Perspectives on Nuclear Coupled-Cluster Theory

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A. Schwenk (TRIUMF), A. Nogga (Julich), …

It is better to know some of the questions than all of the answers.  -- James Thurber
Nothing shocks me. I’m a scientist.  -- Harrison Ford (as Indiana Jones)
Key science drivers of rare isotopes

- Test the predictive power of models by extending experiments to new regions of mass and proton-to-neutron ratio
- Identify new phenomena that will challenge existing many-body theory

- Create and study super heavy nuclei
- Characterize neutron skins and excitation modes
- Constrain r-process site and explosive nucleosynthesis
- Constrain nuclear equation of state (neutron star crusts)
- Societal Applications: Energy, Security
- Beyond ‘Standard Model’: $\beta\beta^0\nu$ decay; Dark Matter, EDM…

ROADMAP
Landscape and consequences

- Stable nuclei
- Nuclei known to exist
- Unexplored Territory
- r-process

Diagram showing the distribution of protons and neutrons, with labeled numbers and regions.
Shell gaps and structure

Digital photography of $^{45}\text{Fe}(2p)$
Nuclear ‘scale separation’ in weakly bound nuclei

\[ T_{1/2} \approx 8.6 \text{ ms} \]

... and mass of $^{11}\text{Li}$: $\Delta m/m = 7 \cdot 10^{-8}$
The challenges of theory for nuclei

“The first, the basic approach, is to study the elementary particles, their properties and mutual interaction. Thus one hopes to obtain knowledge of the nuclear forces. If the forces are known, one should, in principle, be able to calculate deductively the properties of individual nuclei. Only after this has been accomplished can one say that one completely understands nuclear structure....The other approach is that of the experimentalist and consists in obtaining by direct experimentation as many data as possible for individual nuclei. One hopes in this way to find regularities and correlations which give a clue to the structure of the nucleus....The shell model, although proposed by theoreticians, really corresponds to the experimentalist’s approach.”

–M. Goeppert-Mayer, Nobel Lecture

Verfication and Validation (V&V)

Doing the problem right. – Verify
Doing the right problem. – Validate
From the interaction to solving the nuclear many-body problem

Begin with a NN (+3N) Hamiltonian

$$H = -\frac{\hbar}{2} \sum_{i=1}^{A} \frac{\nabla_i^2}{m_i} + \frac{1}{2} \sum_{i<j} V_{2N}(\vec{r}_i, \vec{r}_j) + \frac{1}{6} \sum_{i<j<k} V_{3N}(\vec{r}_i, \vec{r}_j, \vec{r}_k) - T_{cm}$$

Basis expansions:
- Determine the appropriate basis
- Generate $H_{\text{eff}}$ in that basis (or not if basis is large)
- Use many-body technique to solve problem

Bare (GFMC)
(Local only, Av18 plus adjusted 3-body)

Basis expansion
(explain forces)

Substantial progress in many-body developments
- GFMC (ANL, LANL)
- NCSM (Arizona, ISU, LLNL)
- Coupled-cluster theory
(ORNL, UT, Oslo)
(will show some results)

$$|\Psi\rangle = \exp(T)|\Phi\rangle$$
Effective Lagrangian \( \rightarrow \) obeys QCD symmetries (spin, isospin, chiral symmetry breaking)

Lagrangian \( \rightarrow \) infinite sum of Feynman diagrams.

Invoke power counting:
Expand in \( O(Q/\Lambda_{QCD}) \)
Weinberg, Ordonez, Ray, van Kolck

NN amplitude uniquely determined by two classes of contributions: contact terms and pion exchange diagrams.

3-body (and higher) forces are inevitable.

Thus one hopes to obtain knowledge of the nuclear forces. If the forces are known… (MGM)
Effective field theory potentials bring a 3-body force

“...the force should be chosen on the basis of NN experiments (and possibly subsidiary experimental evidence...) (Bethe)

Challenge: Deliver the best NN and NNN interactions with their roots in QCD (eventually from LQCD, see Ishii, Aoki and Hatsuda, PRL99, 022001 (2007))
Renormalize interaction to model space

Project H into large basis;
Perform Lee-Suzuki (NCSM)
Use $\text{Heff}$ as 2-(+3) body interaction

$\text{Heff}$ has one-, two, three-, … A-body terms

Recovers Bare A-body in large space
Requires addition of 3-body force
for experimental binding (adjust to He-4)
Challenge: slow convergence

No exact reproduction of N eigenvalues

\[
\frac{d}{d\Lambda} V_{\text{low}}^\Lambda (k', k) = \frac{2}{\pi} \frac{V_{\text{low}}^\Lambda (k', \Lambda) T^\Lambda (\Lambda, k; \Lambda^2)}{1 - (k/\Lambda)^2}
\]

• Renormalize at a momentum cutoff $\Lambda$
• Project onto oscillator basis
• Preserves phase shifts to the cutoff
• “reasonable” convergence

Challenges:
• Does not recover bare result
• Requires 3-body force for experimental binding
  …adjust to He-4
• $\Lambda$-independence

Schwenk, Bogner, Furnstahl,…
Coupled Cluster Theory in a nutshell

\[ |\Psi\rangle = \exp(T)|\Phi\rangle \]

Correlated Ground-State wave function

Correlation operator

Reference Slater determinant

\[ T = T_1 + T_2 + T_3 + \cdots \]

\[ T_1 = \sum_{i<a \atop i < \varepsilon_f} t_{ai} a_i^+ a_i \]

\[ T_2 = \sum_{ij<\varepsilon_f \atop ab>\varepsilon_f} t_{abij} a_i^+ a_j^+ a_i a_j \]

Energy

\[ E = \langle \Phi | \exp(-T)H \exp(T)|\Phi\rangle \]

Amplitude equations

\[ \langle \Phi_{ij \cdots} | \exp(-T)H \exp(T)|\Phi\rangle = \langle \Phi_{ij \cdots} | H |\Phi\rangle = 0 \]

- Fully Size Consistent
- Fully Size Extensive
- Systematically improvable
- CCSD = Coupled-Clusters in Singles and Doubles
- CCSDT = CCSD and Triples
- EOM for densities and excited states
The binding energy of a nucleus is an extensive quantity: \( \text{BE} \propto A \)

Goldstone’s linked cluster theorem (1955): Formal diagrammatic proof of Brueckner’s conjecture that perturbation theory is size consistent. Only linked diagrams contribute to the energy of a (closed shell) nucleus.

Unlinked diagrams do not scale with mass number \( A \), and the sum of all unlinked diagrams is zero.

Theories that maintain a consistent scaling with size (“size-extensive”):
• Many-body perturbation theory
• “Exact” methods like matrix diagonalization within a full model space
• Coupled-cluster theory (CCSD, CCSDT, …)

Theoretical approaches that are not size extensive:
• Diagonalization in a space of np-nh excitations (\( n < A \)). (CISD, CISDT…)
Size (extensivity) matters!

Only size extensive theories produce a result and an error that scale as $A$. 

Our Coupled-Cluster history curve

- 1997/8 → Dean/Hjorth-Jensen collaborations start
- 2001 → Dean/Papenbrock collaborations start
- 1999 → DJD involved with chemists and materials people at Lab
- 2000 → Morten and collaborators start computational project at Oslo (leading to CMA)
- Oct 2007 → Dean to Director’s Office
- Jan 2008 → Hagen joins ORNL R&D staff
Benchmarking in light nuclei using $V_{\text{lowk}}$

1. Smaller $\hbar \omega \rightarrow$ perturbation theory breaks down (need non-iterative corrections)
2. He results are all with $l \leq 7$
3. In larger model spaces, the (T) correction is consistent
4. CoM 0.01 MeV (large model space)
Results in $^{16}\text{O}$

Approximately 1 MeV extrapolation error between (T) and T-1 (out of 140 MeV from CCSD)
$^{40}$Ca and pulling it all together

10$^{63}$ many-body basis states

How does this compare with importance truncated CI calculations?

SAME interaction (we supplied)

$^{16}$O at 4p-4h: -142.8 MeV

$^{40}$Ca at 3p-3h: -461.2 MeV

$^{40}$Ca at 4p-4h: -471.0 MeV

$\langle H_{cm} \rangle < 0.2$ MeV for $^{40}$Ca

Error estimate: $<< 1\%$ $< 1\%$ $1\%$

<table>
<thead>
<tr>
<th></th>
<th>$^4$He</th>
<th>$^{16}$O</th>
<th>$^{40}$Ca</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_0$</td>
<td>-11.8</td>
<td>-60.2</td>
<td>-347.5</td>
</tr>
<tr>
<td>$\Delta E_{CCSD}$</td>
<td>-17.1</td>
<td>-82.6</td>
<td>-143.7</td>
</tr>
<tr>
<td>$\Delta E_{CCSD(T)}$</td>
<td>-0.3</td>
<td>-5.4</td>
<td>-11.7</td>
</tr>
<tr>
<td>$E_{CCSD(T)}$</td>
<td>-29.2</td>
<td>-148.2</td>
<td>-502.9</td>
</tr>
<tr>
<td>exact (FY)</td>
<td>-29.19(5)</td>
<td></td>
<td></td>
</tr>
</tbody>
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Hagen, Dean, Hjorth-Jensen, Papenbrock, Schwenk, PRC76, 044305 (2007)

Dean, Hagen, Hjorth-Jensen, Papenbrock, Schwenk, comment submitted
The Hamiltonian is normal-ordered w.r.t. the vacuum state $|\Phi\rangle$.

$$
H = \sum_{pq} \varepsilon_{pq} \hat{a}^+_p \hat{a}_q + \frac{1}{4} \sum_{pqrst} \langle pr||sr\rangle \hat{a}^+_p \hat{a}^+_q \hat{a}_r \hat{a}_s \\
= \sum_i \varepsilon_{ii} + \frac{1}{2} \sum_{ij} \langle ij||ij\rangle \\
+ \sum_{ij} \left( \varepsilon_{pq} + \sum_i \langle pi||qi\rangle \right) \{ \hat{a}^+_p \hat{a}_q \} + \frac{1}{4} \sum_{pqrst} \langle pq||sr\rangle \{ \hat{a}^+_p \hat{a}^+_q \hat{a}_r \hat{a}_s \}
$$

Similarly, the Hamiltonian of the $3NF$ becomes

$$
\hat{H}_3 = \frac{1}{6} \sum_{ijk} \langle ijk||ijk\rangle + \frac{1}{2} \sum_{ijp} \langle ijp||ijq\rangle \{ \hat{a}^+_p \hat{a}_q \} \\
+ \frac{1}{4} \sum_{ipqrs} \langle ipq||irs\rangle \{ \hat{a}^+_p \hat{a}^+_q \hat{a}_s \hat{a}_r \} + \hat{h}_3 ,
$$

Vacuum energy and density-dependent one-body terms

Density-dependent two-body terms

Residual three-body terms

Note:
1. The form of the Hamiltonian is different for each nucleus under consideration.
3. “Density-dependent” terms are coherent sums over two- and three-body matrix elements.
Progress: inclusion of full TNF in CCSD: F-Y comparisons in $^4$He

Solution at CCSD and CCSD(T) levels involve roughly 67 more diagrams.....

Hagen, Papenbrock, Dean, Schwenk, Nogga, Wloch, Piecuch
PRC76, 034302 (2007)
CC results with $V_{\text{lowk}}$ from N3LO NN-interaction.
Small model space (N=3)
Only contact term at the $N^2$LO is retained in the 3-nucleon force.
3NF fitted to reproduce binding energy of $^4$He

$$H^A = T - T_{CM} + V_2(\Lambda) + V_3(\Lambda) + \cdots + V_A(\Lambda) \approx T - T_{CM} + V_2(\Lambda) + V_3(\Lambda)?$$

Testing $\Lambda$-dependence (preliminary)
Code parallelism

Memory distribution across processors

\[ t_2(ab, ij) = \sum_{kl<\epsilon_f} V(kl, cd) t_{ij}^{cd} t_{kl}^{ab} \]

Partial sum \( t_2 \) reside on each processor

Global reduce (sum) \( t_2 \), distribute

\[ V(ab, c1, d1) V(ab, c1, d2) V(ab, c2, d1) (a, b, c2, d2) \]

\( t_2 \) partial sum \( t_2 \) partial sum \( t_2 \) partial sum \( t_2 \) partial sum

+…
Implemented a CCSD J-coupled (Hagen) code for heavier nuclei:

- Scaling at CCSD goes from \( O(n_o^2 n_u^4) \) to \( O(n_o^{4/3} n_u^{8/3}) \)
- Can do up to 14 complete major shells on a single node.
- CCSDT ➔ Gold standard for these heavier nuclei (developing)
- Enables specified calculations for heavy nuclei
- The large model spaces mean that we can approach BARE interactions!
  - Must start with a spherical HF basis

- Is it technically feasible to go further? (YES)
- Does size extensivity work in the nuclear case? (YES)
- Opens some interesting doors for future research….
Ca isotopes from bare chiral NN potential at N³LO (no 3-body yet)

Chiral NN potential at N³LO underbinds by ~1MeV/nucleon. (Size extensivity at its best.)

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>ΔE / A [MeV]</th>
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<tbody>
<tr>
<td>⁴He</td>
<td>1.08 (0.73⁹⁸)</td>
</tr>
<tr>
<td>¹⁶O</td>
<td>1.25</td>
</tr>
<tr>
<td>⁴⁰Ca</td>
<td>0.84</td>
</tr>
<tr>
<td>⁴⁸Ca</td>
<td>1.27</td>
</tr>
<tr>
<td>⁴⁸Ni</td>
<td>1.21</td>
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$$\lambda \approx 3.5$$

$${\Delta E / A}$$
We will advance computational capability by 1000x over the next decade

<table>
<thead>
<tr>
<th>Mission: Deploy and operate the computational resources required to tackle global challenges</th>
<th>Vision: Maximize scientific productivity and progress on the largest scale computational problems</th>
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<tr>
<td>• Deliver transforming discoveries in materials, biology, climate, energy technologies, etc.</td>
<td>• Providing world-class computational resources and specialized services for the most computationally intensive problems</td>
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<tr>
<td>• Ability to investigate otherwise inaccessible systems, from supernovae to energy grid dynamics</td>
<td>• Providing stable hardware/software path of increasing scale to maximize productive applications development</td>
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**Future system: 1 EF**

- **Cray “Baker”:** 1 PF Leadership-class system for science
- **DARPA HPCS:** 20 PF Leadership-class sustained PF system
- **100-250 PF**
- **Future system:** 1 EF
Nuclear Coupled Cluster Theory Perspectives

Opportunity:
- Capitalize on CC developments to realize an ab initio foundation for nuclear structure (including the shell model) and reactions with calculations reaching into heavy nuclei
- Develop the CC technology to include powerful tools for investigating the relationship between ab initio approaches and DFT
- Enable future experimental directions through ab initio predictions of nuclear properties in uncharted regions

Resources:
- CC theory implementations described in this talk: CCSD, CCSD(T), CCSDT-1, V3-CCSD(T), Gamow-based CCSD(T), CCSDT, (some under development in J-scheme)
- Excited state calculations
- Effective (and now BARE) interaction expertise
- Software development at scale
- Dynamic and promising interface of nuclear theory and computational science
- Broad collaboration base
- Longstanding partnerships with DOE (NP and ASCR), Oslo/CMA among others

Strategy:
- Develop and deploy all necessary elements to calculate nuclear masses, excitation energies, and transition properties
- Develop ‘shell-model’ like effective interactions from CC theory
- Leverage ultrascale computing and nuclear theory expertise to solve a wide range interesting problems within the CC framework
- Develop ‘one-off’ problems for nurturing of post-docs and students (NRC grant)

Outcome: A cross-cutting theory for understanding and building nuclei from the ground up