Coupled cluster computations of atomic nuclei on lattices

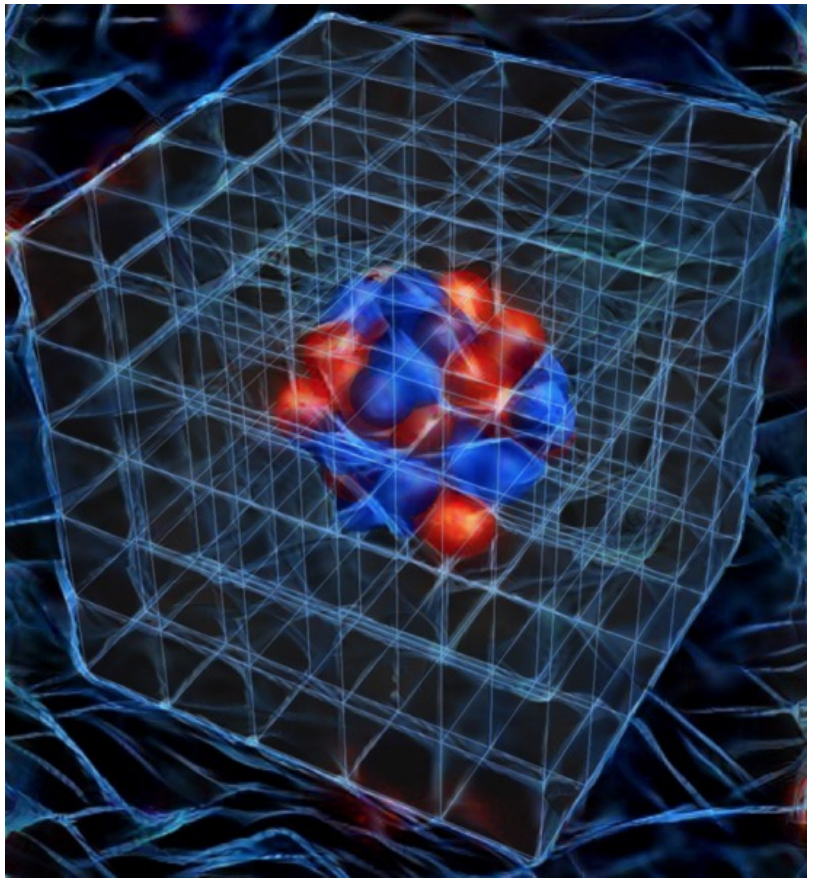


Image credit: Laboratory for Nuclear Science, MIT

Thomas Papenbrock, University of Tennessee & Oak Ridge National Laboratory, tpapenbr@utk.edu

Many-body theory: nuclear physics meets quantum chemistry

MITP Mainz, Aug. 31, 2026

Work supported by the US Department of Energy

U.S. DEPARTMENT of ENERGY

NUCLEI Nuclear Computational Low-Energy Initiative

Coupled-cluster computations of deformed atomic nuclei

Hagen, Novario, Sun, TP, Jansen, Lietz, Duguet, Tichai, Phys. Rev. C 105, 064311 (2022)
Sun, Ekström, Forssén, Hagen, Jansen, TP , Phys. Rev. X 15, 011028 (2025)

How do we compute deformed nuclei?

Input: Nucleon-nucleon and three-nucleon forces from chiral effective field theory:

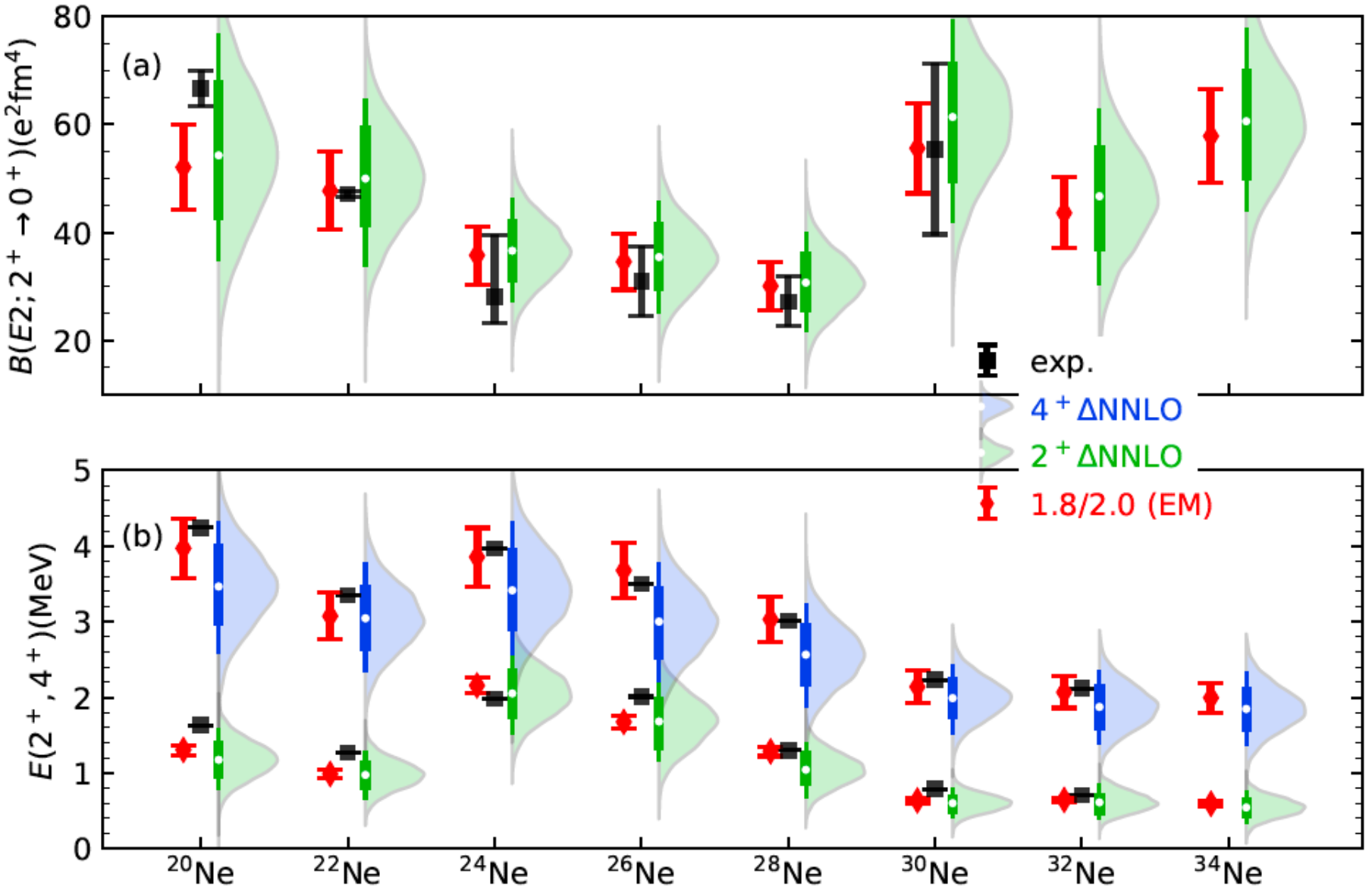
1.8/2.0(EM) from [Hebeler at al, Phys Rev C (2011)]; and an ensemble of

interactions used for computations of ^{28}O [Kondo et al, Nature 2023]; large model

space consisting of 13 harmonic oscillator shells

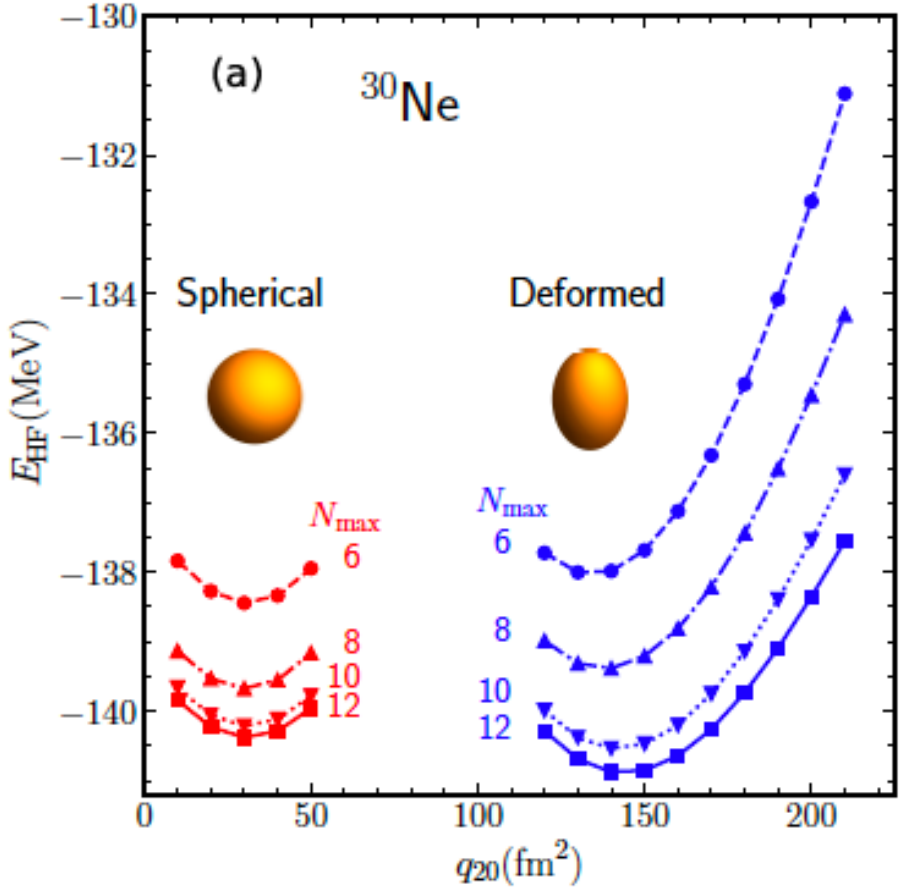
1. Axially-symmetric Hartree-Fock computations with quadrupole constraint
2. Normal-ordered two-body approximation [Hagen et al 2007; Roth et al 2012; Ripoche et al 2020; Frosini et al., 2021; Hebeler 2023]
3. Coupled-cluster computations based on deformed reference state
4. Angular momentum projection of deformed coupled-cluster state based on the disentangled formalism $e^V e^T = e^W$ [Qiu, Henderson, Scuseria; Duguet, …]

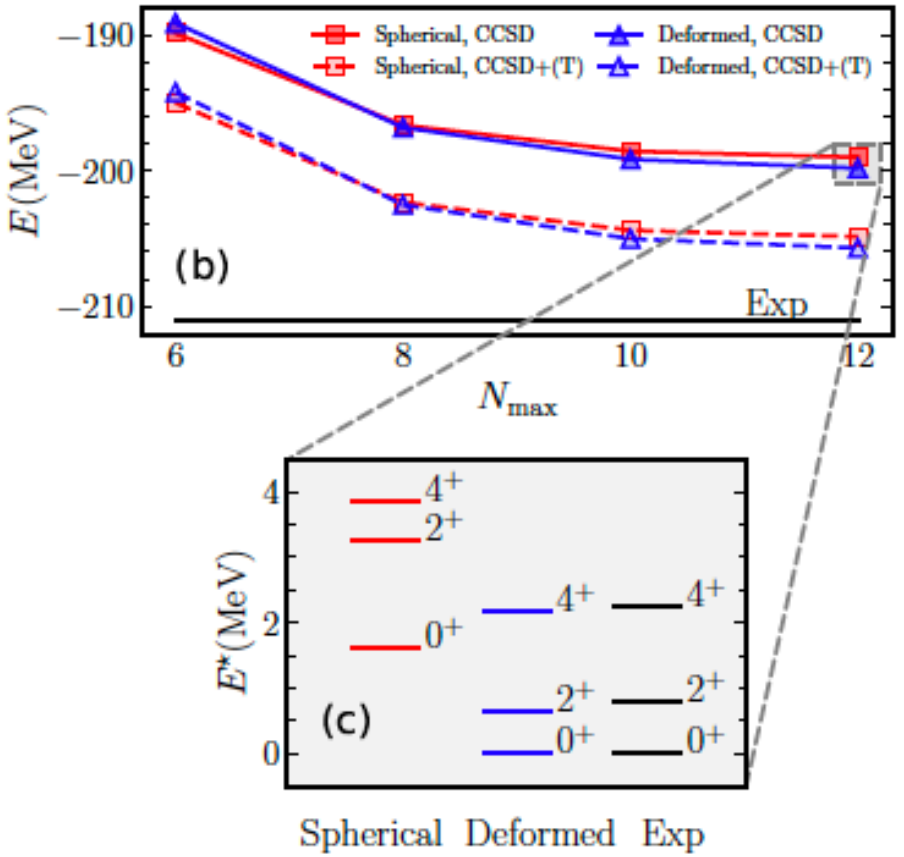
Collectivity of neon nuclei



Zhonghao Sun, Ekström, Forssén, Hagen, Jansen, TP, Phys. Rev. X (2025)

Prediction: Shape coexistence in ^{30}Ne



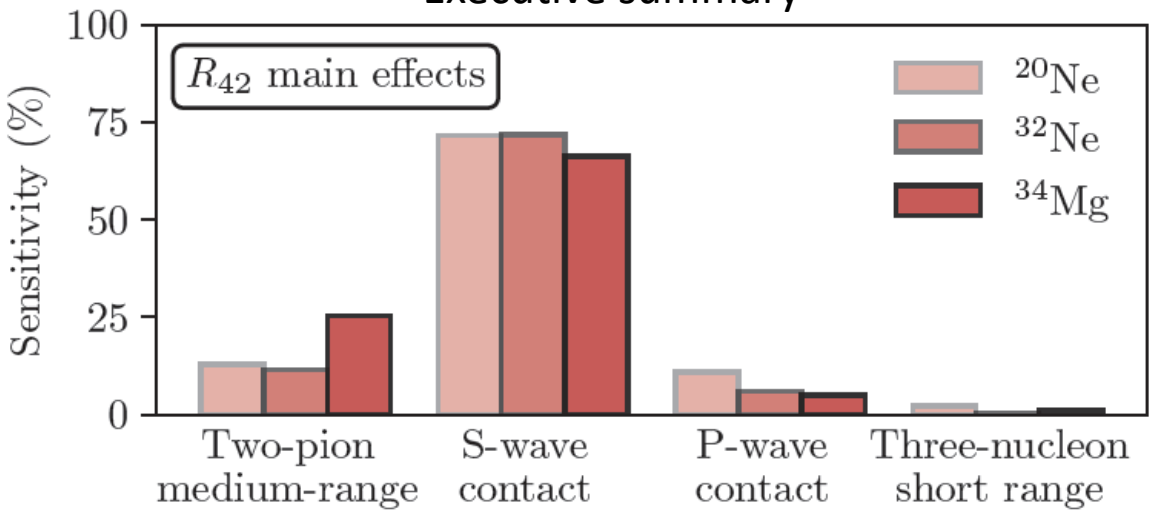


Zhonghao Sun, Ekström, Forssén, Hagen, Jansen, TP, Phys. Rev. X (2025)

What drives nuclear deformation?

Executive summary

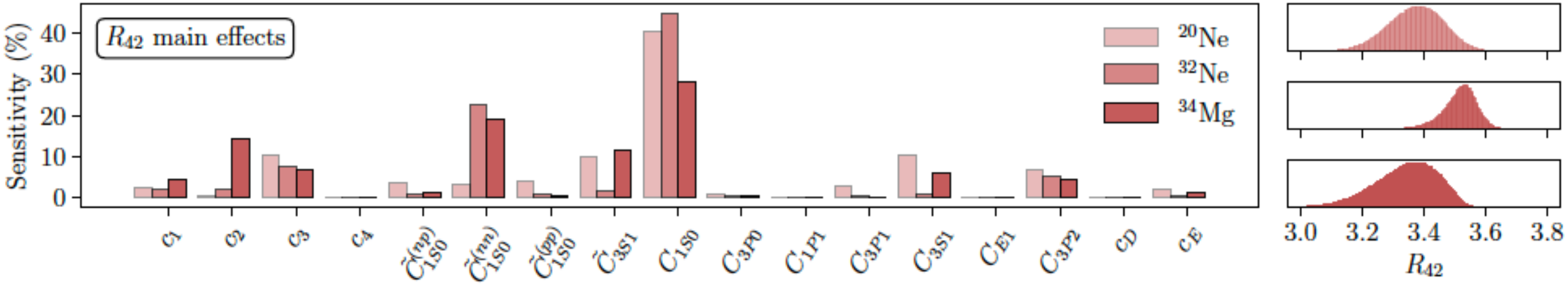
Global sensitivity analysis based on Hartree-Fock emulators used to compute R_{42}



No d-wave contacts at NNLO. (d-wave physics entirely from pion-nucleon couplings)

More detailed view from a Global Sensitivity Analysis

Saltelli, Ratto, Andres, Campolongo, Cariboni, Gatelli, Saisana, Tarantola. Global Sensitivity Analysis. The Primer (2007)



Zhonghao Sun, Ekström, Forssén, Hagen, Jansen, TP, Phys. Rev. X (2025)

NuLattice computations

Collaboration

- Chenyi Gu, Ben Johnson-Toth, Maxwell Rothman (University of Tennessee)
- Francesca Bonaiti, Vivek Booshan, Matthias Heinz, Gaute Hagen (ORNL)
- Oriel Kiss (CERN)

This presentation

M. Rothman, G. Hagen, M. Heinz, and TP, arXiv:2606.12166.
M. Rothman, B. Johnson-Toth, G. Hagen, M. Heinz, and TP, Eur. Phys. J. A 62, 28 (2026); arXiv:2509.08771
M. Rothman, B. Johnson-Toth, F. Bonaiti, G. Hagen, M. Heinz, TP, Phys. Rev. C 112, L051301 (2025); arXiv:2508.01507.
C. Gu, M. Heinz, O. Kiss, TP, Phys. Rev. C 113, 034321 (2026); arXiv:2507.14690.

`https://github.com/NuLattice`

Challenges / opportunities

Ab initio computations of nuclei

- Limitations from the spherical normal-ordered two-body approximation is the obstacle to rare-earth nuclei and actinides

Classical computers now allow us to address beyond-mean-field dynamics

- Study of equilibration / chaos in nuclear dynamics → Francesca Bonaiti's talk
- Ab initio computations of fission and fusion

Quantum computers are here and are becoming more powerful

- Nuclear structure and dynamics

Challenges / opportunities

Ab initio computations of nuclei

- Limitations from the spherical normal-ordered two-body approximation is the obstacle to rare-earth nuclei and actinides

Classical computers now allow us to address beyond-mean-field dynamics

- Study of equilibration / chaos in nuclear dynamics → Francesca Bonaiti's talk
- Ab initio computations of fission and fusion

Quantum computers are here and are becoming more powerful

- Nuclear structure and dynamics

Computing nuclei on lattices

Why work on lattices?

- Exploit short range of interaction
  - For $n = 4L^3$ states, number of two-body matrix elements is $O(n) \cdots O(n^2)$ and not $O(n^3)$
- Makes Hamiltonian more suitable for quantum computing (Baroni, Carlson, Roggero, Stetcu, Weiss; Watson, Childs, Davoudi; …)

Adaptive VQE solutions of few-nucleon systems

→Chenyi Gu, Matthias Heinz, Oriel Kiss, TP, Phys. Rev. C 113, 034321 (2026), arXiv:2507.14690.

System:

- Nucleons on a cubic lattice (L^3 sites, spacing $a = 2$ fm) and periodic boundary conditions
- Hamiltonian from leading-order pion-less effective field theory, $O(L^3)$ Pauli terms

$$\hat{H} = \sum_{\langle \mathbf{l},\mathbf{l}' \rangle} \sum_{\tau s} T^{\mathbf{l}}_{\mathbf{l}'} \hat{a}^\dagger_{\mathbf{l}\tau s} \hat{a}_{\mathbf{l}'\tau s} + \frac{V}{2} \sum_{\mathbf{l}} \sum_{ss'\tau\tau'} \hat{a}^\dagger_{\mathbf{l}\tau s} \hat{a}^\dagger_{\mathbf{l}\tau' s'} \hat{a}_{\mathbf{l}\tau' s'} \hat{a}_{\mathbf{l}\tau s} + W \sum_{\mathbf{l}} \sum_{\tau s} \hat{a}^\dagger_{\mathbf{l}\tau\uparrow} \hat{a}^\dagger_{\mathbf{l}\tau\downarrow} \hat{a}^\dagger_{\mathbf{l}-\tau s} \hat{a}_{\mathbf{l}-\tau s} \hat{a}_{\mathbf{l}\tau\downarrow} \hat{a}_{\mathbf{l}\tau\uparrow}$$

Kinetic energy: Hopping to neighboring lattice sites

Two-body contact: on-site only and SU(4) symmetric

Three-body contact: on-site only

- Adjusted V, W such that the deuteron and triton/^{3}He are acceptable on large lattices

ADAPT VQE solution of nuclei w/ unitary coupled cluster

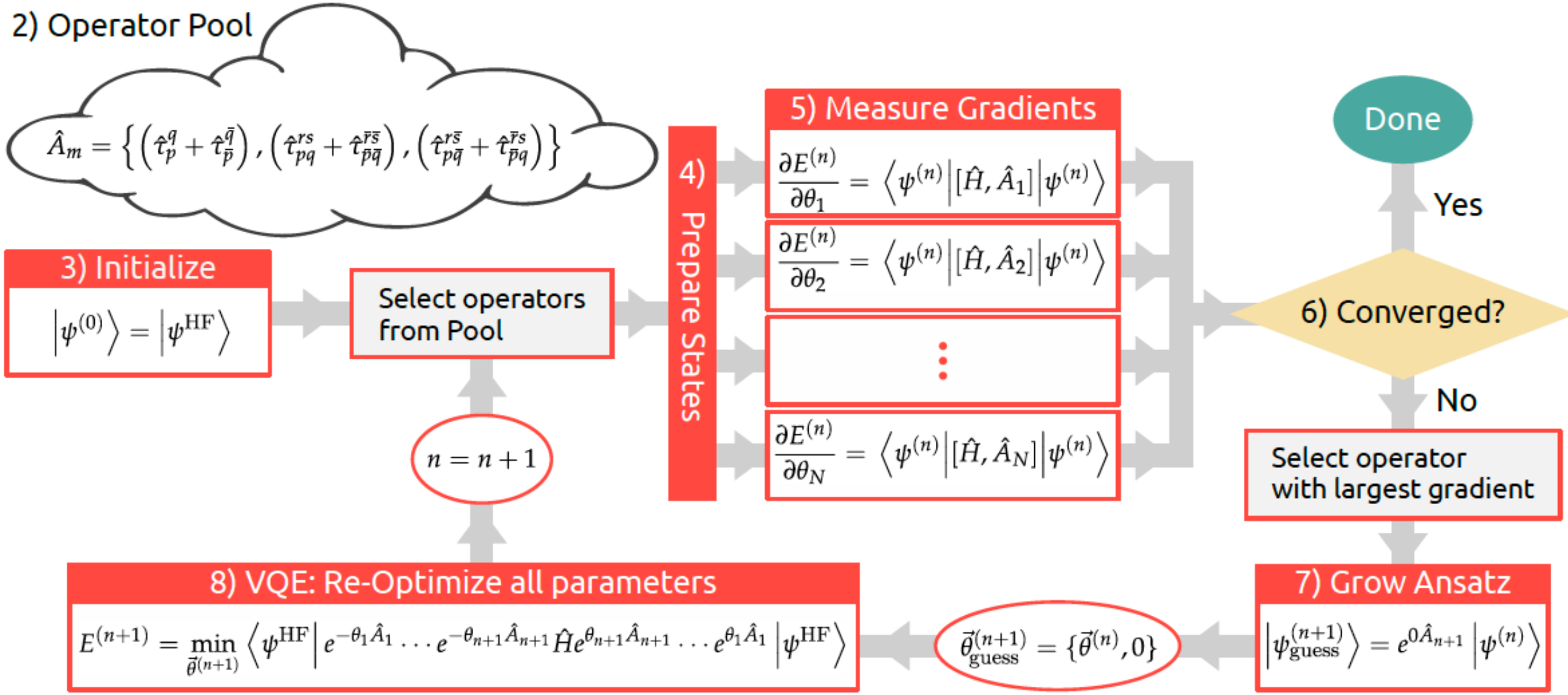
$$|\vec{\theta}\rangle = \prod_{\alpha=1}^{N_e} \exp\left(\sum_{\beta=1}^{N_p} \theta_{\alpha\beta}\hat{A}_{\alpha\beta}\right)|\phi_0\rangle$$

N_e exponentials used

$N_p = 10$ operators used in each epoch;
this was Trotterized;
100 optimization steps to determine $\theta_{\alpha\beta}$
for fixed epoch α.

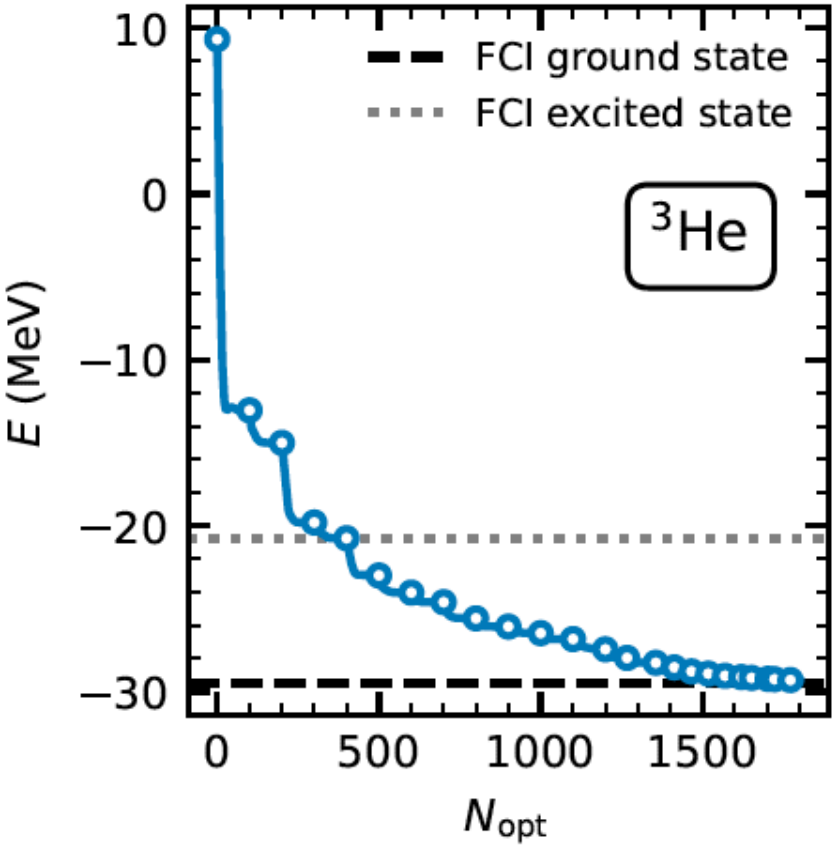
Unitary coupled cluster in quantum computing
Evangelista, Chan, Scuseria, J. Chem. Phys. (2019)
Recent review: Anand et al., arXiv:2109.15176

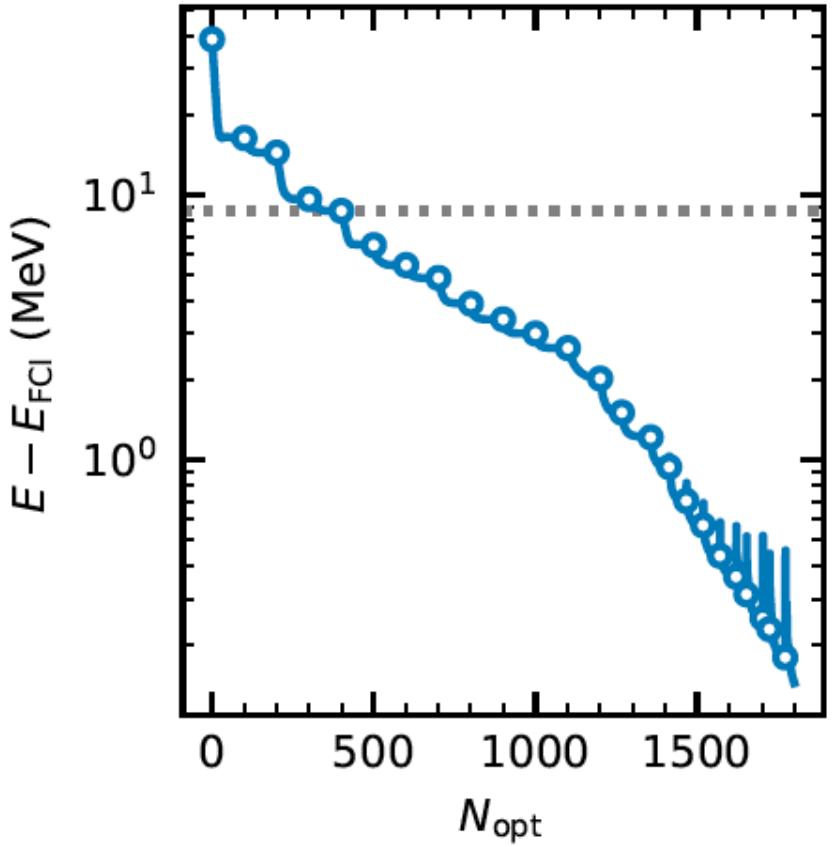
Adaptive VQE based on unitary coupled cluster

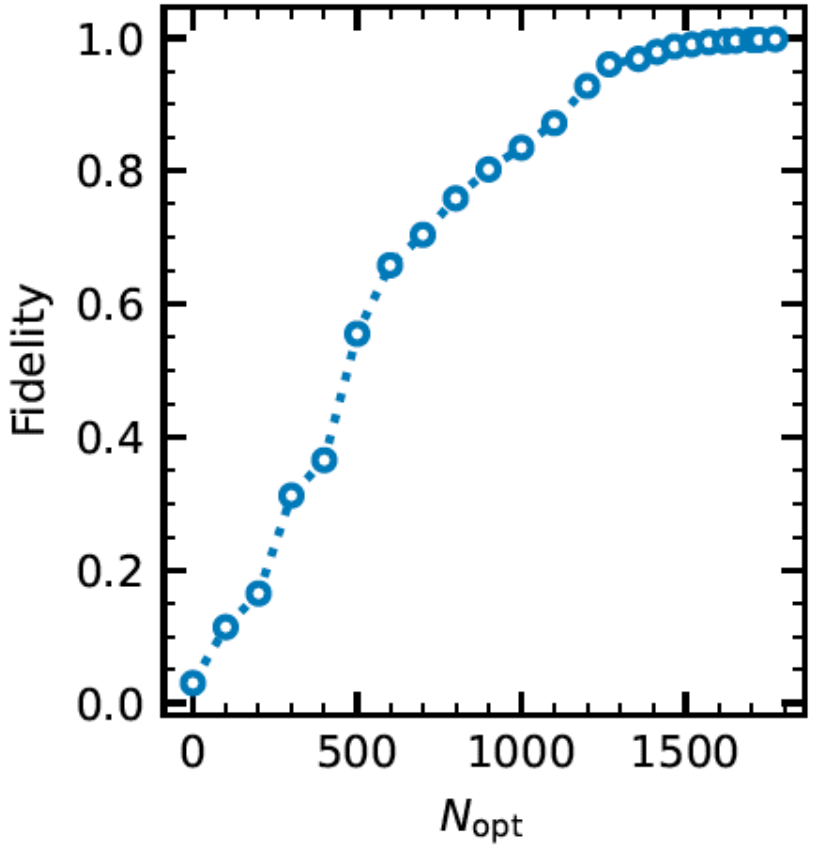


H. R. Grimsley, S. E. Economou, E. Barnes, N. J. Mayhall, Nat. Comm. 10, (2019) 3007

Quantum simulation of ^{3}He on a 2×2×2 lattice







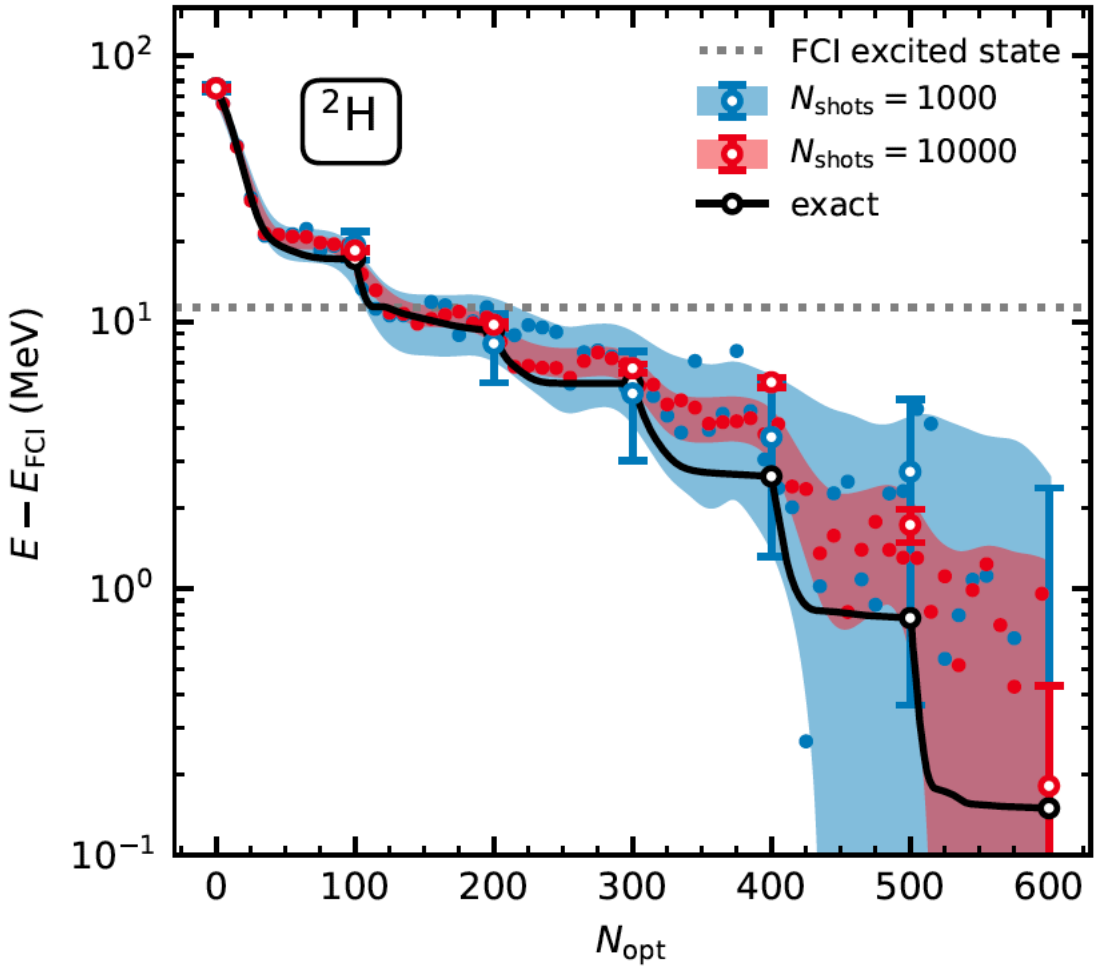
10 operators per epoch
100 optimization steps per epoch
20+ epochs used

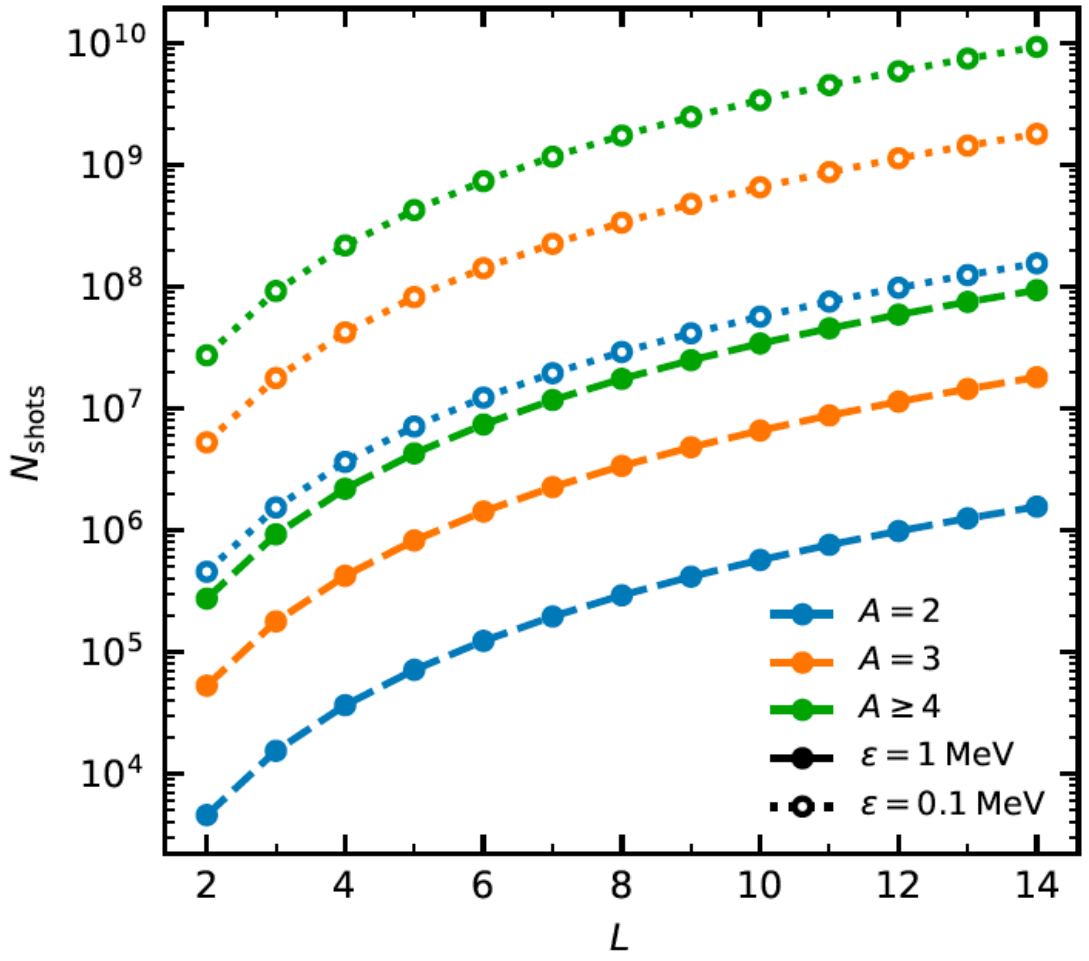
$$|\vec{\theta}\rangle = \prod_{\alpha=1}^{N_{\text{e}}} \exp\left(\sum_{\beta=1}^{N_{\text{p}}} \theta_{\alpha\beta}\hat{A}_{\alpha\beta}\right)|\phi_0\rangle$$

Fidelity: $\left|\langle\vec{\theta}|\psi_{\text{exact}}\rangle\right|^2$

Chenyi Gu, Matthias Heinz, Oriel Kiss, TP, Phys. Rev. C 113, 034321 (2026)

Number of measurements “shots” required



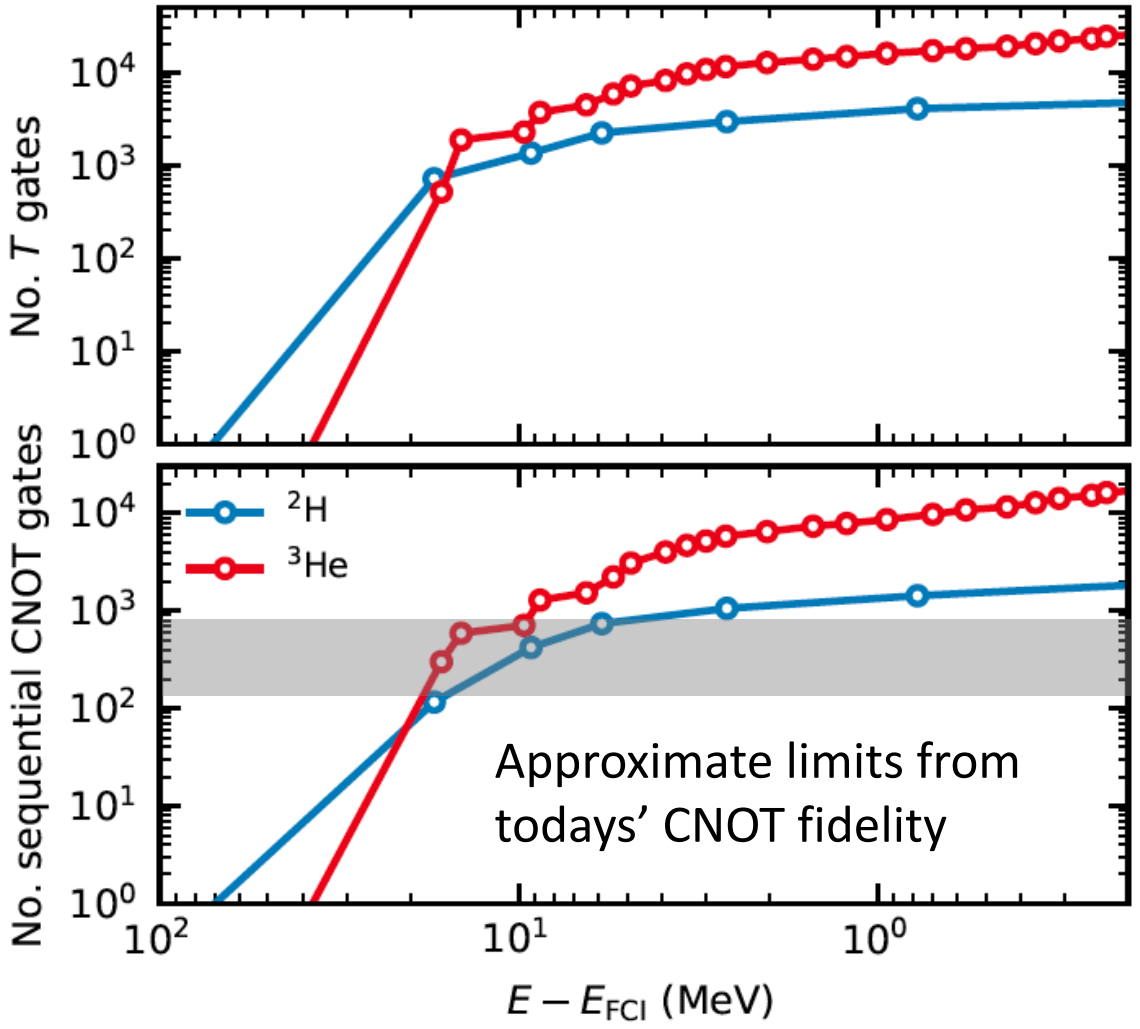


Chenyi Gu, Matthias Heinz, Oriel Kiss, TP, Phys. Rev. C 113, 034321 (2026)

Complexity of the used quantum circuits

Quantum simulations with PennyLane
[V. Bergholm et al., arXiv:1811.04968]

The complexity of circuits is reflected in the number of CNOT and T gates, $T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}$.



Chenyi Gu, Matthias Heinz, Oriel Kiss, TP, Phys. Rev. C 113, 034321 (2026)

Why work on lattices?

- Exploit short range of interaction
  - For $n = 4L^3$ states, number of two-body matrix elements is $O(n) \cdots O(n^2)$ and not $O(n^3)$
- Makes Hamiltonian more suitable for quantum computing (Baroni, Carlson, Roggero, Stetcu; Watson, Childs, Davoudi; …)
- Scrutinize simple Hamiltonians from Nuclear Lattice EFT (Elhatisari, Epelbaum, Lähde, Lee, Lu, Ma, Meissner, …)

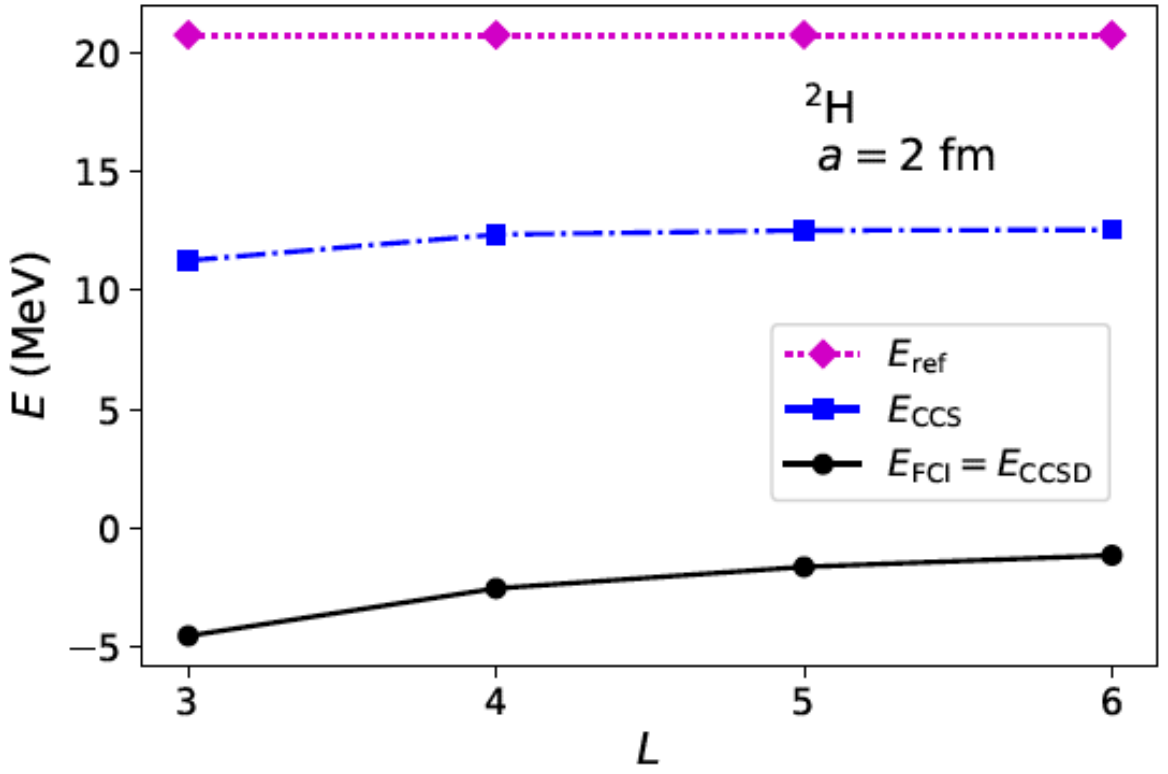
Coupled-cluster results from the lattice
(pionless EFT at leading order)

$$H = T(a) + V_{NN}(v) + W_{NNN}(w)$$

a	v	w	^{4}He	^{3}He	^{2}H
2.5	−9.0	6.0	−29.70	−16.32	−2.48
2.0	−8.0	5.5	−29.45	−14.84	−2.53
1.7	−7.0	4.4	−28.97	−10.82	−2.33

	^{3}He			^{4}He		
a	1.7	2.0	2.5	1.7	2.0	2.5
E_{ref}	10.04	−2.59	−9.95	−2.87	−10.37	−19.91
HF	−4.62	−12.09	−15.18	−26.37	−27.65	−29.06
CCS	−4.09	−11.85	−15.08	−26.82	−28.52	−29.28
CCSD	−4.80	−12.18	−15.22	−26.41	−27.73	−29.11
FCI	−10.82	−14.84	−16.32	−28.97	−29.45	−29.70

Energies converge from below
(tunneling under periodic boundary conditions)
→ Lüscher (1980s); König et al (2010s)



^{3}He: Center of mass important; particularly for small a

^{4}He: HF / CCS yields most of the energy (only kin. energy is off-diagonal)

Nuclear saturation

Really old view:

- Hard core in nucleon-nucleon interaction, i.e. interaction is attractive at low momenta and repulsive at high

EFT/SRG view:

- Repulsive three-nucleon force yield saturation. → Hebeler, Bogner, Furnstahl, Nogga, Schwenk, Phys. Rev. C 83, 031301(R) (2011)

Nuclear Lattice Effective Field Theory:

🤔 Attractive two body alone yields accurate nuclear radii and binding energies
→Elhatisari et al., Phys. Rev. Lett. 119, 222505 (2017); Phys. Rev. Lett. 117, 132502 (2016)

🤔 Attractive two body + attractive three-body yield accurate nuclear radii and binding energies → Bing-Nan Lu et al., Phys. Lett. B 797, 134863 (2019)

Interactions with OPE and two-body contacts

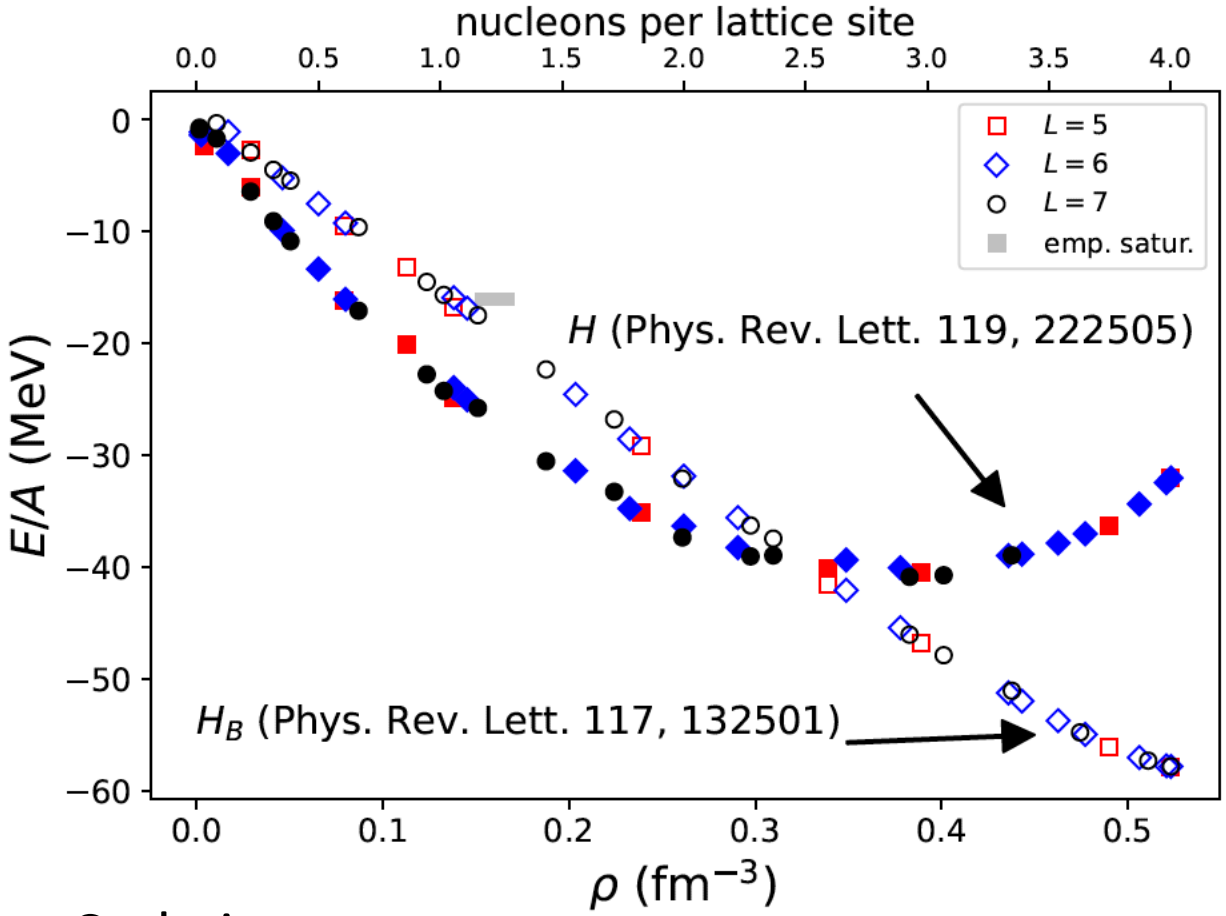
[20] Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, Lee, Rupak, PRL 117, 132501 (2016)

[19] Elhatisari, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)

$$H = T + V_{\rm OPE} + V_0$$

$$H_B = T + V_{\rm OPE} + V_L + V_{NL}$$

Nucl.	H from Ref. [20]		H_B from Ref. [19]		Exp.
	HF	AFMC	HF	AFMC	
^{4}He	−19.81	−25.4	−32.19	−29.2	−28.3
^{8}Be	−63.17	−51.9	−76.37	−59.7	−56.5
^{12}C	−137.28	−83.8	−139.83	−95.0	−92.2
^{16}O	−213.37	−128.2	−222.06	−135.4	−127.6

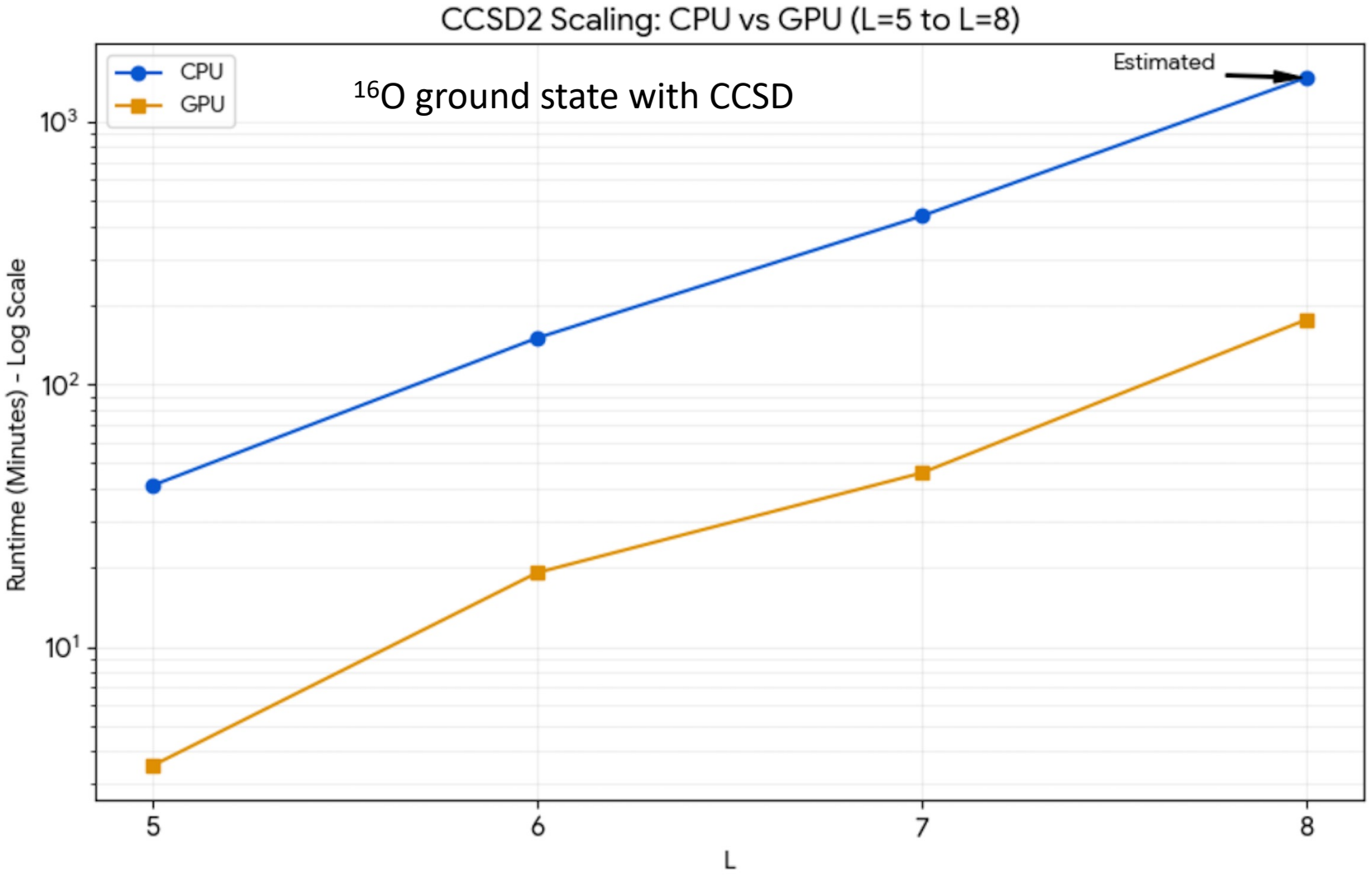


Auxiliary-field Monte Carlo inaccurate

Rothman, Hagen, Heinz, TP, arXiv:2606.12166

NuLattice is going HPC

Vivek Booshan, Matthias Heinz, … are porting NuLattice to Frontier via JAX



Scaling is roughly as $\propto L^9$ in our implementation

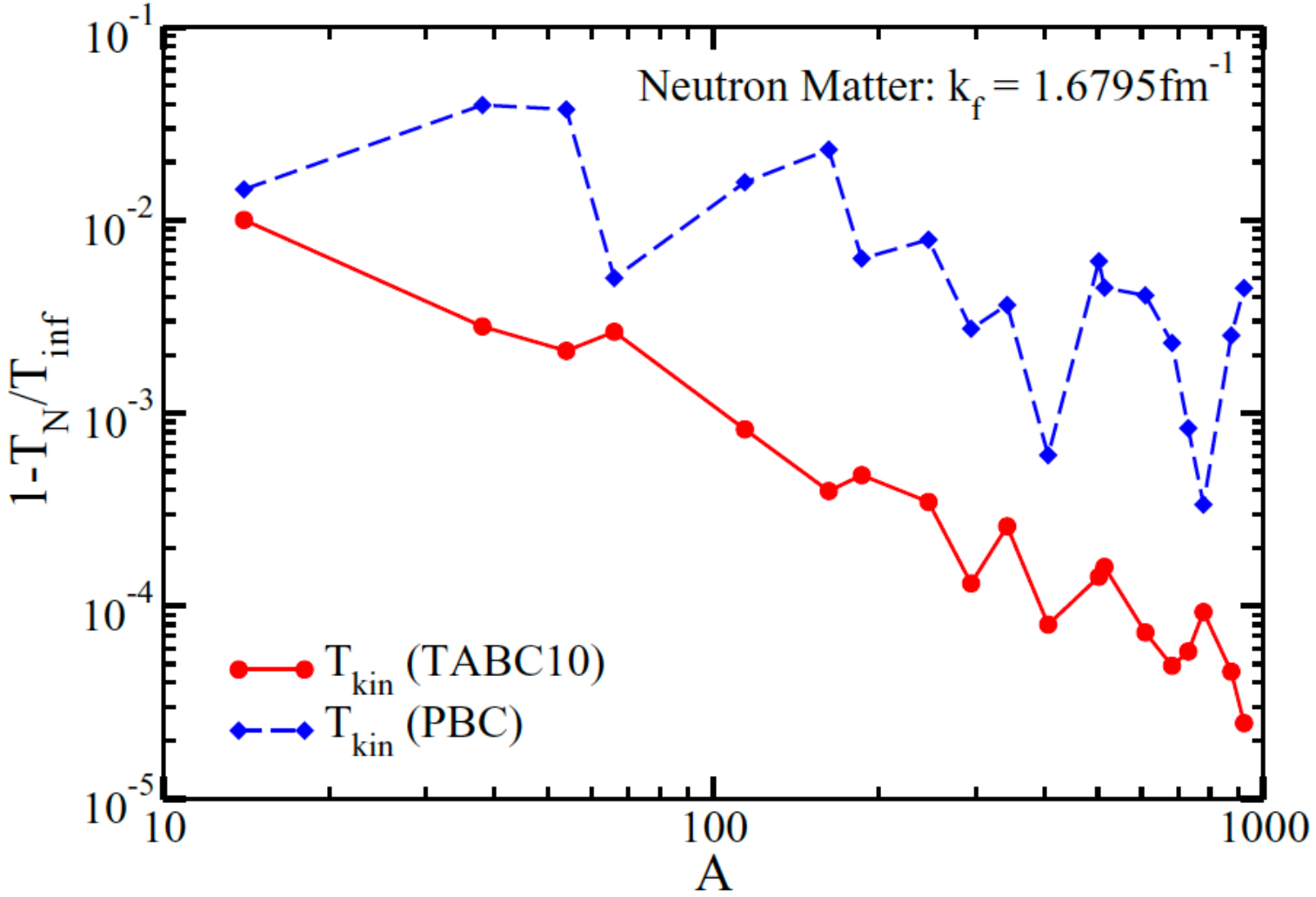
Summary

Computations of atomic nuclei on lattices

- Quantum simulation of ^{3}He via adaptive VQE using 2 & 3-body forces
- Normal-ordered 2-body approximation is exact for zero-ranged forces
- Implemented more sophisticated NLEFT interactions, neutron / nuclear matter EOS
  - Auxiliary-field Monte Carlo simulations did not accurately solve the printed Hamiltonians
  - Saturation on lattices due to dominance of kinetic energy and crowding
  - Questions regarding ab initio alpha clustering are probably still open

Thank you

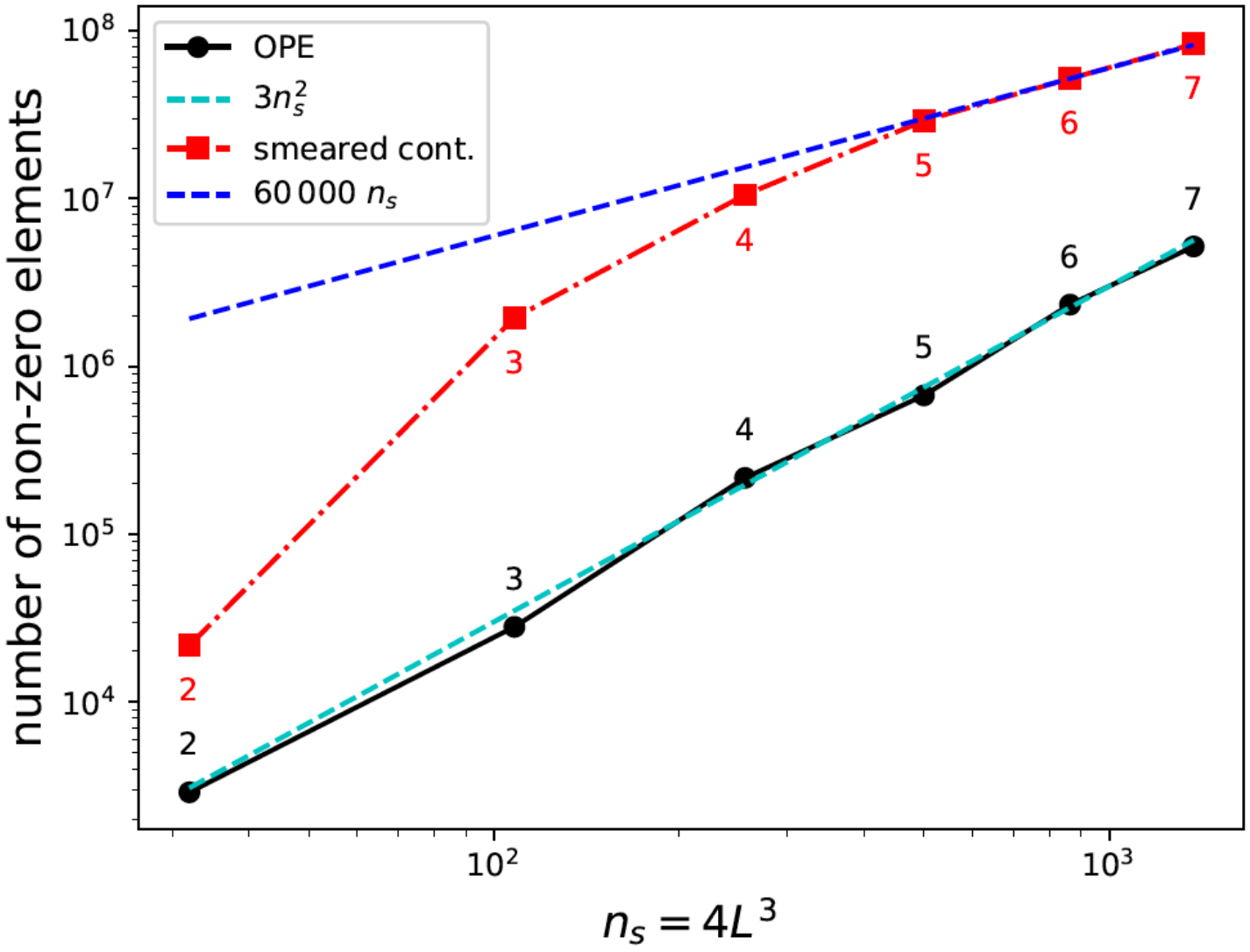
Finite size corrections: periodic boundary conditions



Twist-averaged boundary conditions converge faster to the infinite matter limit than periodic boundary conditions.

[Hagen, TP, Ekström, et al., PRC 89, 014319 (2014); C. Gros, Z. Phys. B C 86, 359 (1992).]

Number of nonzero matrix elements



Interactions from Elhatisari et al., Phys. Rev. Lett. 119, 222505 (2017)