Building Nuclei from the Ground Up: Nuclear Coupled-cluster Theory

Presented by

David J. Dean
Oak Ridge National Laboratory

Nuclear Coupled-cluster Collaboration:
T. Papenbrock, K. Roche, Oak Ridge National Laboratory
P. Piecuch, M. Wloch, J. Gour, Michigan State University
M. Hjorth-Jensen, Oslo
A. Schwenk, Triumf

Funding: DOE-NP, SciDAC, DOE-ASCR
“Given a lump of nuclear material, what are its properties, and how does it interact?”

How do we describe nuclei we cannot measure?

- Robust, predictive nuclear theory exists for structure and reactions.
- Nuclear data needed to constrain theory.
- Goal is the Hamiltonian and nuclear properties:
  - Bare intra-nucleon Hamiltonian.
  - Energy density functional.
- Mission relevant to NP, NNSA.
- Half of all elements heavier than iron produced in r-process where limited (or no) experimental information exits.
- Nuclear reaction information relevant to NNSA and AFCI.
The Leadership Computing Facility effort will

- Enlarge ab-initio square to mass 100
- Enable initial global DFT calculations with restored symmetries

**All Regions:** Nuclear cross-section efforts (NNSA, SC/NP, Nuclear Energy)
Nuclear interactions: Cornerstone of the entire theoretical edifice

- Solved up to mass 12 with GFMC, converged mass 8 with diagonalization. We want to go much further!

- Depends on spin, angular momentum, and nucleon (proton and neutron) quantum numbers. Complicated interactions

\[ H = \sum_{i=1, A} \frac{-\hbar^2}{2M_i} \nabla_i^2 + \sum_{i<j} V(r_i, r_j) + V_{NNN} \]

- Real three-body interactions derived from QCD-based effective theories

- Method of Solution: Nuclear Coupled-Cluster Theory
Coupled-cluster theory: Ab initio in medium mass nuclei

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

**Correlated ground-state wave function**

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

\[ T_1 = \sum_{i<\epsilon_f} t_{ai} a_i^+ a_i \]

\[ T_2 = \sum_{ij<\epsilon_f} t_{abij} a_i^+ a_j^+ a_j a_i \]

**Correlation operator**

**Energy**

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

**Amplitude equations**

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

- It boils down to a set of coupled, nonlinear algebraic equations (odd-shaped tensor-tensor multiply).
- Storage of both amplitudes and interactions is an issue as problems scale up.
- Largest problem so far: \(^{40}\text{Ca}\) with 10 million unknowns, 7 peta-ops to solve once (up to 10 runs per publishable result).
- Breakthrough science: Inclusion of 3-body force into CC formalism (6-D tensor) weakly bound and unbound nuclei.
Coupled cluster theory for nuclei

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

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

\[ E = \langle \Phi | H | \Phi \rangle = \langle \Phi | e^{T H e^T} | \Phi \rangle \]

\[ \langle \Phi_{ij\ldots} | H | \Phi \rangle = 0 \]

\[ R \overline{H} | \Phi \rangle = E^* R | \Phi \rangle \]

\( R = \) excitation operator

POLYNOMIAL SCALING!! (good)
Ab initio in medium mass nuclei

$^4$He

$E(\nu\nu)$ with Fast convergence with cluster rank

$E_{\text{CCSD}}$ and $E_{\text{CCSD(T)}}$

Exact (FY) - 29.19(5)

<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>$\Delta E_{\text{CCSD}}$</td>
<td>-17.1</td>
<td>-82.6</td>
<td>-143.7</td>
</tr>
<tr>
<td>$\Delta E_{\text{CCSD(T)}}$</td>
<td>-0.3</td>
<td>-5.4</td>
<td>-11.7</td>
</tr>
<tr>
<td>$\Delta E_{\text{CCSD(T)}}$</td>
<td>-29.2</td>
<td>-148.2</td>
<td>-502.9</td>
</tr>
</tbody>
</table>

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

Inclusion of full TNF in CCSD: F-Y comparisons in $^4\text{He}$

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

Challenge: Do we really need the full 3-body force, or just its density dependent terms?

Coupling of nuclear structure and reaction theory (microscopic treatment of open channels)

Introduction of continuum basis states (Gamow, Berggren)
Ab initio weakly bound and unbound nuclei

Single-particle basis includes bound, resonant, non-resonant continuum, and scattering states. ENORMOUS SPACES...almost 1k orbitals. $10^{22}$ many-body basis states in $^{10}\text{He}$

Challenge: Include 3-body force

[feature article in Physics Today (November 2007)]
Solution of coupled-cluster equation

Basic numerical operation:

\[ t_{new}(ab, ij) = \sum_{k,l=1,n}^{n} V (kl, cd) t_{old}(cd, ij) t_{old}(ab, kl) \]

- System of non-linear coupled algebraic equations \( \rightarrow \) solve by iteration
- \( n \) = number of neutrons and protons
- \( N \) = number of basis states
- Solution tensor memory
  - \((N-n)^2 \cdot n^2\)
- Interaction tensor memory
  - \( N^4 \)
- Operations count scaling
  - \( O(n^2 \cdot N^4) \)
  - \( O(n^4 \cdot N^4) \) with 3-body
  - \( O(n^3 \cdot N^5) \) at CCSDT

- Many such terms exist.
- Cast into a matrix-matrix multiply algorithm.
- Parallel issue: block sizes of \( V \) and \( t \).
Code parallelism

Memory distribution across processors

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

Partial sum

\( t_2 \) reside on each processor

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

\( V(ab, c1, d1) \)
\( t_2 \) partial sum

\( V(ab, c1, d2) \)
\( t_2 \) partial sum

\( V(ab, c2, d1) \)
\( t_2 \) partial sum

\( V(a, b, c2, d2) \)
\( t_2 \) partial sum

\( + \ldots \)
Future direction

• Current algorithm scales to 1K processors with about 20% efficiency. Attacking problems in mass 40 region is doable with current code.

• Develop algorithm that spreads both the 2-body matrix elements and the CC amplitudes (in collaboration with Ken Roche) → Enables nuclei in the mass 100 region and should scale to 100K processors (under way).

• Designing further parallel algorithms that calculate nuclear properties to calculate densities and electromagnetic transition amplitudes.

• Eventual time-dependent CC for fission dynamics.
Contact

David J. Dean
Physical Sciences Directorate
Nuclear Theory
(865) 576-5229
deanj@ornl.gov

References:
Dean and Hjorth-Jensen, PRC 69, 054320 (2004); Kowalski, Dean, Hjorth-Jensen, Papenbrock, Piecuch, PRL 92, 132501 (2004); Wloch, Dean, Gour, Hjorth-Jensen, Papenbrock, Piecuch, PRL 94, 21501 (2005); Gour, Piecuch, Wloc, Hjorth-Jensen, Dean, PRC (2006); Hagen, Dean, Hjorth-Jensen, Papenbrock, PLB (2007); Hagen, Dean, Hjorth-Jensen, Papenbrock, Schwenk, PRC 76, 044305 (2007); Hagen, Papenbrock, Dean, Schwenk, Nogga, Wloch, Piecuch, PRC 76, 034302(2007); Dean, Physics Today (November 2007)