Coupled-cluster theory within UNEDF

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1. Main accomplishments since last meeting
2. Status regarding high-performance computing
3. Roadmap for remainder of year-3 and for year-4

Annual UNEDF collaboration meeting

Pack Forest, WA, June 22-26 2009

Research partly funded by the US Department of Energy

Main accomplishments since last meeting

Science:

1. Medium-mass nuclei: saturation properties of chiral interactions; computation of densities
2. Solution of the center-of-mass problem
3. Neutron-rich oxygen isotopes

Computing / algorithm developments:

1. Triples correction Λ-CCSD(T) in spherical scheme (rationale: increased precision)
2. Parallelization of j-coupled coupled-cluster code (rationale: ensure convergence of “hard” interactions and/or heavier nuclei)

Publication Summary

Submitted articles

1. *Solution of the center-of-mass problem in nuclear structure calculations*, G. Hagen, T. Papenbrock, and D. J. Dean, arXiv:0905.3167, submitted to PRL (2009)
2. *Helium halo nuclei from low-momentum interactions*, S. Bacca, A. Schwenk, G. Hagen, and T. Papenbrock, arXiv:0902.1696, accepted by Eur. Phys. J. A (2009)
3. *Ab-initio computation of neutron-rich oxygen isotopes*, G. Hagen, T. Papenbrock, D. J. Dean, M. Hjorth-Jensen, and B. Velamur Asokan, to be submitted to Phys. Rev. C (2009).

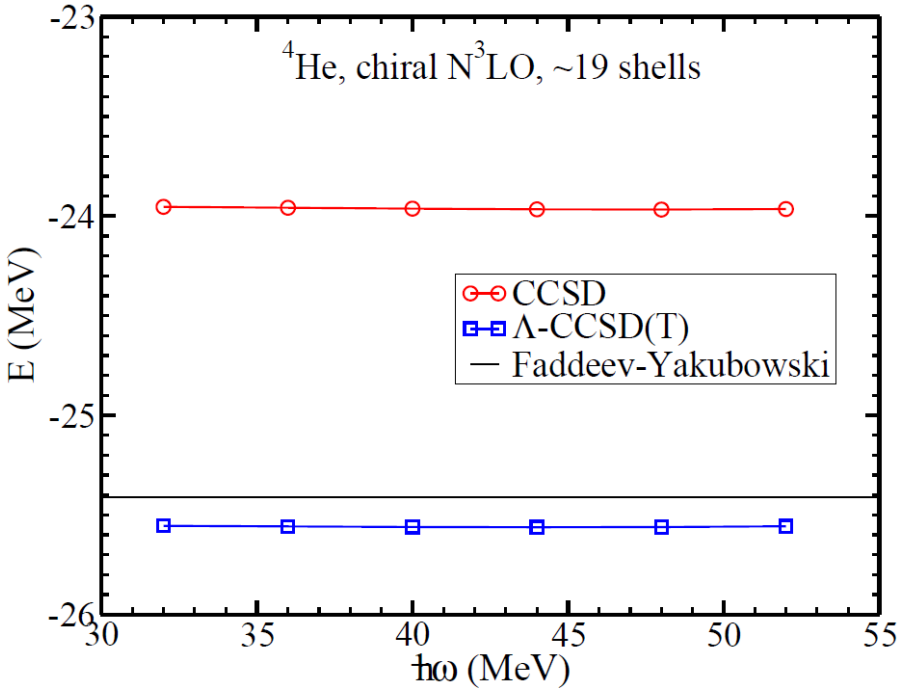
Published since July 2008

1. *Computational aspects of nuclear coupled-cluster theory*, D. J. Dean, G. Hagen, M. Hjorth-Jensen, and T. Papenbrock, Comput. Sci. Disc. 1, 015008 (2008)
2. *Broyden's Method in Nuclear Structure Calculations*, A. Baran, A. Bulgac, M. McNeil Forbes, G. Hagen, W. Nazarewicz, N. Schunck, M. V. Stoitsov, Phys. Rev. C 78, 014318 (2008)
3. *Medium-mass nuclei from chiral nucleon-nucleon interactions*, G. Hagen, T. Papenbrock, D. J. Dean, and M. Hjorth-Jensen, Phys. Rev. Lett. 101, 092502 (2008).
4. *Comment on "Ab Initio study of 40Ca with an importance-truncated no-core shell model",* D. J. Dean, G. Hagen, M. Hjorth-Jensen, T. Papenbrock, A. Schwenk , Phys. Rev. Lett. 101, 119201 (2008).

Invited talks

1. "Coupled cluster theory for nuclei", Symposium on "50 Years of Coupled Cluster Theory" INT program Atomic, Chemical, and Nuclear Developments in Coupled Cluster Methods, Seattle, WA, June 30 - July 2, 2008. (GH)
2. "Coupled cluster theory for medium-mass nuclei", INT program Atomic, Chemical, and Nuclear Developments in Coupled Cluster Methods, Seattle, WA, June 30 - July 2, 2008. (TP)
3. "Coupled-cluster theory for medium-mass nuclei", Heraeus workshop "Ab-initio nuclear structure - Where do we stand?", Bad Honnef, Germany, July 2008 (TP)
4. "Nuclear Coupled-Cluster approach", ENAM'08 on Exotic Nuclei and Atomic Masses. September 7-13 2008, Ryn, Poland (GH)
5. “Nuclear coupled-cluster theory”, Kernz 08, Queensland, New Zealand, Dec 1-5, 2008. (DJD)
6. “Coupled-cluster methods for medium heavy nuclei”, From ab initio methods to density-functional theory, CMA-CTCC workshop on computational quantum mechanics, January 13, 2009, UiO, Norway (GH)
7. "Coupled-cluster theory for nuclei", 3rd LACM-EFES-JUSTIPEN Workshop, Joint Institute for Heavy Ion Research, Oak Ridge National Laboratory February 23-25, 2009 (GH)
8. "Ab-initio Coupled Cluster Theory for Nuclei", INT Program "Effective Field Theories and the Many-Body Problem", Seattle, WA, April 2009 (GH)
9. “Tentative solution to the center-of-mass problem", INT Program "Effective Field Theories and the Many-Body Problem", Seattle, WA, May 2009 (TP)
10. "Coupled-cluster theory for nuclei", CEA Workshop on Many-Body open quantum systems, Saclay, May 18, 2009 (GH)
11. "Coupled-cluster theory for medium-mass nuclei", 8^{th} international conference on Radioactive Ion Beams (RNB-8), Grand Rapids, MI, May 26-30, 2009 (TP)

Accuracy & precision: ^{4}He from a chiral N^{3}LO [Entem & Machleidt]



[Hagen, TP, Dean, arXiv:0905.3167]

1. Results exhibit practically no dependence on the employed model space.
2. The coupled-cluster method, in its Λ-CCSD(T) approximation, 150keV over binding.
3. Independence of model space of N major oscillator shells with frequency ω:

   $N\hbar\omega > \hbar^2\lambda^2/ m$ to resolve momentum cutoff λ

   $\hbar\omega < N\hbar^2/(mR^2)$ to resolve nucleus of radius R

Summary: CCSD results with a chiral N^{3}LO (NN only)

Nucleus	E/A	V/A	$\Delta E/A$	R	$R_{\rm exp}$
^{4}He	-5.99	-22.75	1.08	1.86	1.64
^{16}O	-6.72	-30.69	1.25	2.71	2.74
^{40}Ca	-7.72	-36.40	0.84	3.24	3.48
^{48}Ca	-7.40	-37.97	1.27	3.22	3.47
^{48}Ni	-6.02	-36.04	1.21	3.50	

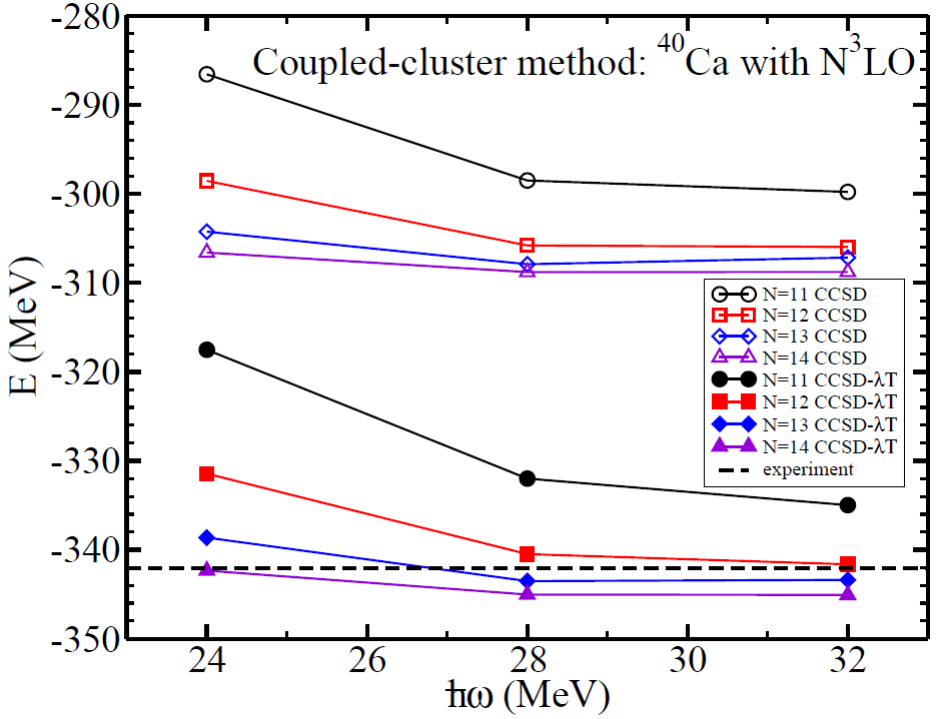
[Hagen, TP, Dean, Hjorth-Jensen, PRL 101, 092502 (2008)]

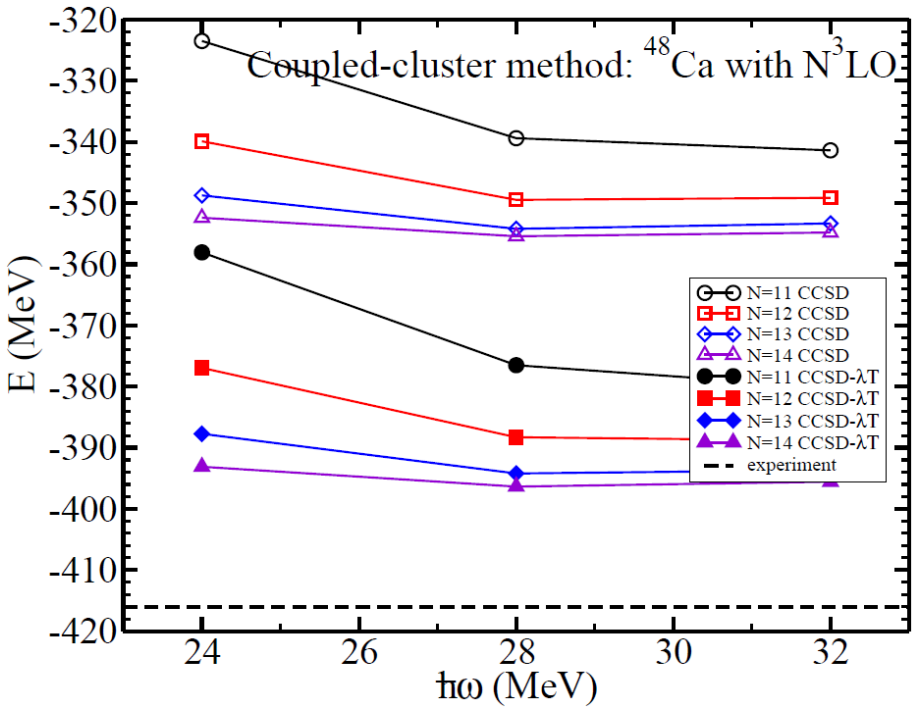
Main results

1. Well converged CCSD results with respect to size of model space (< 1% change in binding energy when going from 14 to 15 oscillator shells.
2. Three-nucleon force and triples corrections expected to yield ~1MeV additional binding?
3. Mirror nuclei ^{48}Ca and exotic ^{48}Ni differ by 1.38 MeV / A → close to mass-table predictions

How do corrections due to three-body clusters modify this picture?

Triples corrections:





- Triples add about 10% of the CCSD correlation energy; ~0.8 MeV per nucleon
- Entem & Machleidt's N^{3}LO nucleon-nucleon only comes closer than expected (from power counting) to experiment
- **Possible show case: ^{48}Ca with triples corrections and three-nucleon forces**

Center-of-mass problem

Intrinsic nuclear Hamiltonian

$$\begin{aligned} H_{\rm in} &= T - T_{\rm cm} + V \ , \\ &= \sum_{1\le i<j\le A} \left(\frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + V(\vec{r}_i - \vec{r}_j) \right) \end{aligned}$$

H_{in} is invariant under translations; it commutes with <u>any</u> center-of-mass Hamiltonian H_{cm}.

Approach that preserves translational and rotational invariance:

☺ Jacobi coordinates

☹ Antisymmetrization scales as A! → limited to A<8 or so.

Antisymmetrization best dealt within second quantization:

☹ No single-particle basis available that consists of simultaneous eigenstates of the angular momentum operator and the momentum operator.

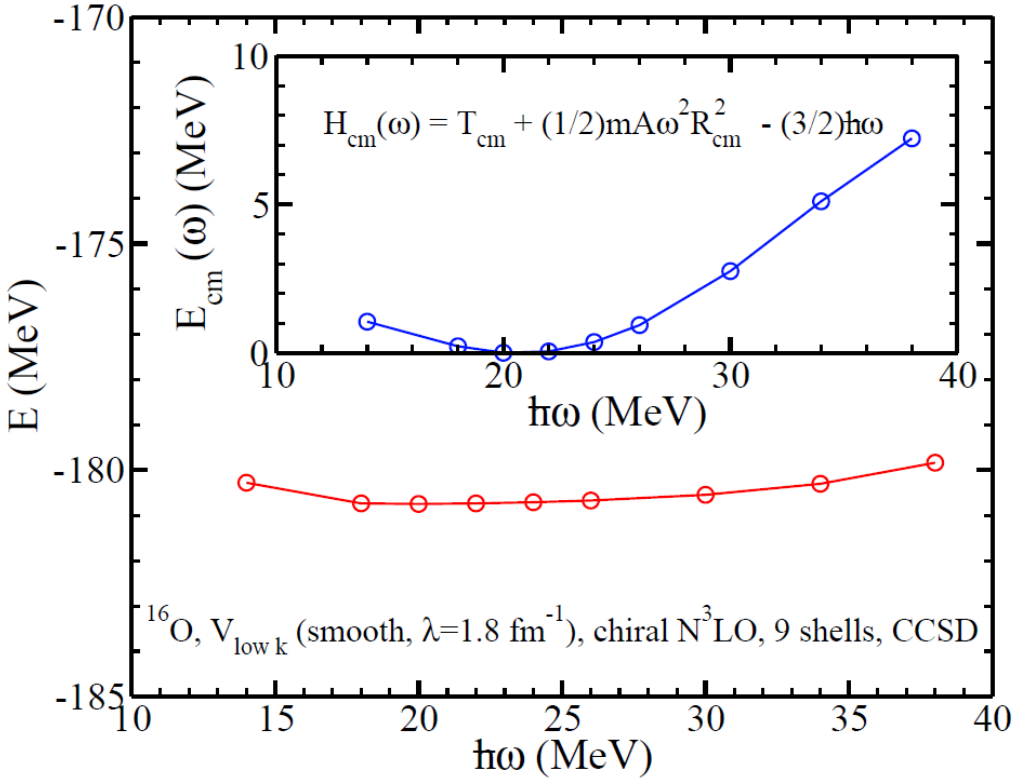
☺ Within a complete $N\hbar\omega$ oscillator space, the wave function is guaranteed to factorize

Intrinsic wave function ψ_{in} invariant under translation

Center-of-mass wave function ψ_{cm} is Gaussian whose width is set by the oscillator length of the employed oscillator basis

Please note: The factorization is key. The form of ψ_{cm} is irrelevant. It only needs to be the ground state of a suitably chosen center-of-mass Hamiltonian.

^{16}O with V_{lowk} (1.8/fm, smooth) within CCSD



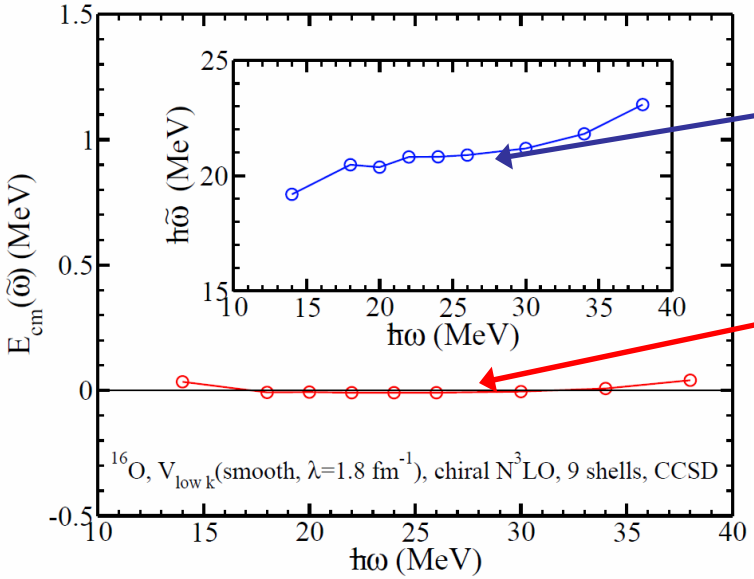
1. Hartree-Fock basis used. Not an $N\hbar\omega$ space
2. Ground-state energy varies little with frequency of oscillator basis.
3. Ground-state energy obviously independent of center-of-mass energy.
4. Center-of-mass energy generally nonzero → coupled-cluster wave function not eigenstate of $H_{cm}(\omega)$. [Beware of misconception: this does not imply that the wave function does not factorize.]

However:

1. Center-of-mass energy $E_{cm}(\omega) \equiv \langle H_{cm}(\omega)\rangle$ vanishes at $\hbar\omega \approx 20$MeV
2. **At $\hbar\omega \approx 20$MeV, the coupled-cluster wave function factorizes**
3. What is ψ_{cm}? **Assume it is a Gaussian with modified width**, i.e. ground state of

$$H_{\rm cm}(\tilde{\omega}) = T_{\rm cm} + \frac{1}{2}mA\tilde{\omega}^2 R^2_{\rm cm} - \frac{3}{2}\hbar\tilde{\omega}$$

Coupled-cluster wave function factorizes to a very good approximation!



Curve becomes practically constant in larger model spaces. Note: spurious CoM excitations are of order 20 MeV ≫ E_{cm}.

E_{cm} is slightly negative (size -0.01 MeV) due to non-variational character of coupled-cluster method.

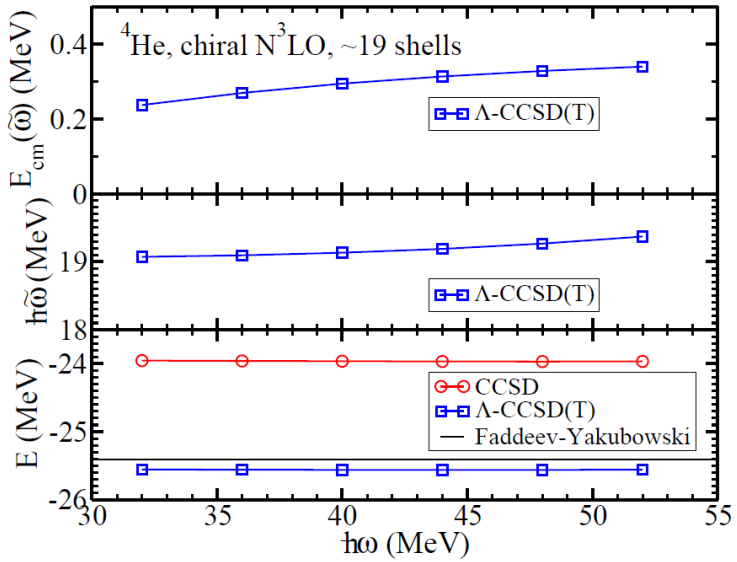
Coupled-cluster state is ground state of suitably chosen center-of-mass Hamiltonian.

Factorization between intrinsic and center-of-mass coordinate realized within high accuracy.

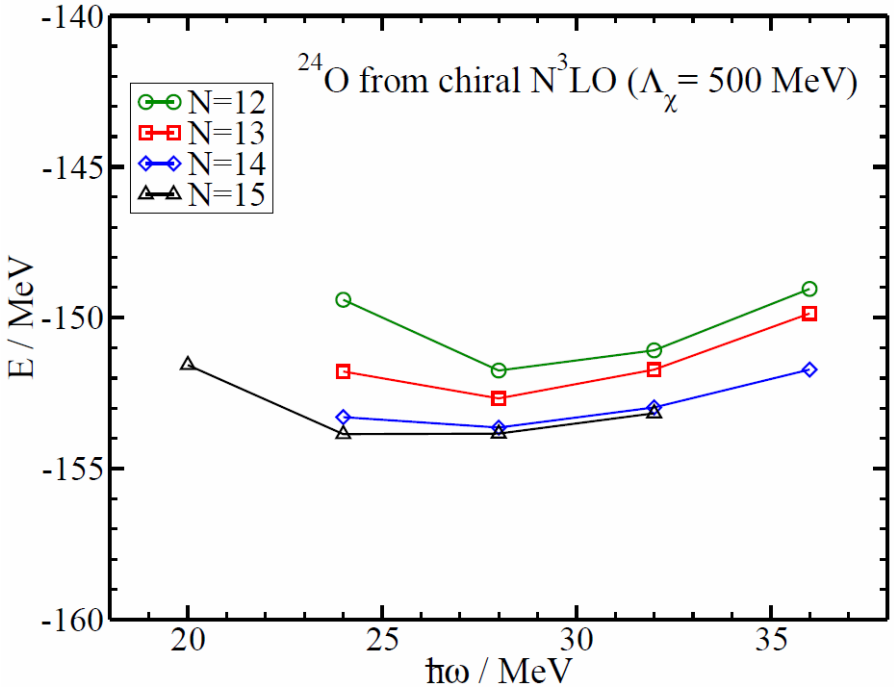
Approximate factorization also observed for “harder” interactions.

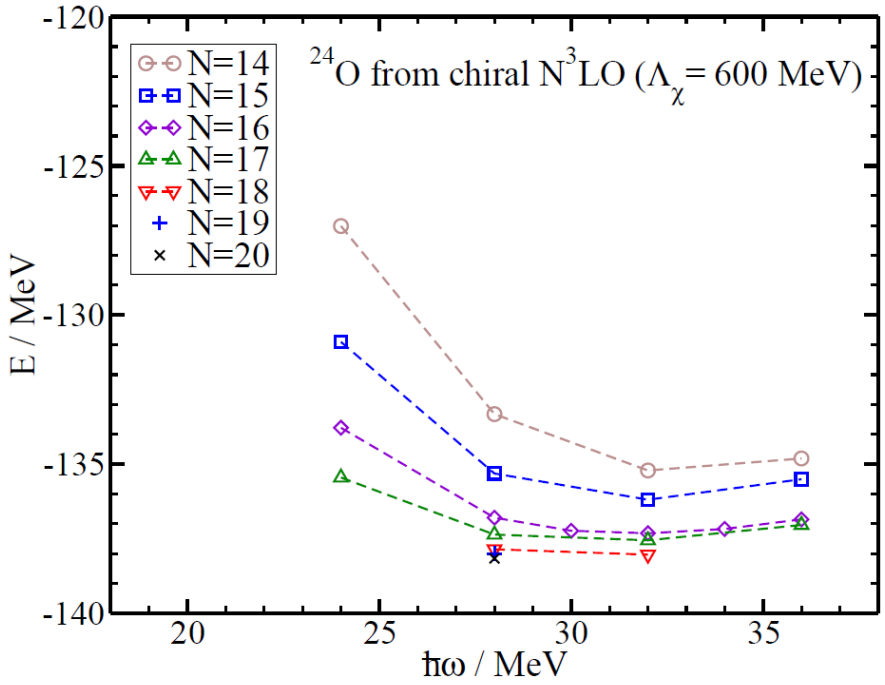
Finding valuable for computation of intrinsic densities.

[Hagen, TP, Dean, arXiv:0905.3167]



Neutron-rich oxygen isotopes





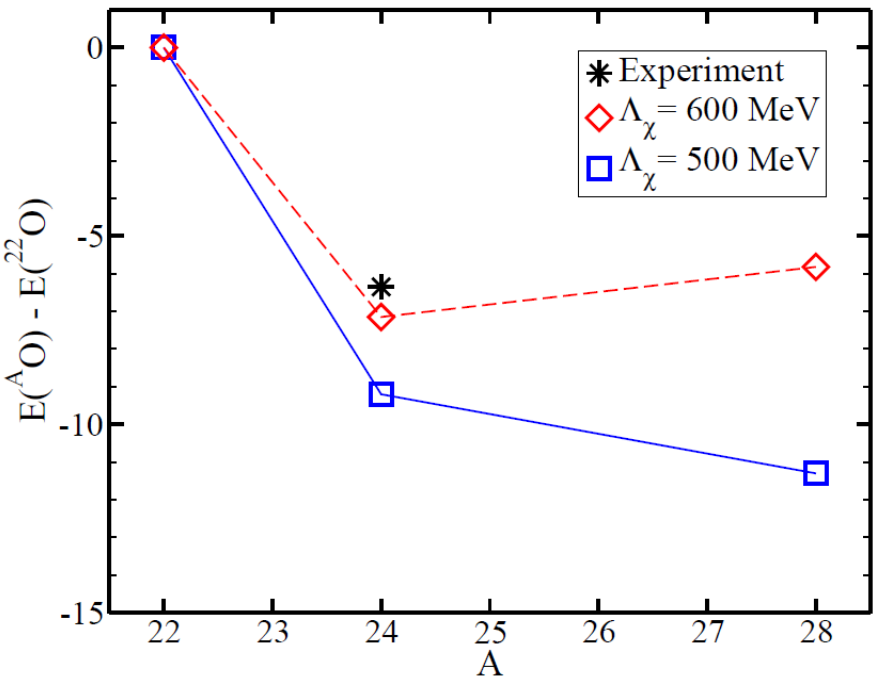
Λ=500 MeV potential converges in about 15 major oscillator shells

Λ=600 MeV potential converges in about 20 shells

Cutoff dependence → dependence of results on short-ranged part of three-nucleon force

Summary of preliminary results

Energies	^{16}O	^{22}O	^{24}O	^{28}O
($\Lambda_\chi = 500$ MeV)				
E_0	24.11	50.37	56.19	71.58
ΔE_{CCSD}	-144.77	-175.79	-190.39	-207.67
ΔE_3	-13.31	-19.22	-19.64	-19.85
E	-120.66	-144.64	-153.84	-155.94
($\Lambda_\chi = 600$ 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	



Estimate of theoretical uncertainties:

1. Finite model space ≲2MeV
2. Truncation at triples clusters ~2MeV (educated guess)
3. Omission of three-nucleon forces (omitted short-range physics ↔cutoff dependence) ~15MeV

Ab-initio theory cannot rule out a stable ^{28}O.

Three-body forces largest potential contribution that decides this question.

Computational status

Data organization

- Interaction spread across processors
- cluster amplitudes stored locally
- oxygen-16 in 20 shells ~ 1500 processor hours per model space

Challenge

- Number of j-coupled matrix elements of interactions fluctuate strongly for given sets of quantum numbers
- load balancing non-trivial: Calculation of estimated computational cost → distribution of data
- scaling (load-balancing) up to few hundred processors
- ideas / input welcome!

Progress for year 3

Proposed work	**Status**
Calculations of Ca and Ni isotopes (energies & densities)	^{16,22,24,28}O and ^{40,48}Ca
Derive and implement triples corrections	Done
Parallelization of spherical coupled-cluster code	Scales to few hundred processors
Interface with DFT: response of energy and density to external potentials; Expansion (DME) of CCSD 1-particle density matrix	Fully possible now within CCSD; more accurate triples corrections not yet
Employ densities for optical potentials (with Ken Amos; with Charlotte Elster)	Under way

Personnel

UNEDF collaborators

D. J. Dean (presently @ 20% time) → Department of Energy

G. Hagen

T. Papenbrock

Jason Holt (TRIUMF → ORNL/UT in summer 2009)

CS support: Badri Velamur Asokan (ORNL → private sector), Hai Ah Nam (ORNL)

Development of coupled-cluster method with relevance for UNEDF (by students co-supervised by Hagen and Hjorth-Jensen)

Oyvind Jensen (student at University of Bergen; spectroscopic factors)

Gustav Jansen (student at University of Oslo; closed shell ±2 nucleons)

Johannes Rekkedal (student at University of Oslo; coupled cluster for nuclear matter)

Future plans (remainder of year 3 and for year 4)

1. Interface with DFT (response of density to external potentials, check DME)
2. Toward ab-initio reactions
    1. Spectroscopic factors
    2. CC densities as microscopic input for optical potentials / g-folding methods
    3. Lorentz integral transform
3. Role of three-nucleon forces in medium-mass nuclei