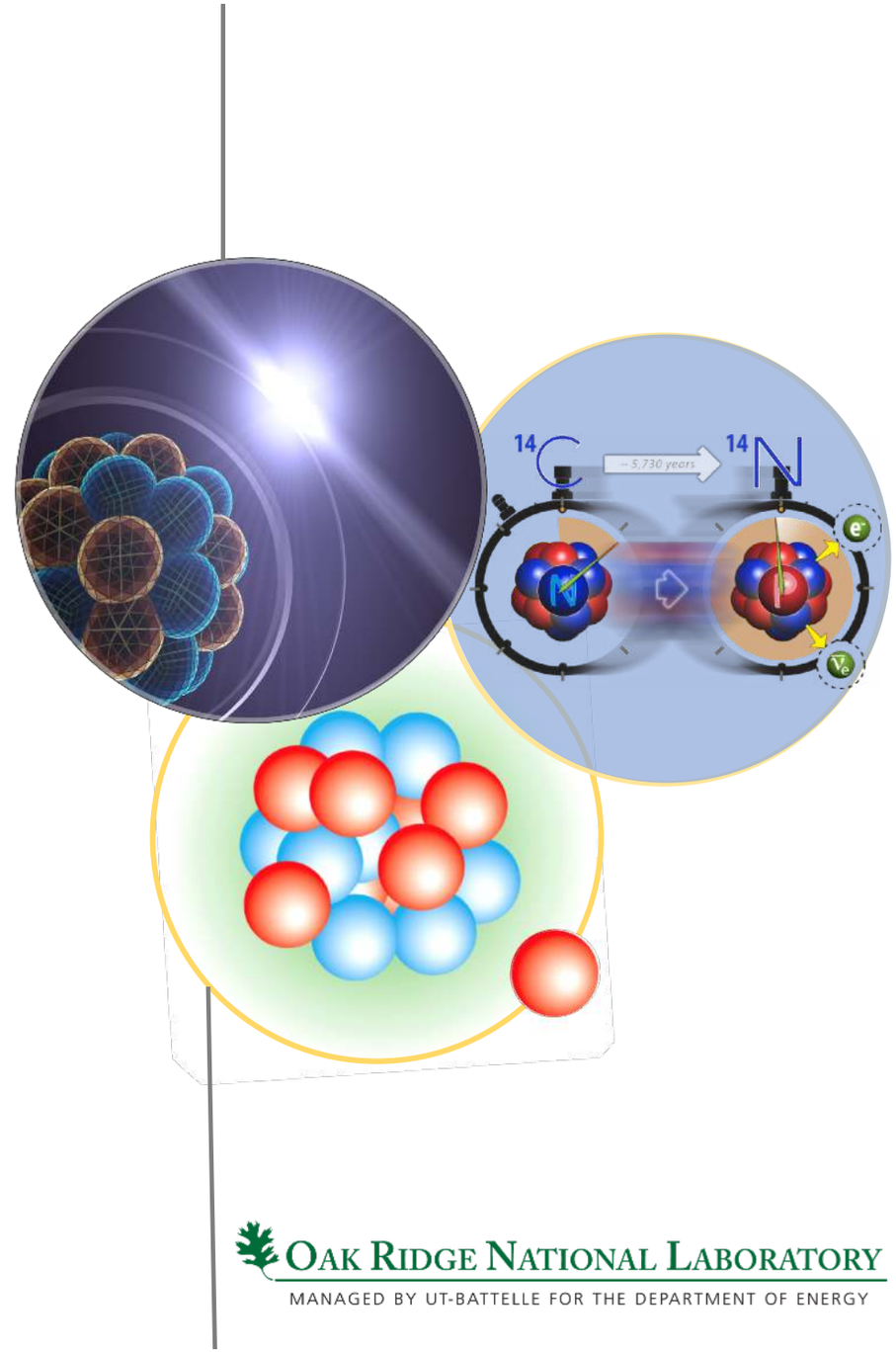
Advances in coupled-cluster computations of nuclei

Gaute Hagen
Oak Ridge National Laboratory

Recent Progress in Many-Body Theories XXI

Chapel Hill, September 14th, 2022



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**, G. R. Jansen, T. Morris, **Z. H. Sun**, T. Papenbrock

@ ANL: S. R. Stroberg

@ CEA/Saclay: T. Duguet

@ Chalmers: A. Ekström, C. Forssén, **W. G. Jiang**

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

@ LANL: **S. Novario**

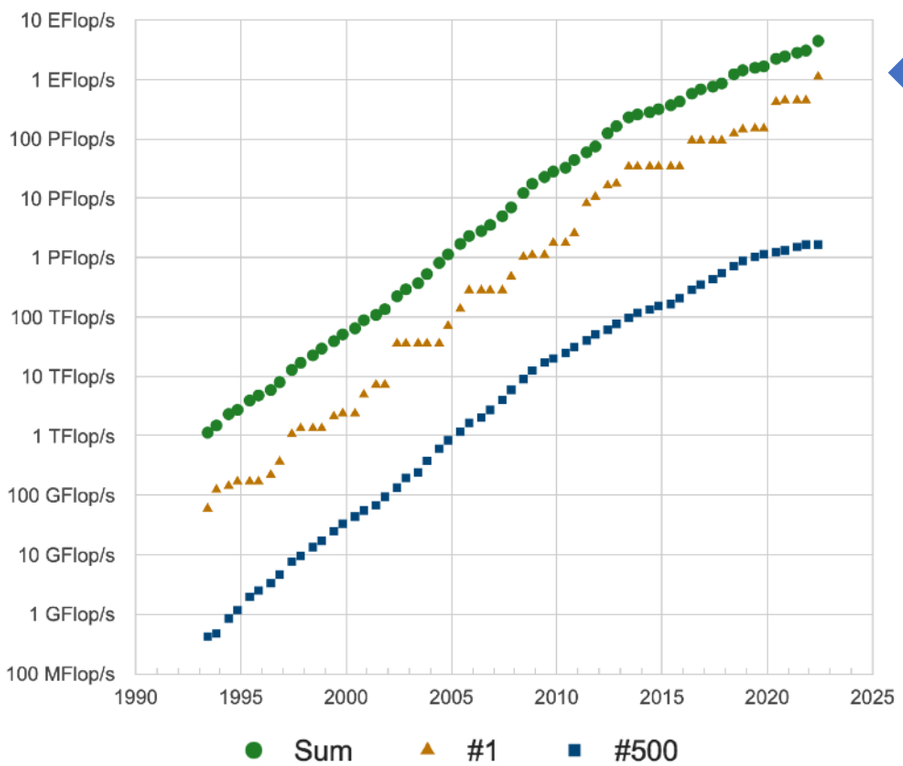
@ TRIUMF: **Baishun Hu**, **P. Gysbers,** J. Holt, P. Navratil

@ TU Darmstadt: **T. Miyagi, A. Tichai**

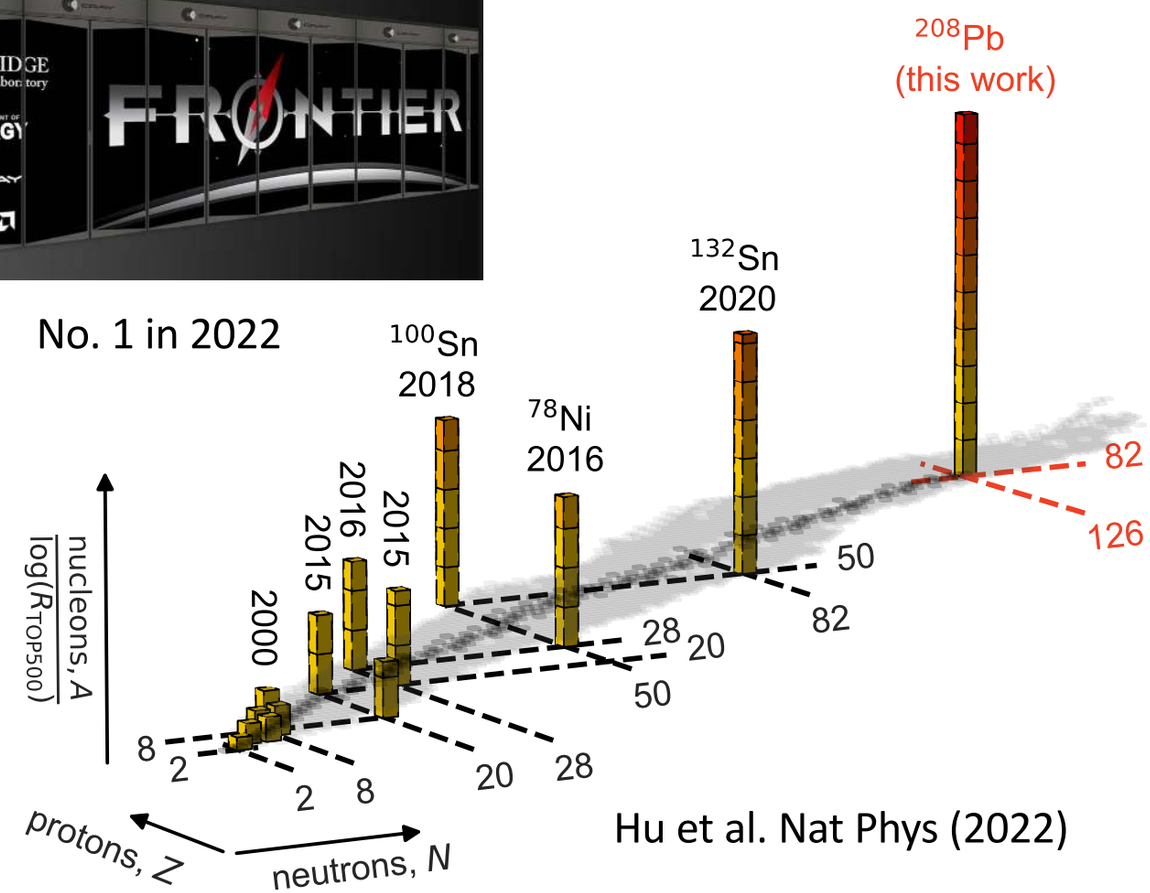
Trend in realistic ab-initio calculations

- Tremendous progress in recent years because of ideas from EFT and the renormalization group
- Computational methods with polynomial cost (coupled clusters 🙂quantum computing 🤔)
- Ever-increasing computer power?

Development with time (top500.org)

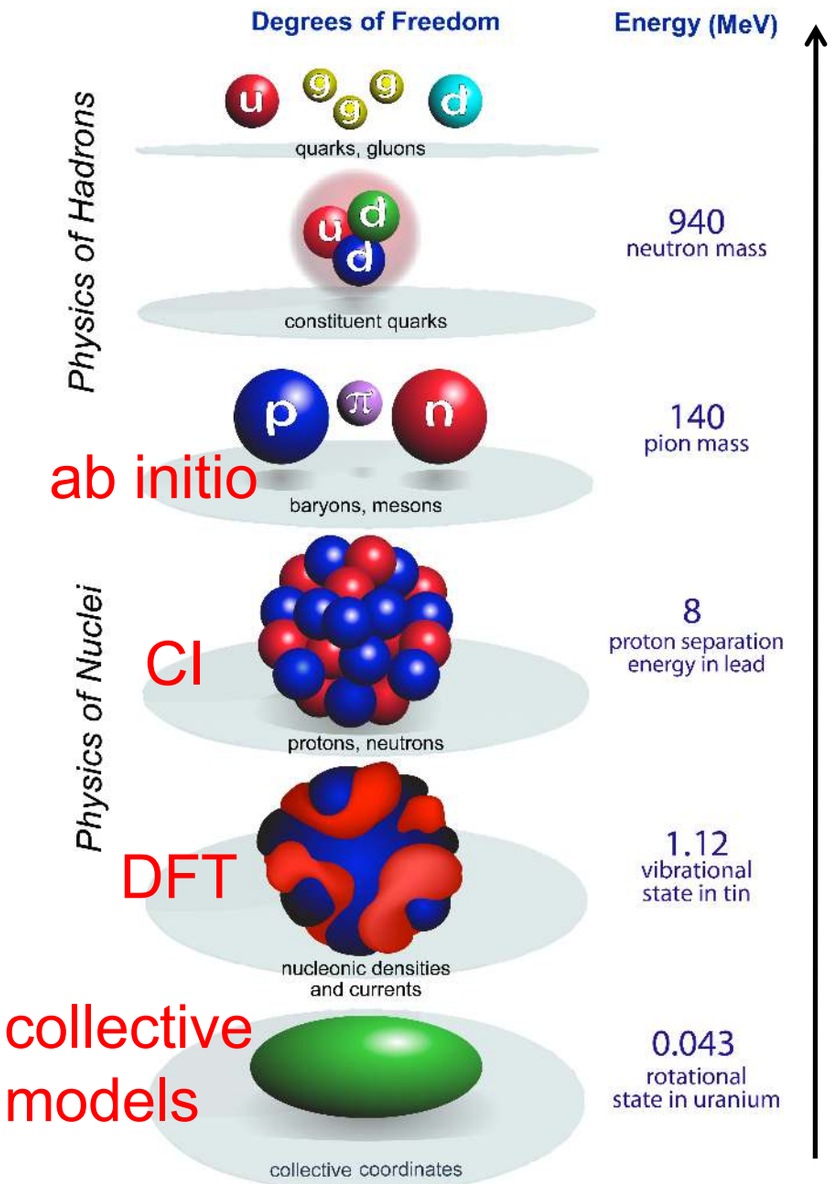


No. 1 in 2022



Hu et al. Nat Phys (2022)

Energy scales and effective field theories



Energy or Resolution

Chiral EFT

Pion-less EFT

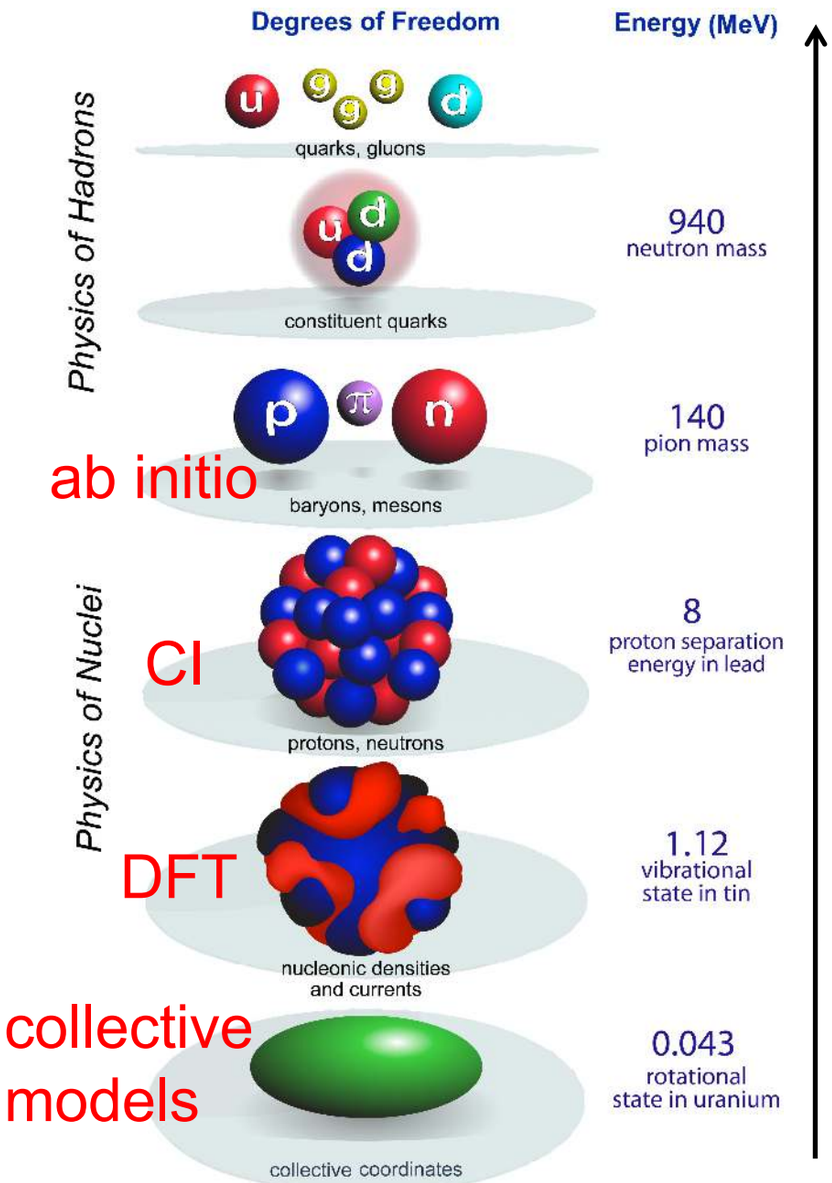
Effective field theories provide us with model independent approaches to atomic nuclei

Key: Separation of scales

Ab-initio low-energy nuclear physics deals with nucleons (and pions) as dynamical degrees of freedom

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

Energy scales and effective field theories



Energy or Resolution

Interactions from chiral EFT

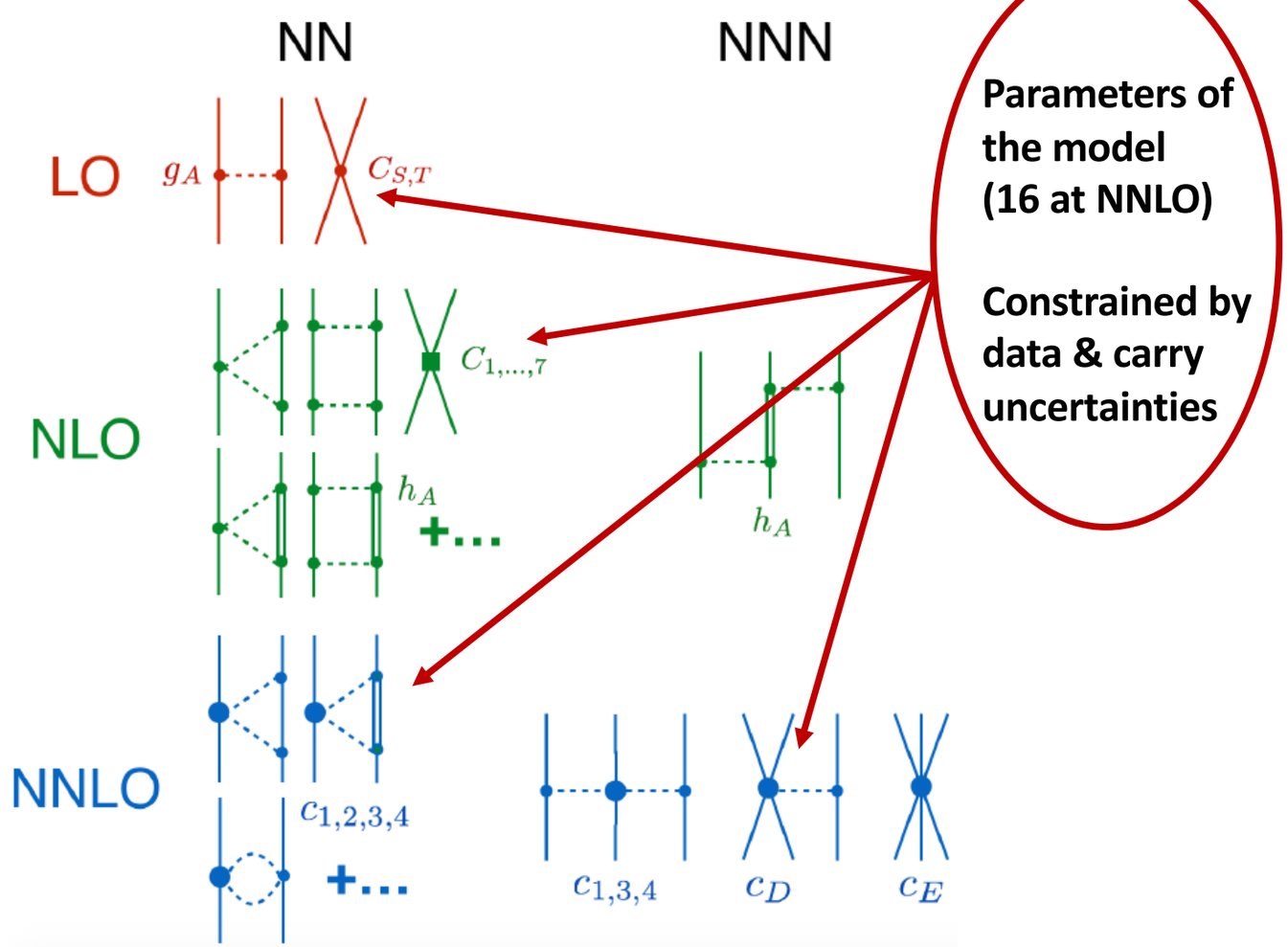
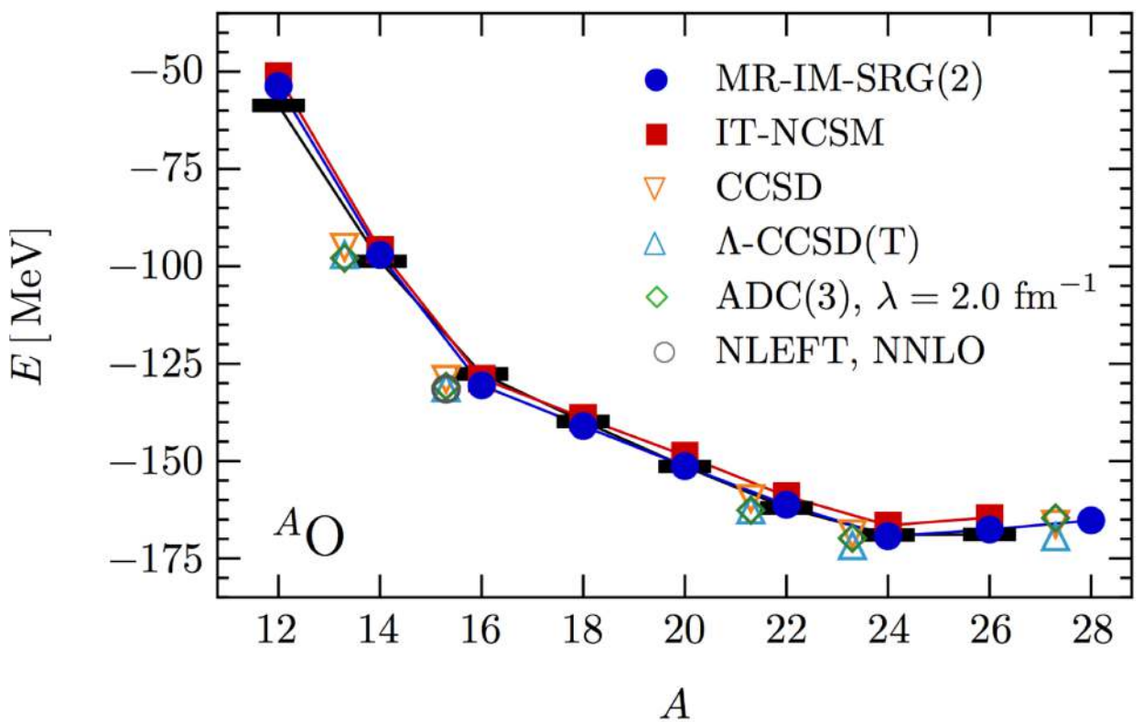


Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

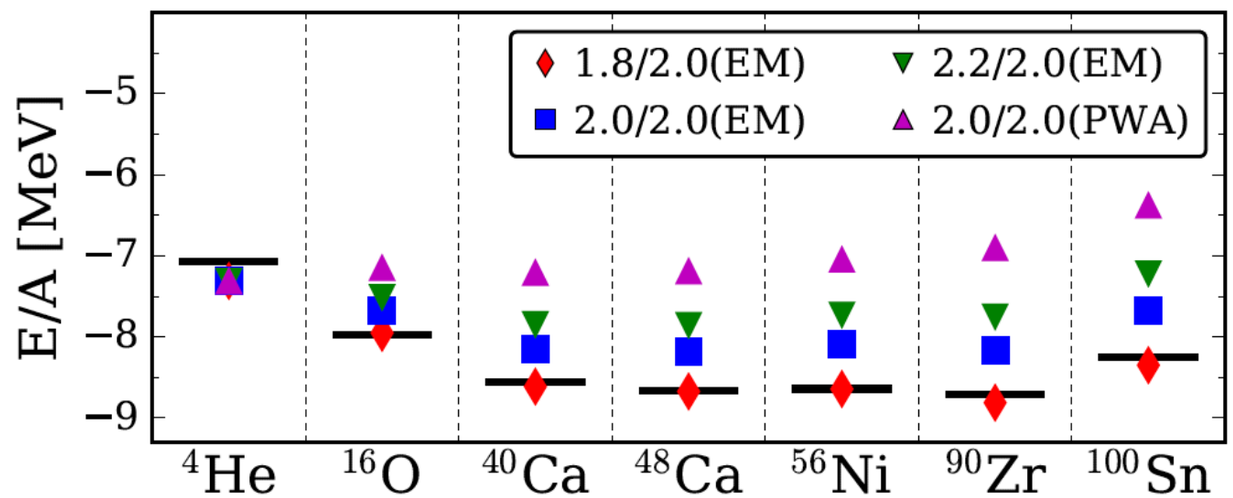
What precision/accuracy can we aim for in ab-initio calculations of nuclei?

Different many-body approaches (CC, IMSRG, SCGF,…) agree with each for binding energies and radii (challenges exist for transitions, isotope shifts, and deformed shapes)



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

Some chiral potentials (models) work better than others



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

How to compute nuclei in an affordable way using interactions from effective field theories

1. Compute Hartree-Fock reference state
   - Nontrivial vacuum state informs us about emergent breaking of symmetries
   - Yields normal-ordered two-body Hamiltonian
2. Include dynamical (extensive) correlations via coupled-cluster theory
   - (or via IMSRG, or Gorkov methods, or Green's functions)
   - Cost increases polynomial with mass number
3. Perform symmetry projections
   - Non-extensive contributions to the energy
   - Often relevant for transition matrix elements
4. Repeat (even-even nuclei for this presentation)

See poster by Pepijn Demol on recent developments on Bogoliubov coupled-cluster

See Thomas Duguet's talk on Friday

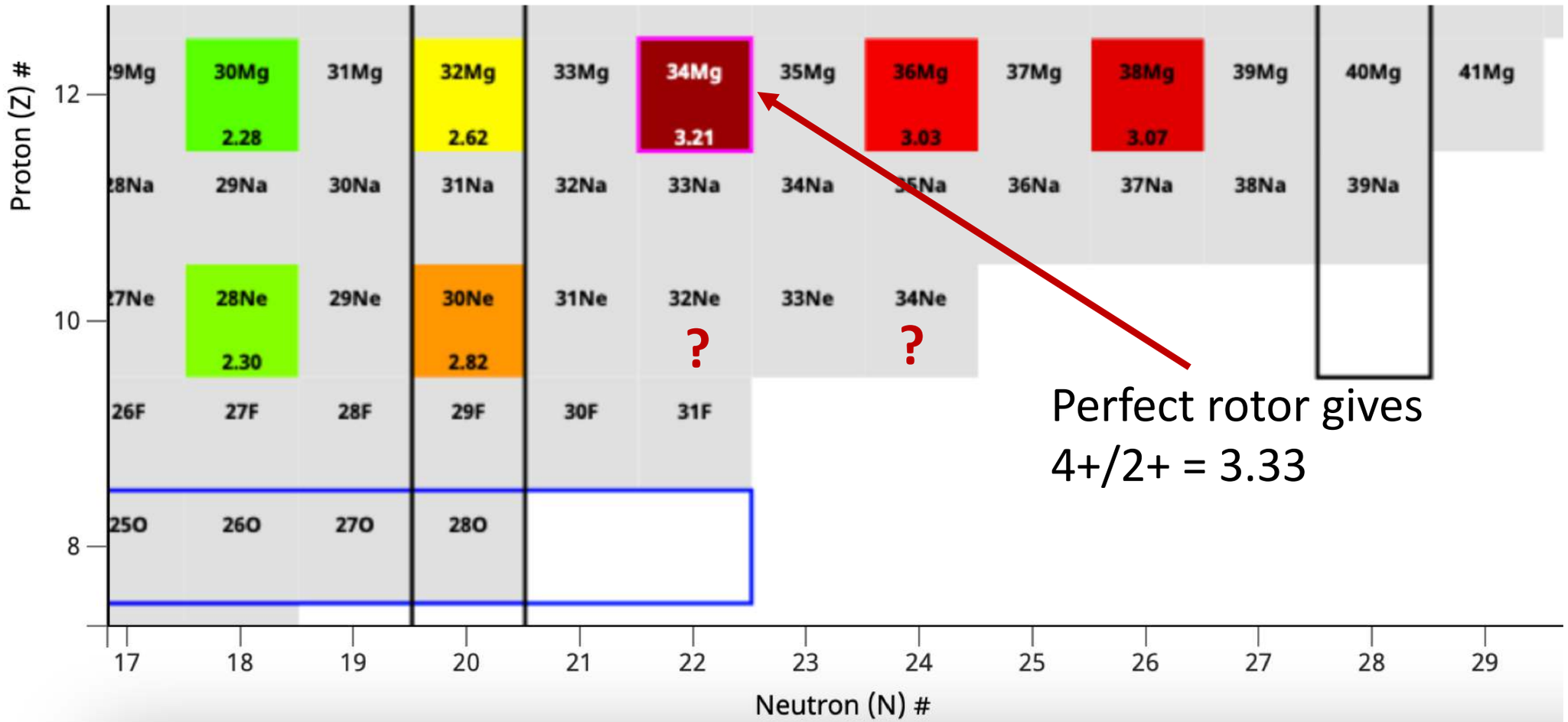
The total energy of a nucleus

Dynamic correlation (large contribution and requires size-extensive methods)

Static correlation (can use non size-extensive methods)

$$E = E_{\mathrm{ref}} + \Delta E_{\mathrm{CCSD}} + \Delta E_{\mathrm{CCSDT-1}} + \delta E$$

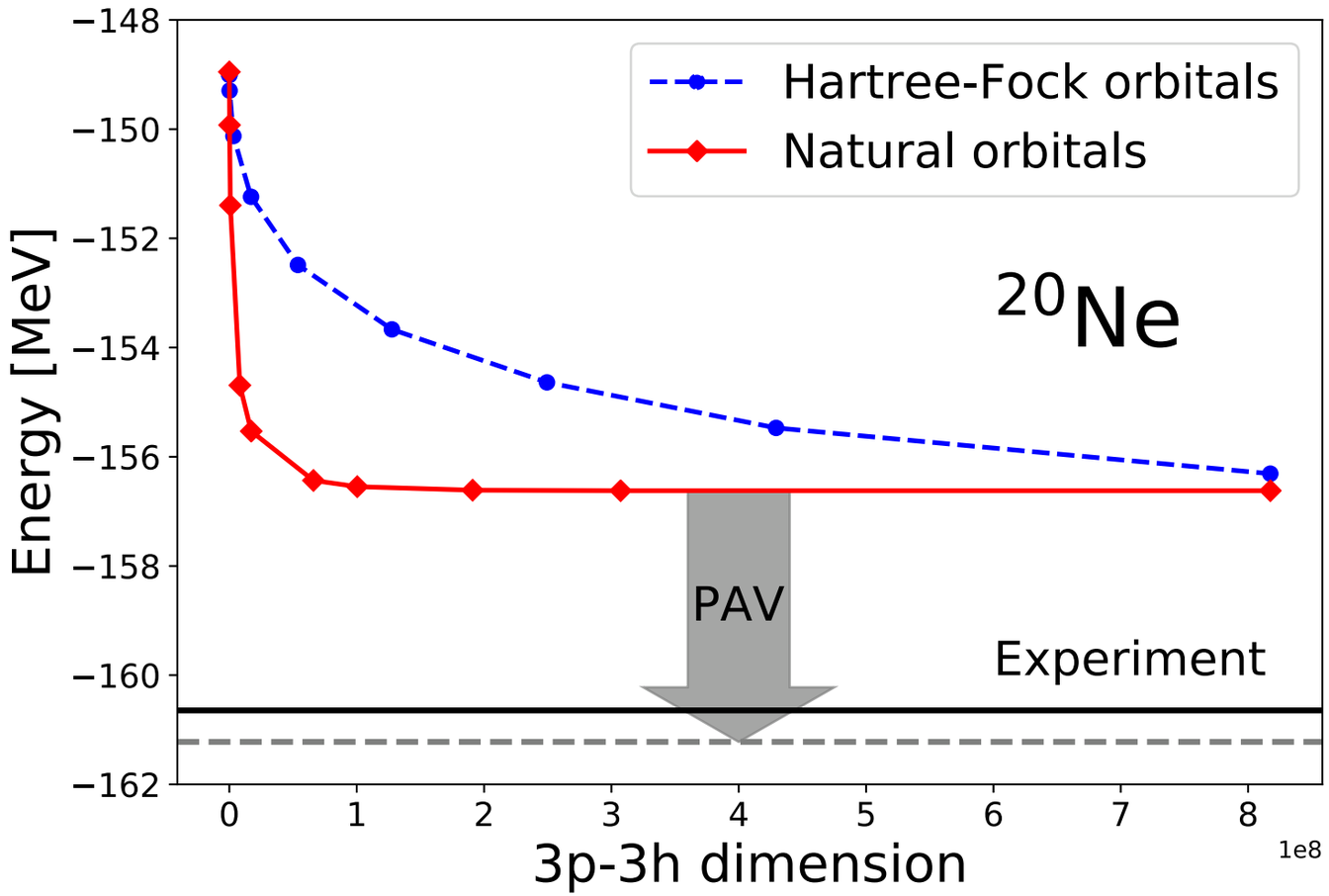
Coupled-cluster computations of deformed nuclei



G. Hagen, S. J. Novario, Z. H. Sun, T. Papenbrock, G. R. Jansen, J. G. Lietz, T. Duguet, A. Tichai Phys. Rev. C 105, 064311 (2022)

S. J. Novario, G. Hagen, G. R. Jansen, T. Papenbrock, Phys. Rev. C 102, 051303 (2020)

Coupled-cluster computations of deformed nuclei – natural orbitals

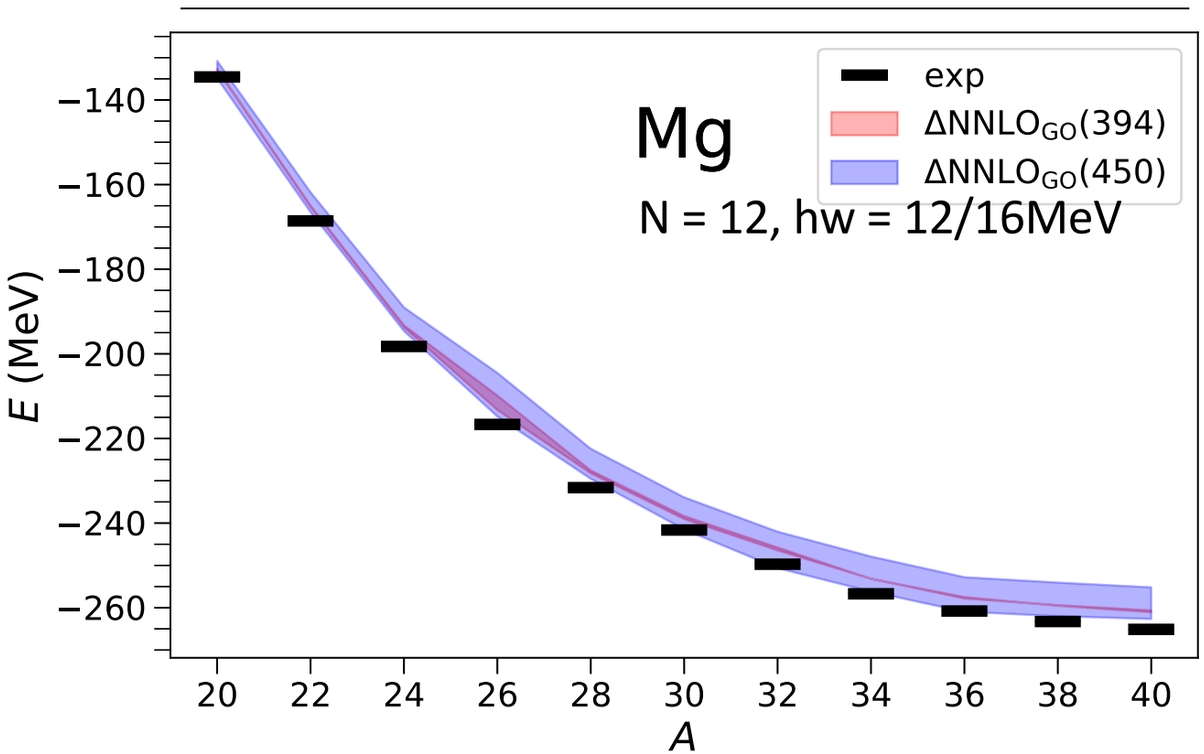


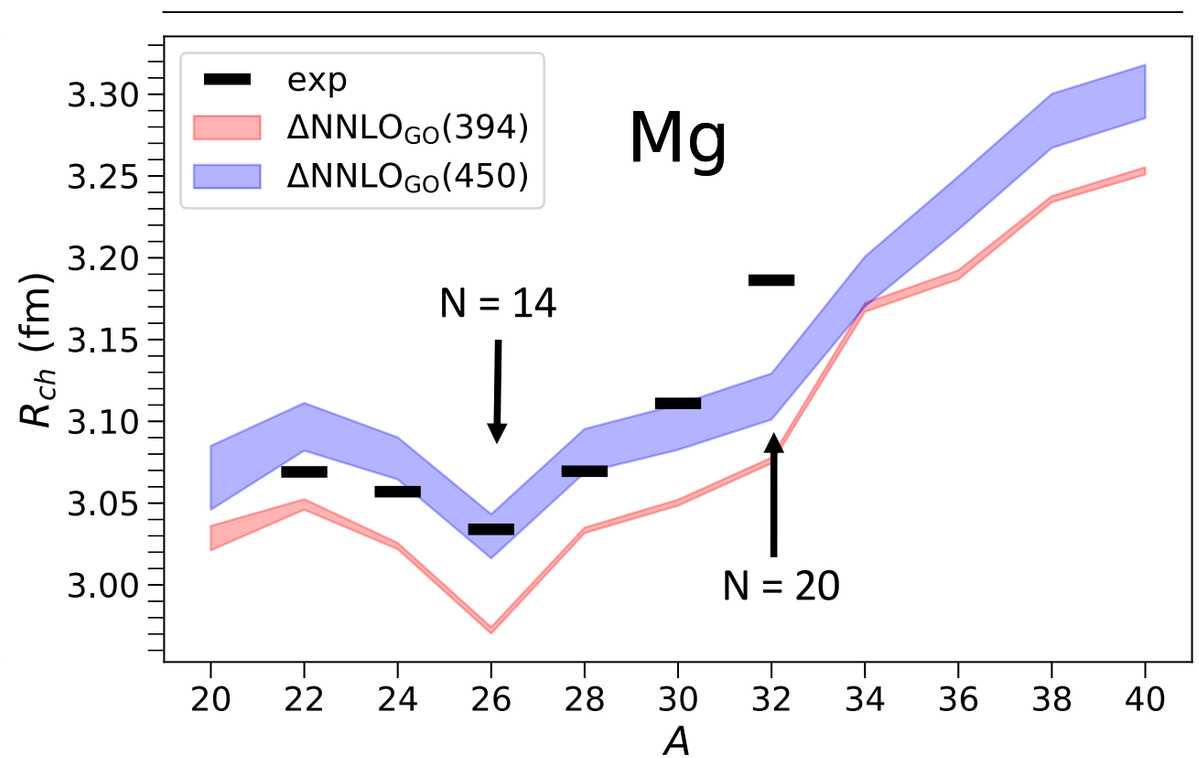
- Coupled-cluster calculations from axially symmetric reference states
- Natural orbitals from many-body perturbation theory [A. Tichai, et al PRC (2019)] yields rapid convergence with respect 3p3h excitations in CCSDT-1
- Hartree-Fock with projection after variation (PAV) gives upper bound on the energy gain from symmetry restoration

S. J. Novario, G. Hagen, G. R. Jansen, T. Papenbrock, Phys. Rev. C 102, 051303 (2020)

Computations of magnesium isotopes

- Symmetry broken reference states allow us to address open-shell/deformed nuclei
- Dripline predicted at ^{40}Mg – continuum may impact the location of the dripline
- Charge radii predicts shell closures at N = 8, N = 14, and at N = 20
- The bands indicate uncertainties from model-space truncations





S. J. Novario, G. Hagen, G. R. Jansen, T. Papenbrock, Phys. Rev. C 102, 051303 (2020)

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 as:

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

Bi-variational | Naïve | Hermitian

Image credit: Wikimedia Commons

The total energy of a nucleus

Dynamic correlation (large contribution and requires size-extensive methods)

Static correlation (can use non size-extensive methods)

$$E = E_{\mathrm{ref}} + \Delta E_{\mathrm{CCSD}} + \Delta E_{\mathrm{CCSDT-1}} + \delta E$$

Technical aspects

G. Hagen, S. J. Novario, Z. H. Sun, T. Papenbrock, G. R. Jansen, J. G. Lietz, T. Duguet, A. Tichai Phys. Rev. C 105, 064311 (2022)

Projected energies

$$E^{(J)} = \frac{\int_0^\pi \mathrm{d}\beta \sin\beta d^J_{00}(\beta)\mathcal{H}(\beta)}{\int_0^\pi \mathrm{d}\beta \sin\beta d^J_{00}(\beta)\mathcal{N}(\beta)}$$

We follow:

- Qiu, Henderson, Scuseria, …
- Tsuchimochi & Ten'no
- Duguet, …

Coupled cluster kernels (naïve ansatz)

$$\mathcal{N}(\beta) = \langle\Phi|R(\beta)|\Phi\rangle\langle\Phi|e^V e^T|\Phi\rangle\,,$$
$$\mathcal{H}(\beta) = \langle\Phi|R(\beta)|\Phi\rangle\langle\Phi|e^V H e^T|\Phi\rangle$$

Disentangled formalism

$$e^V e^T|\Phi\rangle \equiv e^{W_0+W_1+W_2+\cdots}|\Phi\rangle$$

Hermitian kernels

$$\mathcal{N}_H(\beta) \equiv \langle\Psi|R(\beta)|\Psi\rangle\,,$$
$$\mathcal{H}_H(\beta) \equiv \langle\Psi|R(\beta)H|\Psi\rangle$$

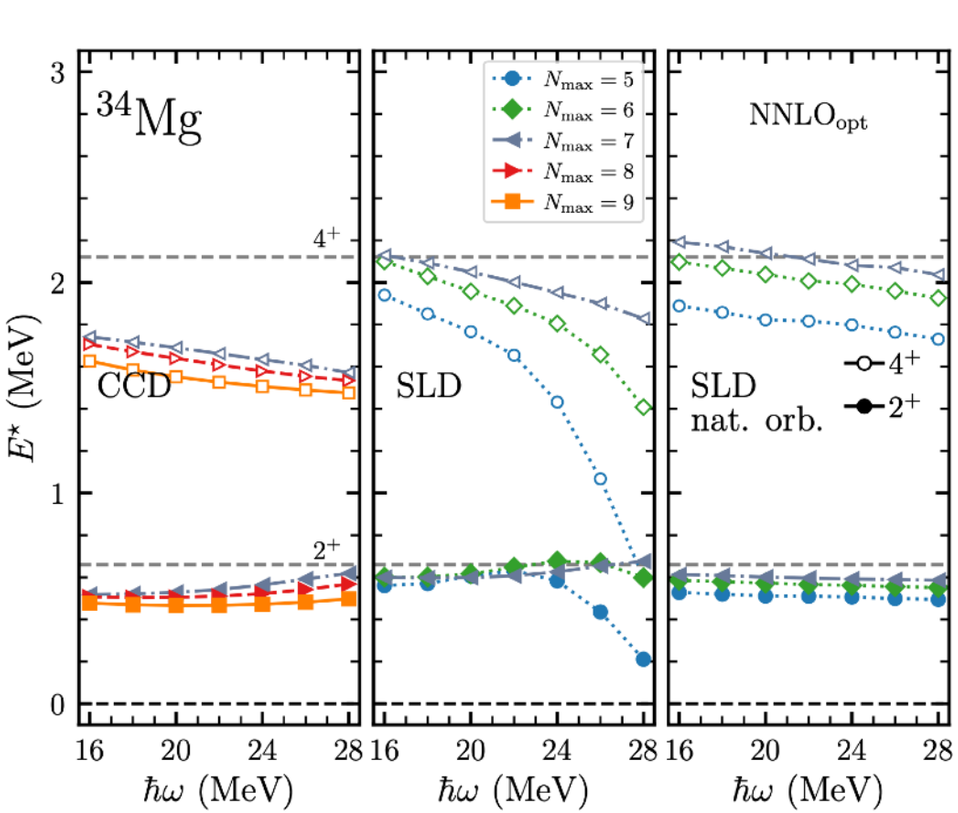
$$|\Psi_{\mathrm{SQD}}\rangle \equiv e^{T_1}\left(1 + T_2 + \frac{1}{2}T_2^2\right)|\Phi\rangle$$

$$|\Psi_{\mathrm{SLD}}\rangle \equiv e^{T_1}\left(1 + T_2\right)|\Phi\rangle$$

Rotational bands from projected coupled-cluster

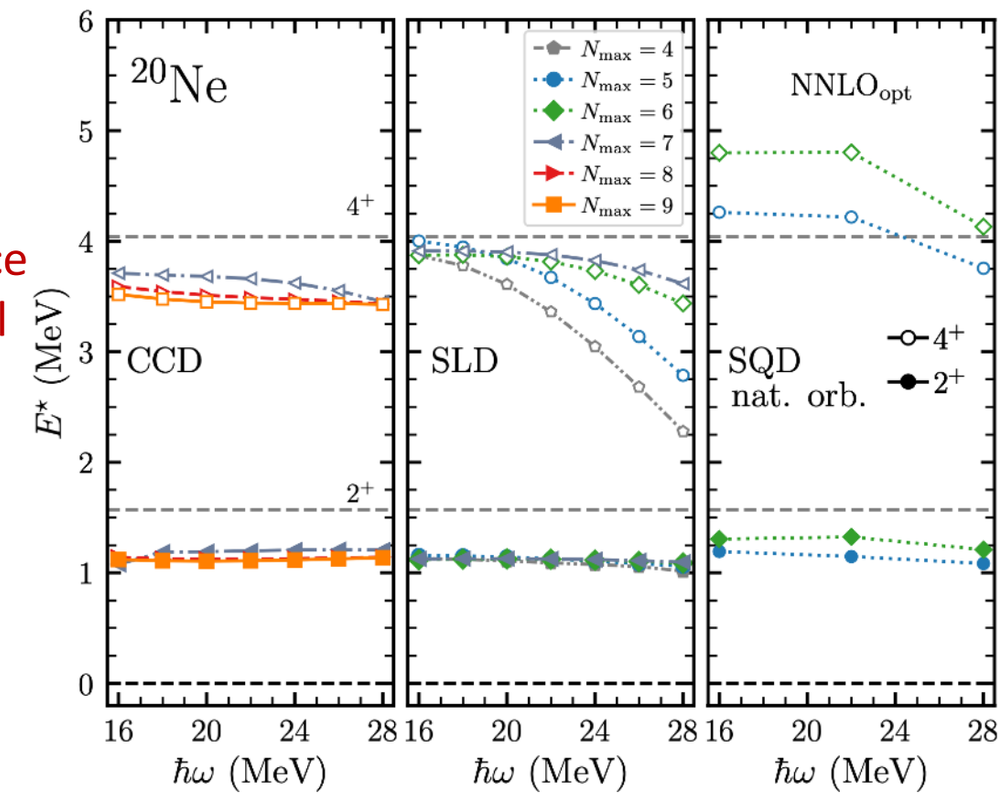
G. Hagen, S. J. Novario, Z. H. Sun, T. Papenbrock, G. R. Jansen, J. G. Lietz, T. Duguet, A. Tichai Phys. Rev. C 105, 064311 (2022)

CCD spectra a bit too compressed due to approximate left state



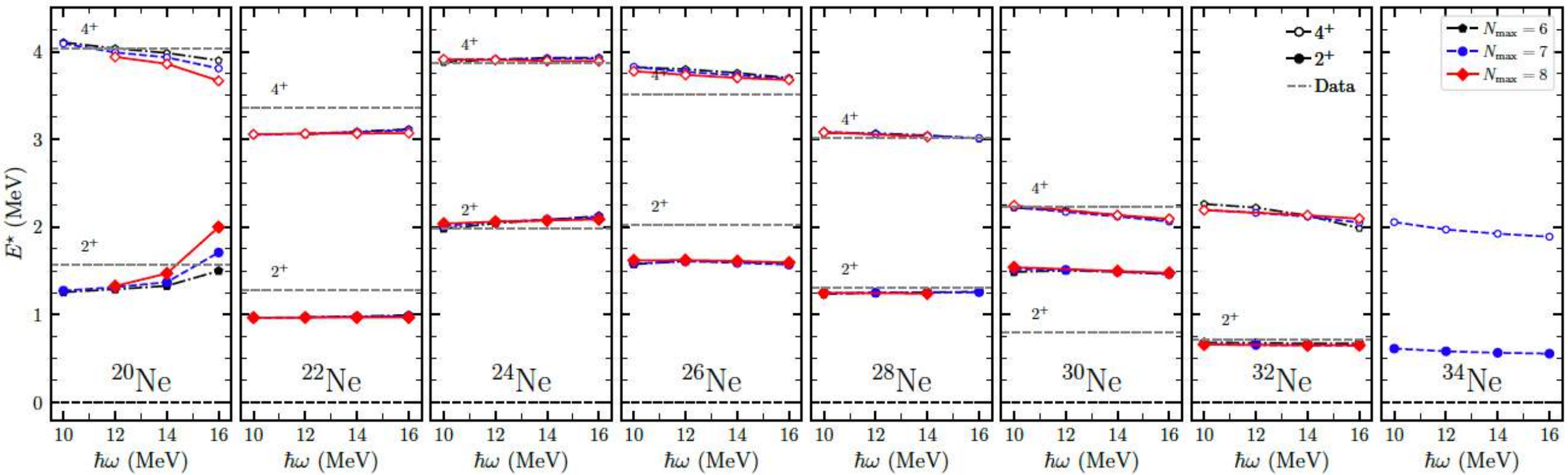
Reproduce rotational structure of ^{34}Mg

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



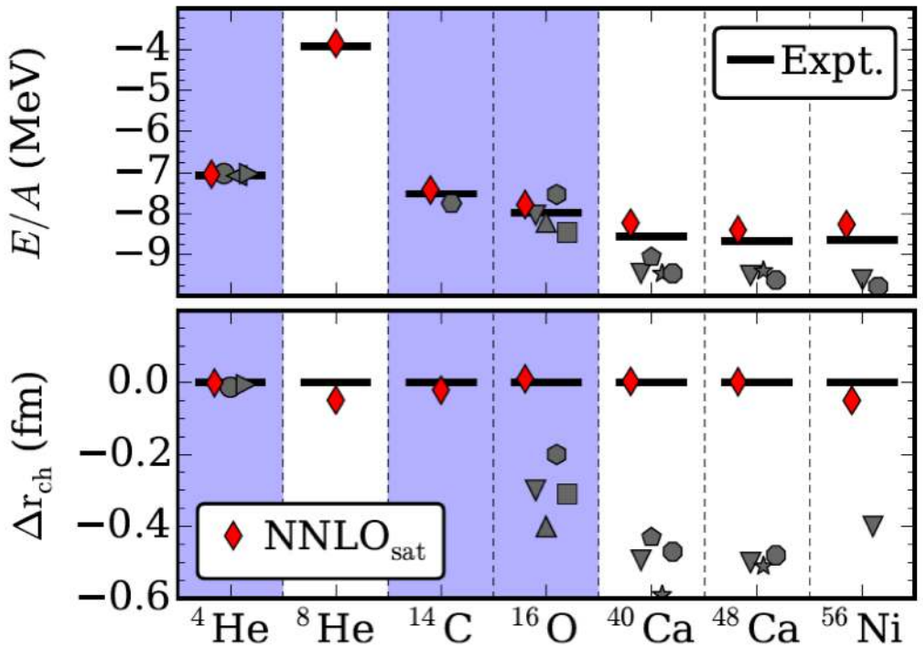
Neon isotopes: Inclusion of three-body forces and more accurate left state

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)

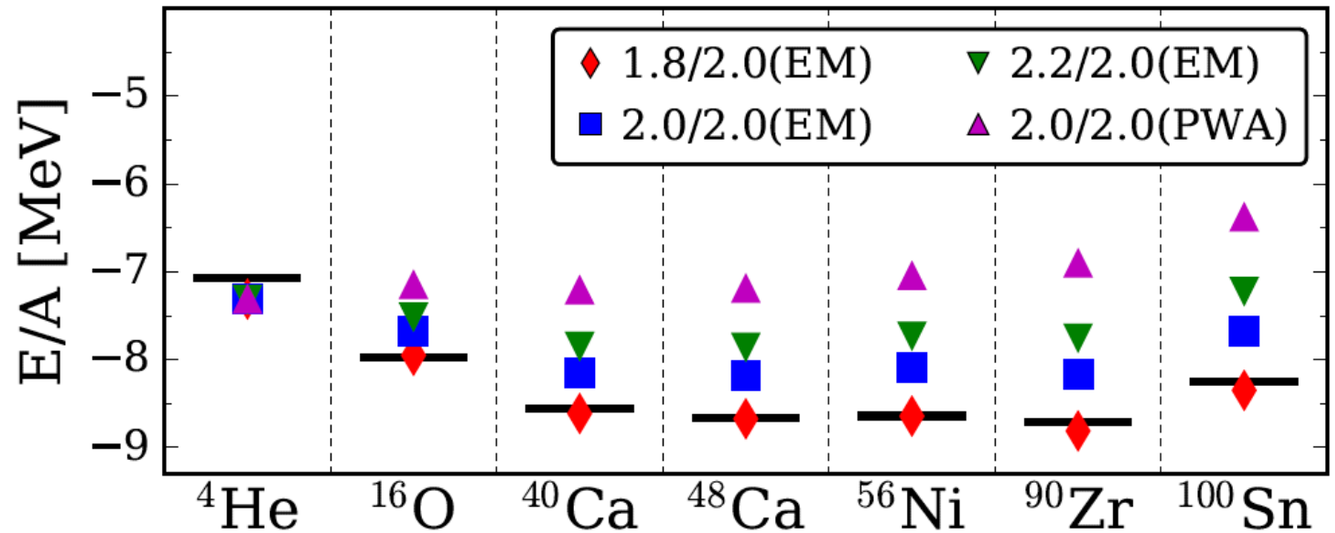


Interaction 1.8/2.0(EM) from Hebeler et al (2012) over-emphasizes *N=20* shell closure
^{32,34}Ne are as rotational as ^{34}Mg

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 the radius and binding energy of 16-O

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.

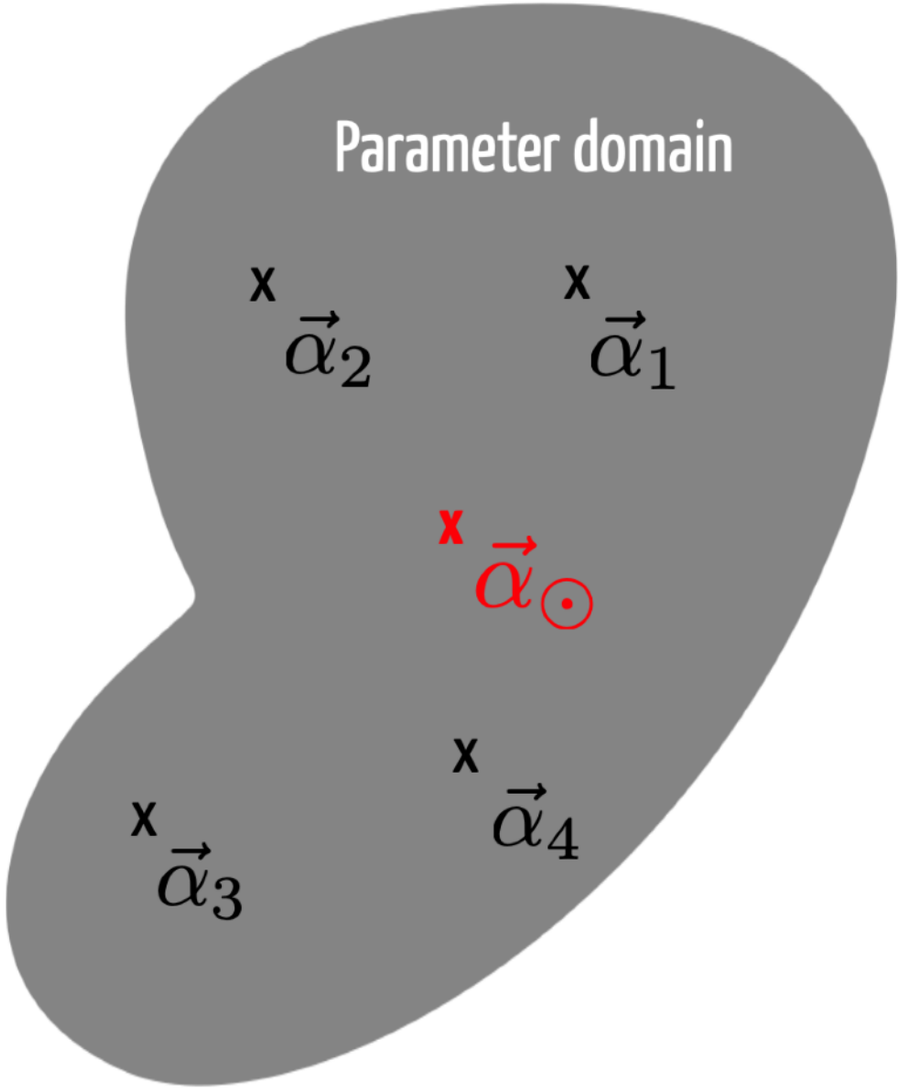
Computational bottleneck

A global sensitivity analyses of the 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)



- Generalization of the eigenvector continuation method [Frame D. et al., Phys. Rev. Lett. 121, 032501 (2018)]
- Write the Hamiltonian in a linearized form

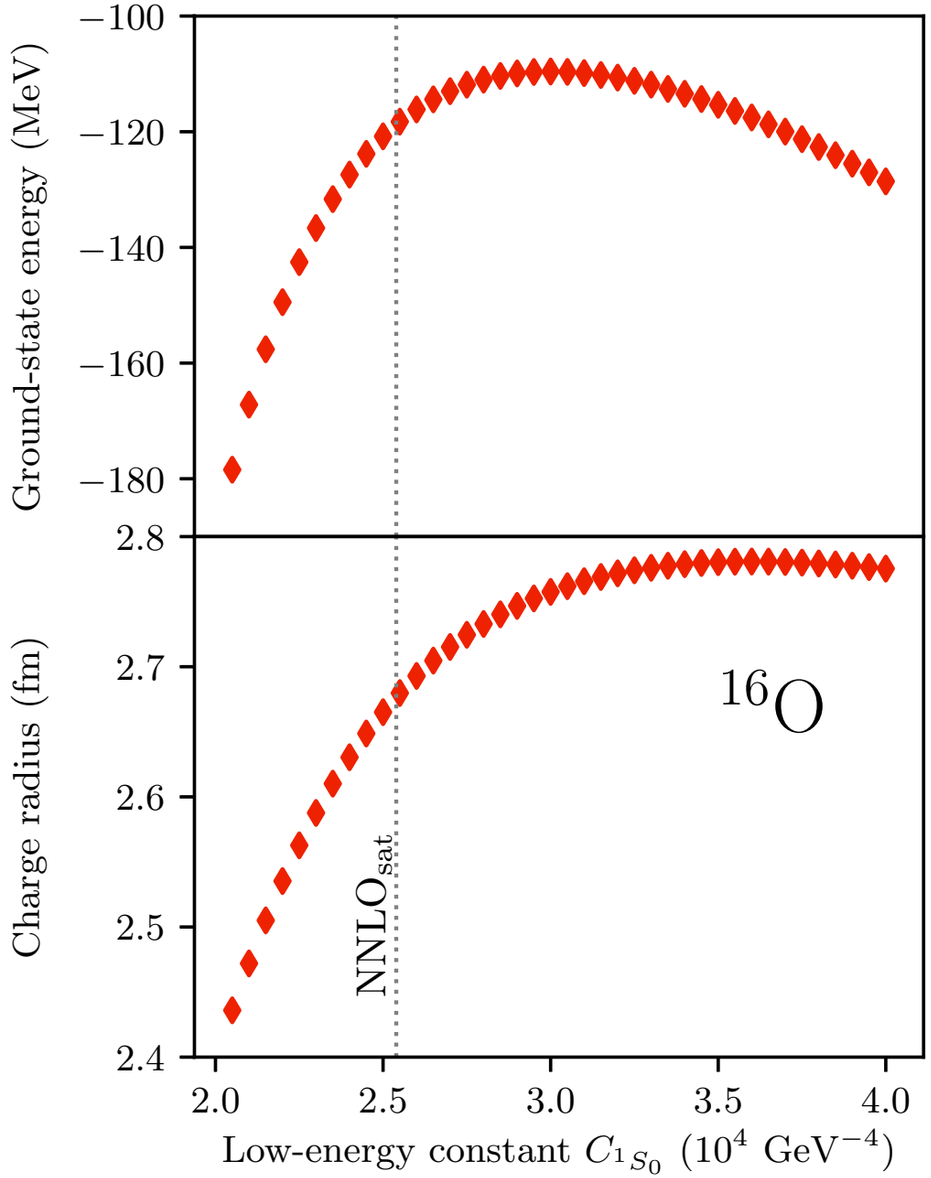
$$H(\vec{\alpha}) = \sum_{i=0}^{N_{\mathrm{LECs}}=16} \alpha_i h_i$$

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

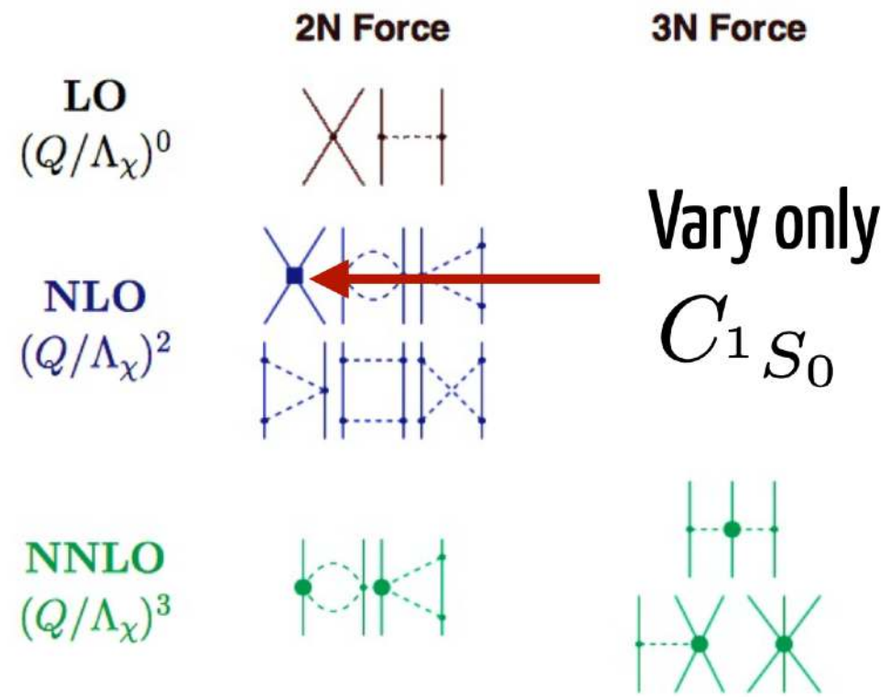
$$\mathbf{H}(\vec{\alpha}_\odot)\,\vec{c} = E(\vec{\alpha}_\odot)\,\mathbf{N}\,\vec{c}$$

Emulating ab-initio coupled-cluster calculations

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

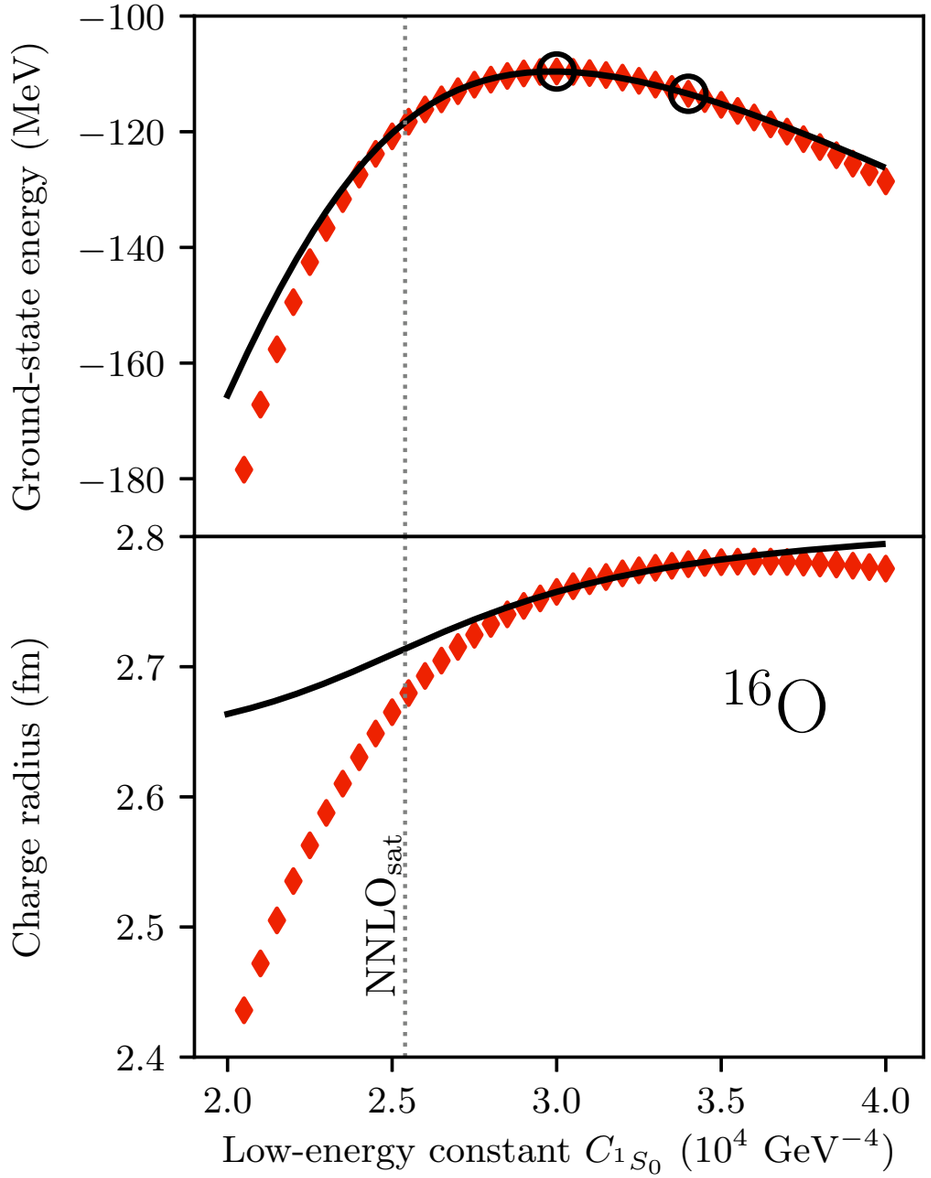


Exact coupled cluster calculations at the singles and doubles level



Emulating ab-initio coupled-cluster calculations

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



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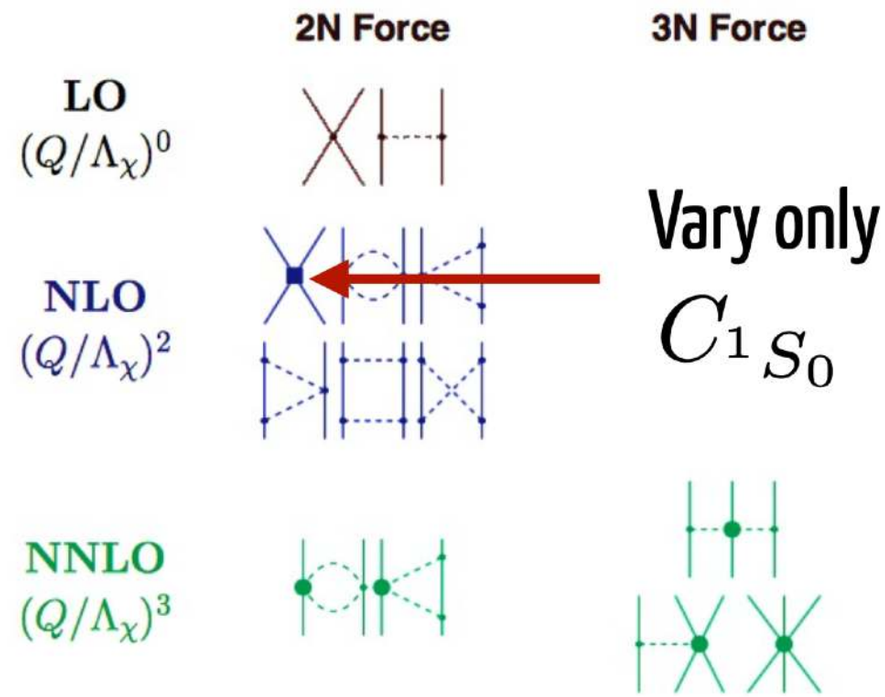

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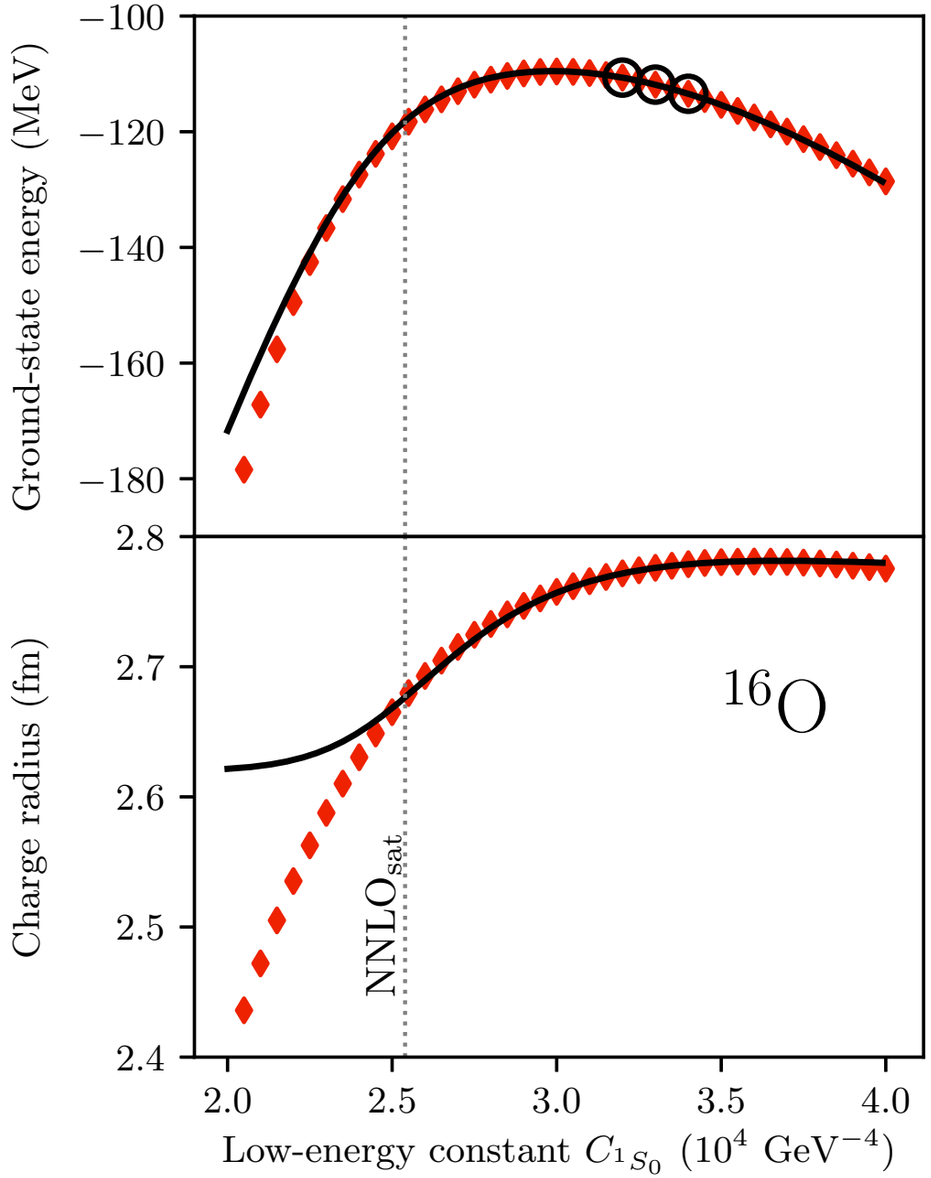
Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)



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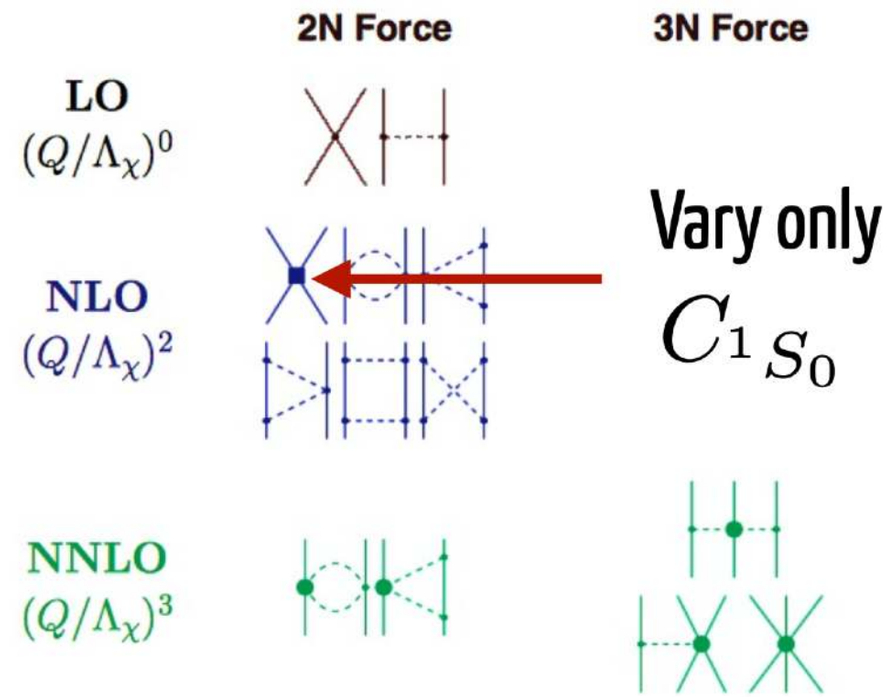

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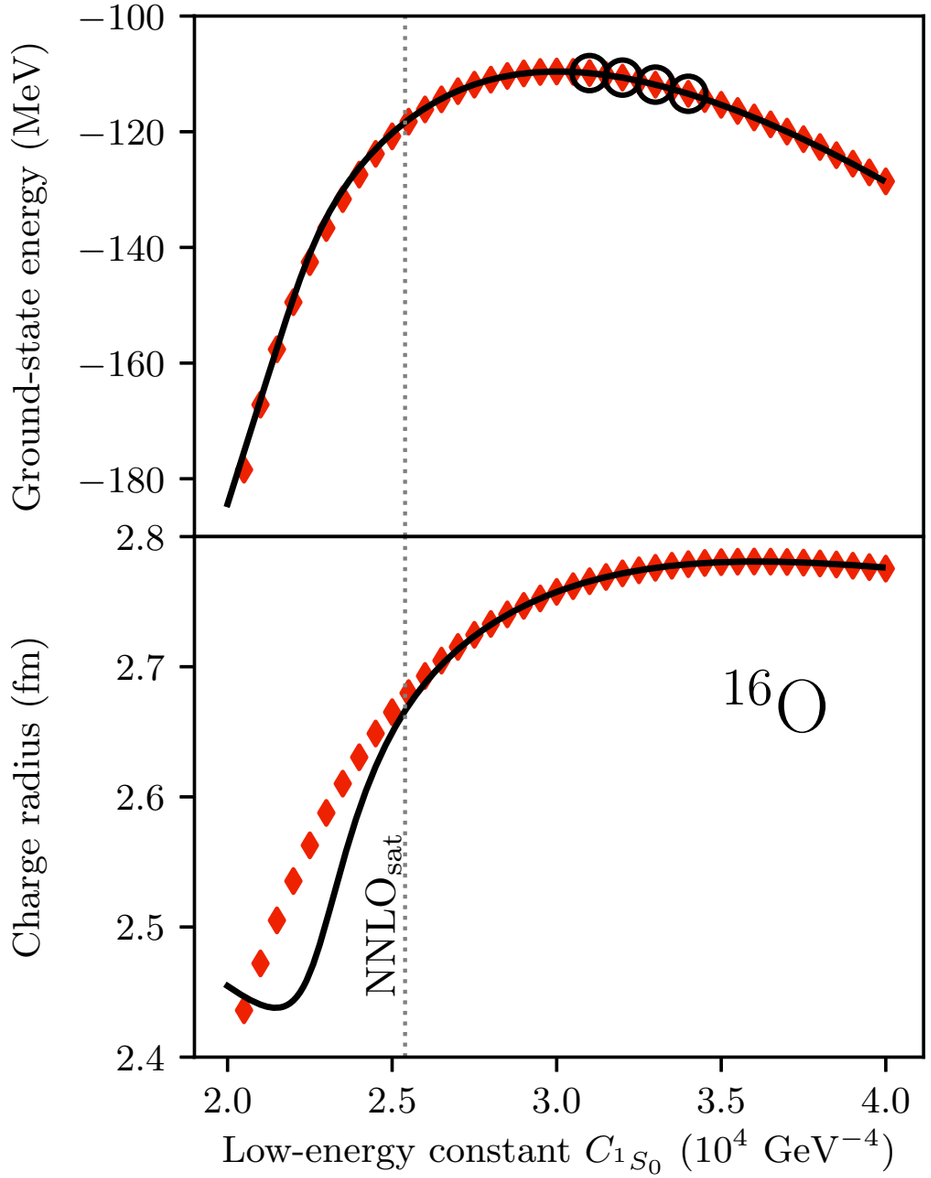

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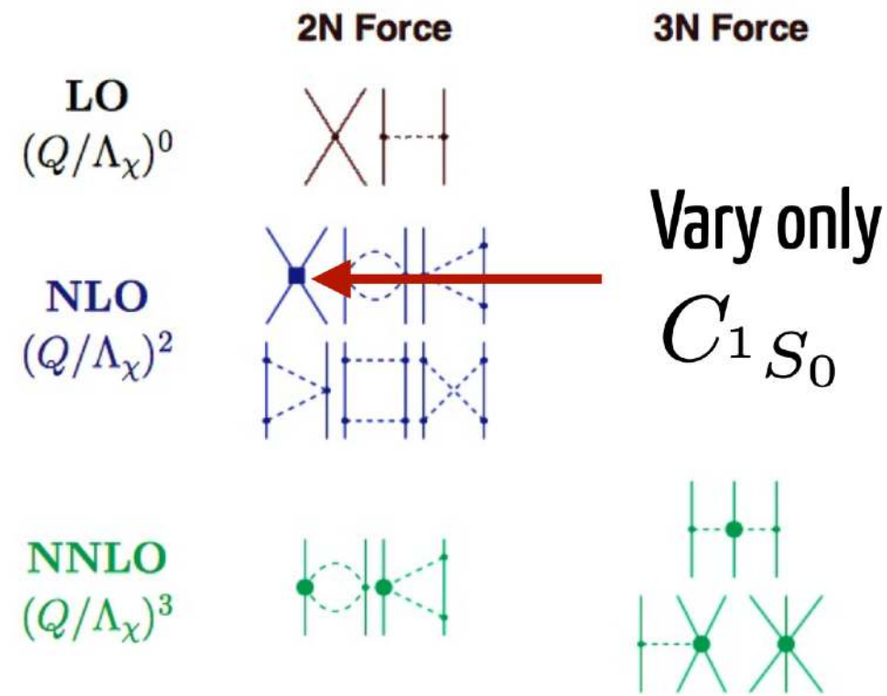

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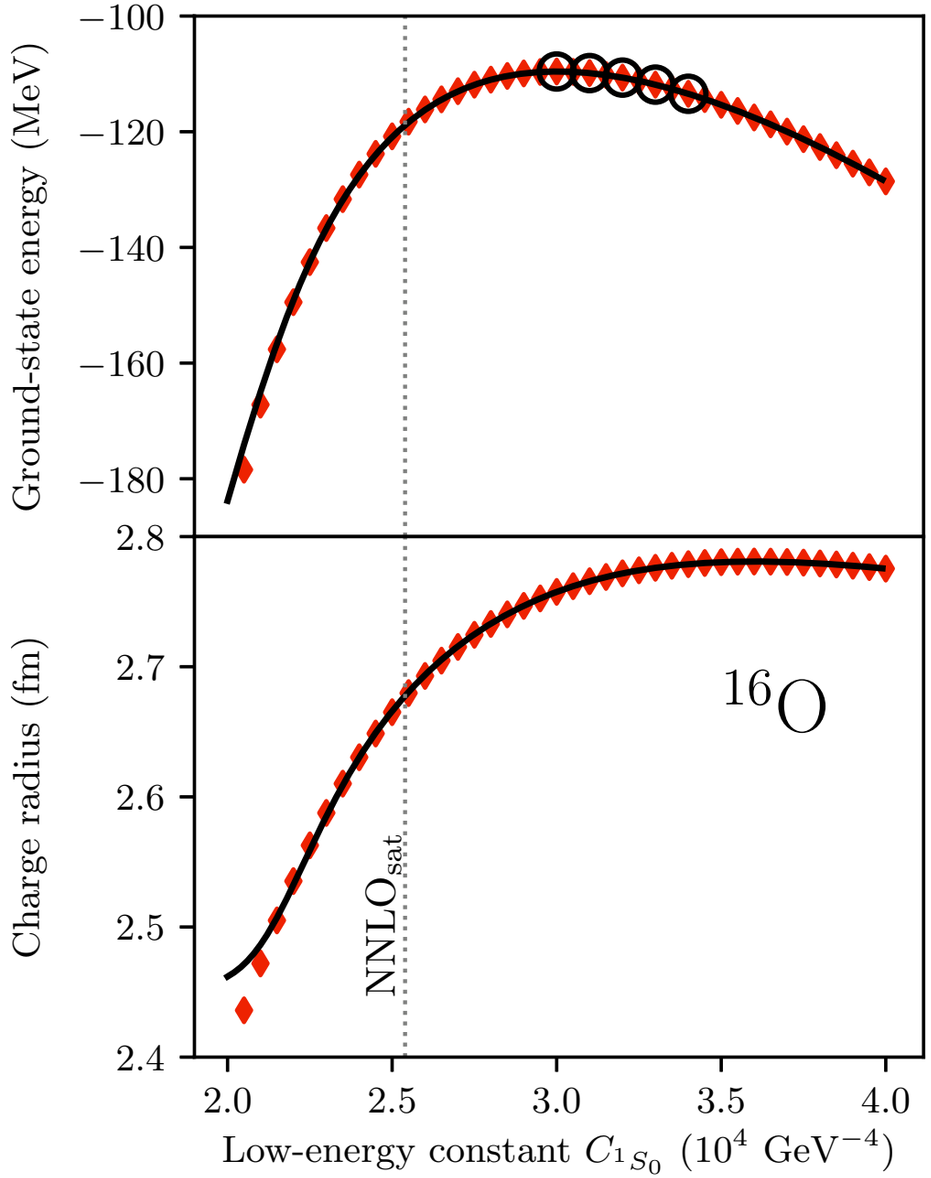

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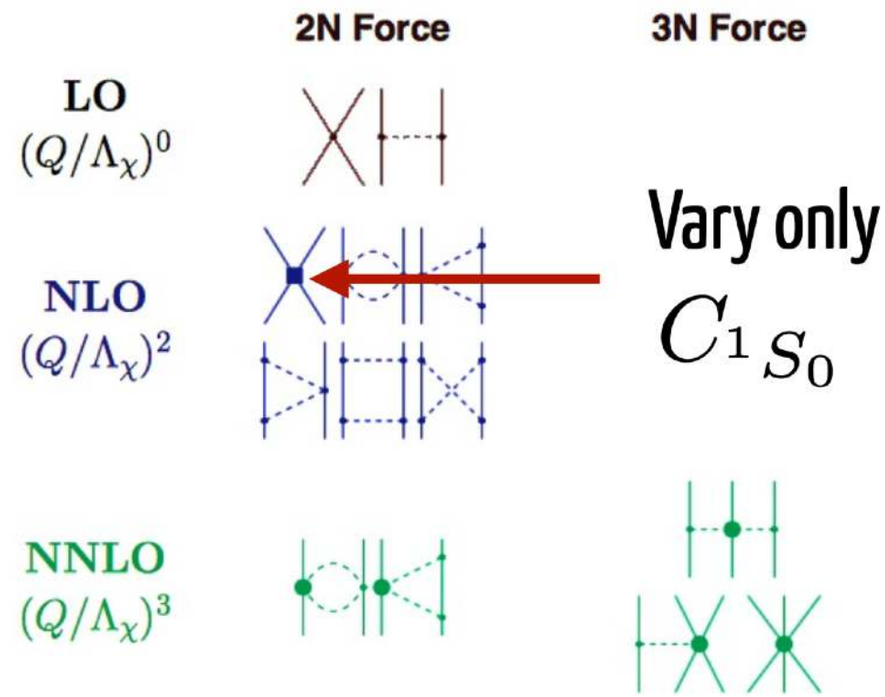
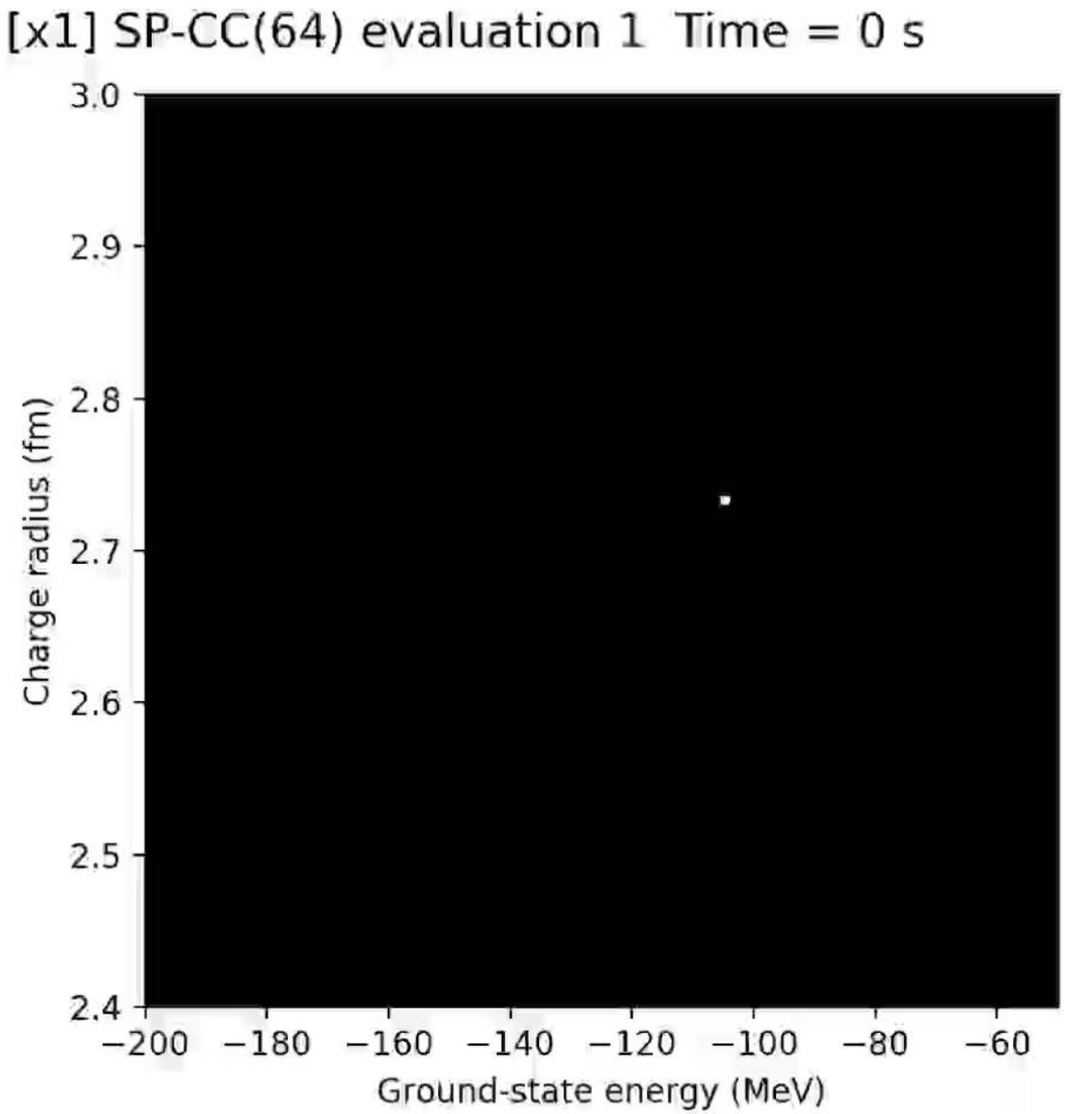


Computing nuclei at lightning speed

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



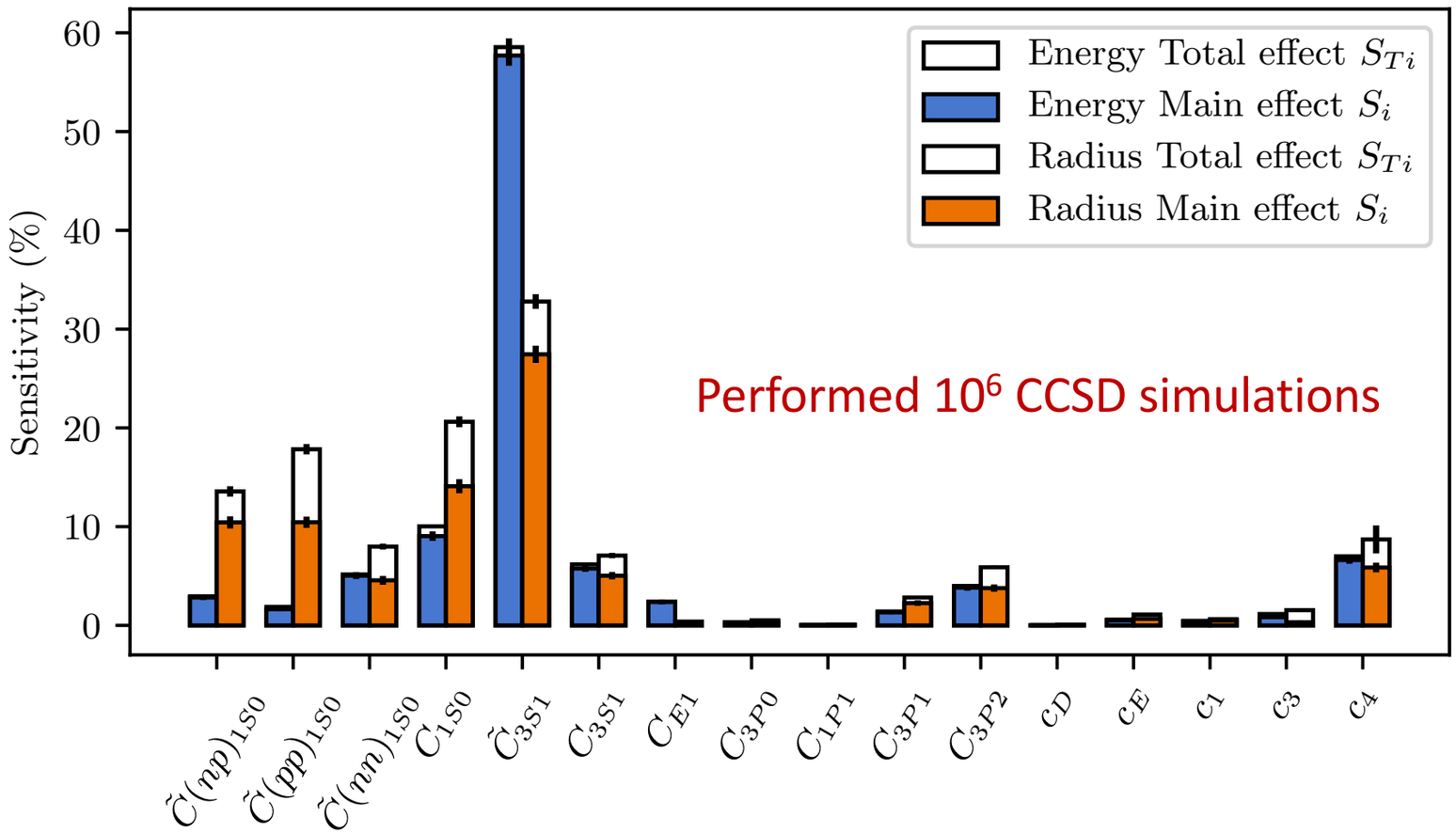
Realtime speed and accuracy of emulated ground-state energy and charge radius of ^{16}O for different values of interaction parameters

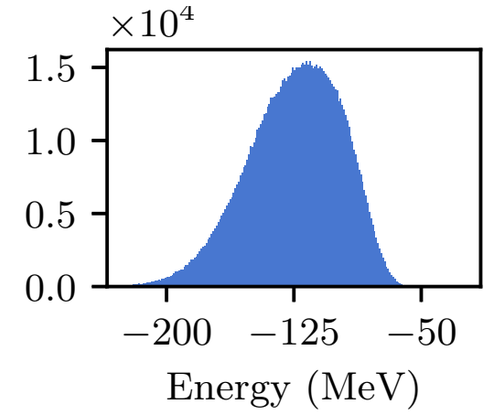
$$H(\vec{\alpha}) = \sum_{i=0}^{N_{\mathrm{LECs}}=16} \alpha_i h_i$$

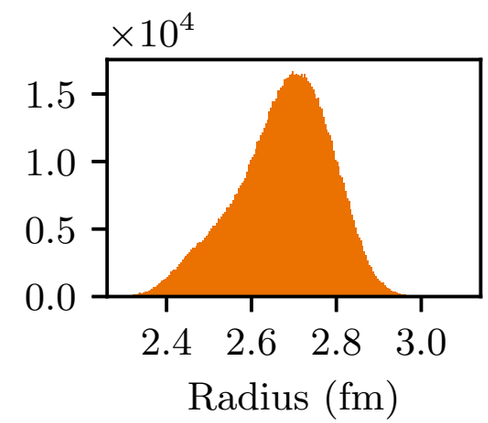
Accuracy: roughly the pixel size

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

The neutron skin of ^{208}Pb

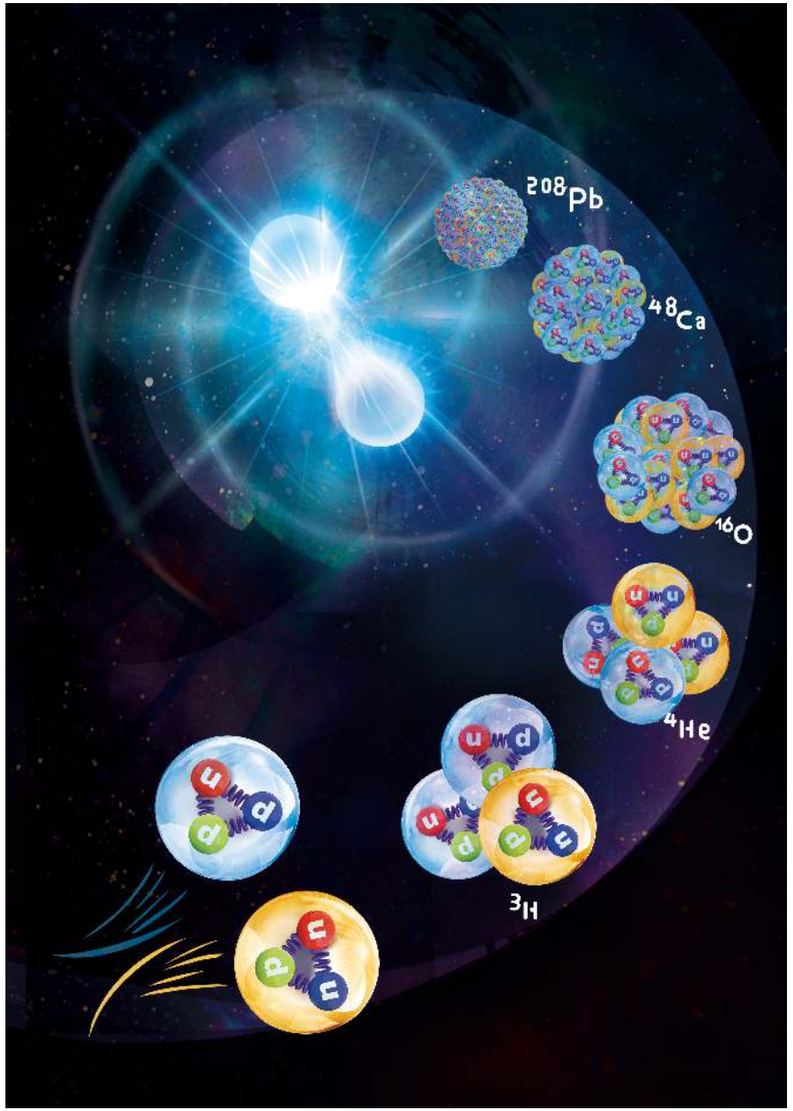


Image credit: Jing Chen

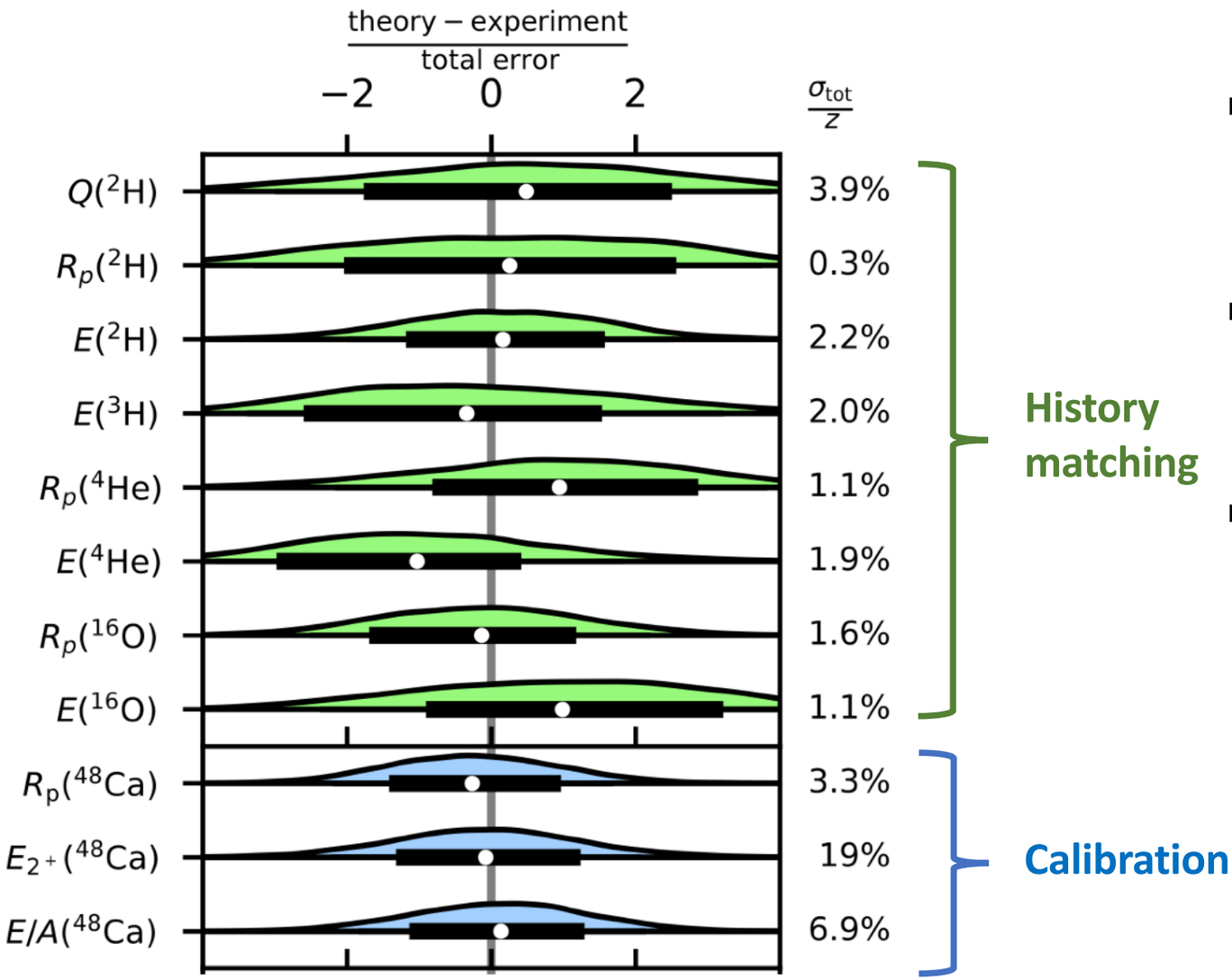
Neutron skin = Difference between radii of neutron and proton distributions

Relates atomic nuclei to neutron stars via neutron EOS

Correlated quantity: dipole polarizability

Recent (model-dependent) extractions of neutron skin (PREX-2/CREX) from parity-violating electron scattering at JLab

The neutron skin of ^{208}Pb

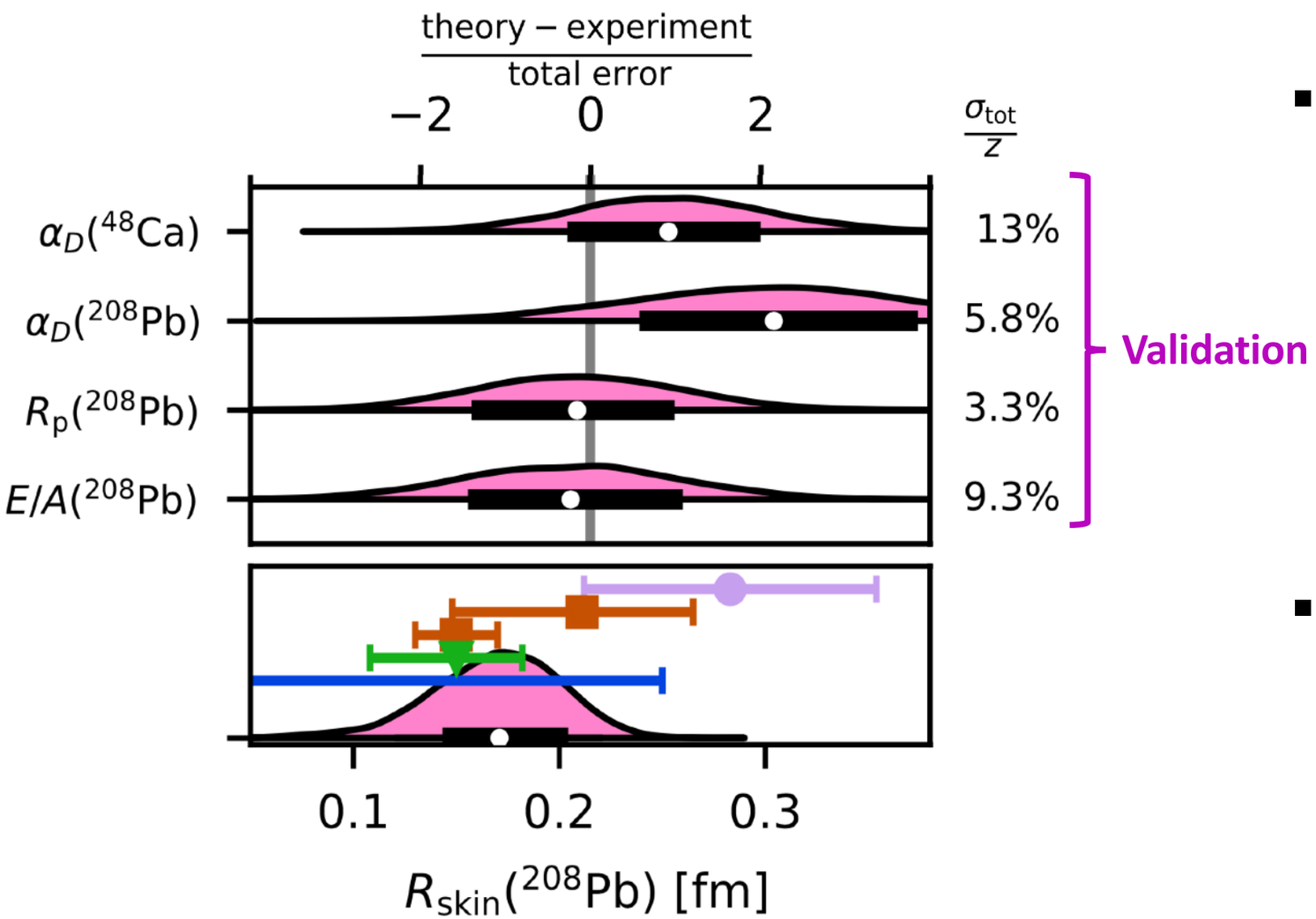


- Emulators allows for billions of ab-initio simulations of selected nuclei
- Opens up new ways for making predictions and addressing uncertainties
- History matching – identify parameters of the model that give results consistent with data

Explored 10^9 different parametrizations and found 34 non-implausible interactions
Calibration on ^{48}Ca yields weighted samples for which we can use for quantified predictions of ^{208}Pb

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

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)

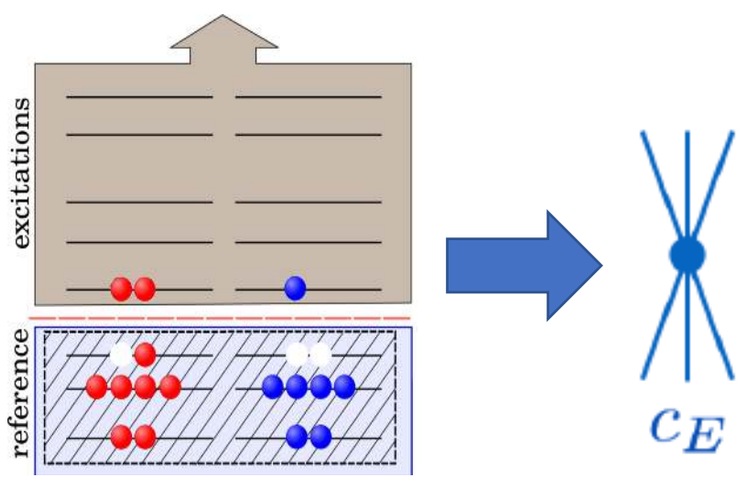
Renormalizing CCSD computations

Proposal: Apply Lepage's insights to many-body computations

- CCSD lacks triples (3p-3h excitations)
- Hypothesis: Energy gain from triples are dominated by short-range correlations; renormalize via three-body contact, following Lepage (1997)

Interaction	Name	c_E
A	1.8/2.0(EM)	−0.12 [52]
A renorm.		−0.0665
B	ΔNNLO$_{\rm GO}$(394)	−0.002 [67]
B renorm.		0.11

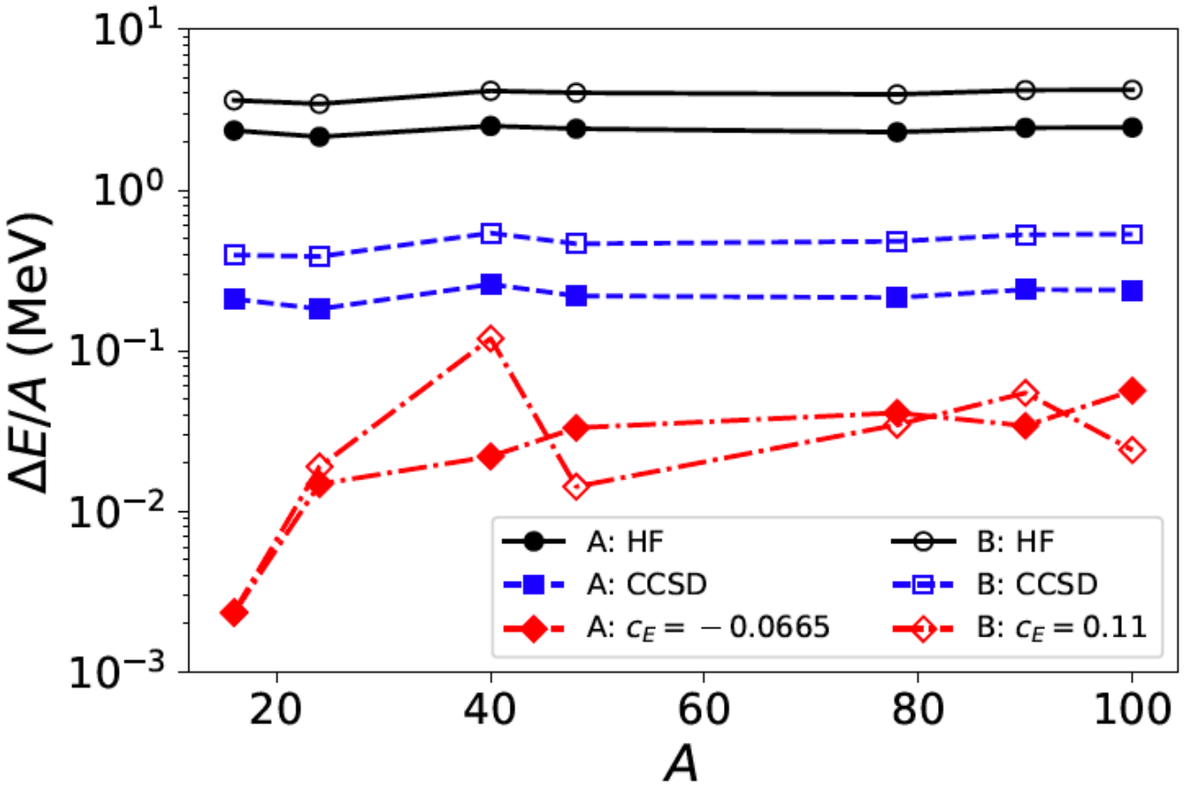
	Interaction and method				Exp.
	A renorm. CCSD	A Λ-CCSD(T)	B renorm. CCSD	B CCSDT-1	
^{16}O	127.8	127.8	127.5	127.5	127.62
^{24}O	166	165	169	169	168.96
^{40}Ca	346	347	341	346	342.05
^{48}Ca	420	419	419	420	416.00
^{78}Ni	642	638	636	639	641.55
^{90}Zr	798	795	777	782	783.90
^{100}Sn	842	836	816	818	825.30



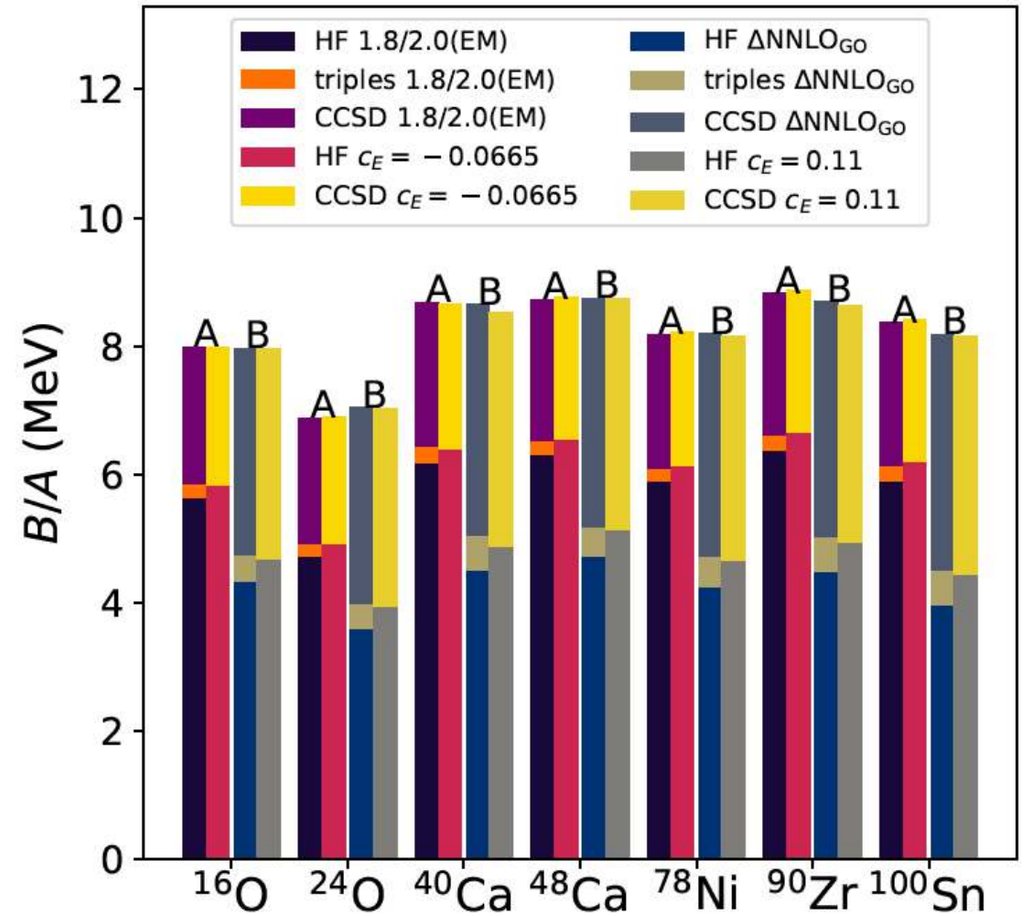
$$e^{-T_3} H e^{T_3} \approx H + V_3$$

Zhonghao Sun, Charles Bell, G. Hagen, T. Papenbrock, arXiv:2205.12990

Renormalizing CCSD computations



ΔE = differences to full triples
Systematic improvement from renormalization



Energy from renormalization essentially goes to HF

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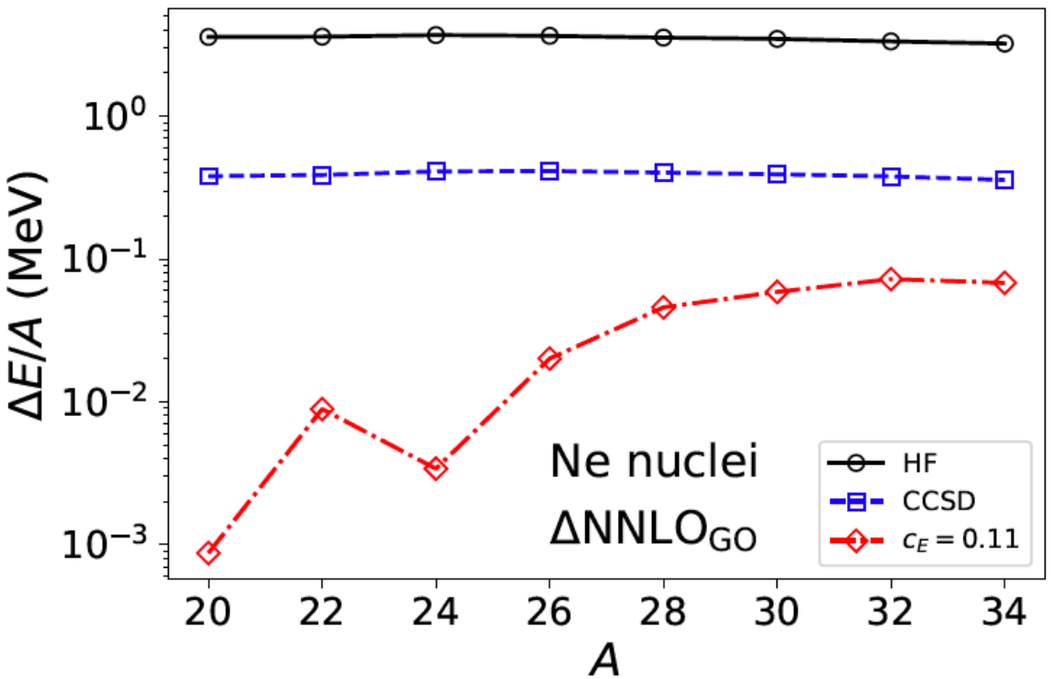
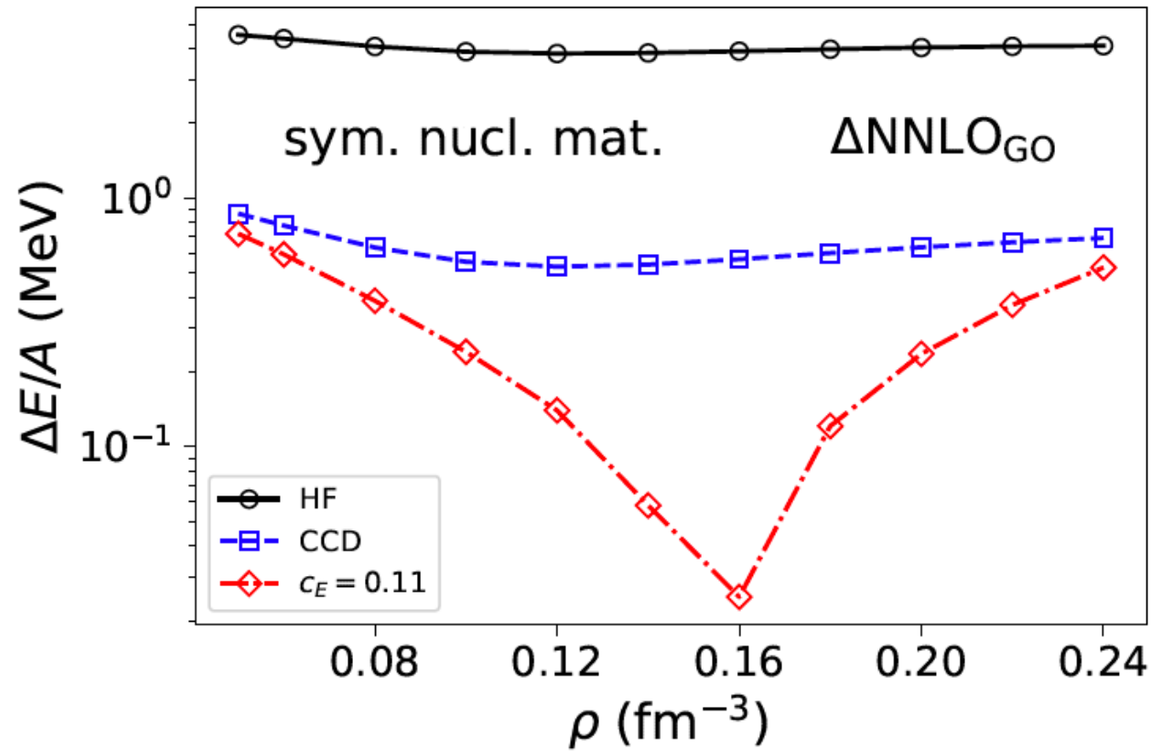
Renormalizing CCSD computations



Renormalization less accurate as the dripline is approached: dilute neutron densities



Nuclear matter only accurate around saturation

Zhonghao Sun, Charles Bell, G. Hagen, T. Papenbrock, arXiv:2205.12990

Summary

- Shell closures predicted at N = 8, 14 in magnesium (and neon)
- Even-even nuclei now possible with symmetry projection: ^{34}Ne is found to be as rotational as ^{32}Ne and ^{34}Mg
- Emulators, novel statistical tools, and Bayesian inference allow us to make accurate predictions with quantified uncertainties
- Neutron skin of ^{208}Pb in mild tension with PREX-2
- Renormalized CCSD reproduces CCSDT by adjusting a three-body contact

Thank you for your attention!