibrated to reproduce nuclear matter saturation, symmetry energy, and slope + $A=2,3,4$ nuclear data, and intermittent guidance by medium-mass energies and radii

Pairing in the calcium isotopic chain

sHFB calculations, varying only C_{1S_0}



History matching: exploring the parameter space

A History Matching analysis using A=2,3,4,16 data

Explore the vast parameter space of χ EFT using emulators and *history matching*.

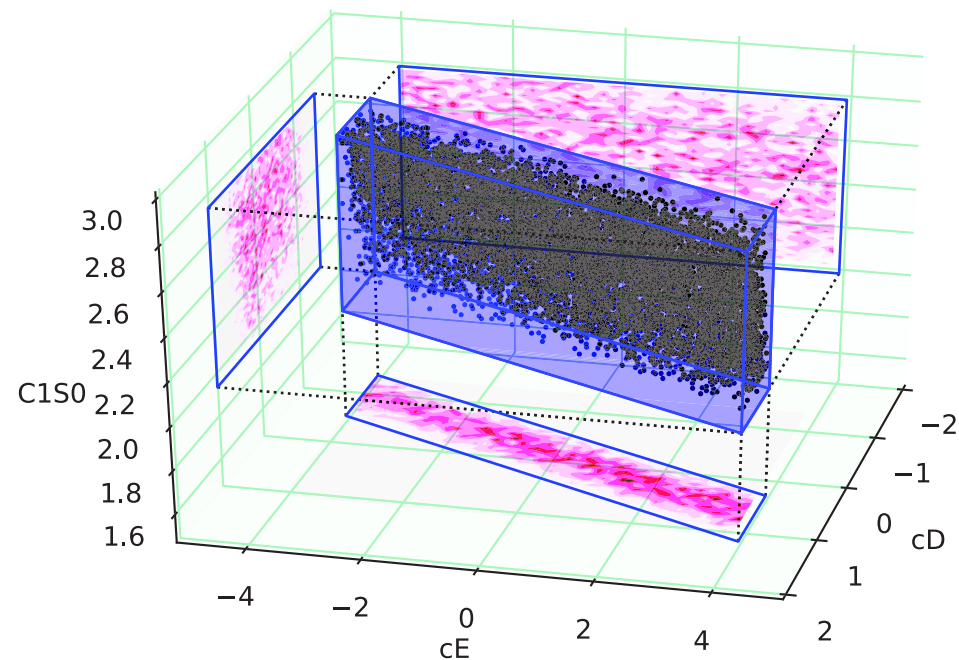
$$M_i(\vec{\alpha}) = \widetilde{M}_i(\vec{\alpha}) + \varepsilon_{\text{emulator},i}$$

$$z_i = \widetilde{M}_i(\vec{\alpha}) + \varepsilon_{\text{exp},i} + \varepsilon_{\text{model},i} + \varepsilon_{\text{method},i} + \varepsilon_{\text{emulator},i}$$

Identify a region in 17-dimensional LEC-space of Δ NNLO(394) where the model reproduces seen (historical) data within specified uncertainties

$$I^2(\vec{\alpha}) = \max_{i \in \mathcal{Z}} \frac{|\widetilde{M}_i(\vec{\alpha}) - z_i|^2}{\text{Var}(\widetilde{M}_i(\vec{\alpha}) - z_i)}$$

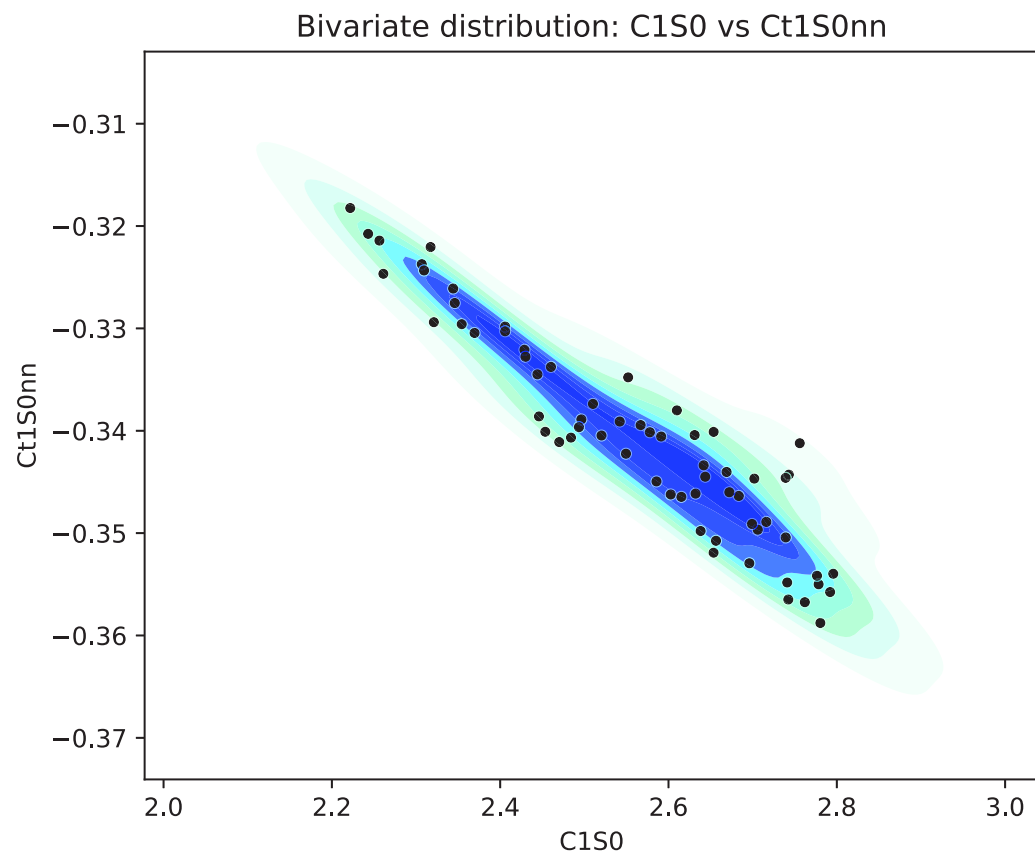
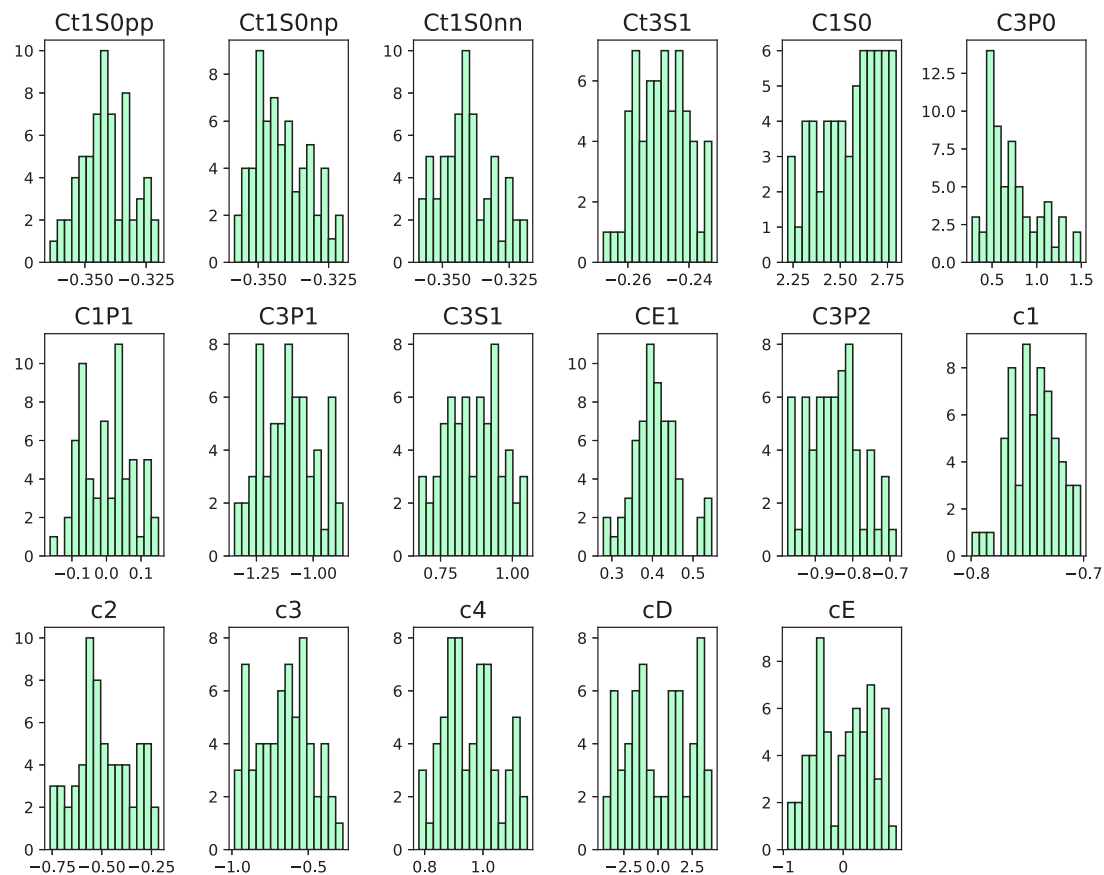
LEC $\vec{\alpha}$ values with $I(\vec{\alpha}) > c = 3$ *implausible*, and reject them!



I. Vernon, et al. Bayesian Anal. 5, 619 (2010)
good intro: I. Vernon, et al. BMC Systems Biology (2018)

64 non-implausible LEC values

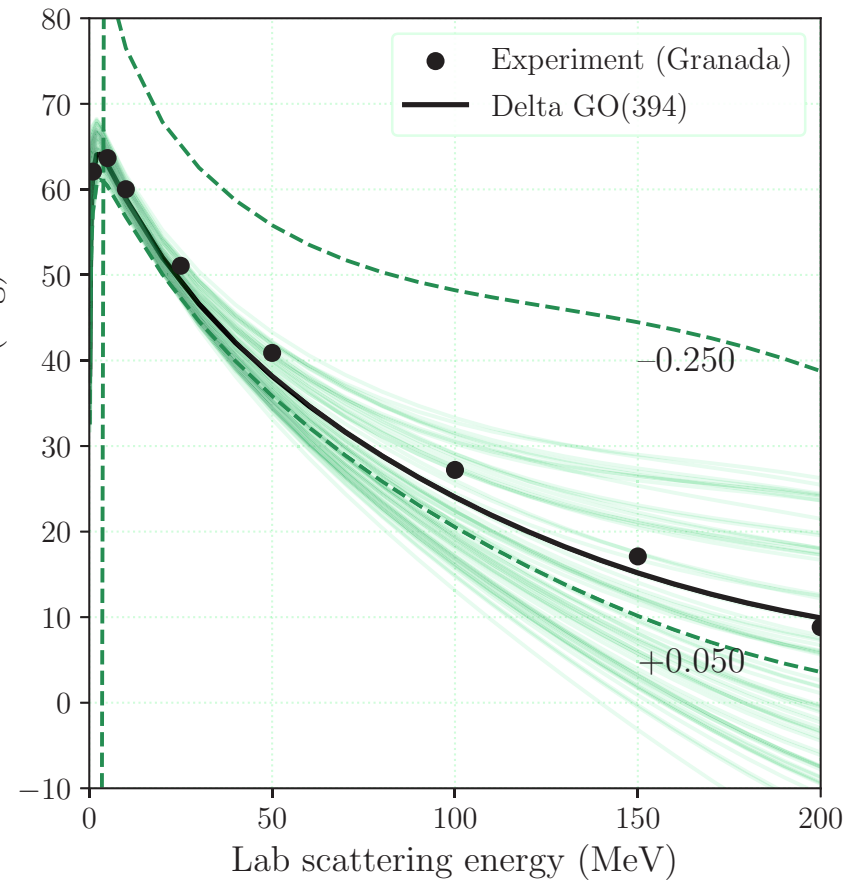
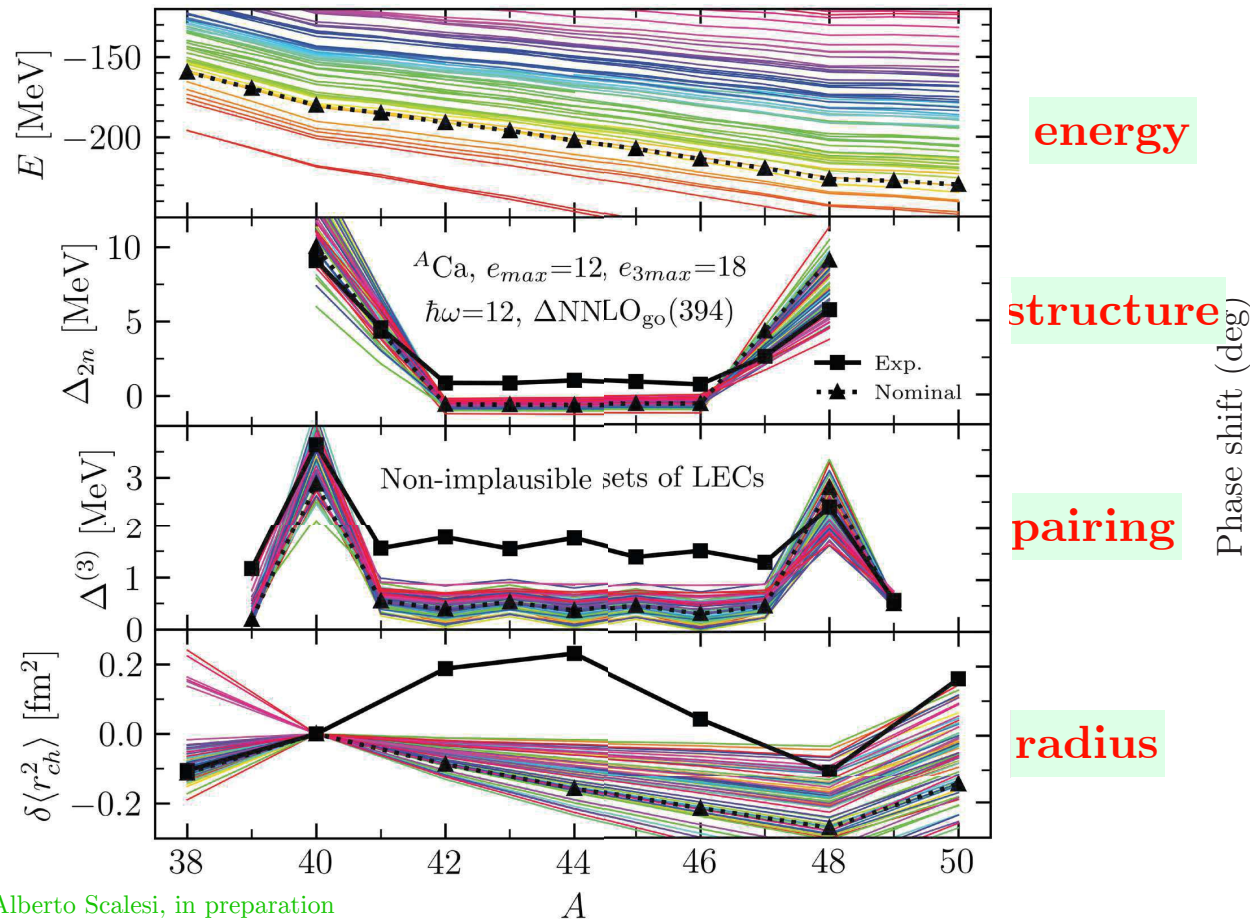
A History Matching analysis using $A=2,3,4,16$ data



Jiang et al Physical Review C 109 (6), L061302
Jiang et al Physical Review C 109 (6), 064314

Pairing in the calcium isotopic chain

sHFB calculations with 64 different sets of LEC values



Summary

- Emulators are essential tools for uncertainty quantification, Bayesian inference, and global sensitivity analysis. Small memory footprint, easy to distribute.
- Global sensitivity analysis of atomic nuclei identify that S-wave contacts strongly impact nuclear deformation and pairing properties.
- Interaction variance might explain $\sim 1/4$ of the observed lack of $\Delta^{(3)}$ in *ab initio* calculations of calcium isotopes.

Thanks for your attention!