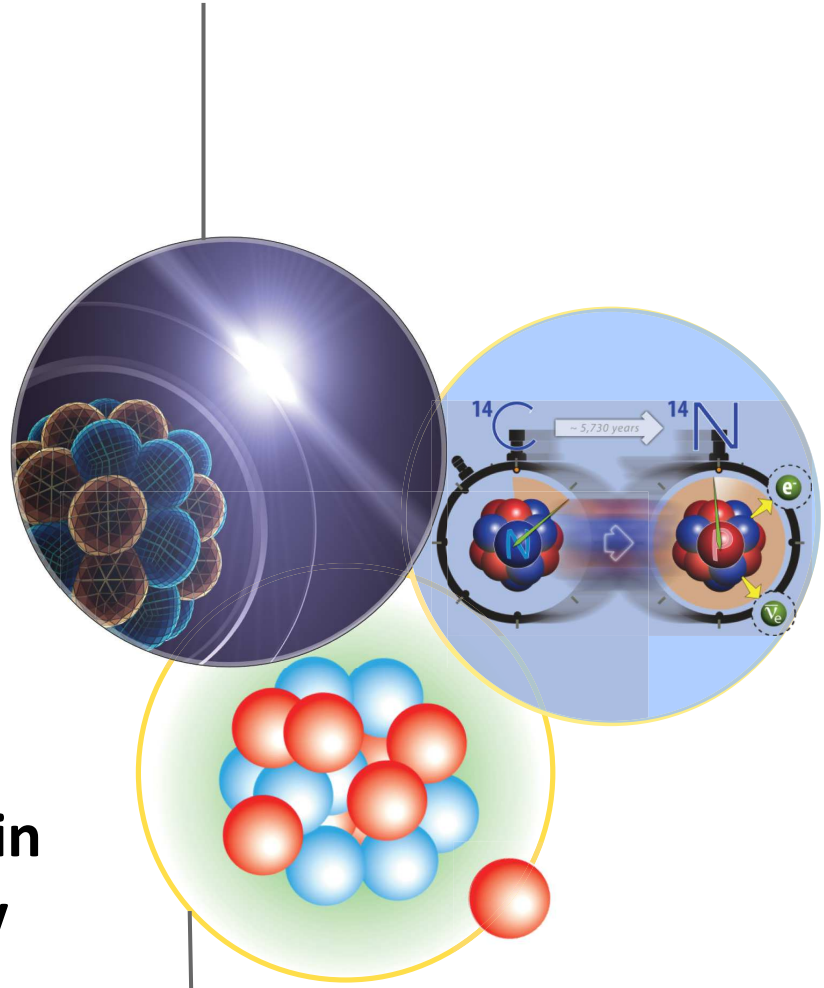
Emulating coupled cluster calculations

Gaute Hagen
Oak Ridge National Laboratory

Workshop on: Eigenvector continuation and related techniques in nuclear structure and reaction theory

CEA/Saclay, May 29th, 2023



U.S. DEPARTMENT OF ENERGY

NUCLEI
Nuclear Computational Low-Energy Initiative

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Collaborators

@ ORNL / UTK: **B. Acharya**, **Baishan Hu**, G. R. Jansen, **Z. H. Sun**, T. Papenbrock

@ UND: S. R. Stroberg

@ CEA/Saclay: T. Duguet

@ Chalmers: A. Ekström, C. Forssén

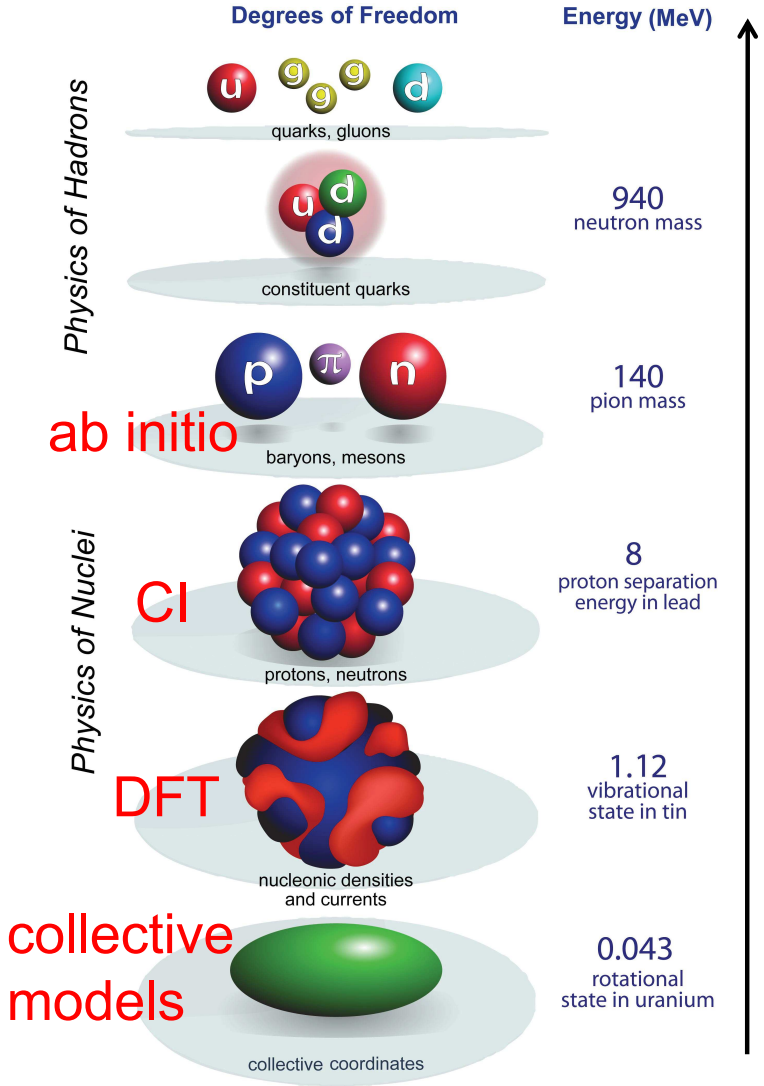
@ Mainz**: F. Bonaiti**, S. Bacca, **J. E. Sobczyk, W. G. Jiang**

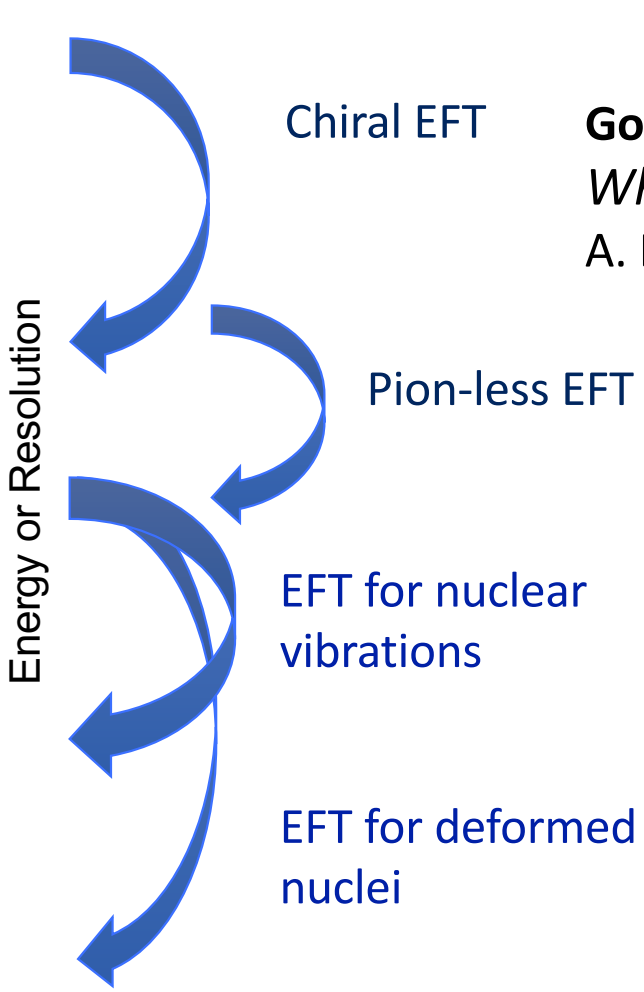
@ LANL: **S. Novario**

@ TRIUMF: **P. Gysbers,** J. Holt, P. Navratil

@ TU Darmstadt: K. Hebeler, **T. Miyagi,** A. Schwenk**, A. Tichai**

What is ab-initio in nuclear theory?





Google: "gruyere and ab initio"
What is ab initio in nuclear theory?
A. Ekström et al, Frontiers (2023)

"we interpret the ab initio method to be a systematically improvable approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities"

Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

Solving the quantum many-nucleon problem

An exponentially hard problem to solve!

$$H|\Psi\rangle = E|\Psi\rangle$$

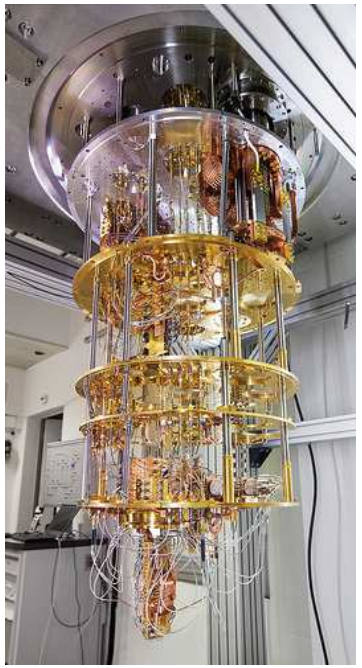
1.1 exaflops

Polynomial scaling

Systematically improvable approaches
with controlled approximations:
Coupled-cluster, IMSRG, Gorkov, SCGF,…

Emulators?

IBM Q Experience



Fault tolerant quantum computing??

$$\Psi = e^T |\Phi\rangle$$

$$T = T_1 + T_2 + \dots$$

$$T_1 = \sum_{ia} t_i^a a_a^\dagger a_i \quad T_2 = \frac{1}{4} \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$$

- ☺ Scales gently (polynomial) with increasing system size
- ☺ Truncation is only approximation
- ☺ A lot of freedom in the choice of reference state (spherical, deformed, pairing,…)

$$\begin{aligned} E &= \langle \Phi | \overline{H} | \Phi \rangle \\ 0 &= \langle \Phi_i^a | \overline{H} | \Phi \rangle \\ 0 &= \langle \Phi_{ij}^{ab} | \overline{H} | \Phi \rangle \end{aligned}$$

CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations

$$\overline{H} \equiv e^{-T} H e^T = \left(H e^T \right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2} HT_1^2 + \dots \right)_c$$

Comparing coupled-cluster with exact CI

$$C_1 = T_1,$$

$$C_2 = T_2 + \tfrac{1}{2}T_1^2,$$

$$C_3 = T_3 + T_1T_2 + T_1^3/3!,$$

$$C_4 = T_4 + T_2^2/2 + T_1T_3 + T_1^2T_2/2 + T_1^4/4!,$$

$$\vdots,$$

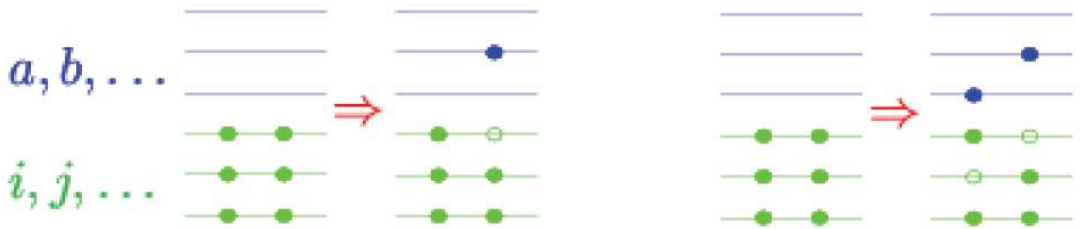
CCSD
CCSDT
CCSDTQ

Exact CI:

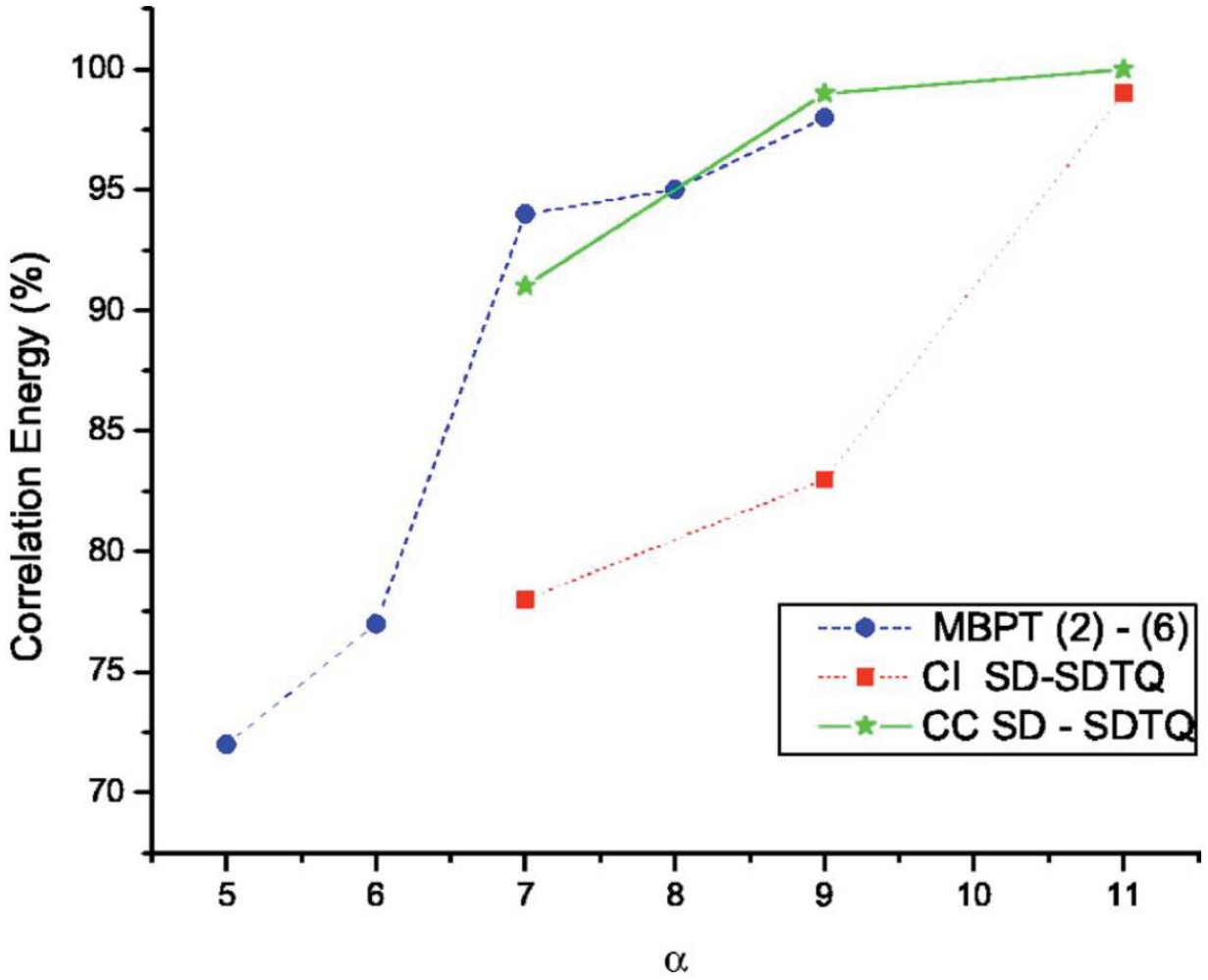
$$|\Psi\rangle = \Omega|\Phi\rangle = (1 + \sum_{i=1}^{A} C_i)|\Phi\rangle$$

- CCSD captures most of the 3p3h and 4p4h excitations (scales as $n_o^2 n_u^4$)
- In order to describe α —cluster states need to include full quadruples (CCSDTQ) (scales $n_o^4 n_u^6$)

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of Ap-Ah excitations included!



Convergence of coupled-cluster method



Bartlett & Musial Rev. Mod. Phys. (2007)

Convergence of coupled-cluster method

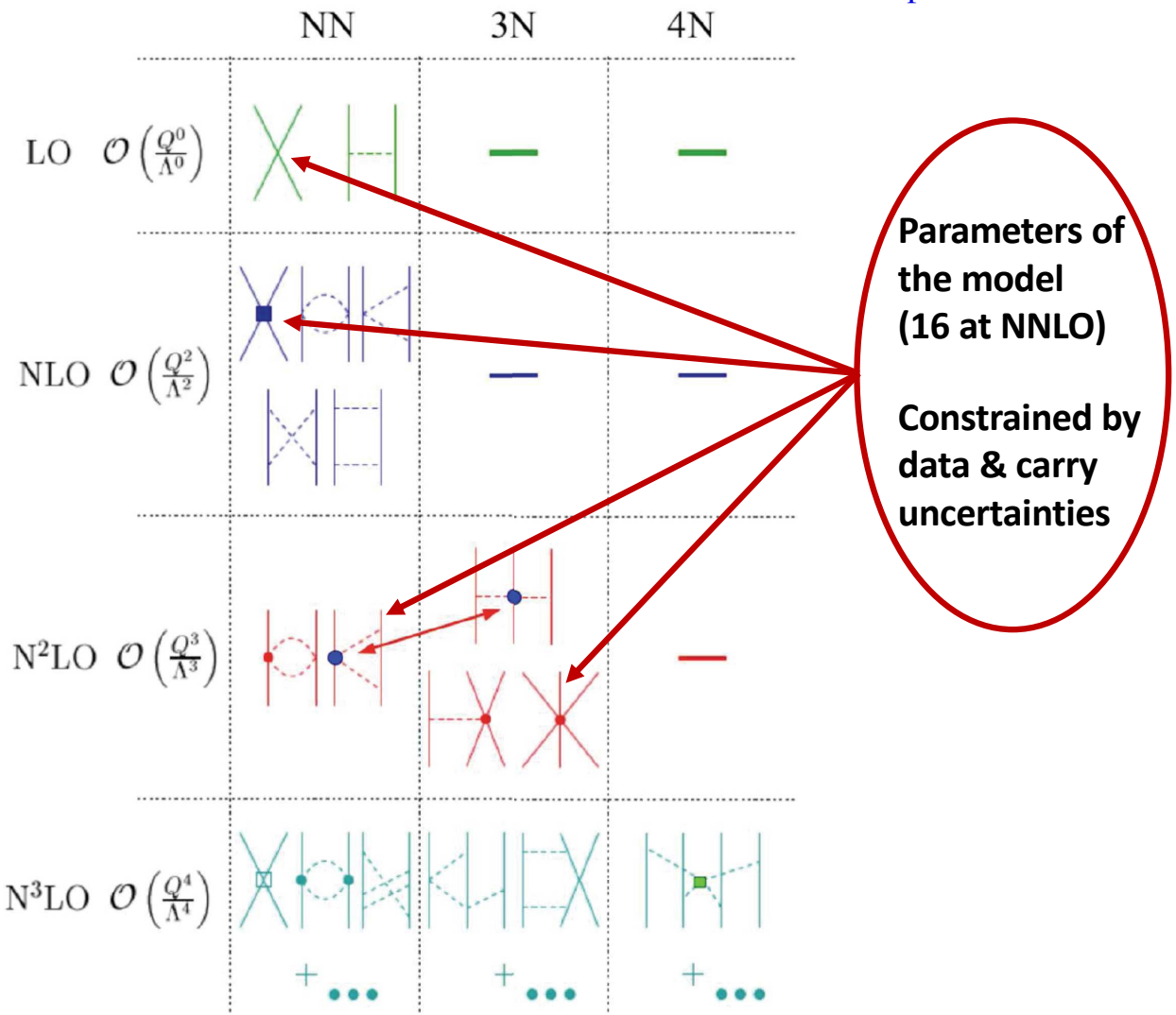
Energies	^{16}O	^{22}O	^{24}O	^{28}O
($\Lambda_\chi = 500$ MeV)				
E_0	25.946	46.52	50.74	63.85
ΔE_{CCSD}	−133.53	−171.31	−185.17	−200.63
ΔE_3	−13.31	−19.61	−19.91	−20.23
E	−120.89	−144.40	−154.34	−157.01
($\Lambda_\chi = 600$ MeV)				
E_0	22.08	46.33	52.94	68.57
ΔE_{CCSD}	−119.04	−156.51	−168.49	−182.42
ΔE_3	−14.95	−20.71	−22.49	−22.86
E	−111.91	−130.89	−138.04	−136.71
Experiment	−127.62	−162.03	−168.38	

G. Hagen, et al, Phys. Rev. C 80, 021306 (2009).

$\Delta E_3 \sim 10 - 13\%$

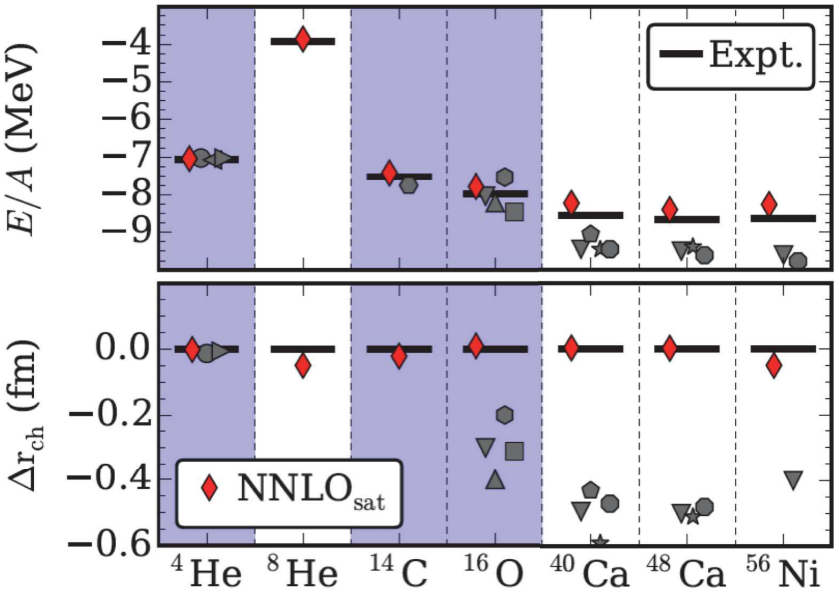
Nuclear forces from chiral effective field theory

[Weinberg; van Kolck; Epelbaum *et al*.; Entem & Machleidt; …]

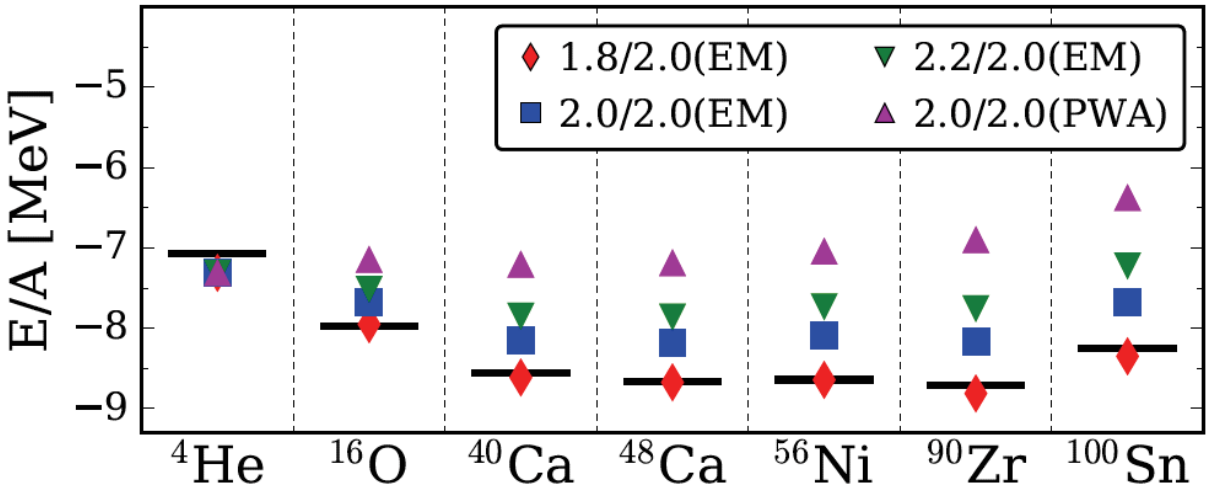


- Developing higher orders and higher rank (3NF, 4NF) [Epelbaum 2006; Bernard et al 2007; Krebs et al 2012; Hebeler et al 2015; Entem et al 2017, Reinert et al 2017…]
- Propagation of uncertainties on the horizon [Navarro Perez 2014, Carlsson et al 2015, Ekström & Hagen 2019, Drischler et al 2020]
- Different optimization protocols [Ekström et al 2013, Carlsson et al 2016]
- Improved understanding/handling via SRG [Bogner et al 2003; Bogner et al 2007]
- local / semi-local / non-local formulations [Epelbaum et al 2015, Gezerlis et al 2013/2014, Binder et al 2018]
- Chiral EFT's with explicit Delta isobars [Krebs et al 2018, Piarulli et al 2017, Ekström et al 2017, Jiang et al (2020)]

Why do some interaction models work better than others?



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



K. Hebeler *et al* PRC (2011).
T. Morris *et al*, PRL (2018).

To answer this we need predictions with rigorous **uncertainty quantification** and **sensitivity analyses** that are grounded in the description of the underlying nuclear Hamiltonian

Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)

Global sensitivity analysis of properties of atomic nuclei

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

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

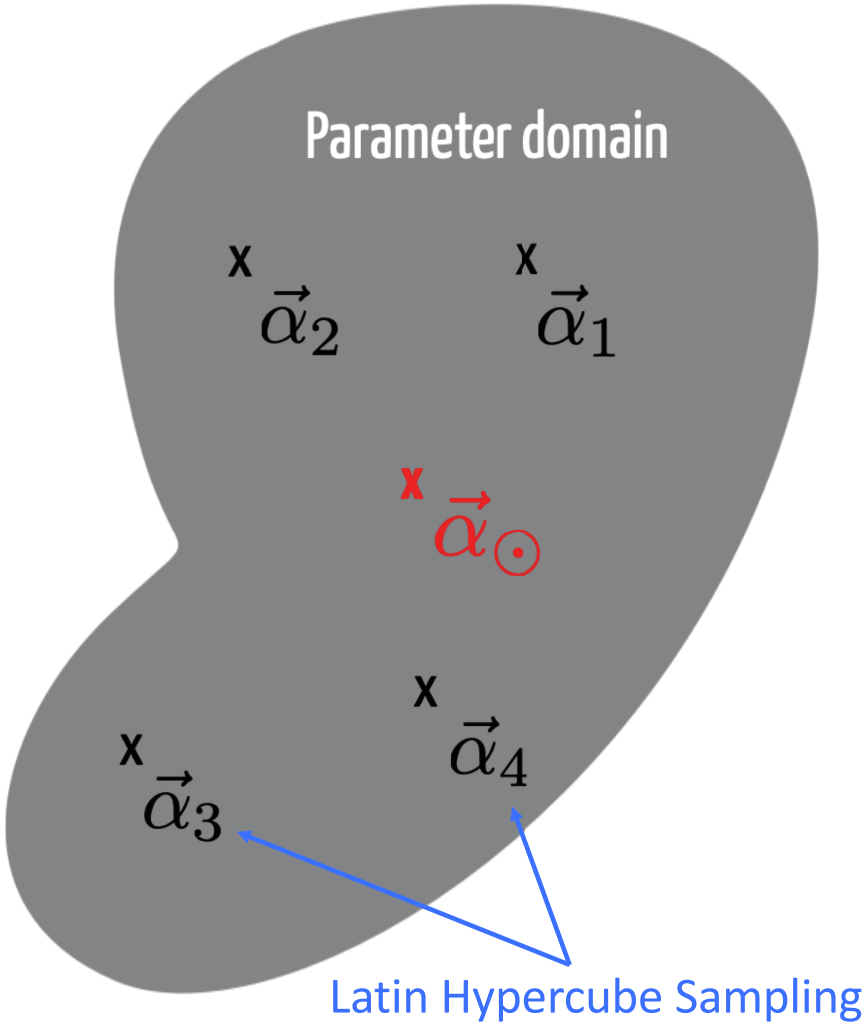
Computational bottleneck

A global sensitivity analyses of binding energy and charge radius of a nucleus like 16-O requires more than one million model evaluations

Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)

Emulating ab-initio coupled-cluster calculations

Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)



- Eigenvector continuation method [Frame D. et al., Phys. Rev. Lett. 121, 032501 (2018), S. König et al Phys. Lett. B 810 (2020) 135814]
- Write the Hamiltonian in a linearized form

$$H(\vec{\alpha}) = \sum_{i=0}^{N_{\mathrm{LECs}}=16} \alpha_i h_i$$

- Select "training points" where we solve the exact problem
- Project a target Hamiltonian onto sub-space of training vectors and diagonalize the generalized eigenvalue problem

$$\mathbf{H}(\vec{\alpha}_\odot)\,\vec{c} = E(\vec{\alpha}_\odot)\,\mathbf{N}\,\vec{c}$$

Emulating ab-initio coupled-cluster calculations

Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)

Physical SPCC vector

$$|\Psi(\vec{\alpha}_{\circledcirc})\rangle = e^{T(\vec{\alpha}_{\circledcirc}))}|\Phi_0\rangle \approx \sum_{i=1}^{N_{\rm sub}} c_i^{\star} e^{T(\vec{\alpha}_i)}|\Phi_0\rangle$$

Solve generalized non-Hermitian eigenvalue problem:

$$\mathbf{H}(\vec{\alpha}_{\circledcirc})\,\vec{c} = E(\vec{\alpha}_{\circledcirc})\,\mathbf{N}\,\vec{c}$$

$$\langle\tilde{\Psi}'|H(\vec{\alpha}_{\circledcirc})|\Psi\rangle = \langle\Phi_0|(1+\Lambda')e^{X}\overline{H}(\vec{\alpha}_{\circledcirc})|\Phi_0\rangle,$$
$$\langle\tilde{\Psi}'|\Psi\rangle = \langle\Phi_0|(1+\Lambda')e^{X}|\Phi_0\rangle,$$

$$e^{X} = e^{-T'+T}$$

Left coupled-cluster state

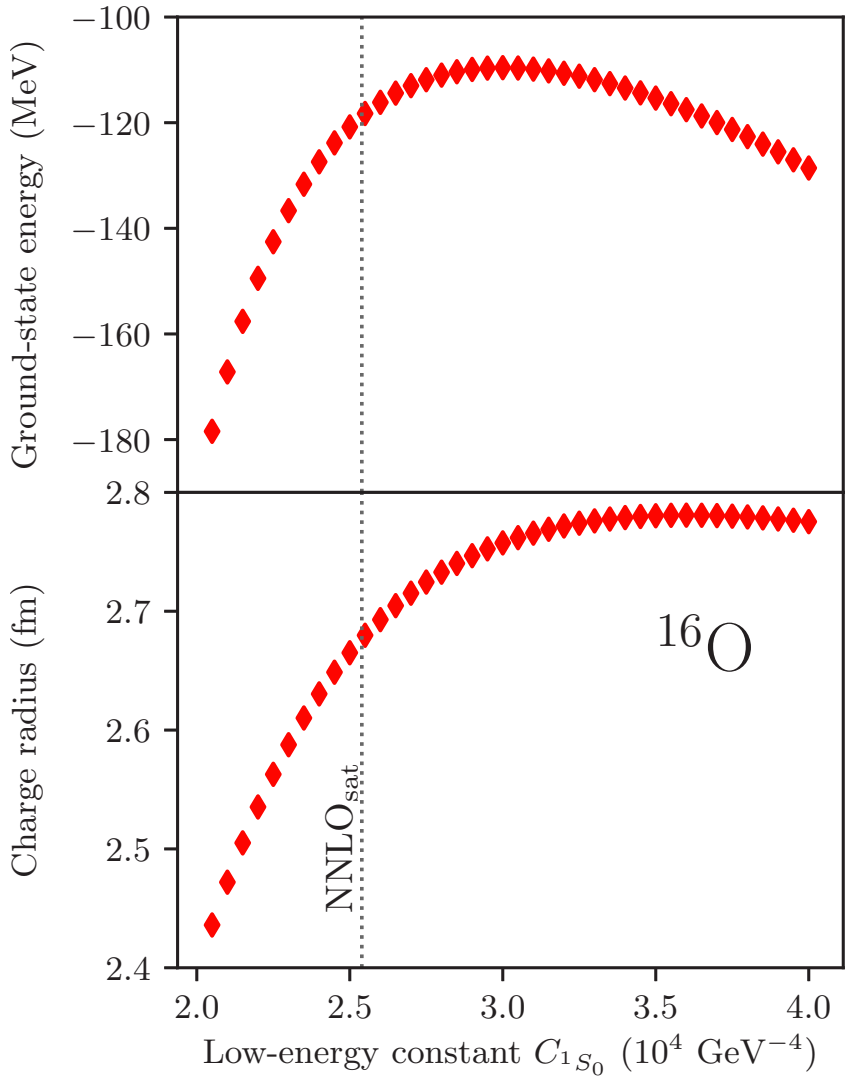
$$\langle\tilde{\Psi}| = \langle\Phi_0|(1+\Lambda)e^{-T}$$

Right coupled-cluster state

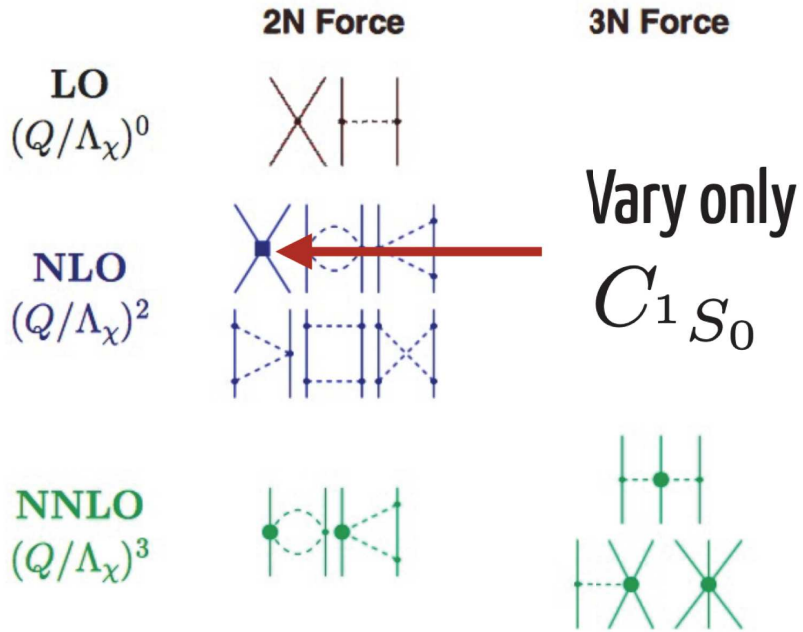
$$|\Psi\rangle = e^{T}|\Phi_0\rangle$$

Emulating ab-initio coupled-cluster calculations

Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)

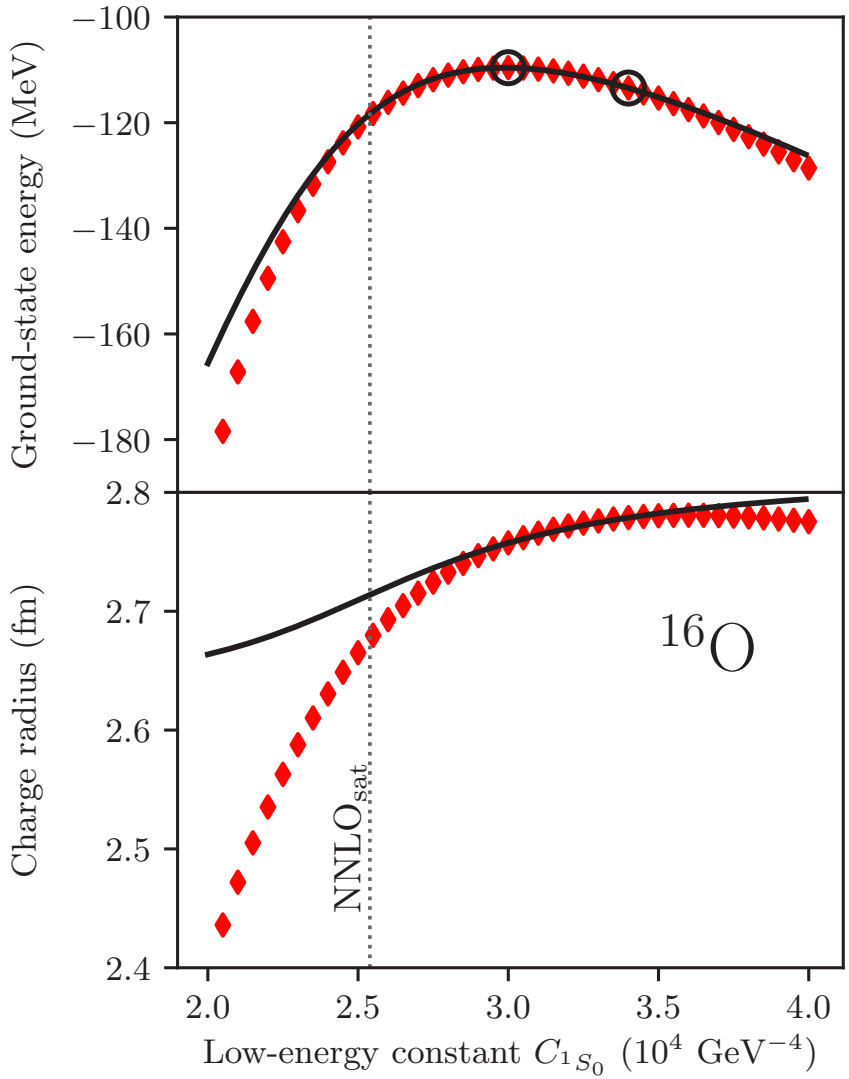


Exact coupled cluster calculations at the singles and doubles level



Emulating ab-initio coupled-cluster calculations

Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)



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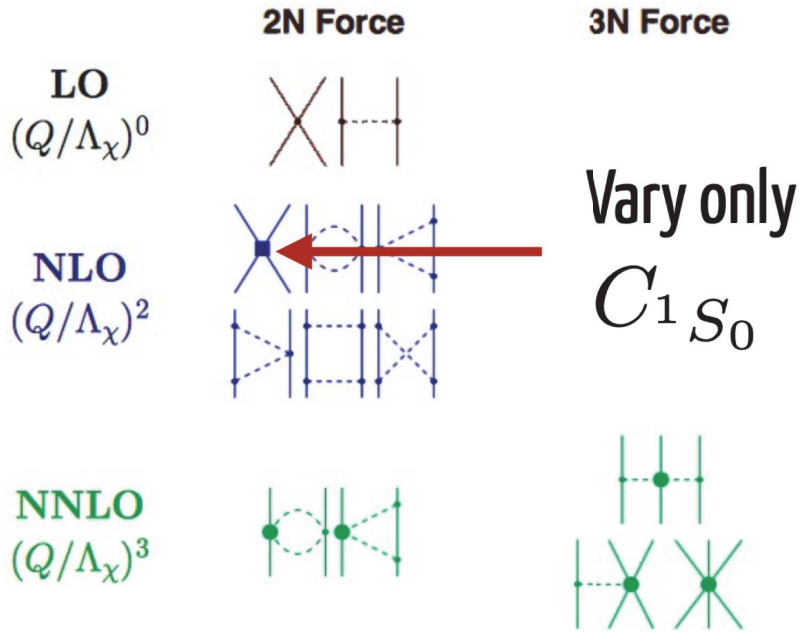

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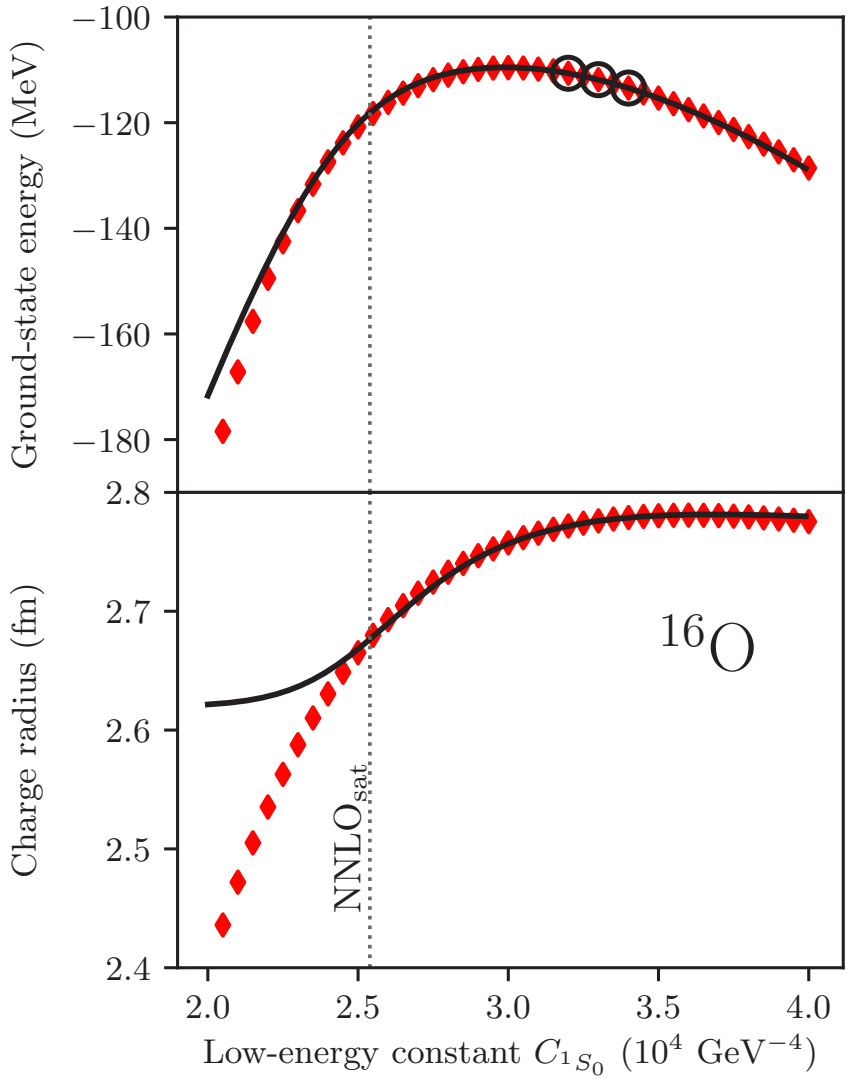

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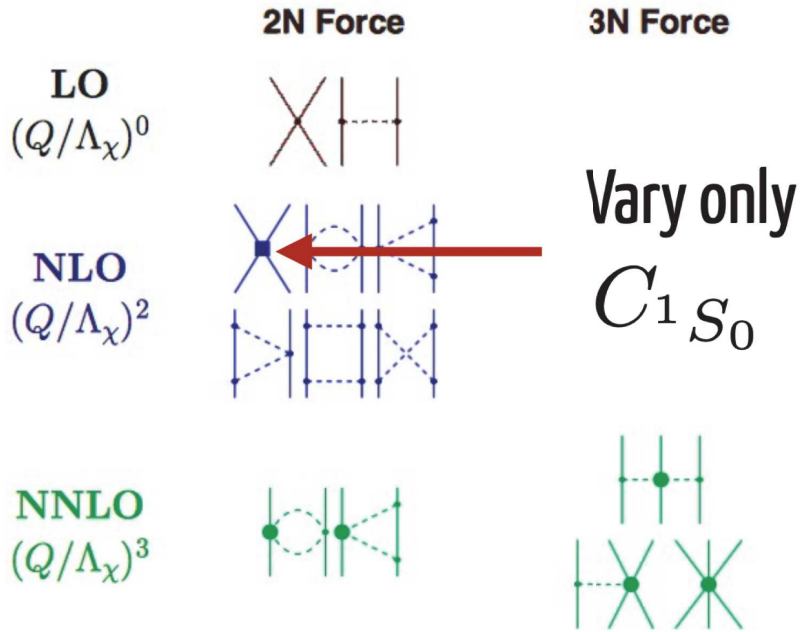

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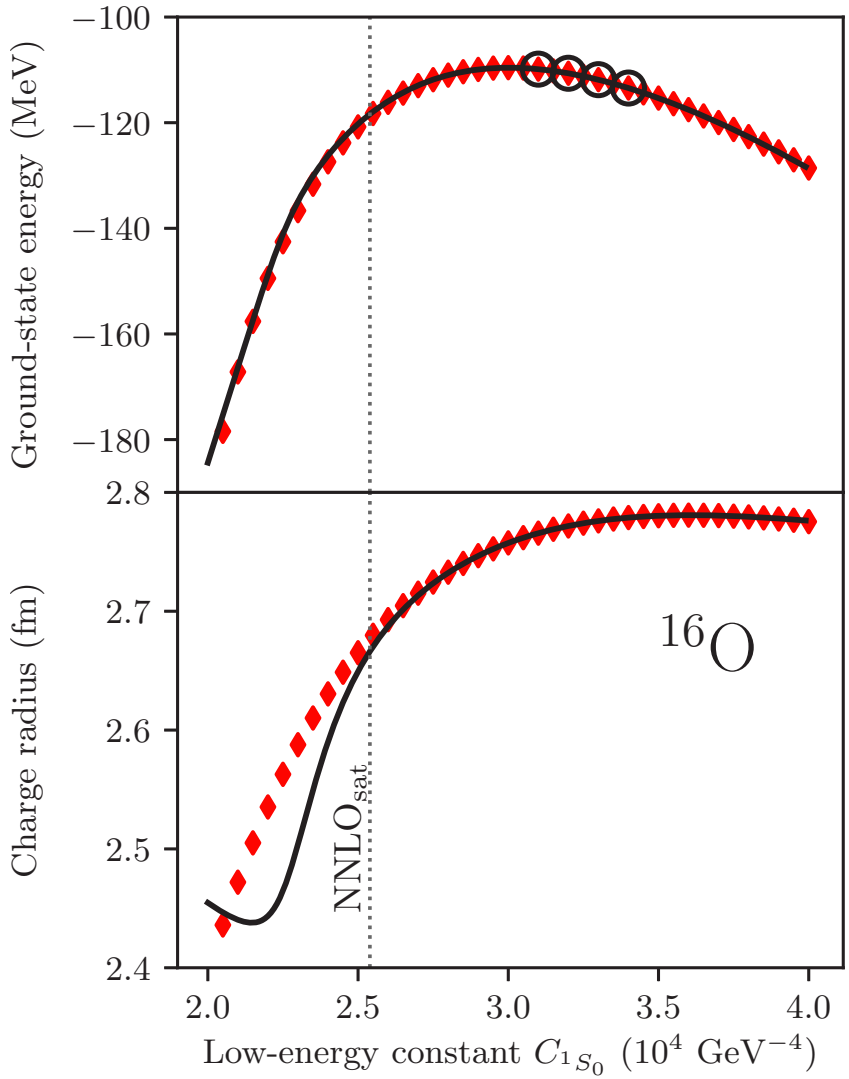

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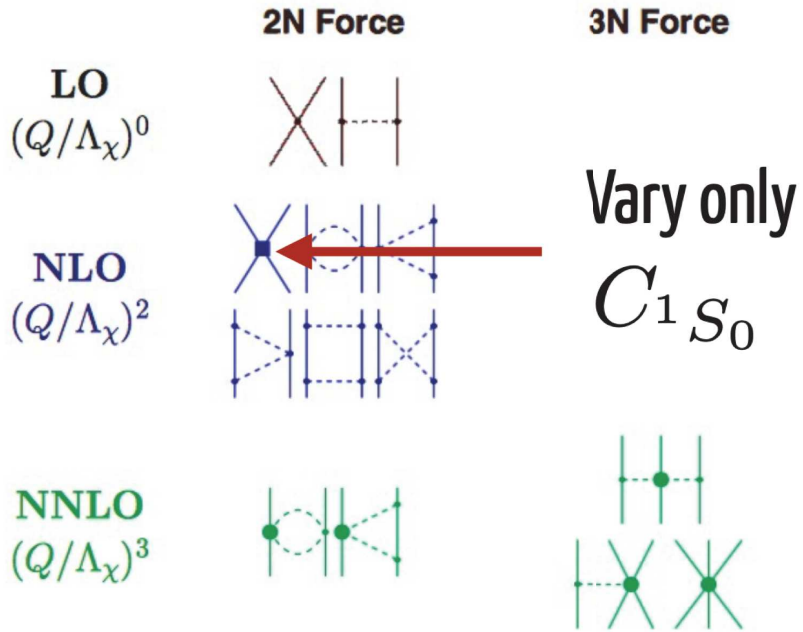

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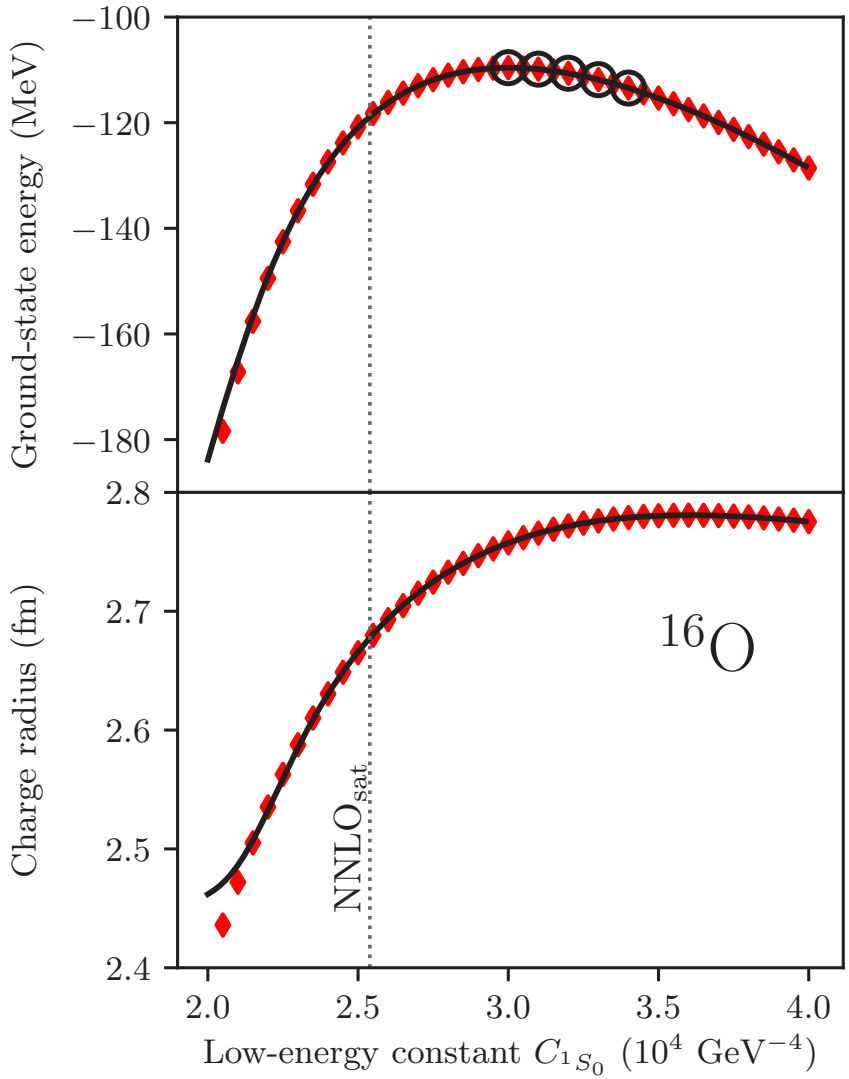

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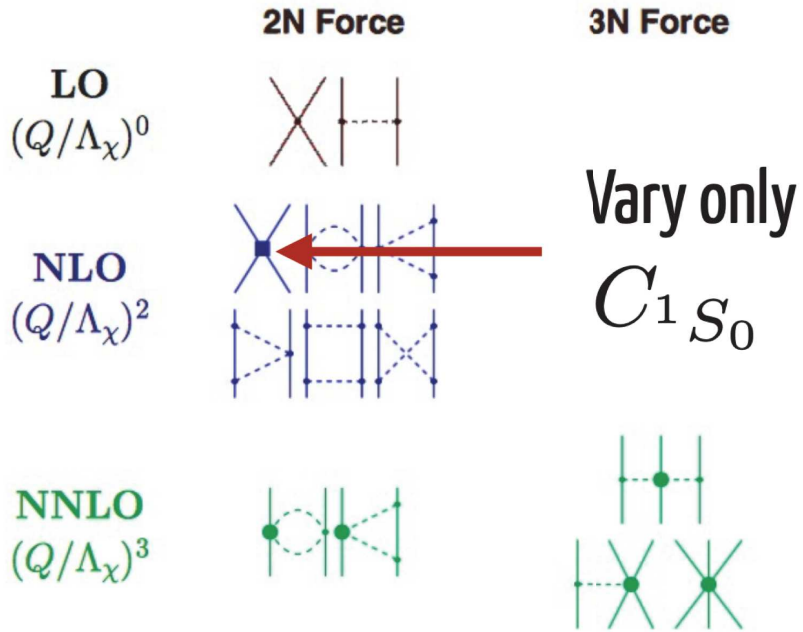
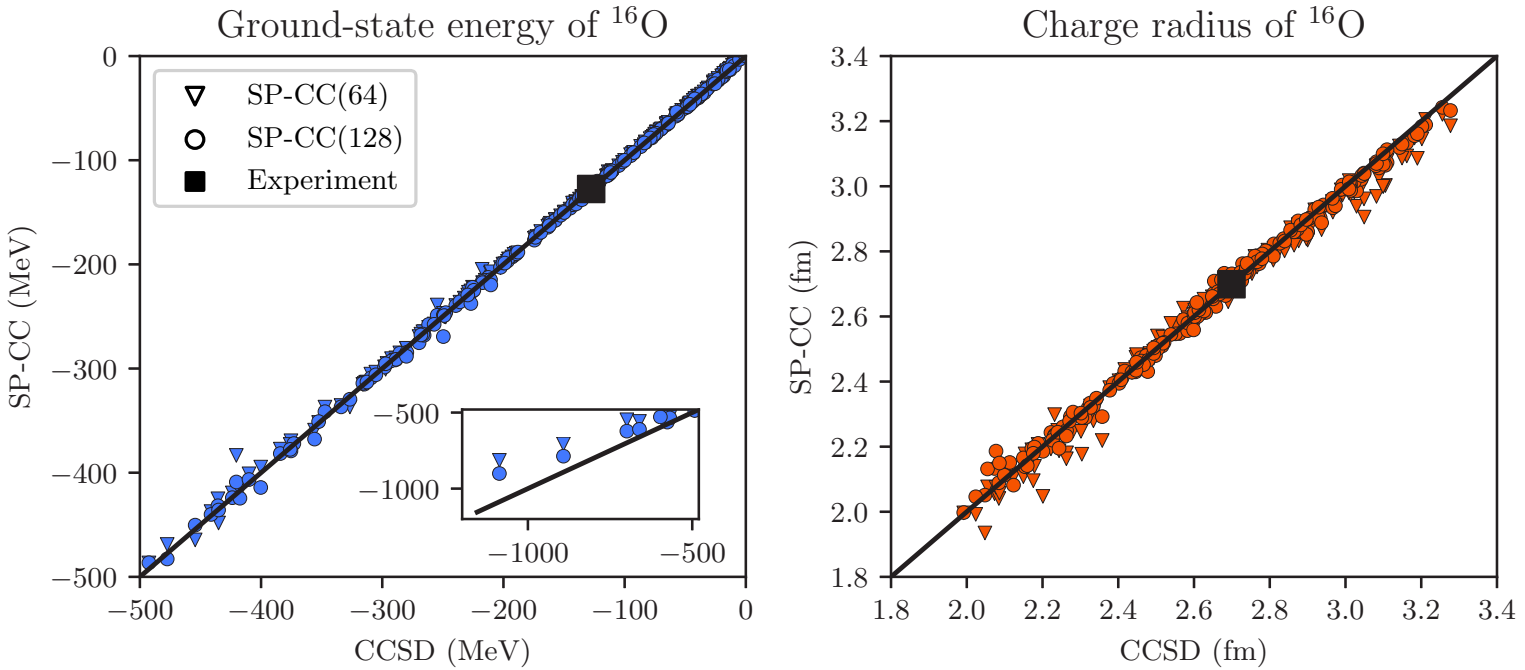


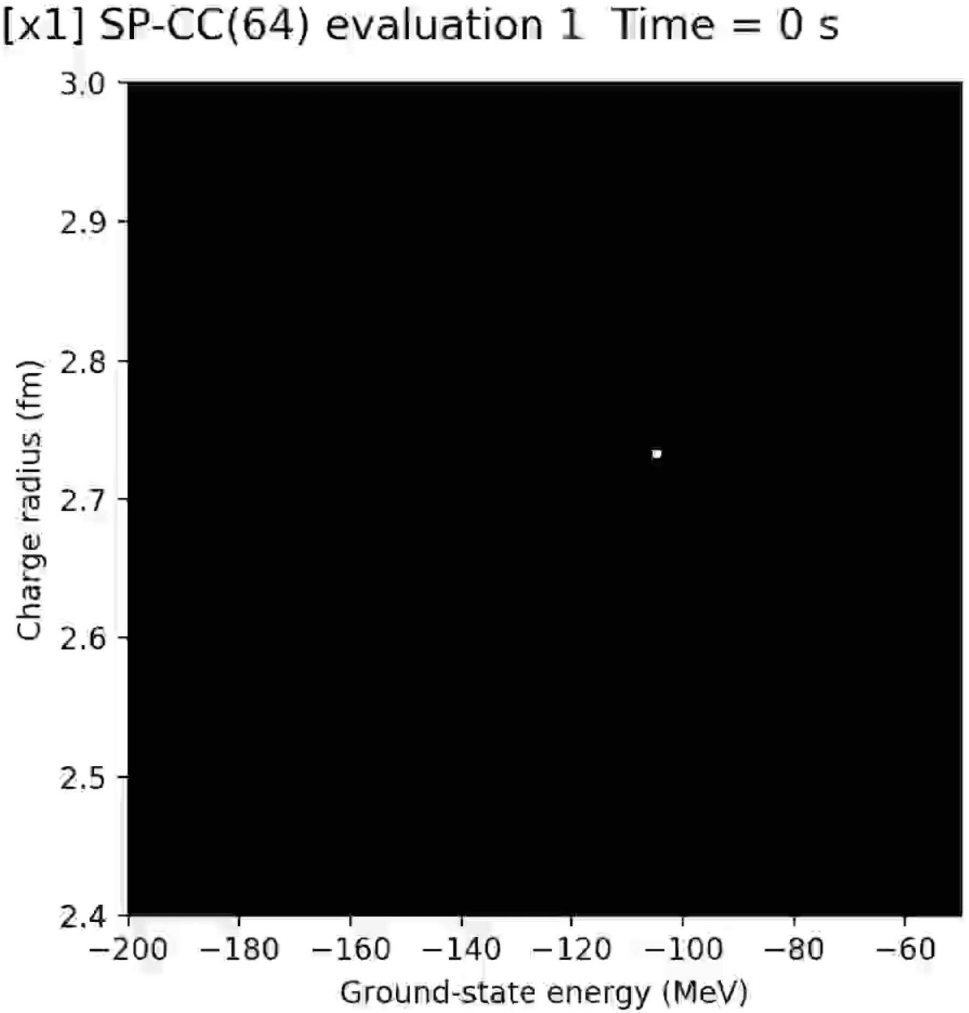
Sub-space projected coupled-cluster – cross validation in 16 dimensions



- Select 64 and 128 sub-space vectors in the 16 dimensional space of LECs using a space-filling latin hypercube design
- Select 200 randomly exact CCSD calculations in a 20% domain around $NNLO_{sat}$
- With 64 subspace vectors we achieve a 1% accuracy relative to exact CCSD solutions

Computing nuclei at lightning speed

(~5 mins: ~10^5 energy/radius calculations of ^{16}O)



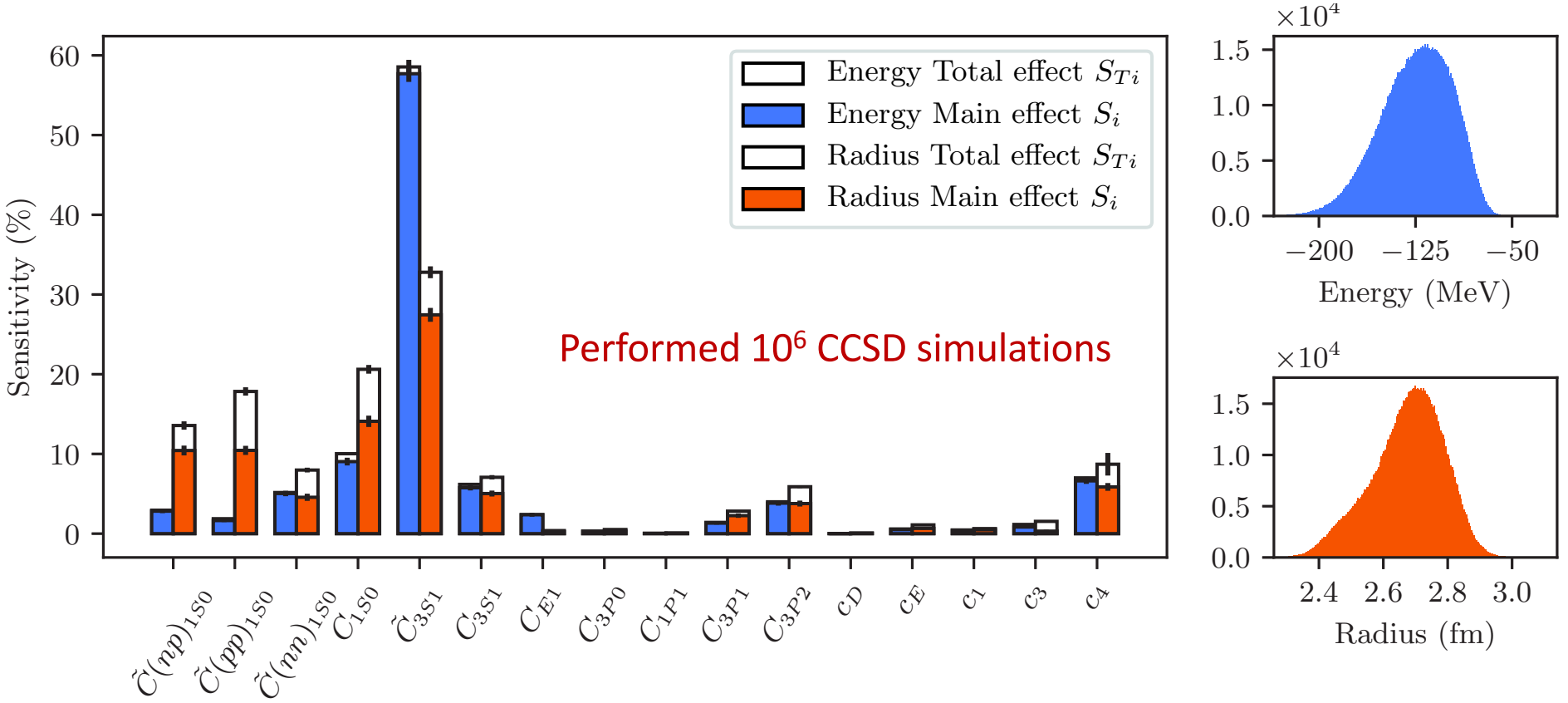
Realtime speed and accuracy of emulated ground-state energy and charge radius of ^{16}O for different values of interaction parameters

$$H(\vec{\alpha}) = \sum_{i=0}^{N_{\mathrm{LECs}}=16} \alpha_i h_i$$

Accuracy: roughly the pixel size

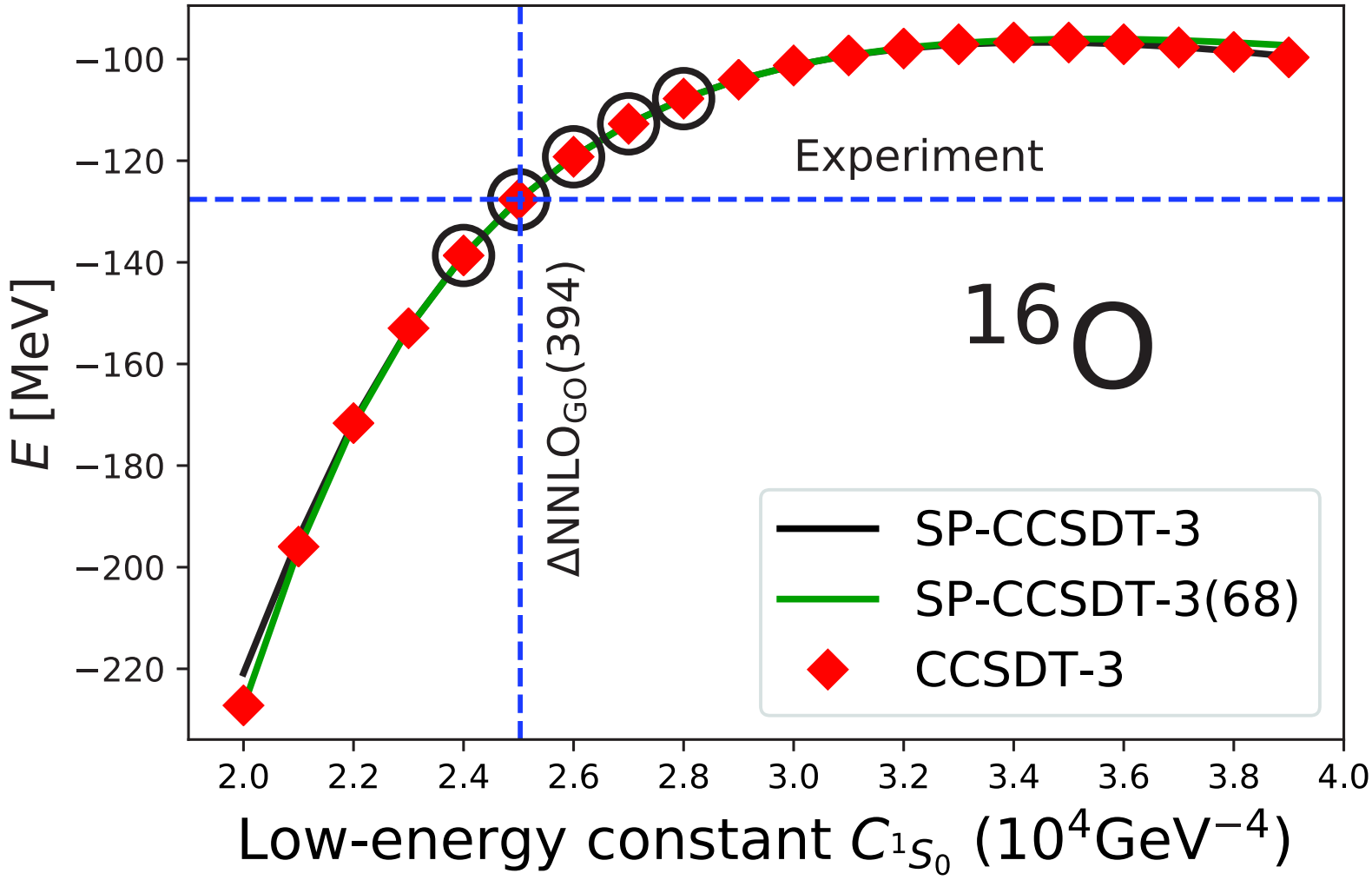
Speedup: 20 years of single node computations can be replaced by a 1 hour run on a laptop

A global sensitivity analysis of the radius and binding energy of ^{16}O

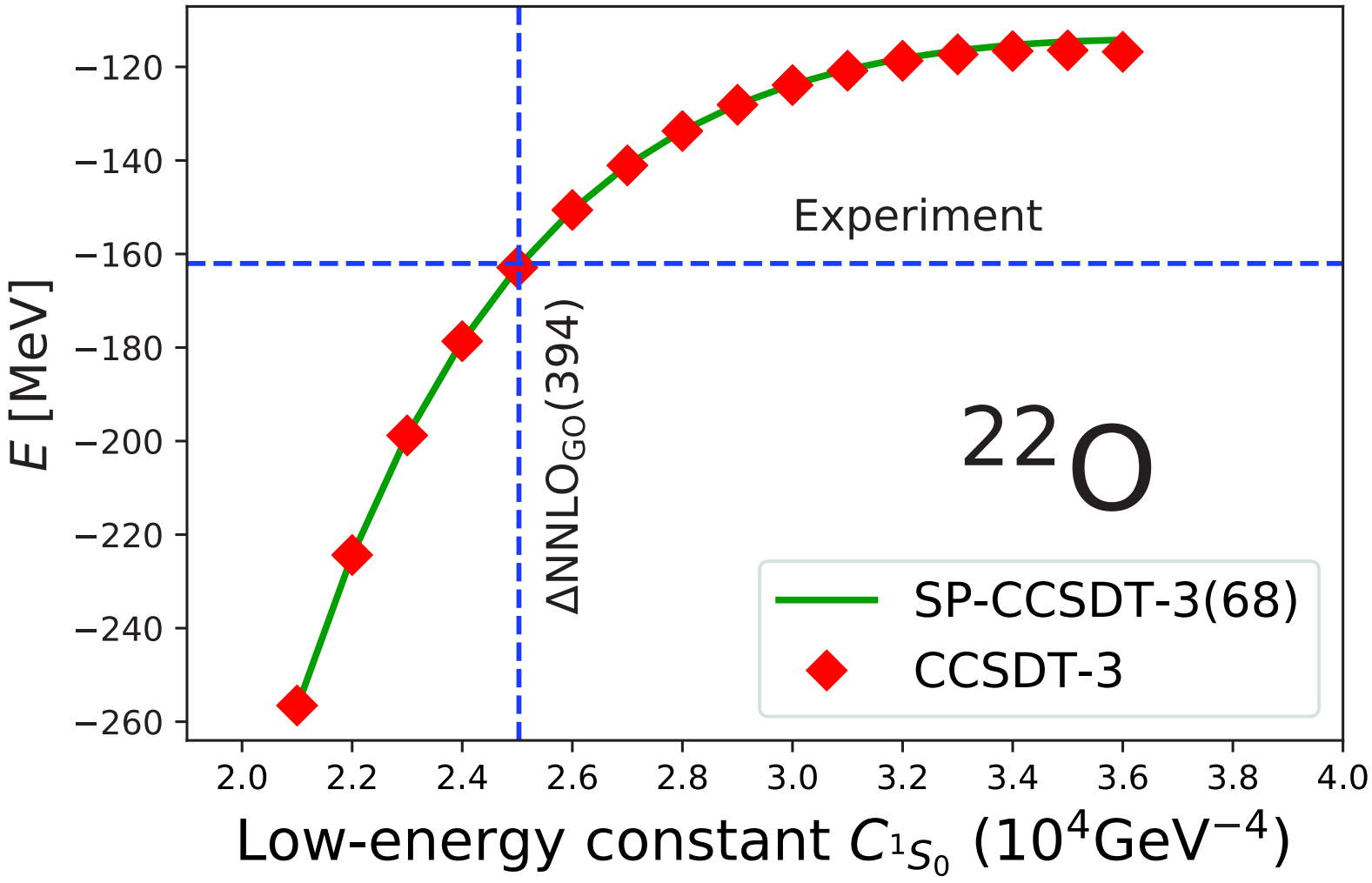


About 60% of the variance in the energy can is attributed to the 3S1-wave, whereas the radius depends sensitively on several LECs and their higher-order correlations

Emulating higher-order coupled-cluster



Emulating higher-order coupled-cluster



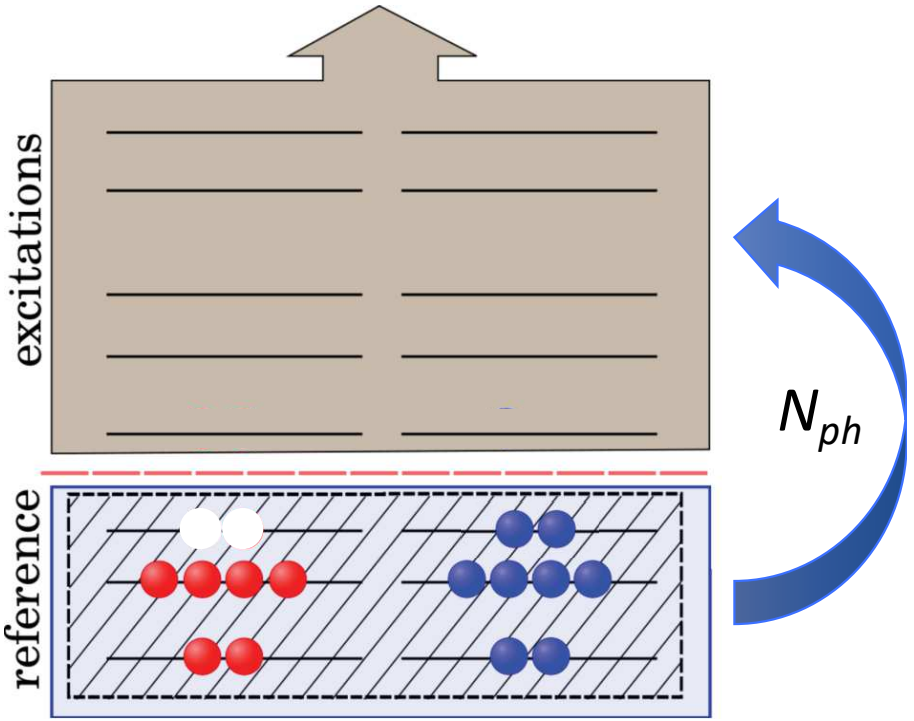
Emulating excited states in coupled-cluster

$$\overline{H} R_\mu |\phi\rangle = E_\mu R_\mu |\phi\rangle \qquad |\psi_\mu\rangle = R_\mu |\phi\rangle$$

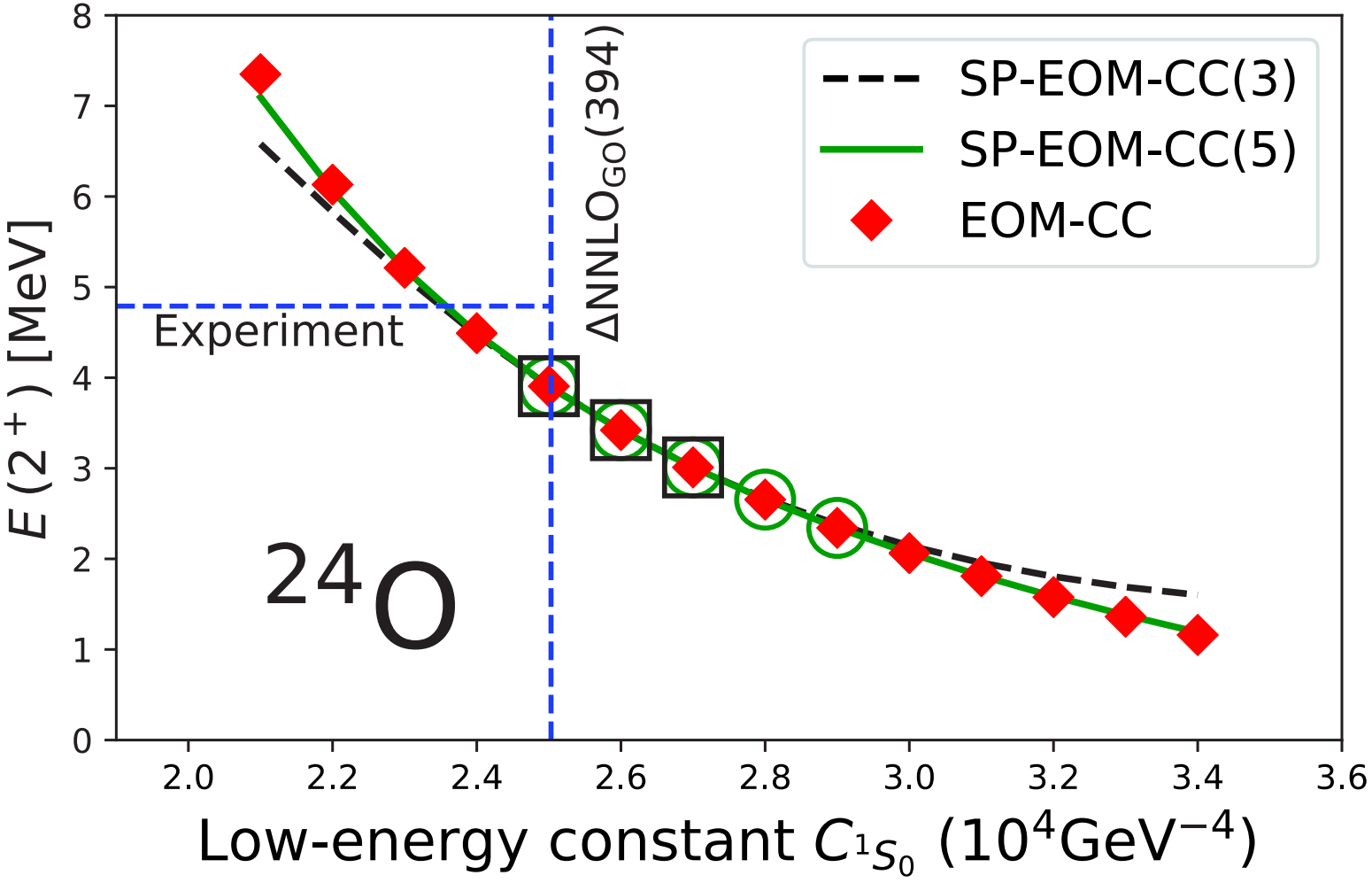
$$R = r_0 + \sum_{ia} r_i^a a_a^\dagger a_i + \frac{1}{4} \sum_{ijab} r_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i + \cdots$$

$$|\psi_\mu(\vec{\alpha}_\circledcirc)\rangle = \sum_j^{n_t} c_j |\psi_\mu^{(j)}\rangle$$

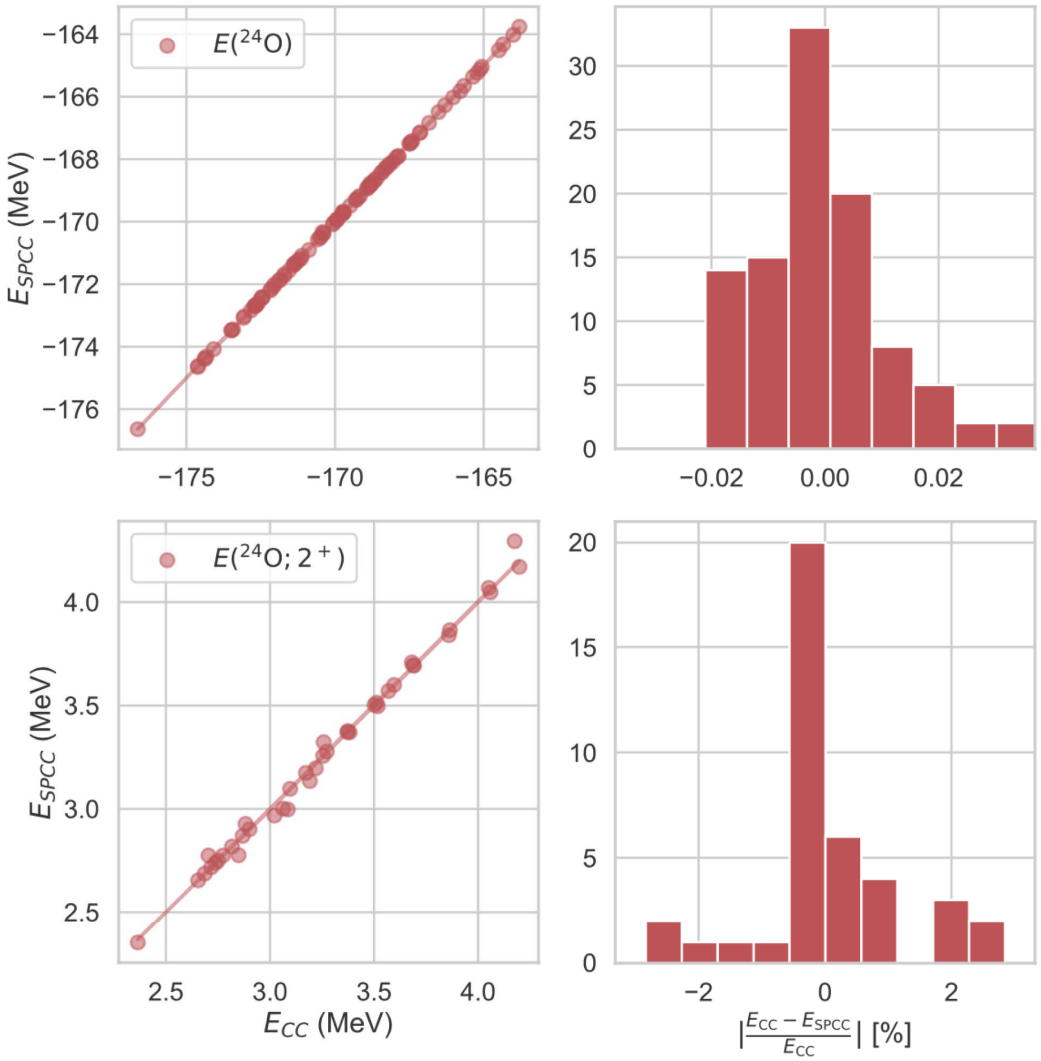
- Solve a generalized non-Hermitian eigenvalue problem
- For now restricted to “training” EOM vectors with the same reference state



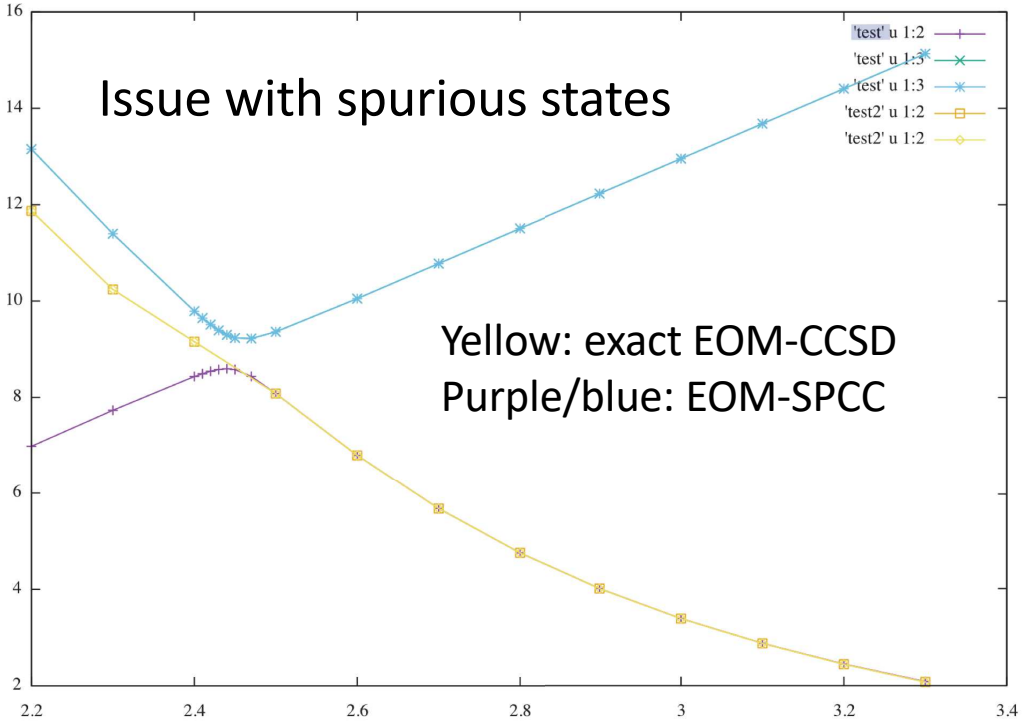
Emulating excited states in coupled-cluster



Emulating excited states in coupled-cluster

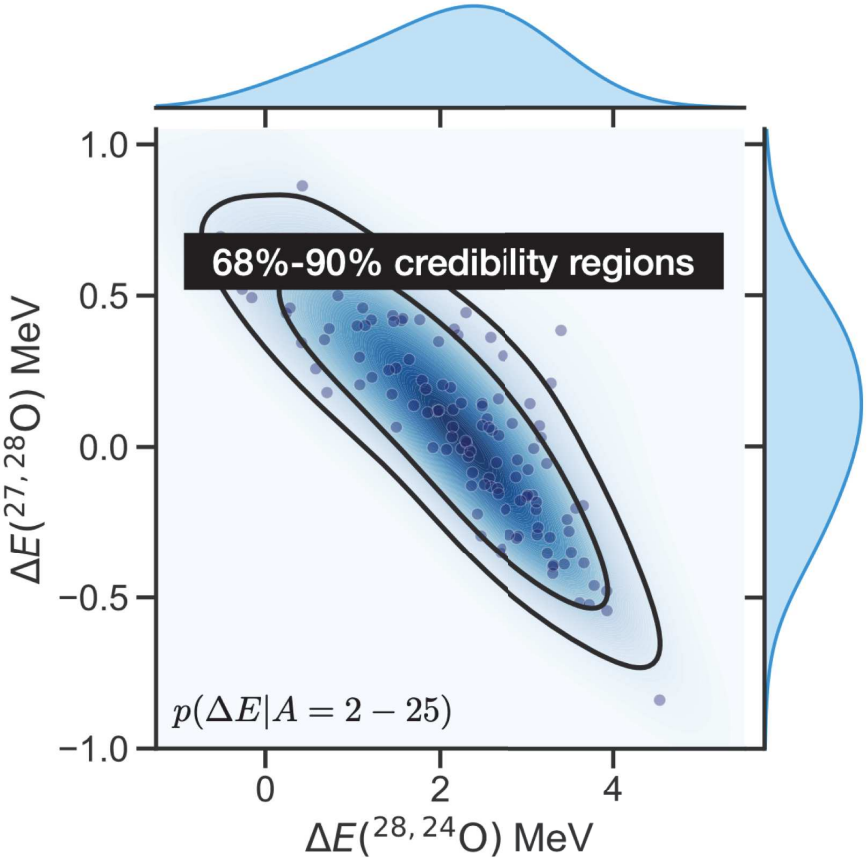


- EOM-CCSDT-3 emulator with 34 training vectors
- Cross validation in ^{24}O for ground-state and excited 2+ state in EOM-CCSDT-3



Does chiral Hamiltonians predict a bound ^{28}O?

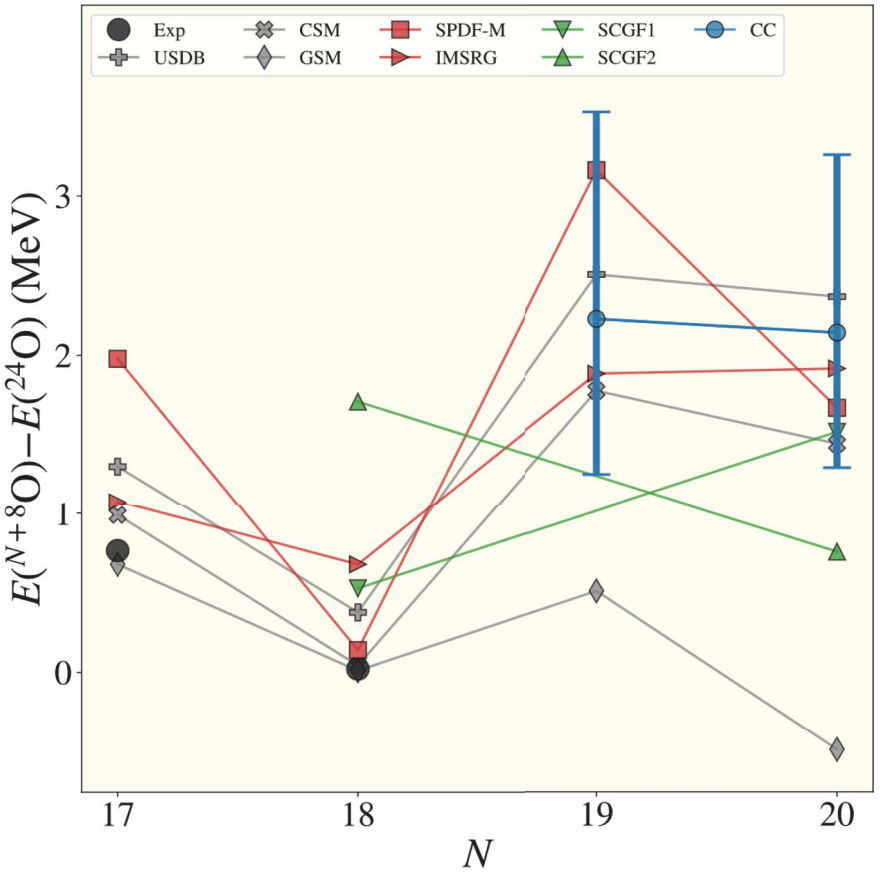
Ekström, Forssén, Hagen, Jiang, Papenbrock, Sun, Vernon



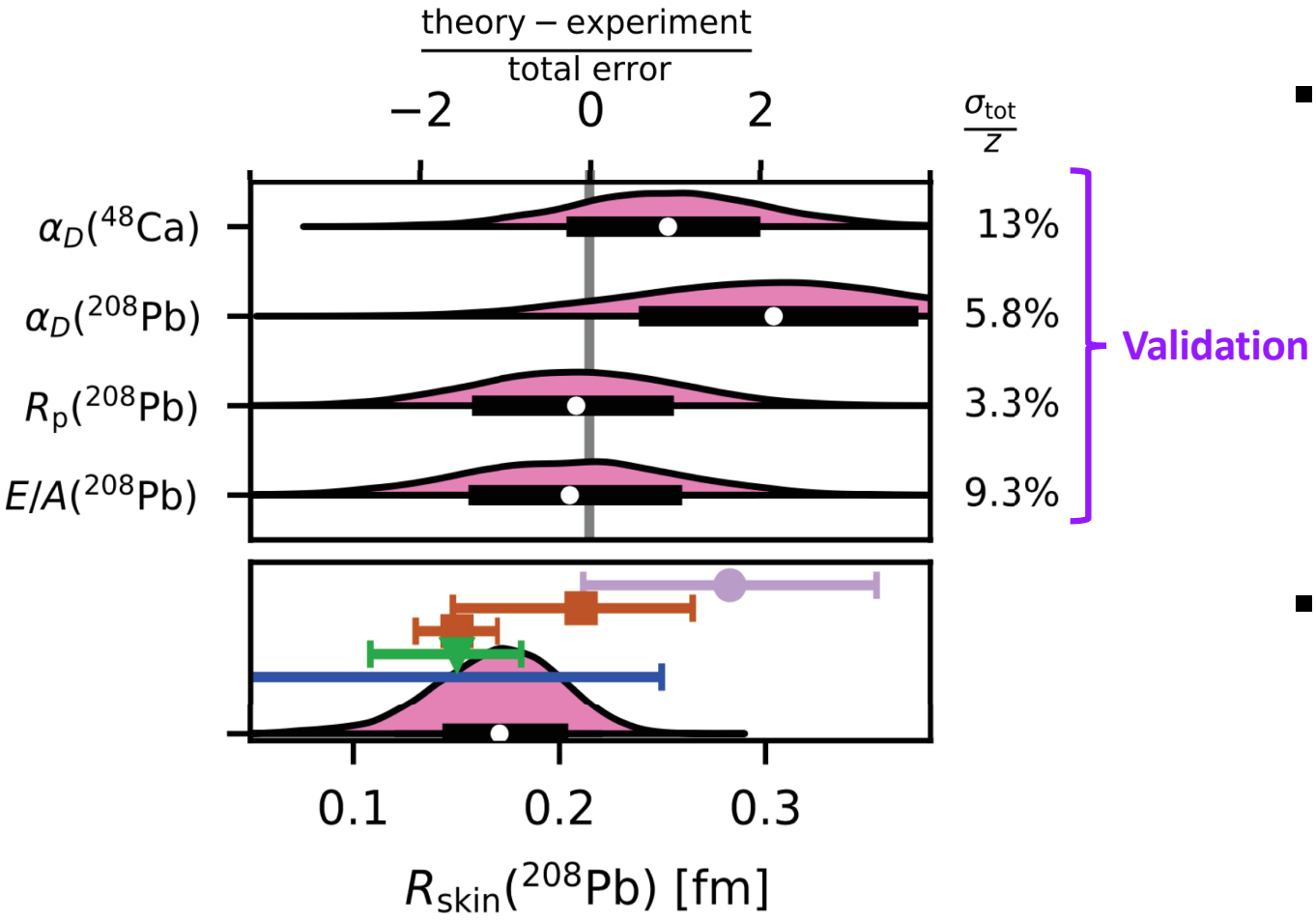
Prediction for 28-O shown as probability distribution where solid lines indicate the 68% and 90% probability density regions

We claim with 98% certainty that 28-O is unbound

Used history matching and performed 10^8 predictions for ground- and excited states of nuclei up to 25-O



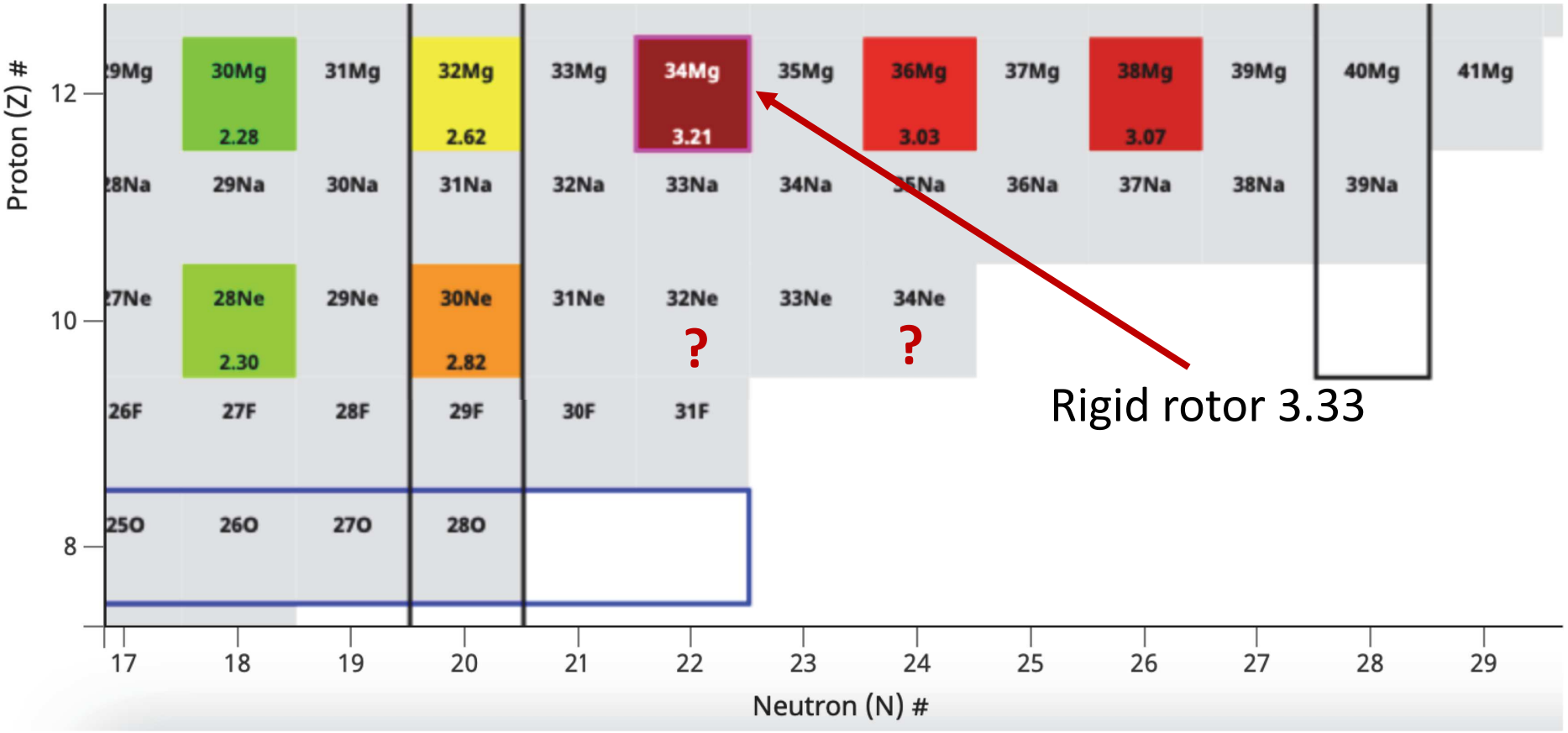
The neutron skin of ^{208}Pb



- Posterior predictive distribution for the neutron skin in ^{208}Pb (experiments: electroweak (purple), hadronic (red), electromagnetic (green), and gravitational waves (blue) probes)
- R_{skin}(208Pb) = 0.14 – 0.20 fm (68% credible interval) exhibits a mild tension with the value extracted from PREX-2

Baishan Hu, Weiguang Jiang, Takayuki Miyagi, Zhonghao Sun, et al Nature Physics (2022)

What drives deformation in atomic nuclei?



Andreas Ekström, Christian Forssén, G. Hagen, G. R. Jansen, T. Papenbrock, Z. H. Sun, arXiv:2305.06955 (2023)

Symmetry restored coupled-cluster theory

Projection after variation (PAV): $$E^{(J)} = \frac{\langle\widetilde{\Psi}|P_J H|\Psi\rangle}{\langle\widetilde{\Psi}|P_J|\Psi\rangle}$$

Right state is parametrized: $|\Psi\rangle = e^T|\Phi_0\rangle$

Left state is parametrized differently:

$\langle\widetilde{\Psi}| = \langle\Phi_0|(1+\Lambda)e^{-T}$ or $\langle\widetilde{\Psi}| = \langle\Phi_0|$ or $\langle\widetilde{\Psi}| = \langle\Psi|$

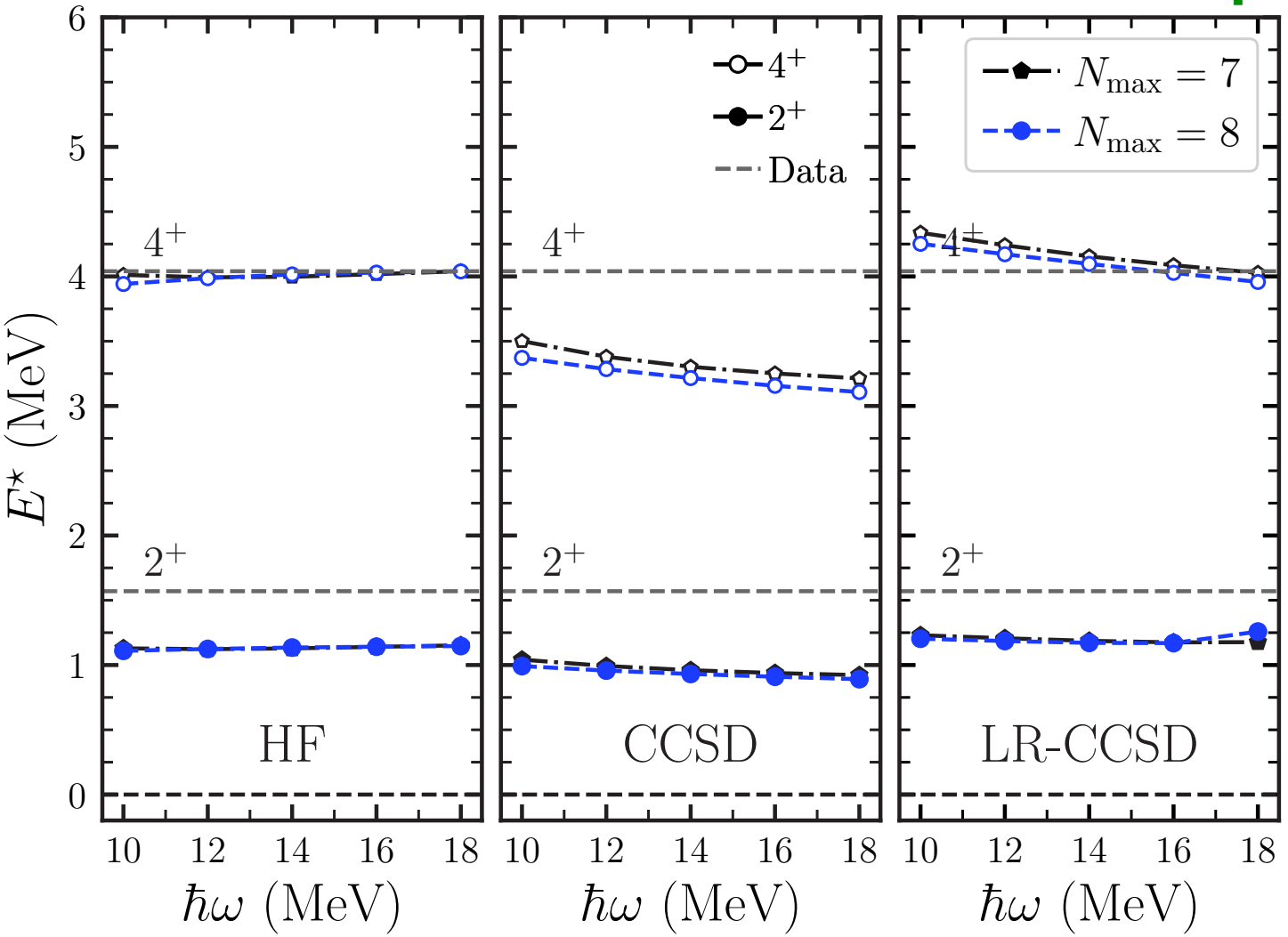
Bi-variational Naïve Hermitian

Image credit: Wikimedia Commons

For axial symmetry around the z-axis the rotation operator is:

$$R(\beta) \equiv e^{i\beta J_y}$$

Projected CCSD with NNLO$_{opt}$ in ^{20}Ne



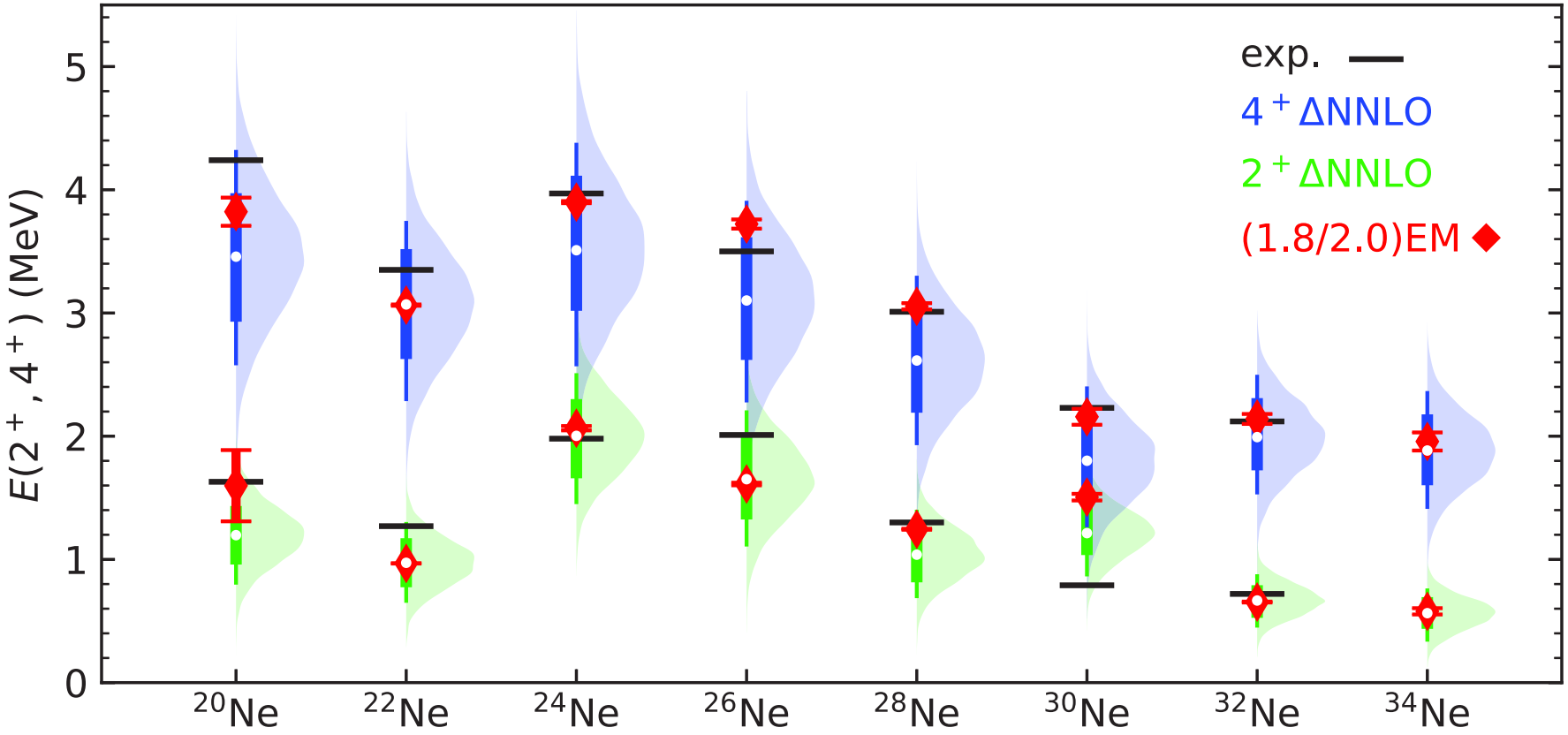
Benchmarks from SA-NCSM
[Dytrych, Launey et al. (2020)]

Andreas Ekström, Christian Forssén, G. Hagen, G. R. Jansen, T. Papenbrock, Z. H. Sun, arXiv:2305.06955 (2023)

Neon iseotopes: Inclusion of three-body forces and more accurate left state

Rotational structure of neutron-rich neon isotopes in good agreement with data

For inclusion of three-nucleon forces we follow Mikael Frosini et al, Eur. Phys. J. A 57 (2021)



Andreas Ekström, Christian Forssén, G. Hagen, G. R. Jansen, T. Papenbrock, Z. H. Sun arXiv:2305.06955 (2023)

Emulating deformation in nuclei

Deformation is long-wave length physics and accurately described at projected Hartree-Fock level

Goal: Construct accurate emulator of projected Hartree-Fock

$$|\phi_\circledcirc\rangle = \sum_i^{n_t} c_i |\phi_i\rangle$$

$$\sum_{ij} \langle\phi_i|H_{\rm HF}(\vec{\alpha}_\circledcirc)|\phi_j\rangle c_j = E_\circledcirc \sum_{ij} \langle\phi_i|\phi_j\rangle c_j$$

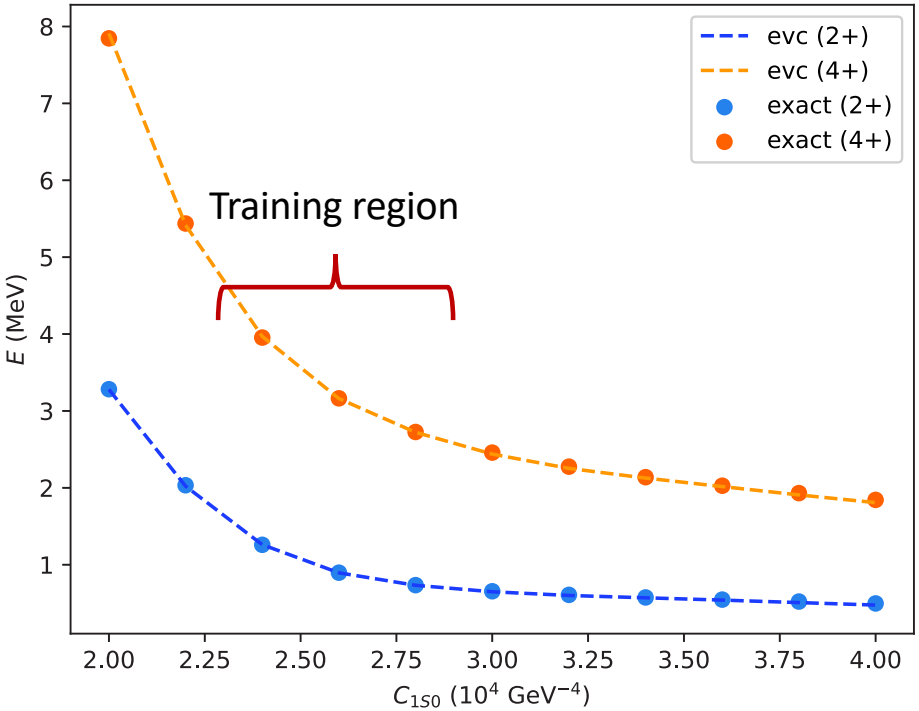
Using Thouless theorem we can evaluate the norm and Hamiltonian kernels between non-orthogonal Hartree-Fock states

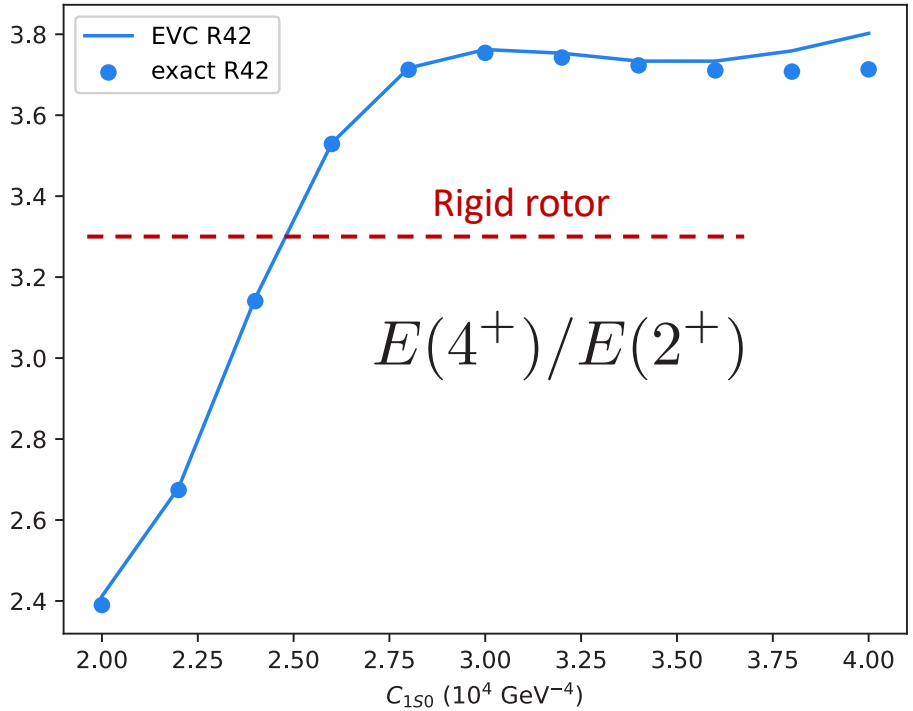
The target rotational states:

$$E^{(J)}_\circledcirc = \frac{\langle\phi_\circledcirc|P_J H(\vec{\alpha}_\circledcirc)|\phi_\circledcirc\rangle}{\langle\phi_\circledcirc|P_J|\phi_\circledcirc\rangle}$$

Emulating rotational structure of ^{20}Ne

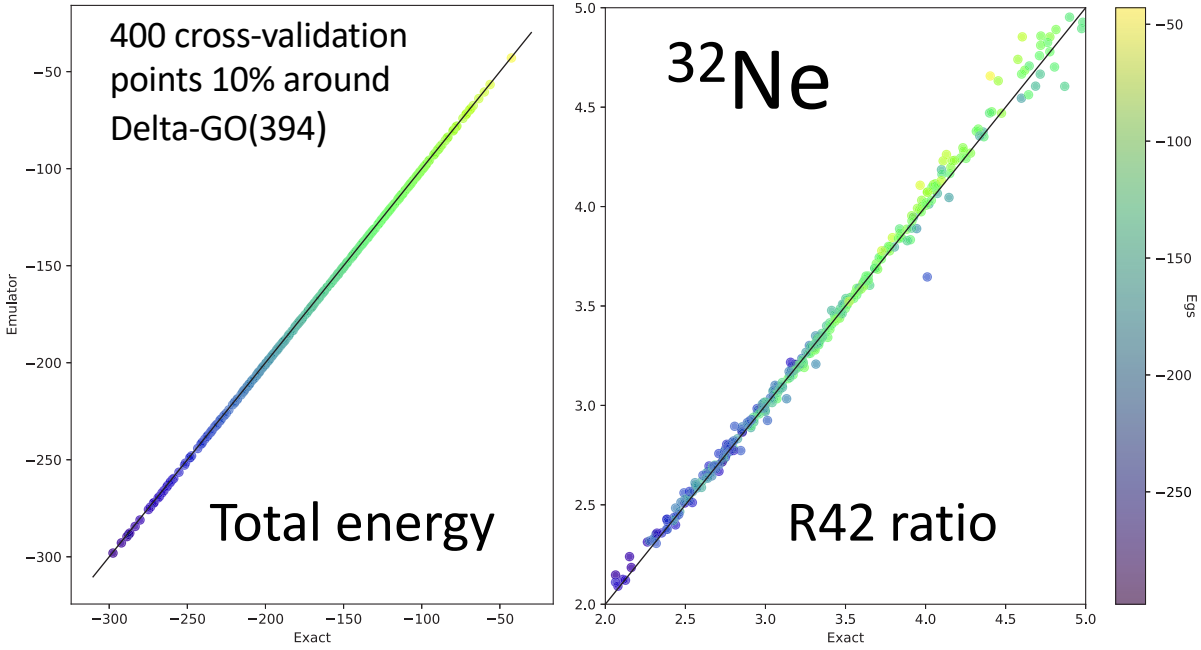
Varying only one parameter: $C_{^1S_0}$



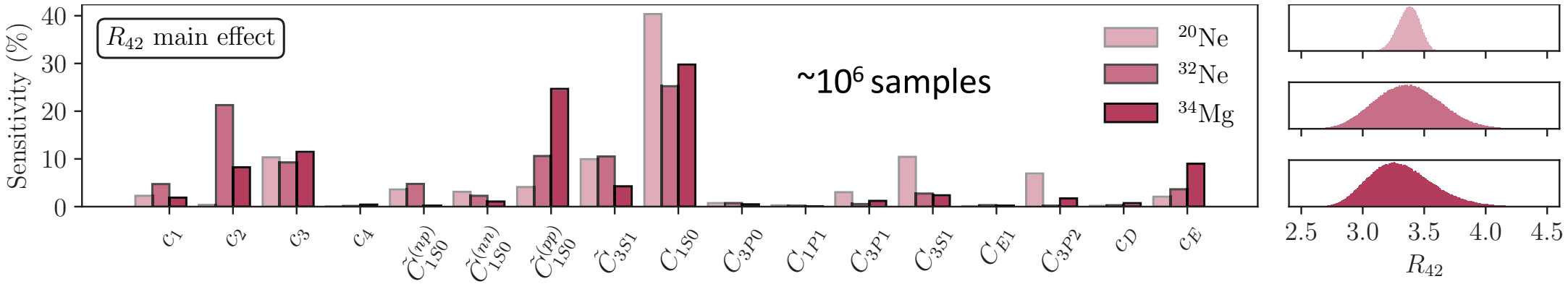


Andreas Ekström, Christian Forssén, G. Hagen, G. R. Jansen, T. Papenbrock, Z. H. Sun, arXiv:2305.06955 (2023)

Linking deformation to nuclear forces

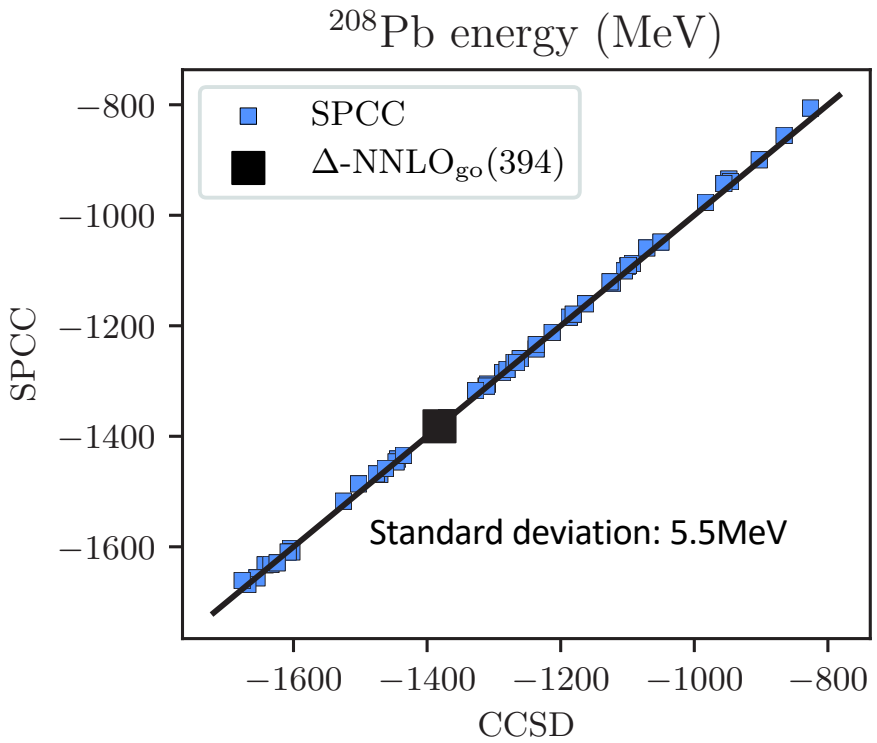


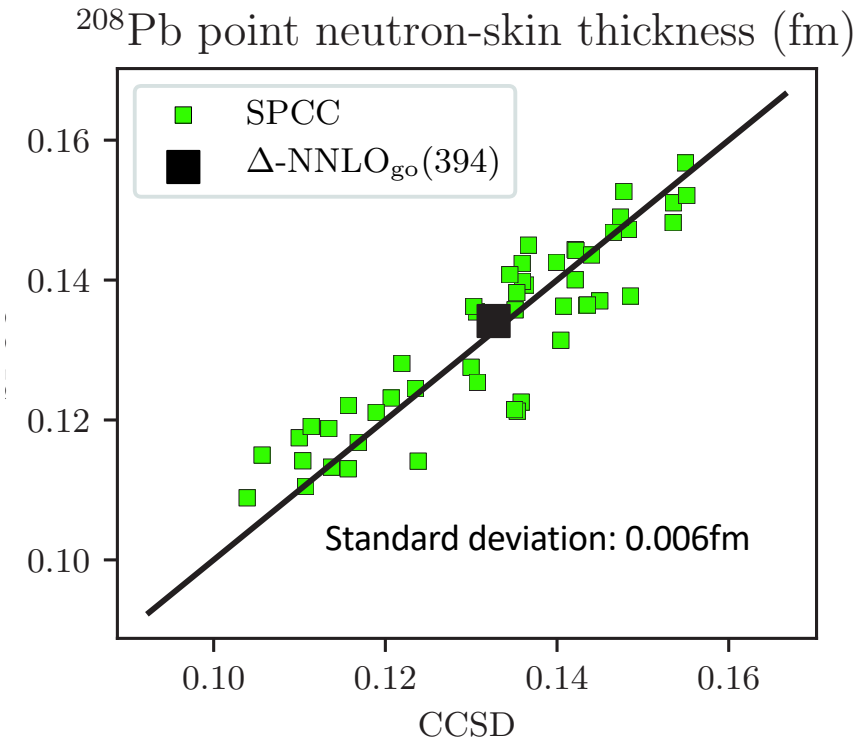
- Constructed emulators of projected HF using 68 training vectors
- Training points obtained by using Latin Hypercube sampling within 20% of original low-energy constants
- Deformation is mainly driven by the pion-nucleon coupling LEC c3 and C1S0
- Short-range three-nucleon forces and the pion-nucleon coupling c2 appear to have increased deformation sensitivities towards the driplines



Emulating heavy nuclei and nuclear matter

- For heavy nuclei/nuclear matter we observe that SPCC can produce spurious states when the number of training vectors increase
- Using ~10 training vectors we constructed an emulator for the computation of the neutron-skin and ground-state energy of 208-Pb
- How can we eliminate/mitigate the occurrence of spurious states?





Removing spurious states

Physical SPCC vector

$$|\Psi(\vec{\alpha}_\circledcirc)\rangle = e^{T(\vec{\alpha}_\circledcirc))}|\Phi_0\rangle \approx \sum_{i=1}^{N_{\rm sub}} c_i^\star e^{T(\vec{\alpha}_i)}|\Phi_0\rangle$$

Coupled-cluster is bi-variational
Arponen Ann. Phys. **151**, 311 (1983)

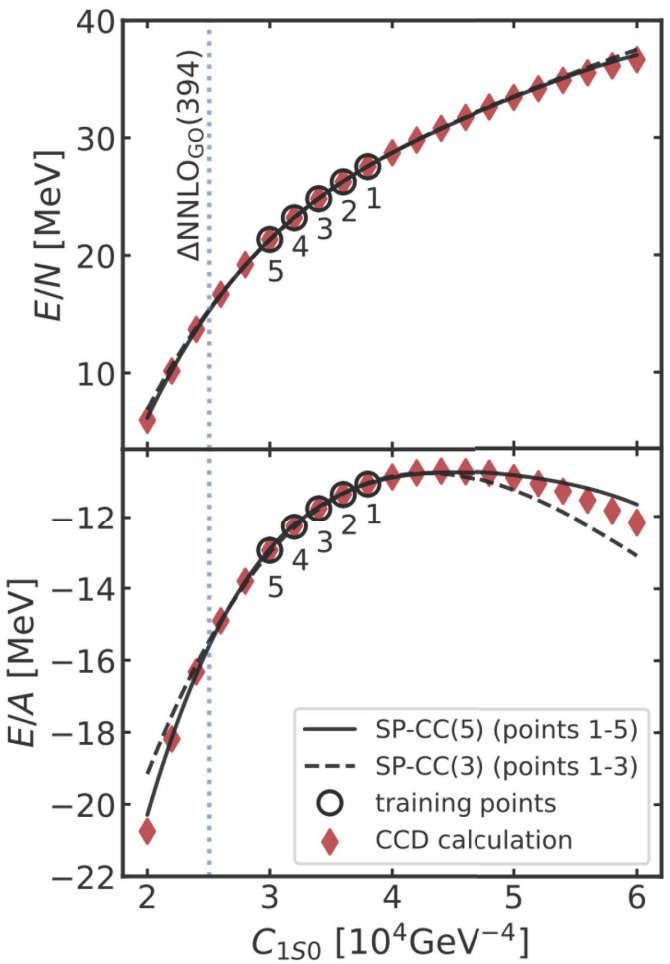
$$\frac{\partial}{\partial \lambda_i}\langle\widetilde{\Psi}(\vec{\alpha}_\circledcirc)|H(\vec{\alpha}_\circledcirc)|\Psi(\vec{\alpha}_\circledcirc)\rangle = 0$$

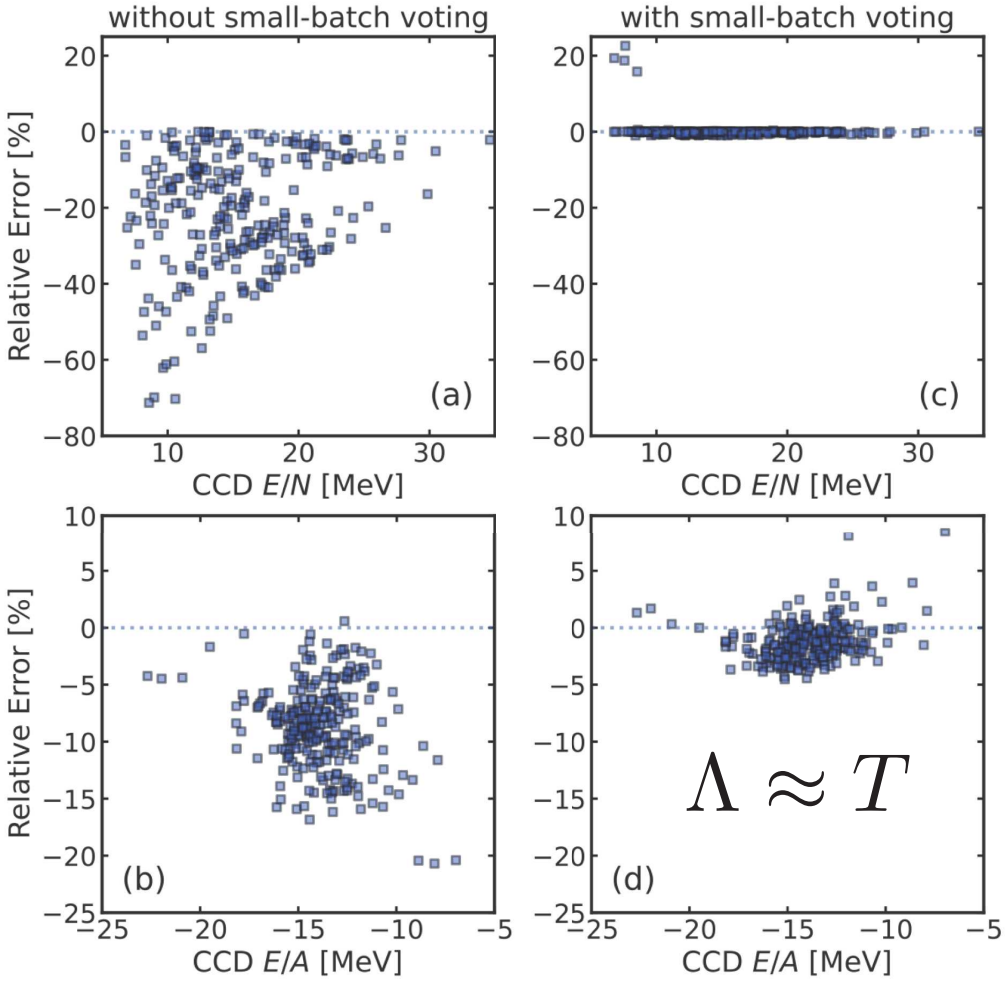
Identify physical state with small batch voting:

- We see that the physical converges rapidly training points
- Physical state is stable with respect to removing small portions of training vectors
- Compare the SPCC spectra for different sized sub-spaces
- Every repeated eigenvalue gets a vote, and the state with most votes is chosen

W. G. Jiang, C. Forssén, T. Djärv, G. Hagen, arXiv:2212.13216; arXiv:2212.13203 (2022)

Emulating nuclear matter





W. G. Jiang, C. Forssén, T. Djärv, G. Hagen, arXiv:2212.13216; arXiv:2212.13203 (2022)

Summary

- Emulators, history matching, and Bayesian inference allow us to make quantified predictions and link properties of nuclei to the underlying microscopic interactions
  - 28-O is unbound with 98% certainty
  - Neutron skin of ^{208}Pb in mild tension with PREX-2
- Developed emulators for projected Hartree-Fock
  - A few low-energy impacts deformation most
  - Even-even nuclei with symmetry projection: ^{34}Ne is found to be as rotational as ^{32}Ne and ^{34}Mg
- Small batch voting removes spurious states for nuclear matter emulators

Thank you for your attention!

SP-CC Hamiltonians occupy very little disk space, and can easily be shared within the nuclear community.

We are happy to share matrix elements, python codes, etc..