Ab initio nuclear predictions

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Hirschegg 2023 - *Effective field theories for nuclei and nuclear matter*, 15-21 January

Presenting work done in collaboration with

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Daniel Phillips

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Sarah Wesolowski

Thomas Papenbrock

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Contents of this talk

What is *ab initio* in nuclear theory

resolution scale & **predictive capability**

systematically improvable

We* interpret the *ab initio* method as a ***systematically improvable approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities.*** In a nuclear physics context, we let nucleons define the beginning.

Lattice quantum chromodynamics might one day be the optimal starting point. However, it currently lacks predictive power for describing atomic nuclei

A. Ekström, C.Forssen, G.Hagen, G. R. Jansen, W. Jiang, and T. Papenbrock arXiv (2022)

What is *ab initio* in nuclear theory

$$D = M(\vec{\alpha}) + \delta D + \delta M$$

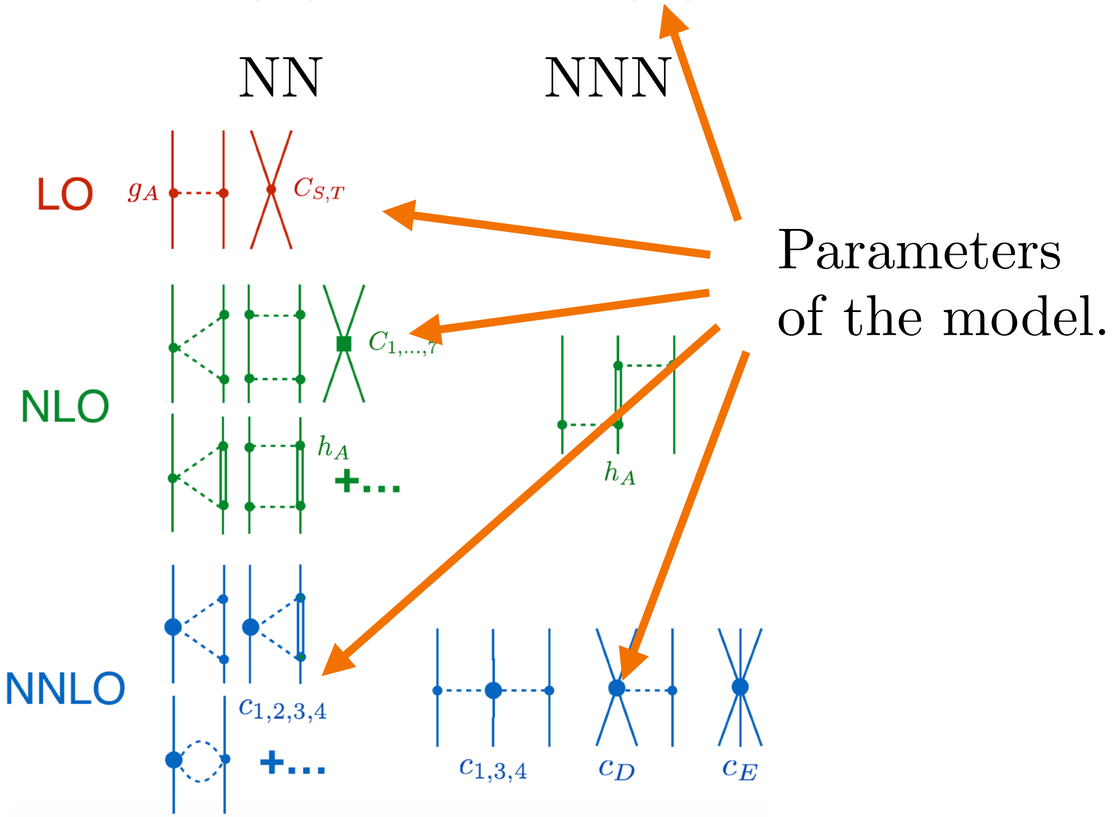
Data — Model parameters — Model discrepancy

The systematicity of the *ab initio* method creates an **inferential advantage.** We can test our assumptions about the model discrepancy as we increase the fidelity of M.

A. Ekström, C.Forssen, G.Hagen, G. R. Jansen, W. Jiang, and T. Papenbrock arXiv (2022)

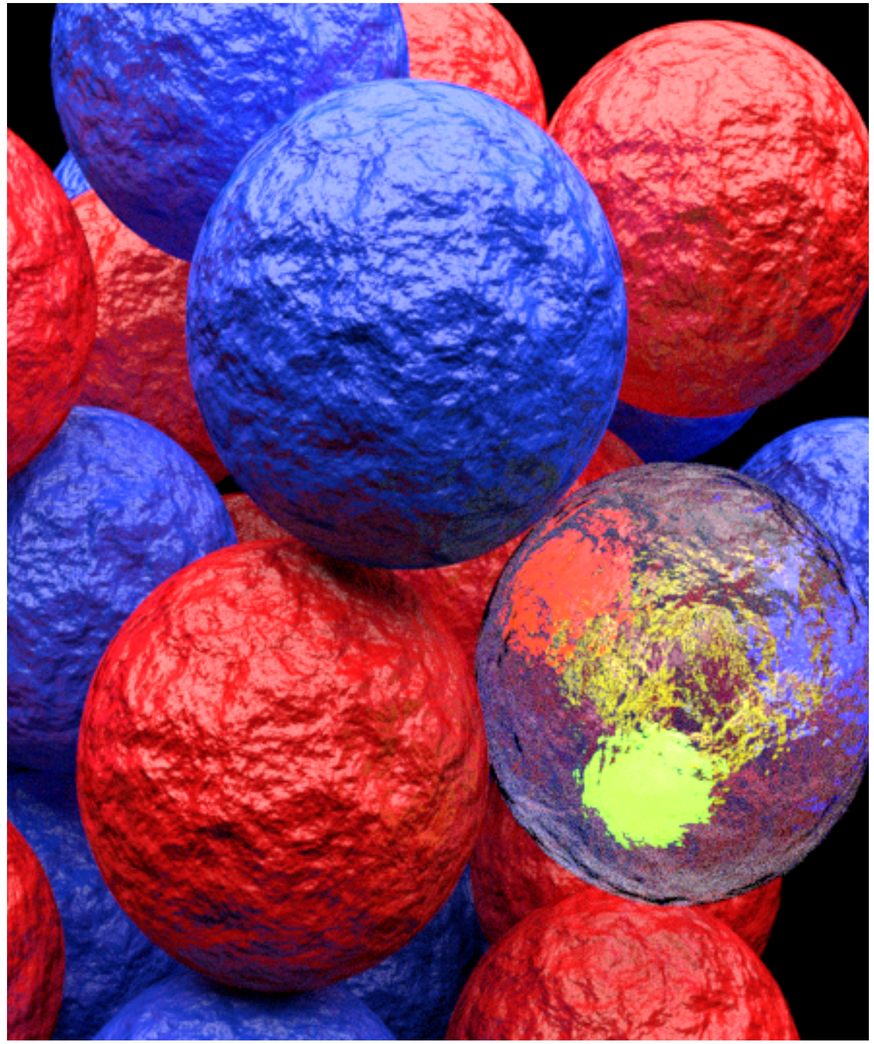
Ab initio modelling of nuclear systems

$$\hat{H}|\Psi_i\rangle = E_i|\Psi_i\rangle$$
$$\hat{H}(\vec{\alpha}) = \hat{T} + \hat{V}(\vec{\alpha})$$



Parameters of the model.

χEFT promises a connection with QCD

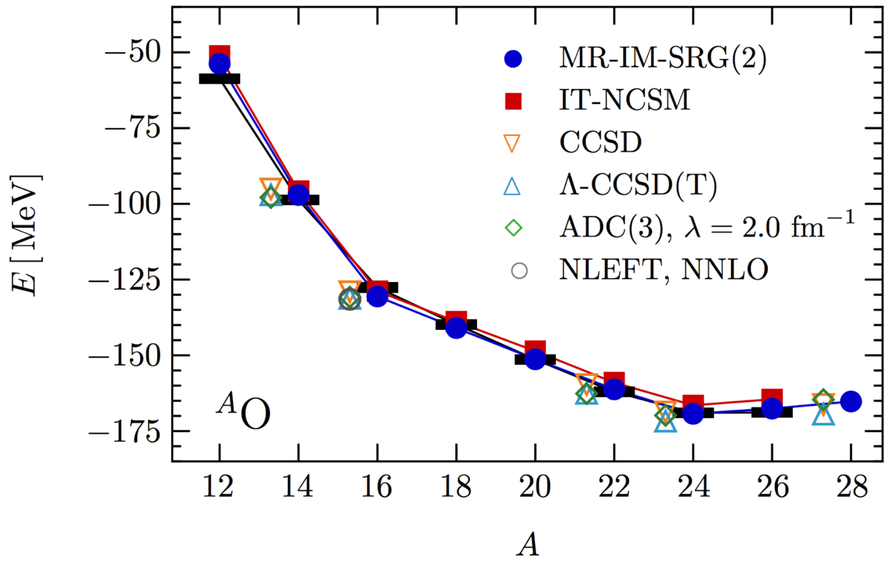


A. Ekström, et al. Phys. Rev **C 97**, 024332 (2018)
W. Jiang, et al. Phys Rev **C 102,** 054301 (2020)

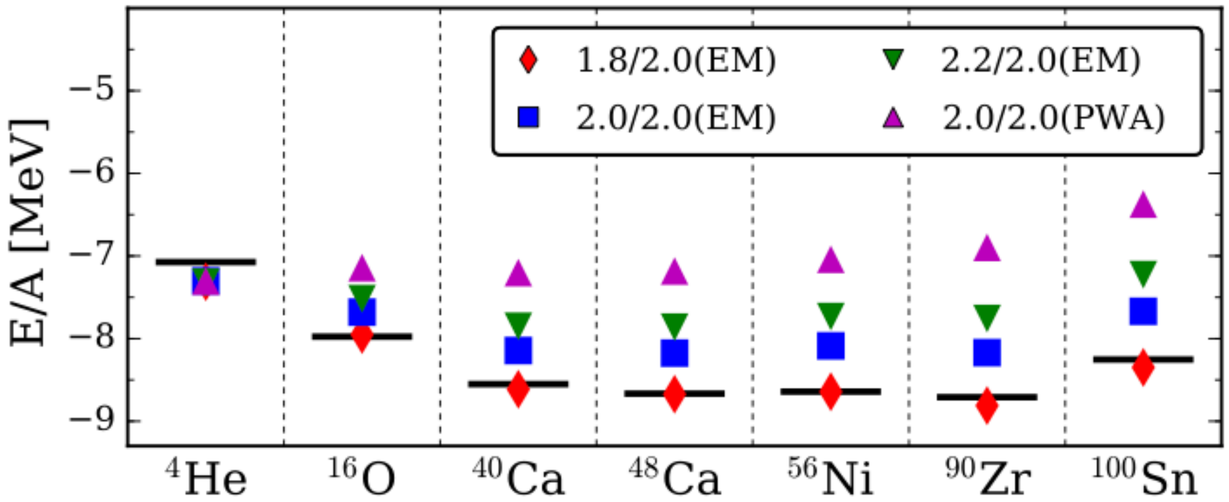
Weinberg, van Kolck, Bernard, Kaiser, Meißner, Epelbaum, Machleidt, Entem, ...

We need to go beyond point-estimate predictions

Different many-body methods agree!



Why do some interactions work better than others?



We can do better than "point-estimate predictions": $M_i(\vec{\alpha}_\star)$

Data $D = M(\vec{\alpha}) + \varepsilon_{\text{exp}} + \varepsilon_{\text{model}} + \varepsilon_{\text{method}} + \varepsilon_{\text{parametric}}$

Model error (e.g. EFT uncertainty)

Method error (e.g. CCSDT-3 is *almost* exact)

T. D. Morris et al. PRL (2018)

H. Hergert Phys. Scripta 92, 023002 (2017)

[7] an overview: Jenný Brynjarsdóttir and Anthony O'Hagan, Inverse Problems **30**, 114007 (2014)

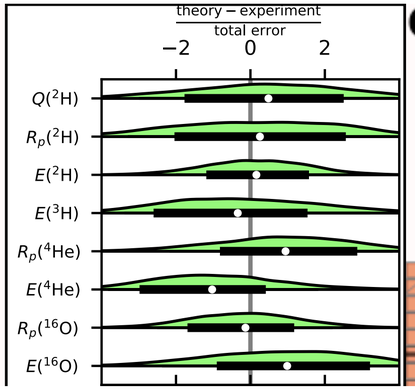
Progress in linking forces to structure and reactions

Breakthroughs in
- effective field theory
- many-body methods
- statistical learning

Lead-208

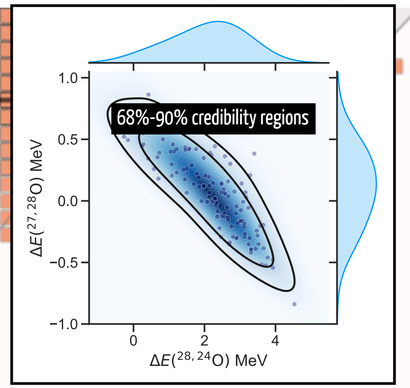
Ab initio progress

History matching



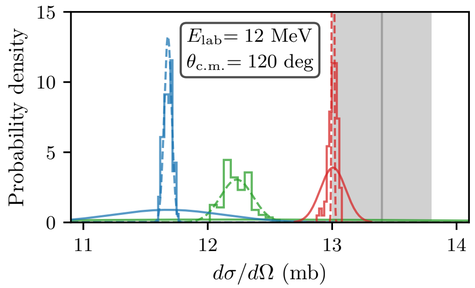
B. Hu et al Nature Physics (2022)

Predicting oxygens



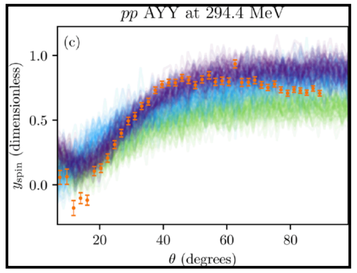
in preparation

nd-scattering



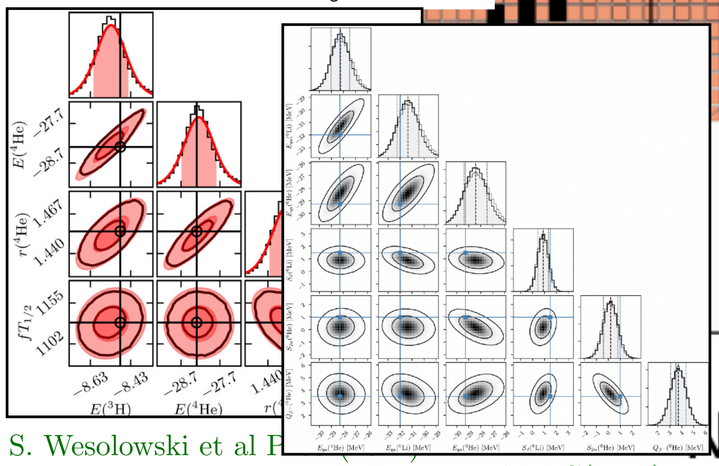
S. B. S. Miller et al PRC (2022)

NN-scattering



I. Svensson et al PRC (2022)

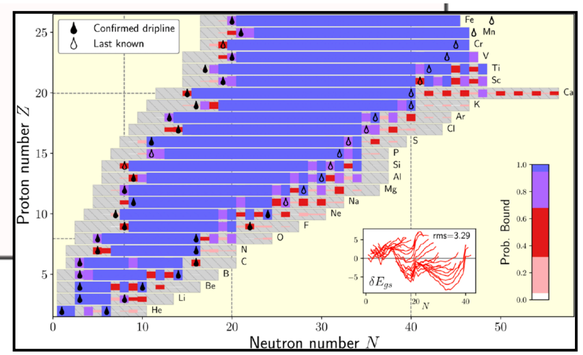
Few-nucleon systems



S. Wesolowski et al P

T. Djärv et al PRC(2022)

Bayesian linear regression



S. R. Stroberg et al PRL (2021)

50

Neutron number N

Sn

O

on number Z

28

The posterior predictive distribution

The fundamental problem of inference is to predict future (or unseen) data F from past data D and your background knowledge I.

Future data F is most definitely uncertain now, so we must describe it using probabilities. **This is the posterior predictive distribution**

$$p(F \,|\, D, I)$$

To enable quantitative statements, we construct a χEFT employing a particular power counting, degrees of freedom & choose a method to solve for observables. This and other assumptions go into I. I will refer to this as a model M. A model comes with parameters $\vec{\alpha}$ that we calibrate using data D.

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

BMM/BMA: See Furnstahl's talk

D. V. Lindley, The Statistician (2000)

Bayes' rule: from likelihood & prior to posterior

- Collect N data points that we gather in a data vector D
- To explain the data, propose some model M, depending on parameters $\vec{\alpha}$
- Apply Bayes' rule

Posterior **Likelihood** **Prior**

$$p(\vec{\alpha}\,|\,D,M,I) = \frac{p(D\,|\,\vec{\alpha},M,I)\cdot p(\vec{\alpha}\,|\,M,I)}{p(D\,|\,M,I)}$$

Marginal likelihood

most likely not Rev. T. Bayes

- The **prior** encodes our knowledge about the parameter values before analyzing the data
- The **likelihood** is the probability of the data given a set of parameters
- The **marginal likelihood** (or model evidence) provides normalization of the posterior
- The **posterior** is the complete inference and resulting probability density for the parameters $\vec{\alpha}$

Inferring LECs up to 4th order in the NN-sector of Δ-less χEFT

We seek a posterior $\mathrm{p}(\alpha_{nn}, \vec{\alpha}_{np,pp} \,|\, a_{nn}^{\mathrm{exp}}, D_{np,pp}, I)$ conditioned on the Granada database of np/pp cross sections and empirical data of the nn scattering length.

In a **first step** we focus on the challenge of sampling the np/pp part of the posterior, i.e., $\mathrm{p}(\vec{\alpha}_{np,pp} \,|\, D_{np,pp}, I)$ at all orders up to N3LO.

$$\mathrm{p}(\vec{\alpha}_{np,pp} \,|\, D_{np,pp}, I) \propto \mathrm{p}(D_{np,pp} \,|\, \vec{\alpha}_{np,pp}, I) \cdot p(\vec{\alpha}_{np,pp} \,|\, I)$$

In a **second step** we extend this posterior to include the isospin breaking nn contact in ${}^1S_0$

$$\mathrm{p}(\alpha_{nn}, \vec{\alpha}_{np,pp} \,|\, a_{nn}^{\mathrm{exp}}, D_{nn,np}, I) = \mathrm{p}(\alpha_{nn}, \,|\, a_{nn}^{\mathrm{exp}}, \vec{\alpha}_{np,pp}, I) \cdot \mathrm{p}(\vec{\alpha}_{np,pp} \,|\, D, I)\,.$$

I. Svensson, et al arXiv:2206.08250

Inferring LECs up to 4th order in the NN-sector of Δ-less χEFT

np/pp likelihood and prior

$$\mathrm{p}(\vec{\alpha}_{np,pp} \,|\, D_{np,pp}, I) \propto \exp\left[-\frac{1}{2}\vec{r}^{\,T}(\Sigma_{exp}+\Sigma_{th})^{-1}\vec{r}\right] \cdot \mathcal{N}(\mu_{NN}, \Sigma_{NN}) \cdot \mathcal{N}(\mu_{\pi N}, \Sigma_{\pi N})$$

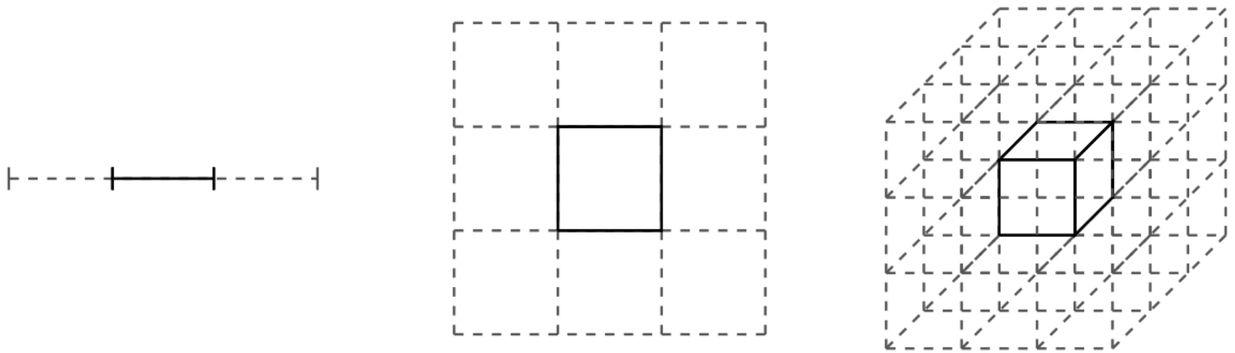
We currently neglect correlations across NN scattering energies and angles. This leads to a **normal likelihood with a diagonal covariance matrix** for the EFT error. Correlated EFT uncertainty in progress. Focus on multivariate inference here.

We place a multivariate normal **prior** on the πN LECs following the Roy-Steiner analysis by *Hoferichter et al.* and an uncorrelated $\mathcal{N}(0,5^2)$ prior (in appropriate units) on the NN contact LECs up to N3LO.

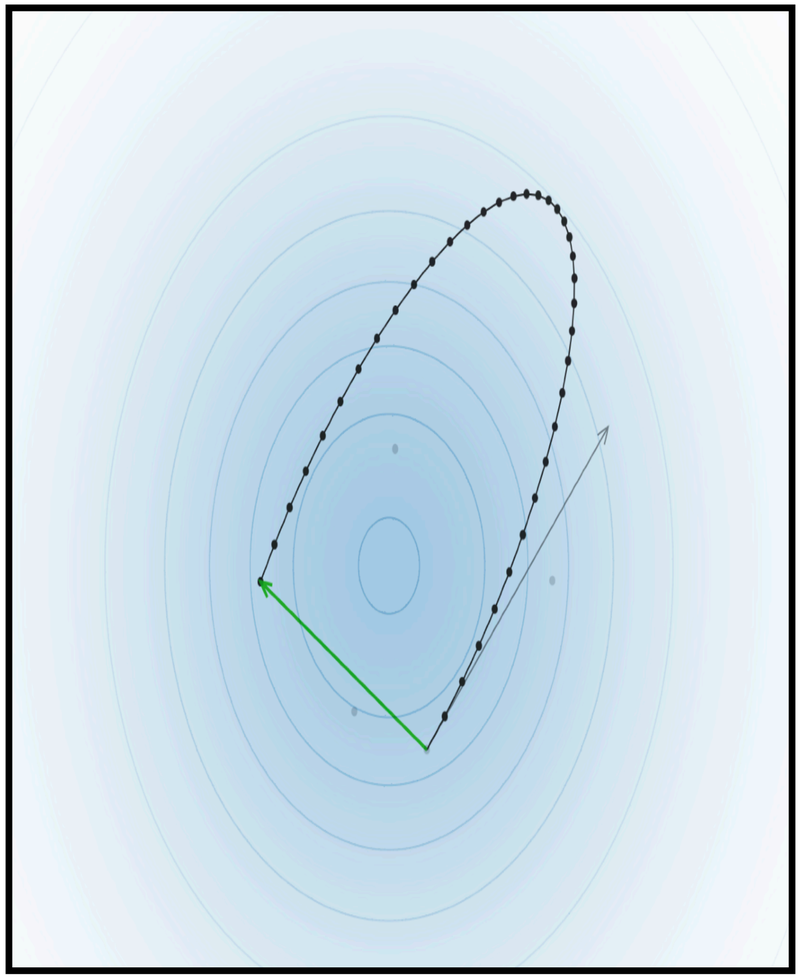
I. Svensson, et al arXiv:2206.08250

Inferring LECs up to 4th order in the NN-sector of Δ-less χEFT

Hamiltonian Monte Carlo (HMC)



credit: M. Betancourt arXiv:1701.02434



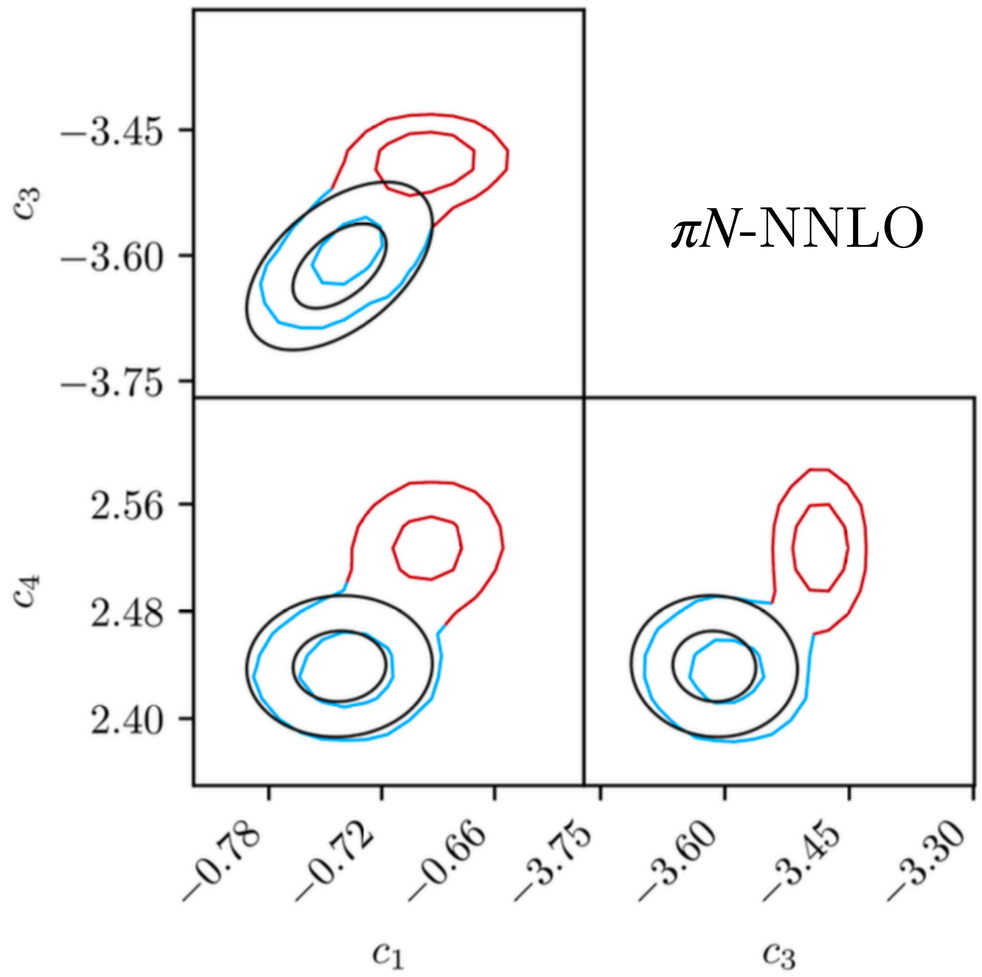
credit: https://chi-feng.github.io/mcmc-demo/

With 10^4 posterior samples per chain, and 10 chains, at each order the HMC sampling passes all convergence tests.

Although we have to compute derivatives and integrate Hamilton's equations at ~ 20 (time) steps for each HMC step, each posterior sample is very informative. This leads to an overall advantage of using HMC.

S. Duane, et al. Phys. Lett B **195,** 216 (1986)
I. Svensson, et al Phys. Rev. C **105**, 014004(2022)

Inferring LECs up to 4th order in χEFT



Black ellipse: Roy-Steiner prior

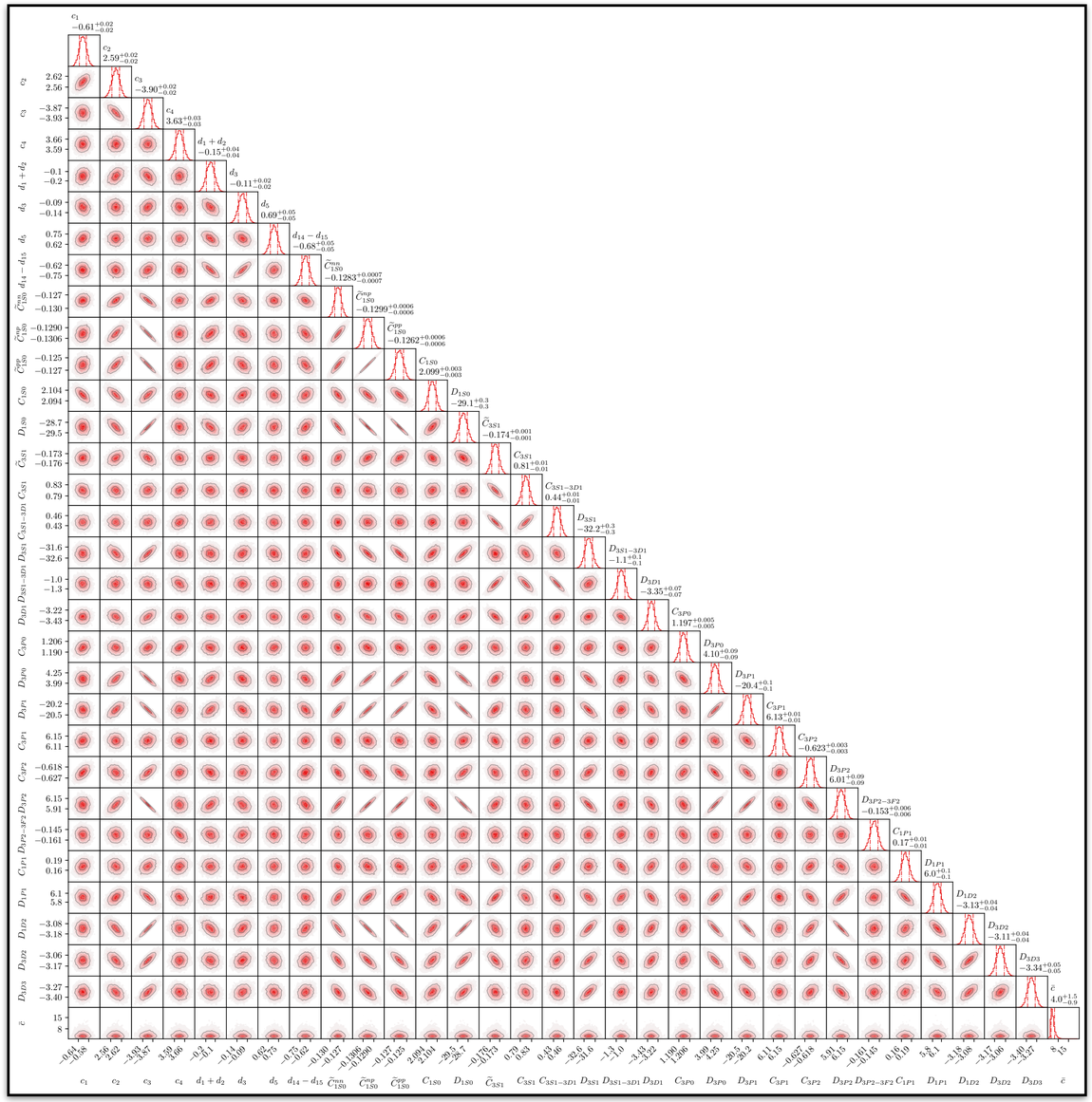
Blue ellipse: πN posterior when conditioning on low-energy NN data ($p_{rel} < m_\pi$)

Red ellipse: πN posterior when conditioning on all NN data with $T_{lab} < 290$ MeV

We observe the same behaviour at N3LO.

I. Svensson, et al arXiv:2206.08250

Inferring LECs up to 4th order in χEFT



Incorporating the *nn* scattering length datum and a straightforward sampling/importance resampling (SIR) yields the following posterior.

A lot of data and a very tight posterior!

If conditioning on low-energy data, the D-wave contacts return the prior.

Some very large contact values, as seen also in many other works.

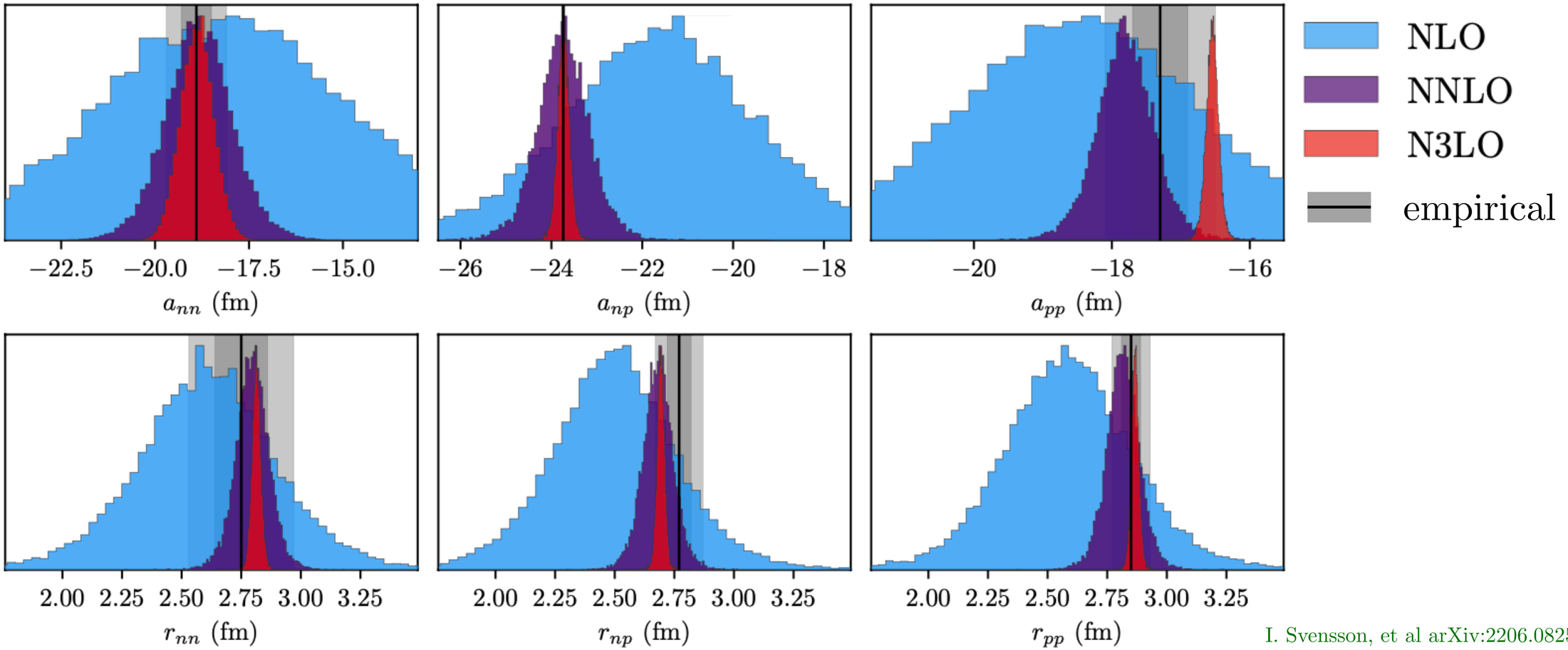
SIR: See Forssen's talk

I. Svensson, et al arXiv:2206.08250

Posterior predictive distribution

NN effective range expansion (electromagnetic effects removed)

Results include estimated EFT truncation errors

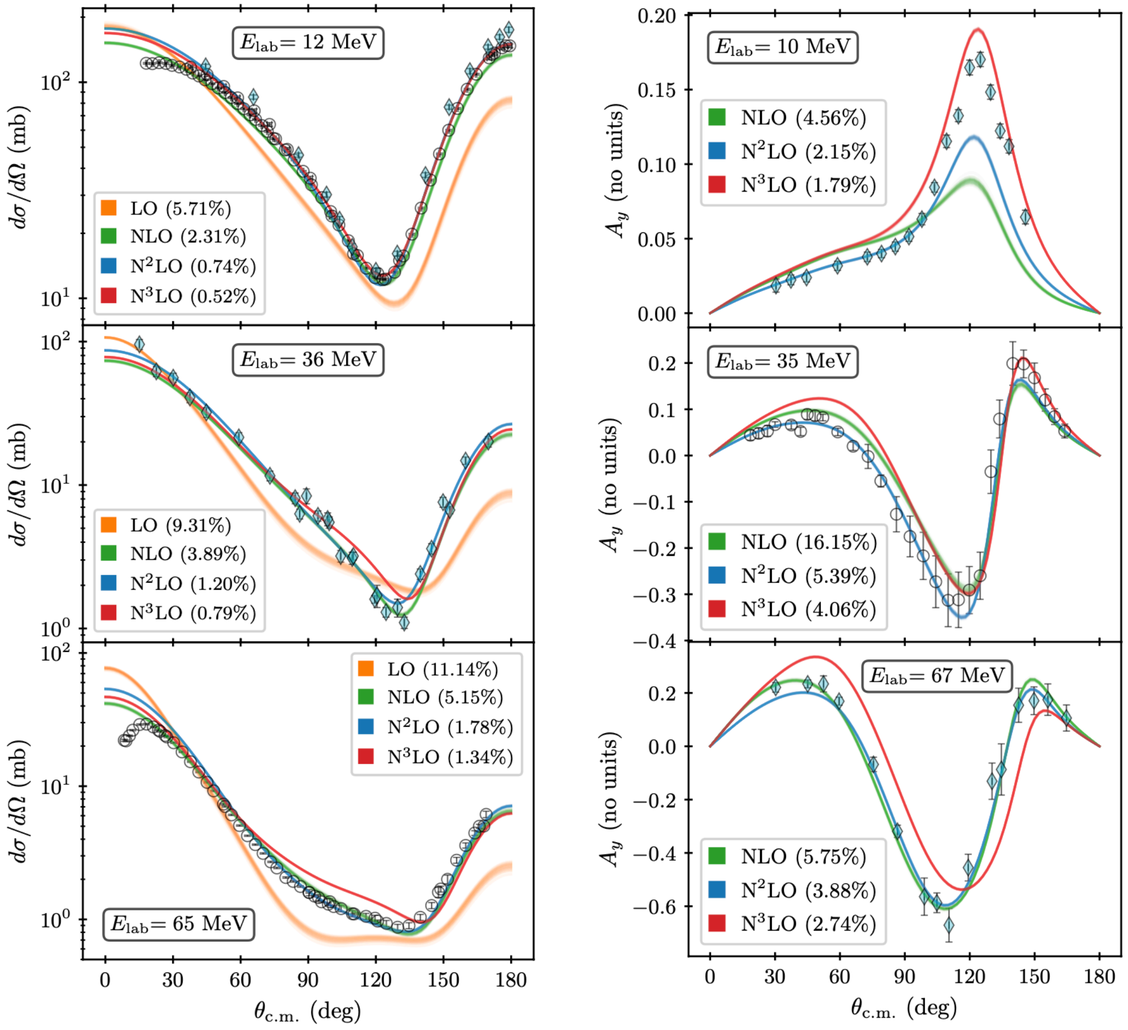


I. Svensson, et al arXiv:2206.08250

S. B. S. Miller et al, Phys. Rev. C **106**, 024001 (2022)

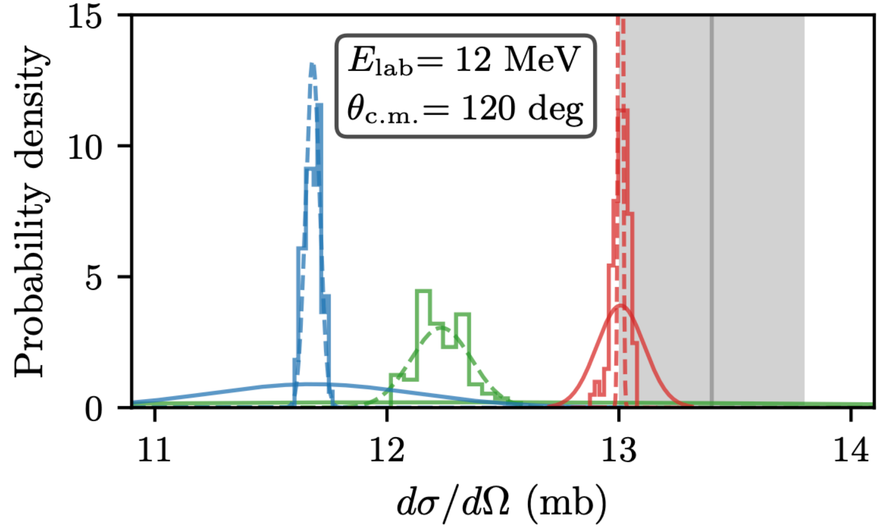
Posterior predictive distribution

Low-energy nd scattering cross sections (NN-only)



Draw 100 samples from the LEC posteriors at LO, ...,N3LO and compute *nd* cross sections.

Does not help resolve the A_y puzzle.



At N3LO, our estimates of the EFT truncation error is comparable to the LEC PPD. Both smaller than experiment (gray).

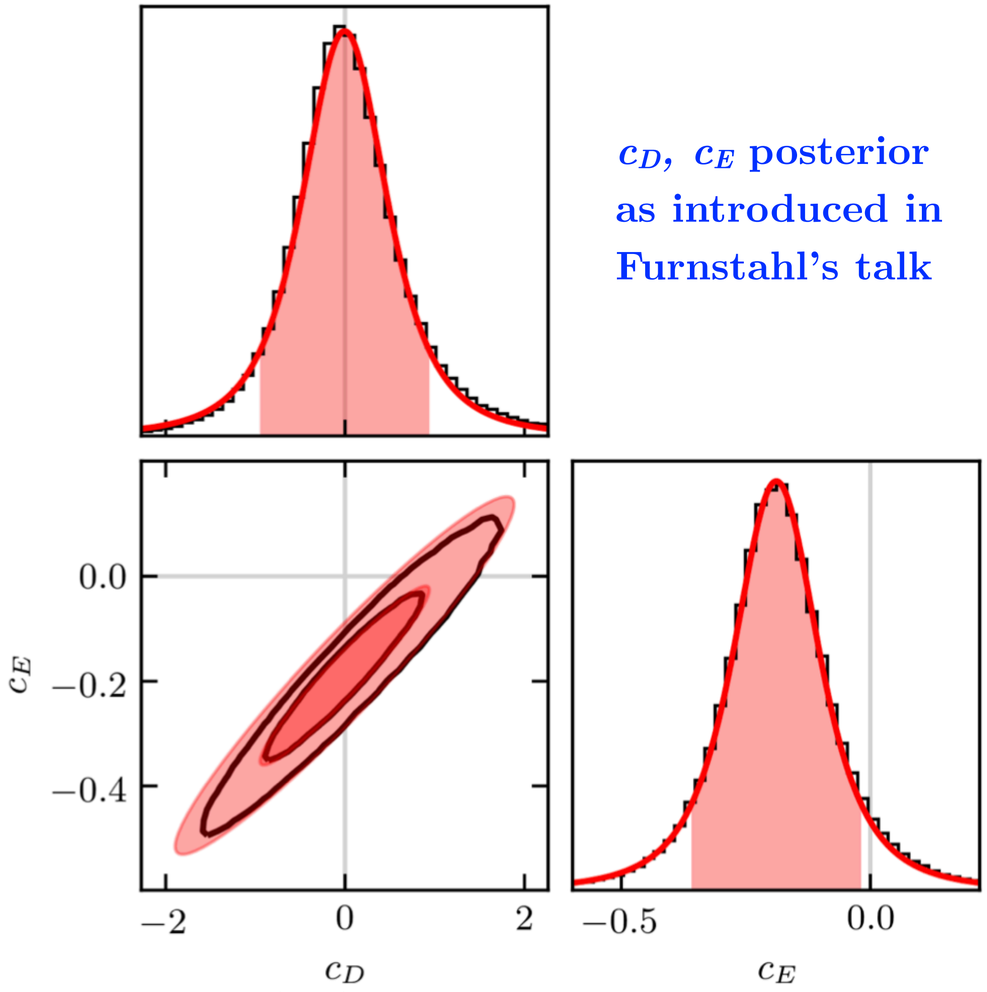
S. B. S. Miller et al, PRC (accepted)

JupiterNCSM *no-core shell model with NN+3N* https://github.com/thundermoose/JupiterNCSM

fastwigxj *fast Wigner symbol computation* http://fy.chalmers.se/subatom/fastwigxj/

Posterior predictive distribution

Low-sample representations can be useful

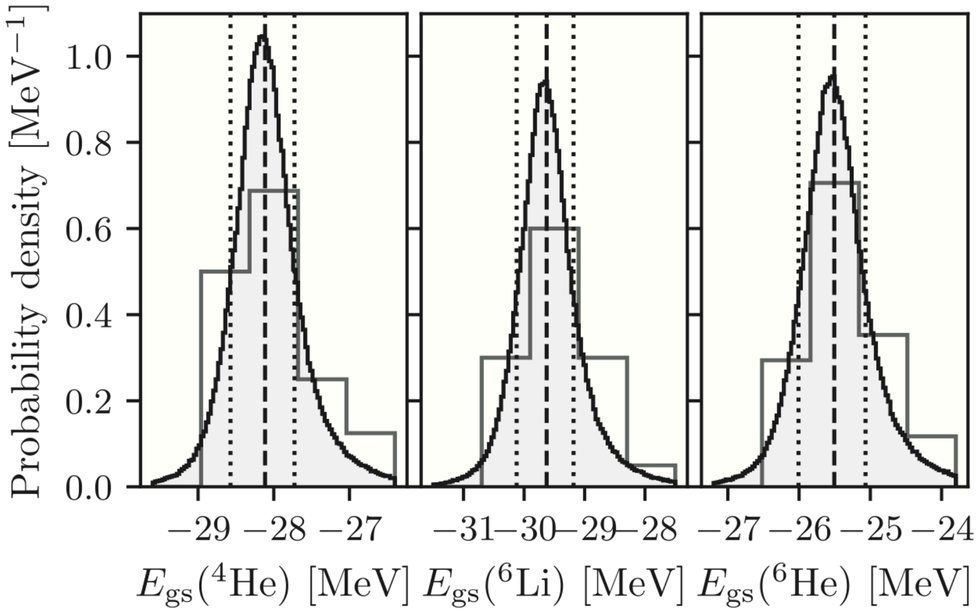


c_D, c_E posterior as introduced in Furnstahl's talk

$$\mathrm{pr}(\boldsymbol{y}_{\mathrm{NCSM}} \mid \mathcal{D}, I) = \int d\vec{a}\, \mathrm{pr}(\boldsymbol{y}_{\mathrm{NCSM}}, \vec{a} \mid \mathcal{D}, I)$$

$$= \int d\vec{a}\, \mathrm{pr}(\boldsymbol{y}_{\mathrm{NCSM}} \mid \vec{a}, \mathcal{D}, I)\mathrm{pr}(\vec{a} \mid \mathcal{D}, I),$$

$$\mathrm{pr}(\vec{a} \mid \mathcal{D}, I) = \delta(\vec{a}_{\mathrm{NN}} - \vec{a}^{*}_{\mathrm{NN}})\delta(\vec{a}_{\pi\mathrm{N}} - \vec{a}^{*}_{\pi\mathrm{N}})\mathrm{pr}(c_D, c_E)$$

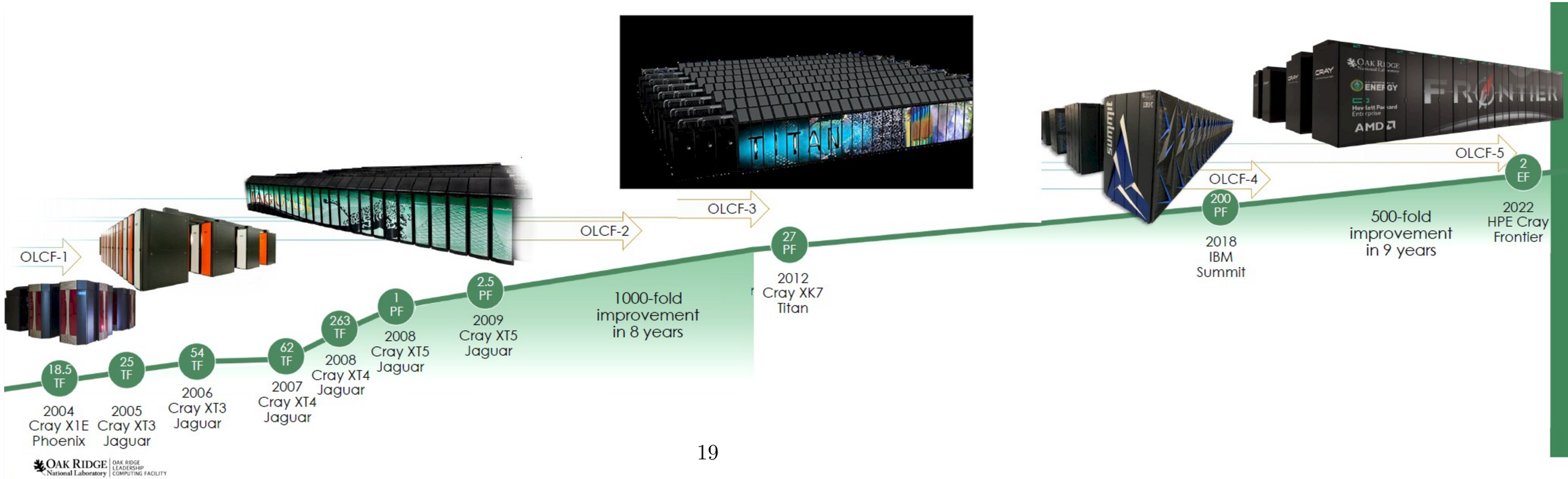


S. Wesolowski, et al. PRC (2021)

T. Djärv et al Phys. Rev. C **105**, 014005 (2022)

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.



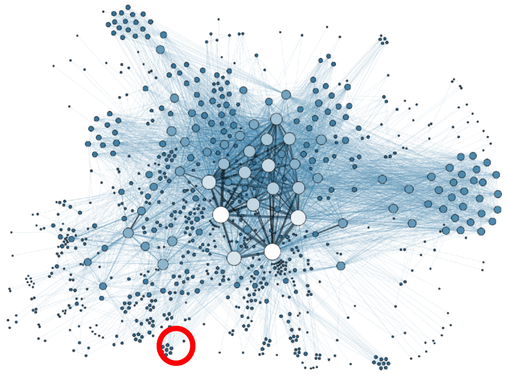
Eigenvector continuation

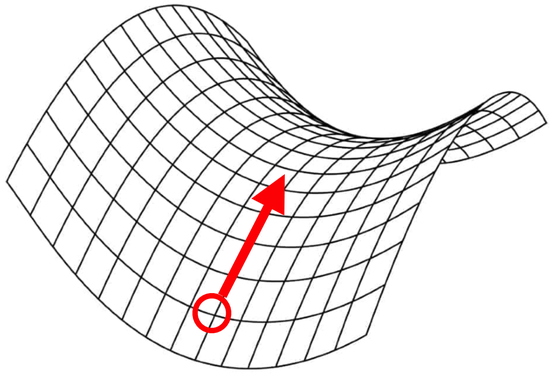
a reduced basis method

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

continuous parameter

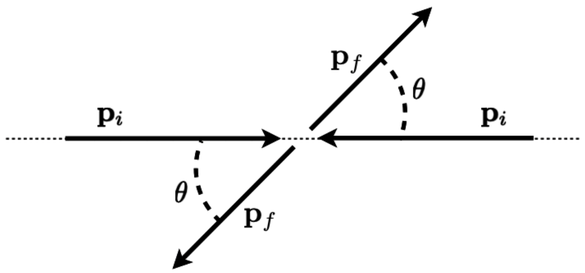
The key insight is that while an eigenvector resides in a linear space with enormous dimensions, the eigenvector trajectory generated by smooth changes of the Hamiltonian matrix is well approximated by a very low-dimensional manifold in many applications.



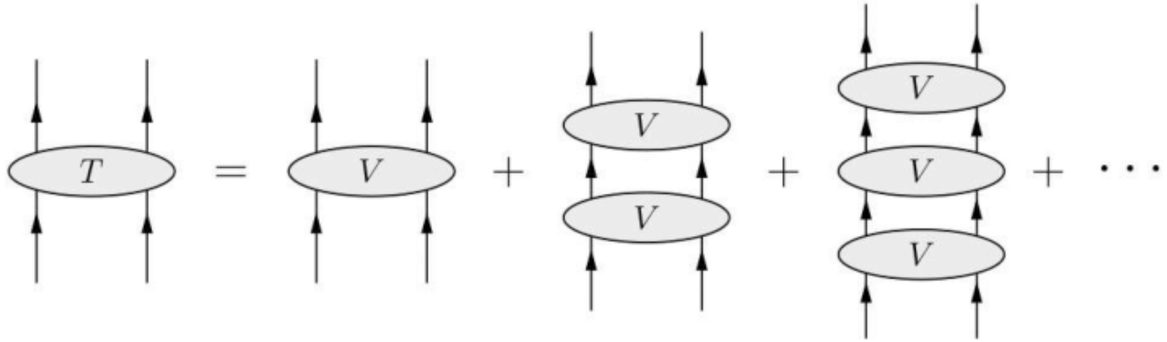


D. Frame, et al. Phys. Rev. Lett. **121**, 032501 (2018)
J. A. Melendez et al 2022 J. Phys. G: Nucl. Part. Phys. 49 102001

Emulating two-body scattering



$$T = V + VGT$$



Newton functional: $S[T] = V + VGT + TGV - TGT + TGVGT$

Assume a trial T-matrix $\widetilde{T} = \sum_{i=1}^{N_t} \beta_i T_i$ ← N_t $\alpha-$snapshots ("training points")

The condition of stationarity $\frac{dS}{d\vec{\beta}} = 0$ yields the following equation for $\vec{\beta}_\star$: $\vec{m} + \mathbf{M}\vec{\beta}_\star = 0$

where $M_{ij} = (T_i[GVG - G]T_j + T_j[GVG - G]T_i)$, $m_i = (VGT_i + T_iGV)$

Inserting solution back into the functional, we approximate the T-matrix by

$$S[T_\star] = V - \frac{1}{2}\vec{m}^T\mathbf{M}^{-1}\vec{m}$$

More on scattering emulators: see Furnstahl's talk

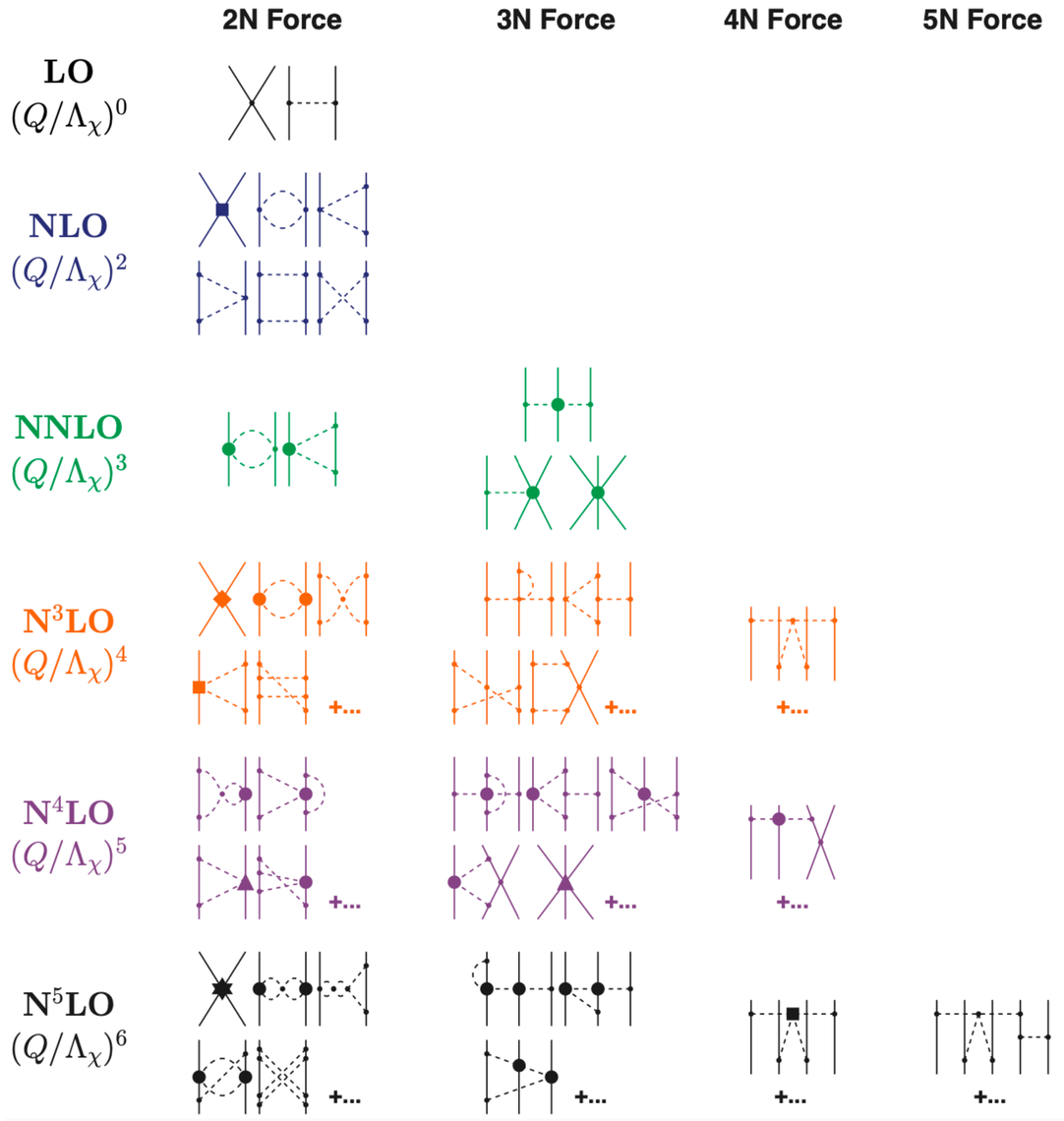
J. A. Melendez, et al Phys. Lett. B 821 136608 (2021)

Linear structure provides easy access to derivatives

$$V(\alpha) = \text{1}\pi + \sum_i h_i(\boldsymbol{\alpha})\ \text{2}\pi + \sum_i g_i(\boldsymbol{\alpha})$$

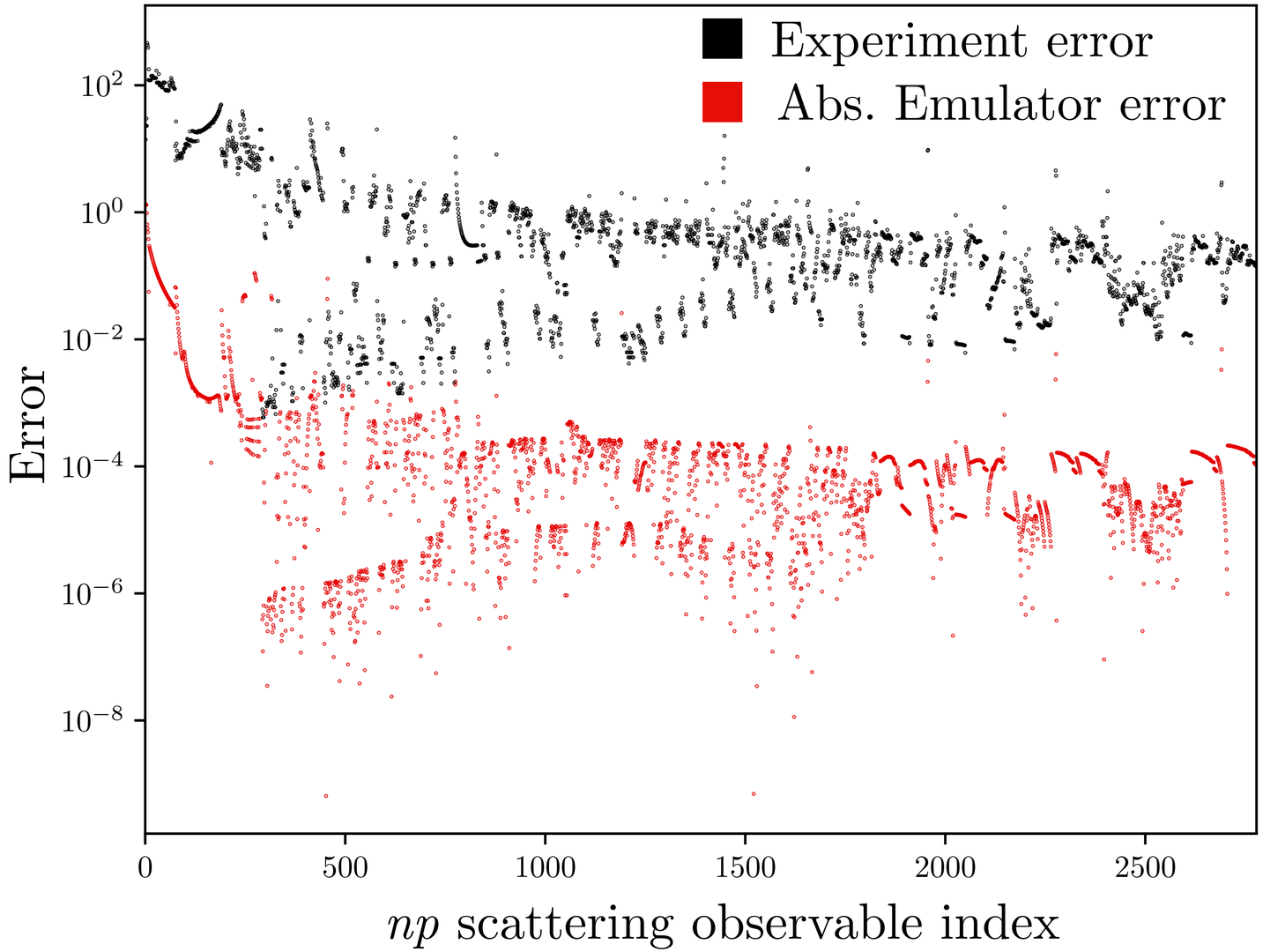
The Hamiltonian up to NNLO is trivially linear in the relevant EFT coupling constants.

Starting at N3LO, there are quadratic dependencies of the $\alpha_i \alpha_j$ due to higher order loop diagrams. Still, it can be factored out of the potential terms



Benchmarking the *NN* scattering emulator

Deltafull NNLO np sector, 8 training points



It takes **0.4 seconds** to evaluate the entire likelihood.

Python implementation accelerated by Google jit-compilation. Provides derivatives via AD as well. *(overhead x2)*

In progress: LEC inference with correlated EFT truncation error.

I. Svensson, et al (in progress, 2023)

Emulating nuclear bound states

The no-core shell-model for nuclei amounts to diagonalizing the nuclear Hamiltonian.Straightforward, although computationally expensive with increasing mass number.

Coupled-cluster (CC) theory exploits a similarity transformed Hamiltonian

$$\bar{H}(\alpha) = e^{-T(\vec{\alpha})} H(\vec{\alpha}) e^{T(\vec{\alpha})}$$

Where in the singles and doubles approximation (CCSD) the truncated cluster operator is

$$T(\vec{\alpha}) = T_1(\vec{\alpha}) + T_2(\vec{\alpha})$$

The sub-space projected coupled-cluster (SP-CC)Hamiltonian, which we end up diagonalizing, is non-hermitian and given by

$$\langle \tilde{\Psi}' | H(\vec{\alpha}_{\text{target}}) | \Psi \rangle = \langle \Phi_0 | (1 + \Lambda(\vec{\alpha}')) e^{-T(\vec{\alpha}') + T(\vec{\alpha})} \bar{H}(\vec{\alpha}_{\text{target}}) | \Phi_0 \rangle$$

small batch voting for SPCC: see Forssen's talk

A. Ekström and G. Hagen Phys. Rev. Lett. **123**, 252501 (2019)

Global sensitivity analysis (GSA)

bulk properties of oxygen 16

A sensitivity analysis addresses the question *'How much does each model parameter contribute to the uncertainty in the prediction?'*

Variance-based methods for GSA decompose the variance of a certain model output in terms of each input and their combinations.

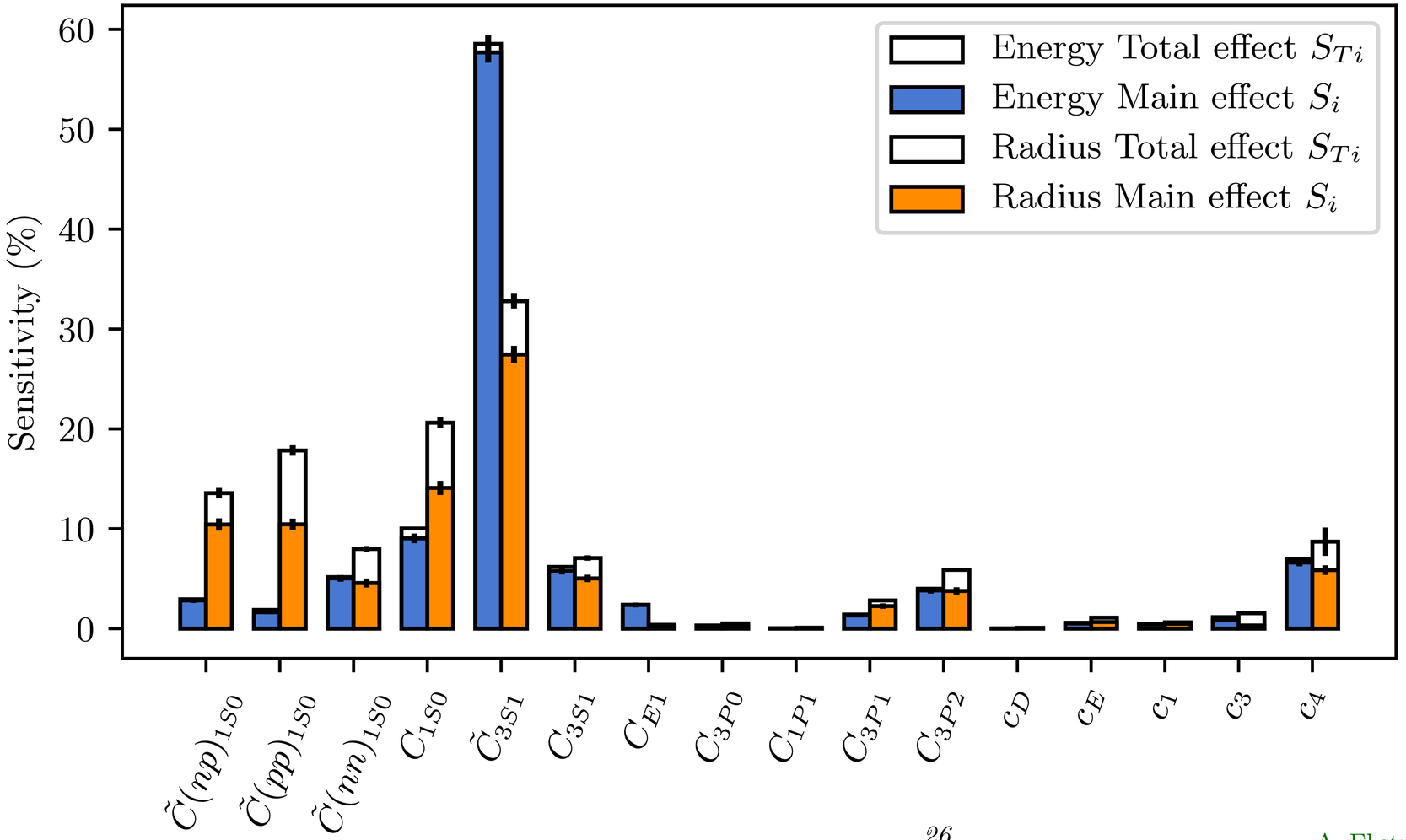
Global methods deal with the uncertainties of the outputs due to input variations over the whole domain.

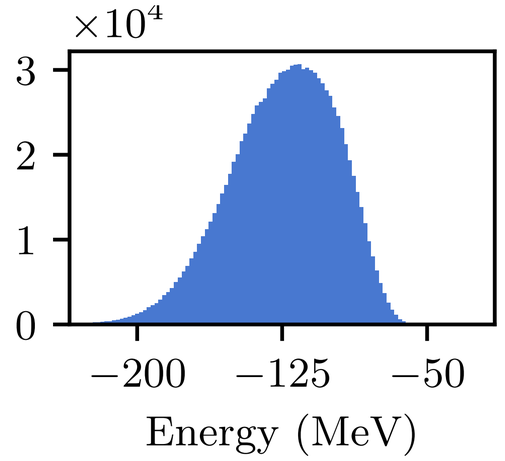
Bottleneck: Converging the MC sampling of the variance integrals require approximately 10^6 samples

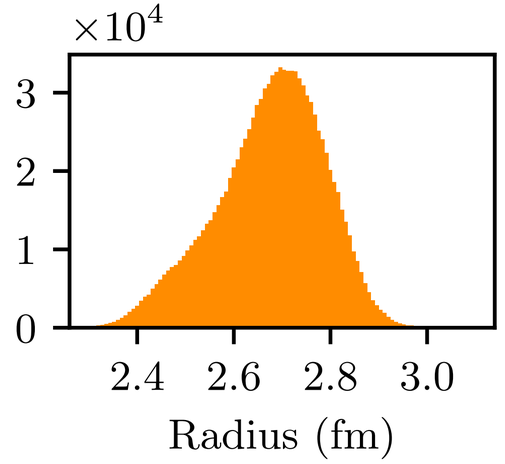
A. Saltelli et al. Global sensitivity analysis: the primer, John Wiley & Sons
A. Ekström and G. Hagen Phys. Rev. Lett. 123, 252501 (2019)

Global sensitivity analysis

bulk properties of oxygen 16





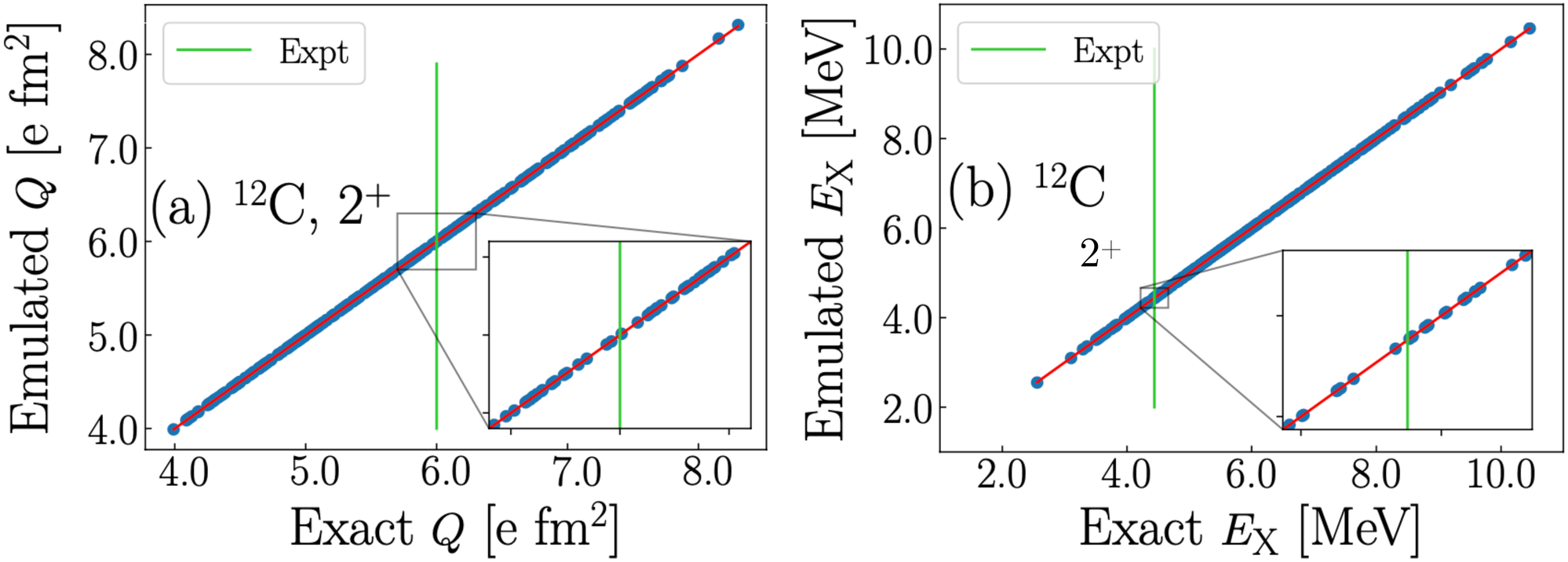


A. Ekström and G. Hagen Phys. Rev. Lett. **123**, 252501 (2019)

Symmetry-adapted eigenvector continuation

analyzing collectivity and clustering (proof of principle)

A two-step approach: (1) Use a Symmetry-Adapted (SA) basis to reduce the complete NCSM space. (2) Setup an EVC subspace to further reduce the SA-NCSM space. Example below: 32 training points, $\mathrm{NNLO_{opt}}$ 10% domain.



K. S. Becker et al, Frontiers (2023)

Symmetry-projected Hartree Fock

G. Hagen et al., PRC (2022)

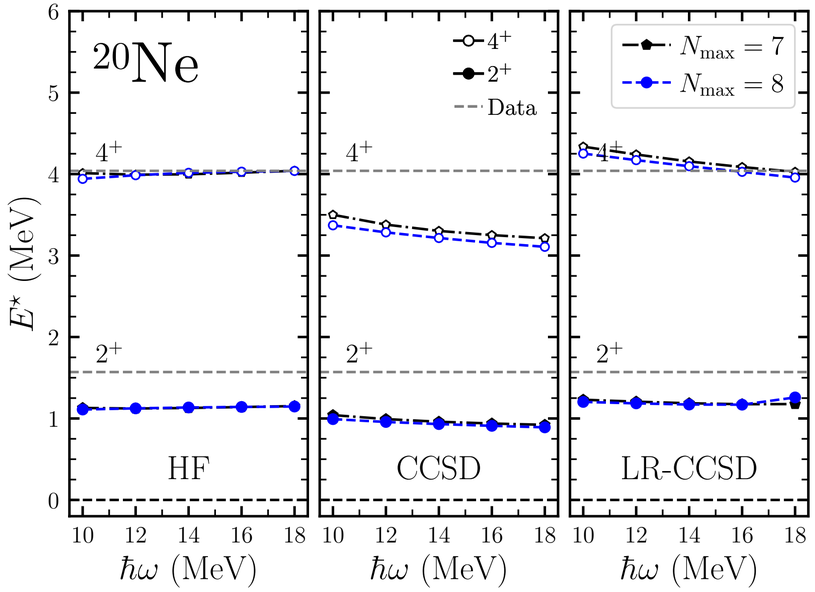
linking deformation to microscopic forces using emulators

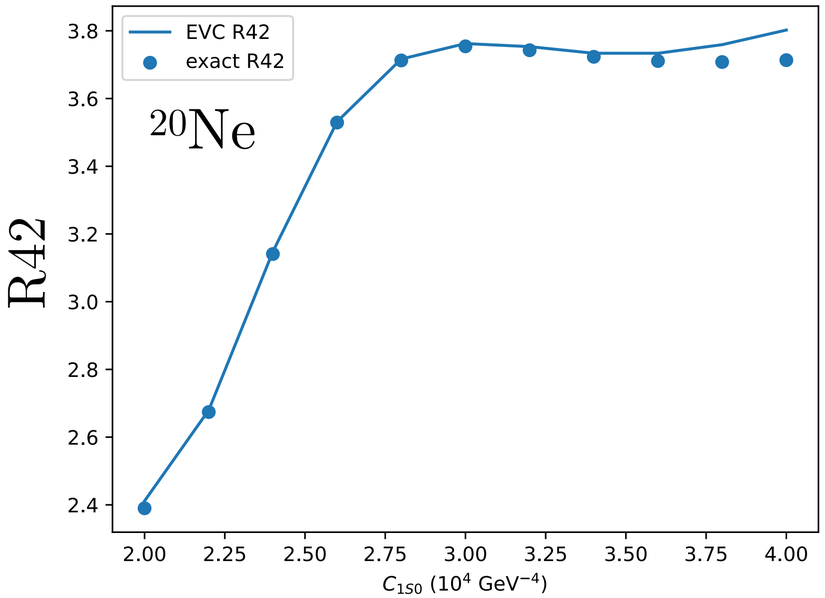
We evaluate the energy in the subspace of HF-solutions $|\Phi\rangle$.

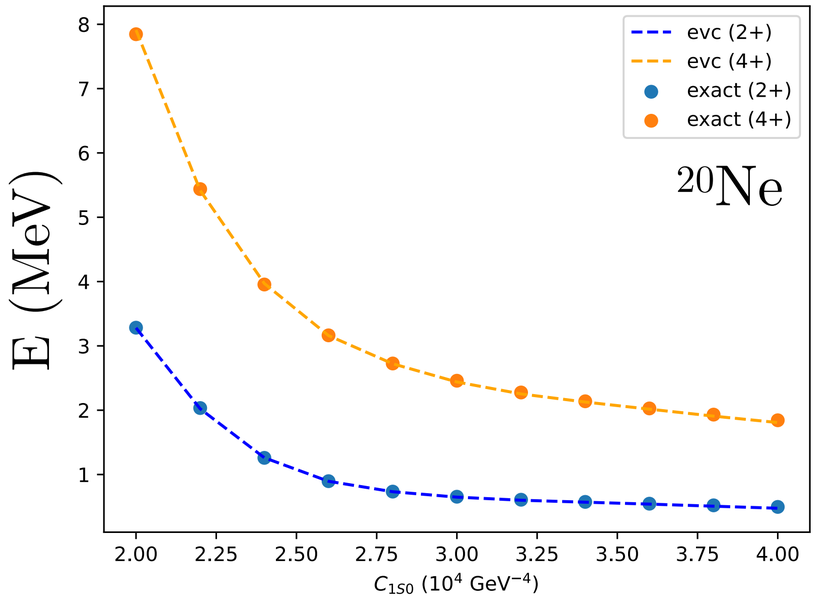
$$\widetilde{E}^{(J)}(\vec{\alpha}) = \frac{\langle \Phi | P_J H(\vec{\alpha}) | \Phi \rangle}{\langle \Phi | P_J | \Phi \rangle}$$

Preliminary

Symmetry-projected Hartree-Fock (HF) is a sufficient approximation for excitation energies and captures the infrared physics of deformation signatures well.



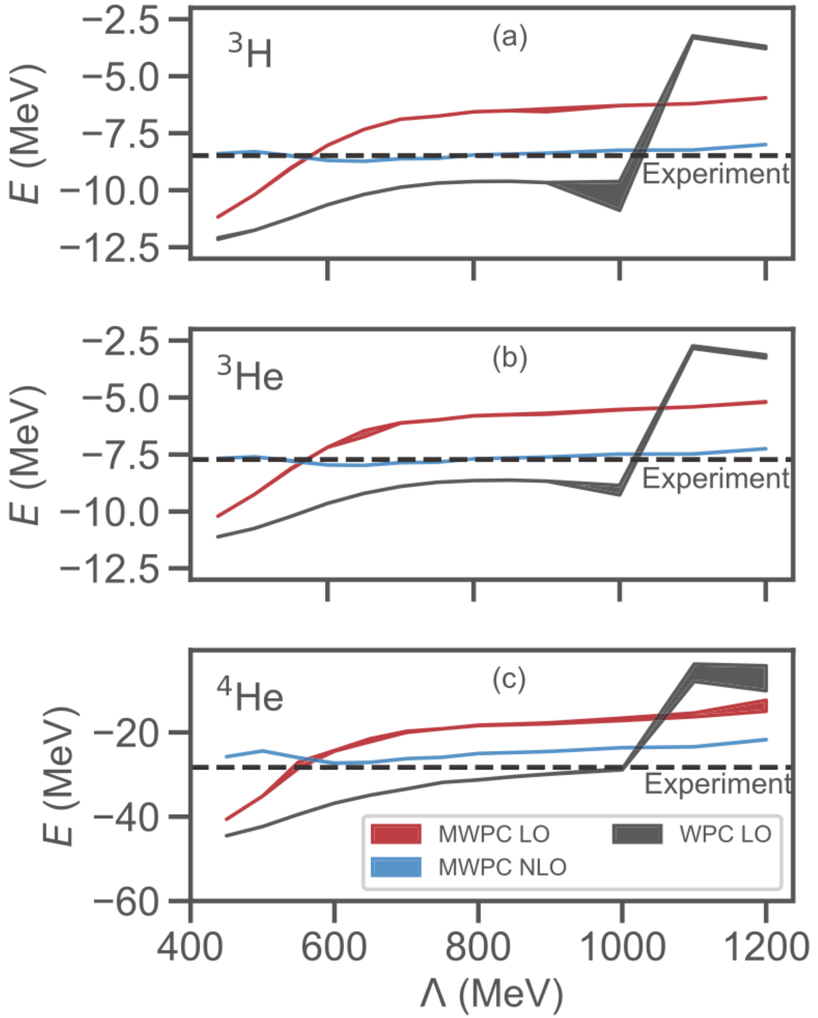




more on collective excitations: see Duguet's talk

Revisiting the leading order of χEFT

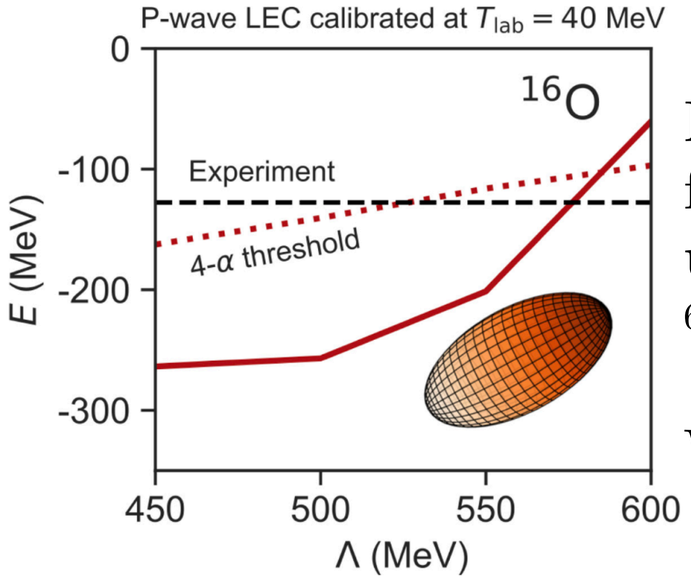
available LO interactions tend to yield unstable/unphysical results for A>4 nuclei



There exists different and sometimes conflicting assumptions regarding the power counting scheme and its meaning.

$$V_{\rm LO}^{\rm WPC}(\mathbf{p},\mathbf{p}') = -\frac{g_A^2}{4f_\pi^2}\tau_1\cdot\tau_2\frac{(\sigma_1\cdot\mathbf{q})(\sigma_2\cdot\mathbf{q})}{m_\pi^2+\mathbf{q}^2} + \tilde{C}_{^1S_0} + \tilde{C}_{^3S_1}$$

$$V_{\rm LO}^{\rm MWPC}(\mathbf{p},\mathbf{p}') = V_{\rm LO}^{\rm WPC}(\mathbf{p},\mathbf{p}') + \left(\tilde{C}_{^3P_0} + \tilde{C}_{^3P_2}\right)pp'$$



MWPC LO typically works fine for $A \leq 4$ but yields unphysical/unstable results for, e.g., ^{6}Li and ^{16}O.

WPC LO yields an unstable ^{16}O

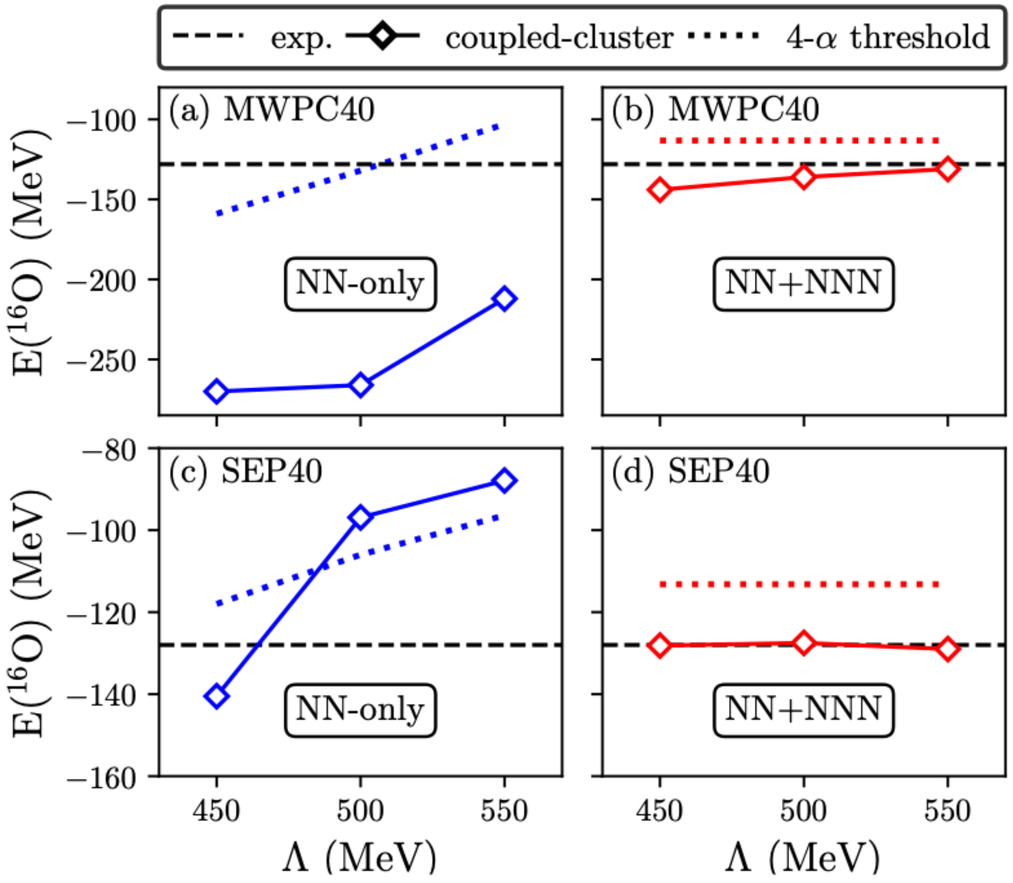
C.-J. Yang, et al Phys. Rev. C **103**, 054304 (2021)

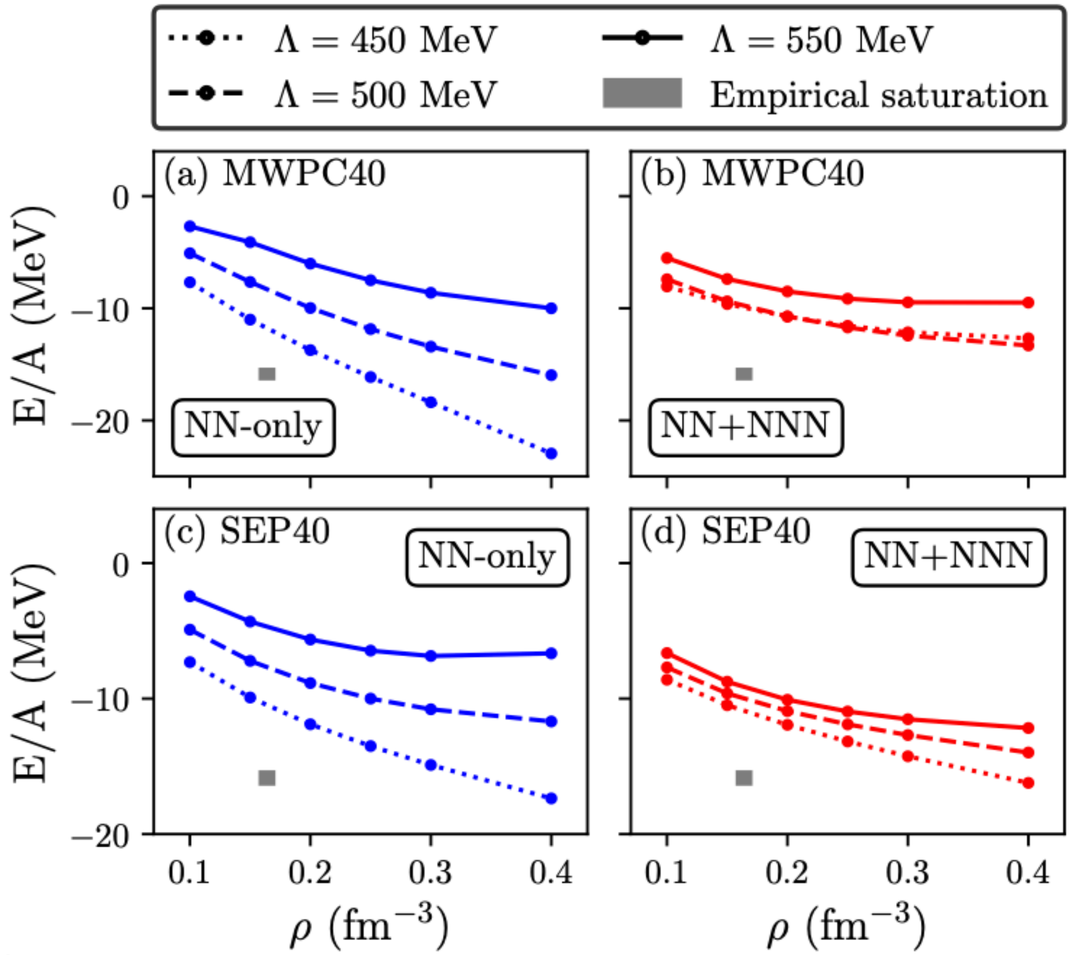
Revisiting the leading order of χEFT

a combinatorial argument: adding a three-nucleon force at LO

need 4NF?!

Realistic E(^{16}O)





C. J. Yang et al., arXiv:2109.13303

Summary

- We have put forward our current interpretation of *ab initio*.
- Converged LEC posteriors up to N3LO using HMC and quantified PPDs for NN,nd - scattering cross sections. Relatively narrow PPDs when considering only LEC-variability. (low-sample realizations can be useful).
- Successfully trained emulators for NN-scattering, SA-NCSM, symmetry-projected HF.
- Available LO χEFT interactions yield unphysical results for nuclei with mass number A$>$4.

Thank you for your attention!