Coupled-cluster theory within UNEDF

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and Oak Ridge National Laboratory

UNEDF: G. Hagen (ORNL), J. Holt, T. Lesinski (UT/ORNL)

CS support: H. A. Nam, B. Velamur Asokan (ORNL)

External collaborators: K. Amos (Melbourne), S. Bacca (TRIUMF), N. Barnea (Jerusalem), D. J. Dean (ORNL), M. Hjorth-Jensen (Oslo)

1. Main accomplishments since last meeting
2. Status regarding high-performance computing
3. Roadmap for remainder of year 4 and for year 5

Annual UNEDF collaboration meeting

East Lansing, MI, June 21-25 2010 Research partly funded by the US Department of Energy
Main accomplishments since last meeting

**Science:**

1. Computation of proton halo state and resonances in A=17 nuclei
2. Computation of spectroscopic factors
3. Long article on nuclear structure with NN interactions from chiral EFT and from $V_{\text{low } k}$ and SRG
4. Progress on interfacing with DFT and reactions (unpublished)
5. Moving toward reactions (optical potentials via g-folding models from ab initio densities; Lorentz integral transform)
6. Inclusion of 3NF (normal ordered contributions to NN within HF basis)

**Computing / algorithm developments:**

1. Inclusion of continuum effects within the spherical coupled-cluster code (rationale: description of open quantum systems)
2. Implementation of spherical equation-of-motion methods for computation of A±1 nuclei (from closed shell nucleus A)
Publication Summary

Submitted articles


Published since July 2009


Talks


2. **Ab-initio approach to nuclei beyond the valley of stability**, ECT Workshop on Confrontation and Convergence in Nuclear Theory, ECT, Trento, Italy, July 27-31, 2009 (GH)


4. **Coupled Cluster Approach to Nuclear Structure**, Internal nuclear physics seminar at the University of Tokyo, Tokyo, Japan, November 10, 2009 (GH)

5. **Three-Nucleon Forces for Medium-Mass Nuclei Towards the Dripline**, Nuclear Theory Seminar University of Tokyo Tokyo, Japan; November 16, 2009 (JH)


7. **Coupled Cluster Approach to Nuclear Structure**, Nuclear physics seminar at RIKEN, Waco, Japan, November 18, 2009 (GH)


11. **Role of the Continuum in Coupled Cluster Theory**, INT workshop on Weakly Bounds Systems in Atomic and Nuclear Physics, INT, Seattle, March 8 - 12, 2010 (GH)


13. **Three-Nucleon Forces and Nuclear Structure in Neutron-Rich Calcium Isotopes**. The 4th LACM-EFES-JUSTIPEN Workshop Joint Institute for Heavy Ion Research Oak Ridge, TN; March 17, 2010 (JH)


15. **Three-Nucleon Forces for Medium-Mass Nuclei Towards the Dripline**, New Quests in Nuclear Structure 10th International Spring Seminar on Nuclear Physics Vietri Sul Mare, Italy; May 22, 2010 (JH)


17. **Three-Nucleon Forces and Fully Microscopic Description of Neutron-Rich Nuclei**, Nuclear Physics Seminar Yukawa Institute for Theoretical Physics; University of Kyoto Kyoto, Japan; June 13, 2010 (JH)

Personnel

UNEDF collaborators: G. Hagen, J. Holt, (T. Lesinski → UW), T. Papenbrock

CS support: Hai Ah Nam (ORNL)

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

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

Gustav Jansen (student at University of Oslo; closed shell ±2 nucleons)
Low lying states in $A=17$ nuclei

- Continuum has to be treated properly
- Our focus is on single-particle states
- Previous study: shell model in the continuum with $^{16}\text{O}$ core
  
Bound states and resonances in $^{17}$F and $^{17}$O

Single-particle basis consists of bound, resonance and scattering states

- Gamow basis for $s_{1/2}$, $d_{5/2}$ and $d_{3/2}$ single-particle states
- Harmonic oscillator states for other partial waves

Computation of single-particle states via “Equation-of-motion CCSD”

- Excitation operator acting on closed-shell reference
- Here: superposition of one-particle and 2p-1h excitations

\[ R_{\mu} = r^a a^+_a + \frac{1}{2} r^b a^+_a a^+_b a_b \]

\[ [\overline{H}, R_{\mu}] |\phi_0\rangle = \omega_{\mu} R_{\mu} |\phi_0\rangle \]

- Gamow basis weakly dependent on oscillator frequency
- $d_{5/2}$ not bound; spin-orbit splitting too small
- $s_{1/2}$ proton halo state close to experiment

Variation of cutoff probes omitted short-range forces

- Proton-halo state ($s_{1/2}$) very weakly sensitive to variation of cutoff
- Spin-orbit splitting increases with decreasing cutoff
CCM results with a chiral $N^3$LO (NN only)

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>CCSD $E/A$</th>
<th>$\Delta E/A$</th>
<th>$\Lambda$-CCSD(T) $E/A$</th>
<th>$\Delta E/A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{16}$O</td>
<td>-6.72</td>
<td>1.25</td>
<td>-7.56</td>
<td>0.41</td>
</tr>
<tr>
<td>$^{40}$Ca</td>
<td>-7.72</td>
<td>0.84</td>
<td>-8.63</td>
<td>-0.08</td>
</tr>
<tr>
<td>$^{48}$Ca</td>
<td>-7.40</td>
<td>1.27</td>
<td>-8.26</td>
<td>0.40</td>
</tr>
</tbody>
</table>

[Hagen, TP, Dean, Hjorth-Jensen, arXiv:1005.2627]

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. $\Lambda$-triples correction adds 0.8MeV per nucleon in binding energy.

3. Three-nucleon force and triples corrections expected to yield 0.4MeV additional binding?
Research proposed at last UNEDF meeting
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
Aim: expansion of density functional up to quadratic terms around CCSD density for a given nucleus.

- Zeroth order: ground-state energy
- 1st order: Kohn Sham potentials reproduce CCSD densities for non-interacting nucleons.
- 2nd order: add small external potentials and extract second derivative of functional from response of density (near future).

\[ J(r) = -i \sum_i \rho_i \phi_i^\dagger(r) \sigma \times \nabla \phi_i(r) \]

**FIG. 1.** Local neutron density in $^{48}$Ca from CCSD and the fit of an external KS potential.

**FIG. 2.** Spin-orbit neutron density in $^{48}$Ca from CCSD and the fit of an external KS potential.

**FIG. 3.** Neutron spin-orbit field $^{48}$Ca the fit of an external KS potential on CCSD results and a naive Skyrme density-gradient shape.
Spectroscopic factors within CCM
nucleon removal from $^{16}\text{O}$

\[ S_{A-1}^A (l j) = \sum_n | \langle A - 1 | \tilde{a}_{nlj} | A \rangle |^2 \]

FIG. 4: (Color online) Spectroscopic factor SF(1/2−) for neutron and proton removal as a function of the oscillator spacing $\hbar \omega$ for nucleon-nucleon interactions with different cutoffs in a model space with $N = 6$.

Ø. Jensen, G. Hagen, TP, D. J. Dean, and J.S. Vaagen, arXiv:1004.2611
Densities and elastic reaction cross sections
(in collaboration with Ken Amos; figures by Ken Amos)

- Optical potential based on CC density computed with an N$^3$LO potential.
- $g$-folding model employs different potential (coordinate space; Yukawa terms)

Densities based on one-body density matrix – no center-of-mass correction yet.
Lorentz integral transform – preliminary results
(in collaboration with S. Bacca and N. Barnea)

Cross section for monopole excitations of $^4$He

- Artificial broadening by 4MeV
- Elastic peak around zero frequency
- Inelastic peak at high energies 20-30MeV

To do
- Role of center-of-mass corrections
- Dipole excitations

$$R(\omega) = \sum_f |\langle f | \Theta | 0 \rangle|^2 \delta(E_f - E_0 - \omega)$$

$$\mathcal{L}(\sigma_R, \sigma_I) = \int d\omega \frac{R(\omega)}{(\omega - \sigma_R)^2 + \sigma_I^2}$$

$$\mathcal{L}(\sigma_R, \sigma_I) = \langle \tilde{\Psi} | \tilde{\Psi} \rangle$$

$$(H - E_0 - \sigma_R - i\sigma_I) |\tilde{\Psi}\rangle = \Theta |0\rangle$$
Computational status

Data organization
• Interaction spread across processors
• Cluster amplitudes stored locally
• Oxygen-16 in 20 shells ~ 1500 processor hours per model space
• Proton halo state in $^{17}$F: total cost of about 100,000 CPU hours on Jaguar.

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
# Progress for years 3-4

<table>
<thead>
<tr>
<th>Proposed work</th>
<th>Status</th>
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<tbody>
<tr>
<td>Interface with DFT: response of energy and density to external potentials</td>
<td>First results available</td>
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<tr>
<td>Spectroscopic factors</td>
<td>(^{15}\text{O}, {^{15}\text{N}}\text{ (m-scheme)}) In progress: spherical scheme</td>
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<tr>
<td>Employ densities for optical potentials (with Ken Amos)</td>
<td>First results</td>
</tr>
<tr>
<td>Lorentz integral transform (w/ Sonia Bacca and Nir Barnea)</td>
<td>First results (monopole excitations)</td>
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<td>Role of three-nucleon forces in medium-mass nuclei (w Sonia Bacca and Achim Schwenk)</td>
<td>Hartree-Fock transformation with 3NF implemented</td>
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<tr>
<td>Equation-of-motion techniques for computation of A ±1 nuclei from closed-shell nucleus A</td>
<td>Implemented: (^{17}\text{F}, {^{17}\text{O}})</td>
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Project is reasonably well on track
Future plans (remainder of year 4 and for year 5)

1. Interface with DFT, and toward ab initio reactions
   1. Intrinsic ground-state densities (w/ CoM corrections)
   2. CC densities as microscopic input for optical potentials / g-folding methods
   3. Lorentz integral transform (proof of principle)

2. Role of three-nucleon forces in medium-mass nuclei
   → Ab initio computation of $^{48}$Ca with 3NF as possible highlight

3. Toward ab-initio reactions
   1. Spectroscopic factors in j-coupled code
   2. Lorentz integral transform (applications)

4. Nuclear matter (PhD student Gustav Baardsen from UiO)