

Coupled-Cluster theory for UNEDF

G. Hagen (ORNL), D. J. Dean(ORNL) and T. Papenbrock (UT/ORNL)

OAK RIDGE NATIONAL LABORATORY and



Collaborators:

**S. Bogner, R. J. Furnstahl, O. Jensen, P. Maris ,
A. Schwenk, J. Vary and B. Velamuri Asokan**



Pack Forest UNEDF meeting 2008



Publications

Published since August 2007:

1. *Coupled cluster theory for three-body Hamiltonians*, G. Hagen, T. Papenbrock, D. J. Dean, A. Schwenk, A. Nogga, M. Wloch and P. Piecuch, Phys. Rev. C 76, 034302 (2007)
2. *Benchmark calculations for ^3H , ^4He , ^{16}O and ^{40}Ca with ab-initio coupled-cluster theory*, G. Hagen, D. J. Dean, M. Hjorth-Jensen, T. Papenbrock and A. Schwenk, Phys. Rev. C 76 044305 (2007).
3. *Beyond the nuclear shell model*, D. J. Dean, Physics Today 60 (2007).
4. *Progress and challenges in the theory of nuclei*, D. J. Dean, Nucl. Phys. A 805, 145 (2008)
5. *Computing Atomic Nuclei: the Universal Nuclear Energy Density Functional*, G. F. Bertsch, D. J. Dean and W. Nazarewicz, SciDAC Review, December, (2007)

Submitted/in Preparation:

1. *Medium mass nuclei from chiral nucleon-nucleon interactions*, G. Hagen, T. Papenbrock, D. J. Dean and M. Hjorth-Jensen, submitted to Phys. Rev. Lett.
2. *Broyden's method in Nuclear Structure Calculations*, A. Baran, A. Bulgac, M. M. Forbes, G. Hagen, W. Nazarewicz, N. Schunk and M. V. Stoitsov, submitted to Phys. Rev. C
3. *Comment on "Ab initio study of ^{40}Ca with an importance truncated no-core shell model"*, D. J. Dean, G. Hagen, M. Hjorth-Jensen, T. Papenbrock and A. Schwenk, arxiv:0709.0449, submitted to Phys. Rev. Lett.

Invited talks at international workshops/conferences

1. *Coupled-Cluster theory for medium-mass nuclei*, Nuclear Many-Body Approaches for the 21st Century, Institute for Nuclear Theory, Seattle, October 2007 (TP)
2. *Coupled-Cluster approach to nuclear structure*, Theory network for nuclear structure and reactions, ECT*, Trento, Italy, January 2008 (GH)
3. *Coupled-Cluster theory for medium-mass nuclei*, International Workshop XXXVI on Gross Properties of Nuclei and Nuclear Excitations, Hirschegg/Austria, January 2008 (TP)
4. *Ab-initio coupled-cluster theory for weakly bound and unbound nuclear states*, Halo08, TRIUMF/Vancouver, March 2008 (GH)
5. *Atomic nuclei – computational challenges in an ab-initio approach*, International conference Nuclear Structure at the Extremes, Paisley/Scotland May 2008 (DJD)
6. *Ab-initio calculations of stable and weakly bound nuclei with coupled-cluster theory*, From quarks to the nuclear many-body problem, Oslo/Norway, May 2008 (GH)
7. *Progress and challenges in the physics of nuclei*, From quarks to the nuclear many-body problem, Oslo/Norway, May 2008 (DJD)

Past accomplishments

1. [Benchmark calculations \(aim: validation of method\)](#)
2. [Spherical CCSD code \(aim: converged for medium mass nuclei\)](#)
3. [Computation of densities and one-body observables \(aim: interface with DFT\)](#)

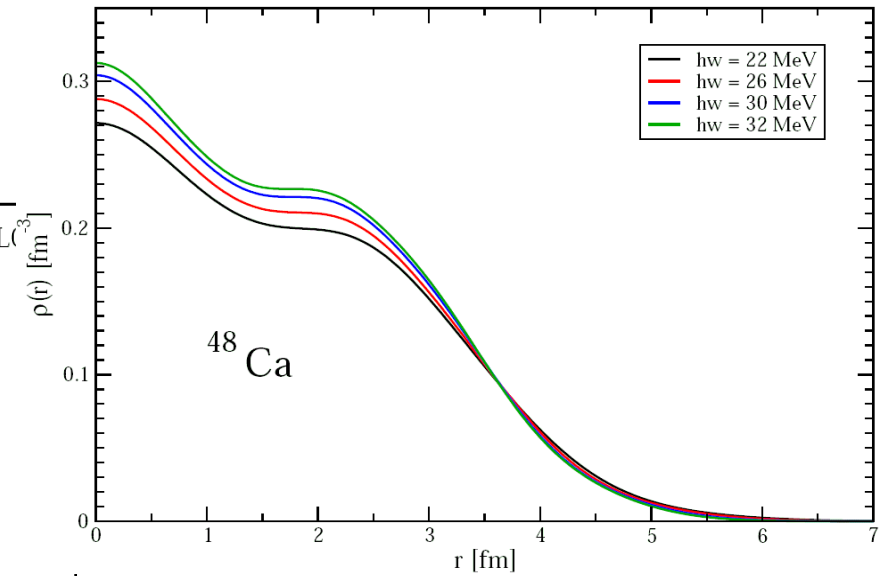
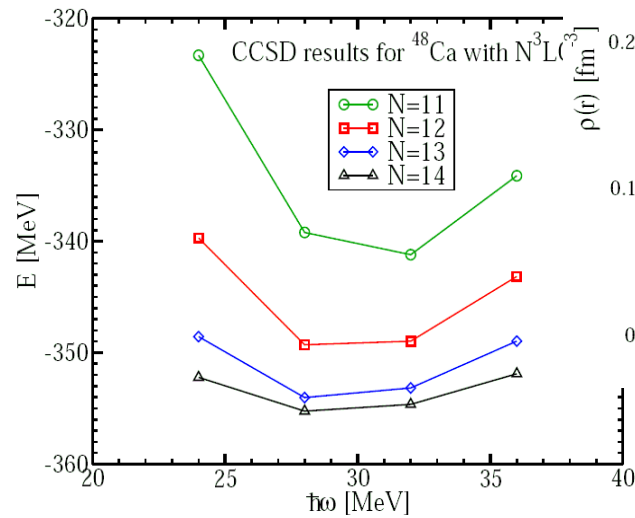
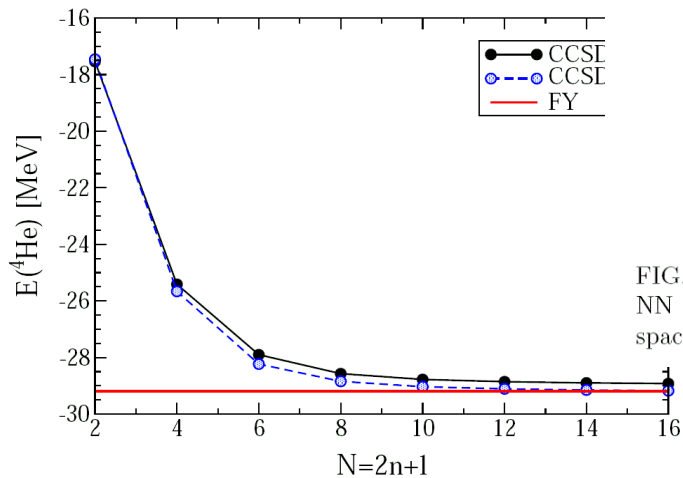
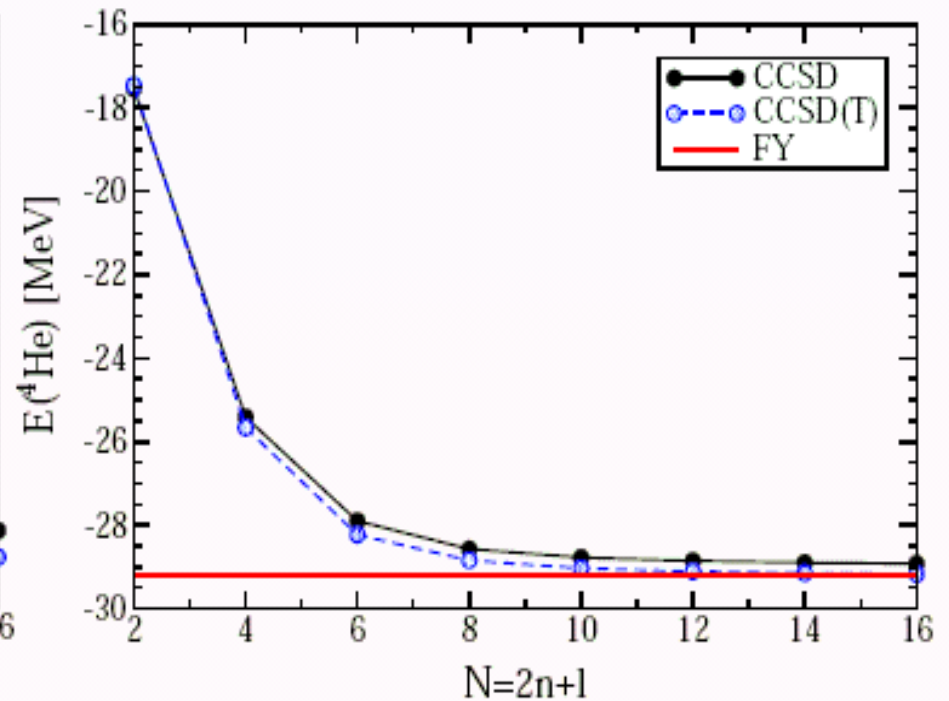
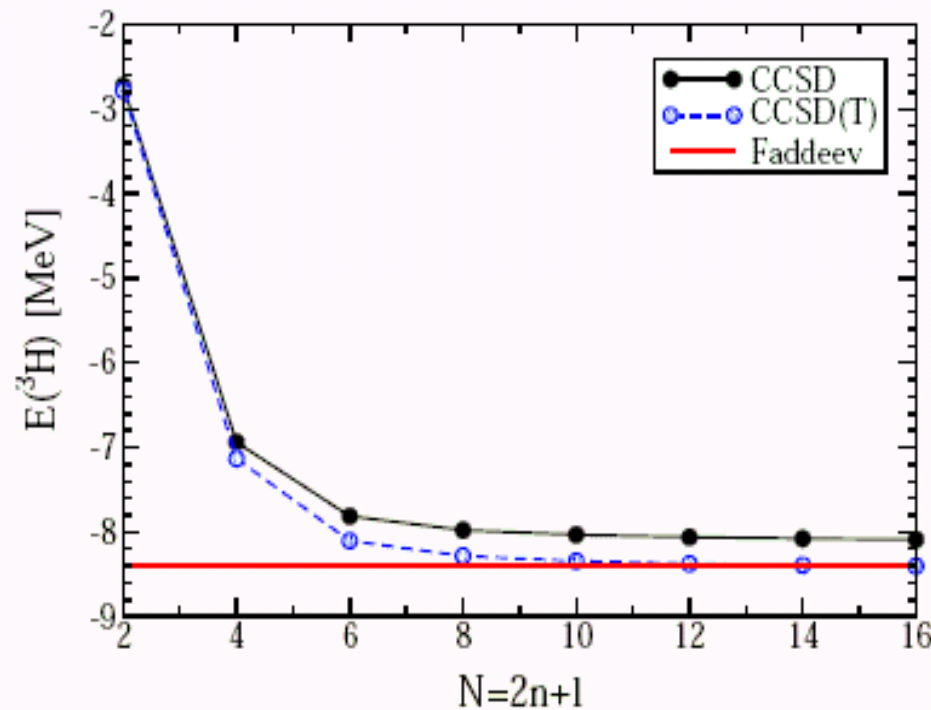


FIG. 4: (Color online) CCSD results for ^{48}Ca from the chiral NN potential at order $N^3\text{LO}$ as a function of the oscillator spacing $\hbar\omega$ and the size of the model space.

1. Coupled-Cluster meets benchmarks of ${}^3\text{H}$ and ${}^4\text{He}$!

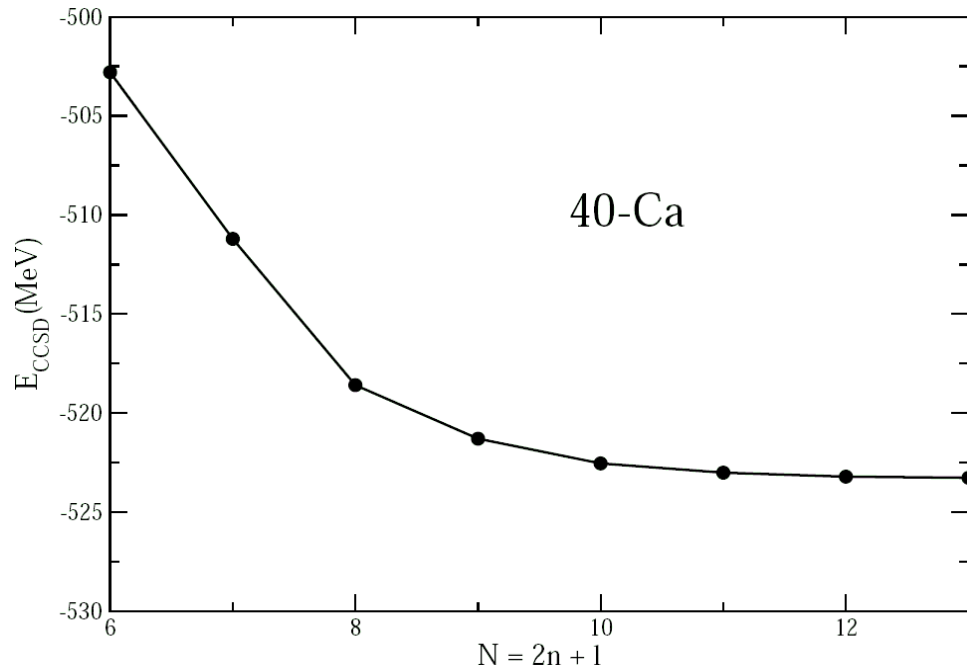
CCSD(T) and Faddeev (-Yakubovsky) results for ${}^3\text{H}$ and ${}^4\text{He}$ using $V_{\text{low}-k}$ from AV18 with $\Lambda = 1.9\text{fm}^{-1}$. **CCSD(T) are within the errors (50 keV) of the Faddeev results!** (G. Hagen et al., Phys. Rev. C 76, 044305 (2007))



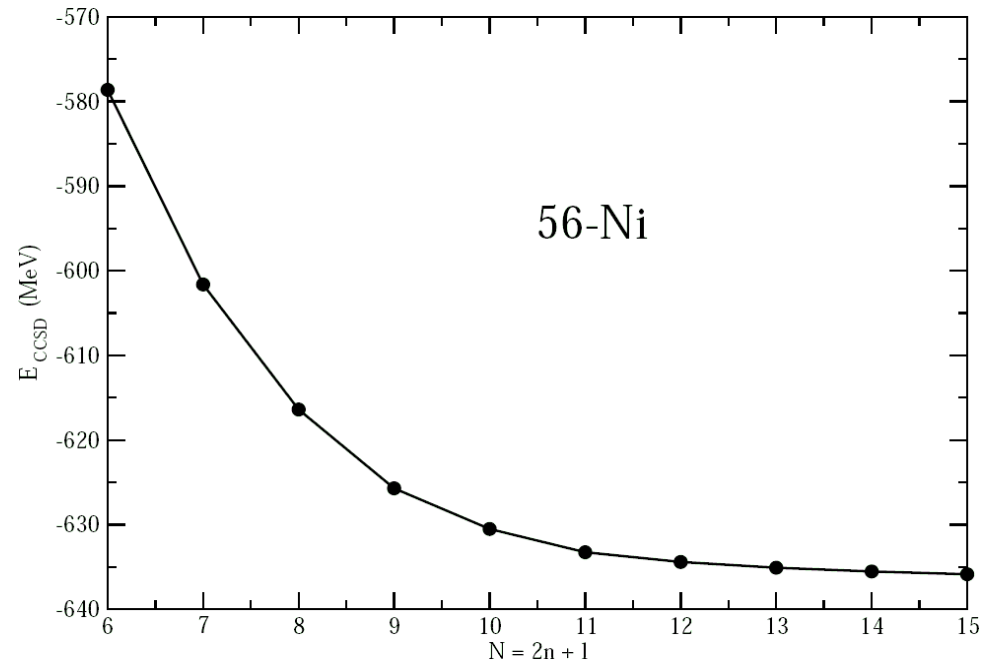
2. Utilize the nuclear spherical symmetry to push further Towards 'ab initio' calculations of heavy nuclei

- Implemented a CCSD J-coupled 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 15 complete major shells on a single node.
- CCSDT “Gold standard” for these heavier nuclei in reach with supercomputing (developing)
- Enables specified calculations for heavy nuclei
- The large model spaces mean that we can do “bare” interactions!
- One-body observables

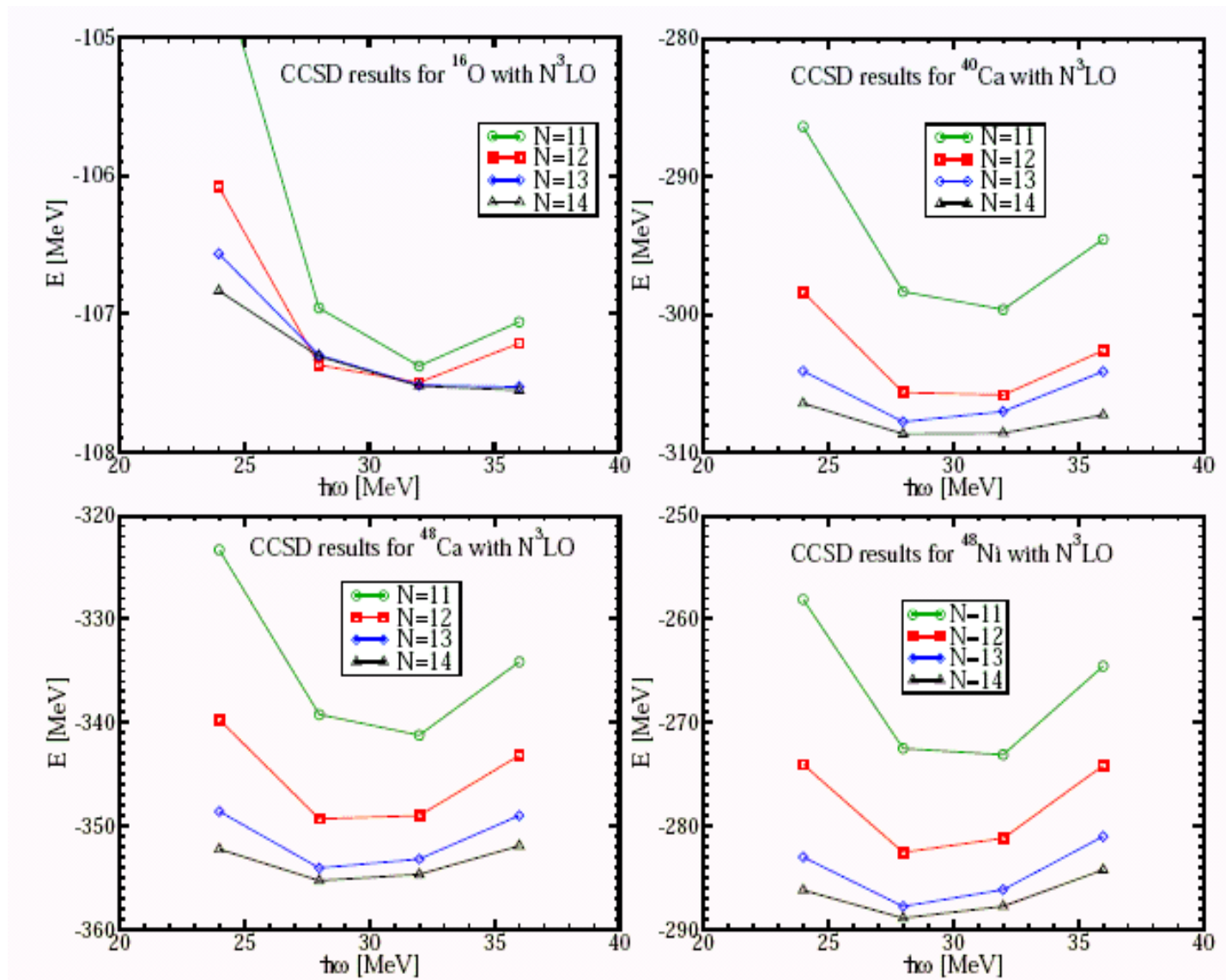
2. Cont'd: ^{40}Ca and ^{56}Ni with SRG at cutoff $\Lambda = 2.5\text{fm}^{-1}$



Large overbinding due to neglected three-body forces



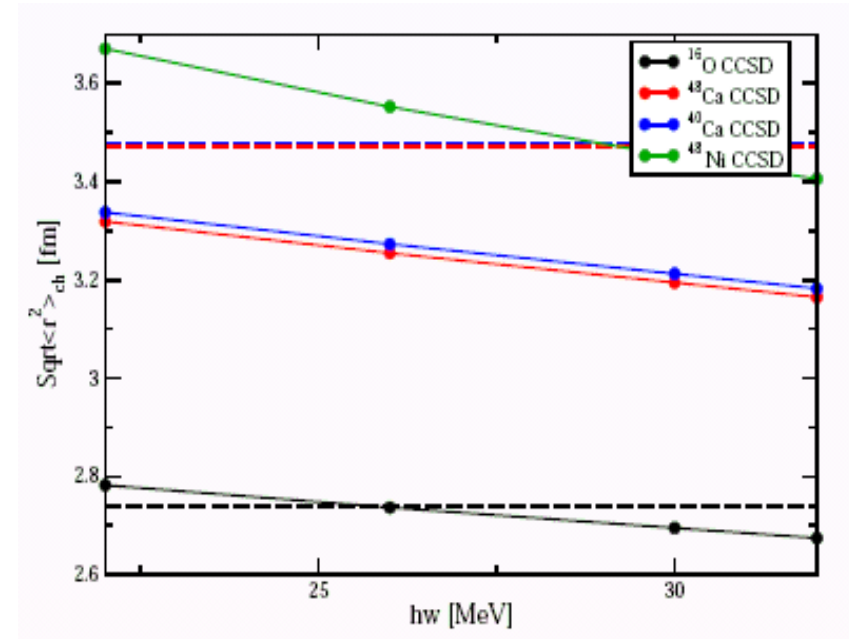
2. Cont'd: Convergence of ^{16}O , ^{40}Ca , ^{48}Ca and ^{48}Ni CCSD ground state energies with the nucleon-nucleon N³LO



2. Cont'd: Charge and matter radii/Summary of results

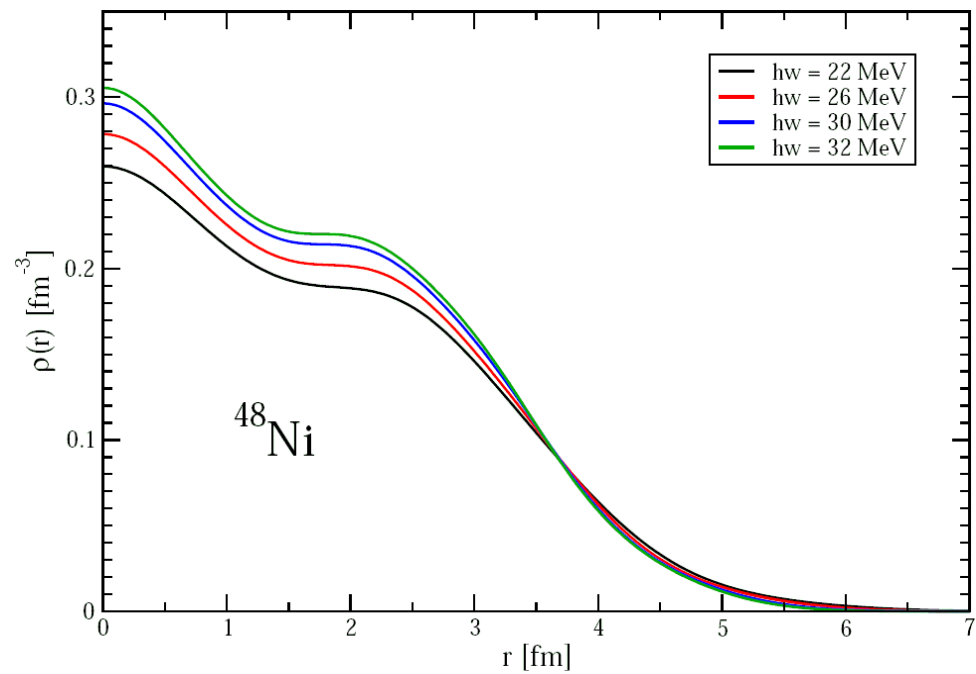
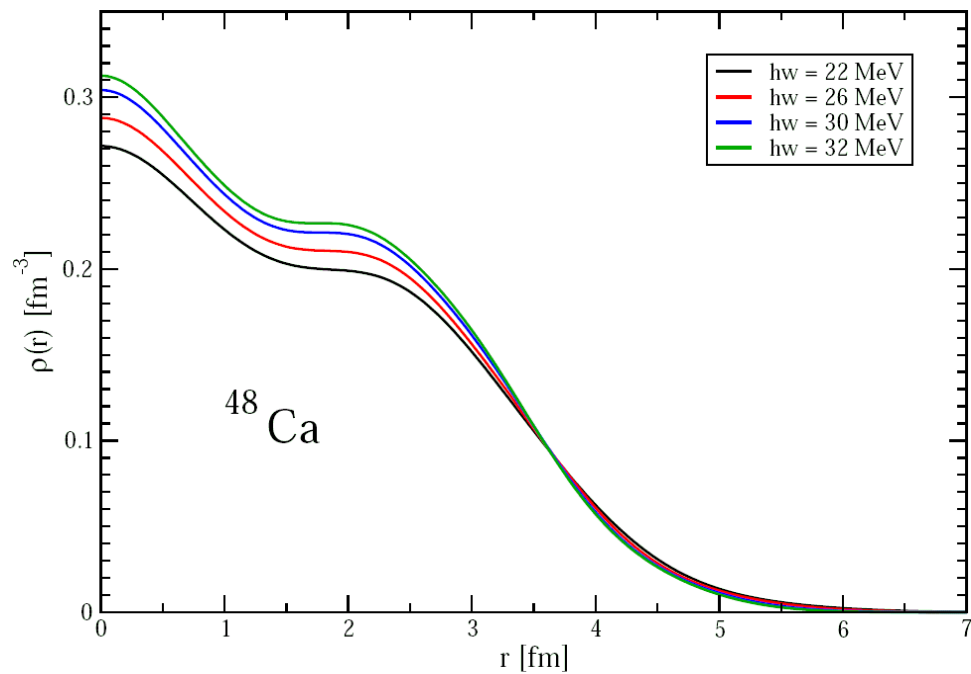
Charge radii for various nuclei using N3LO nucleon-nucleon interaction.

~1MeV missing binding energy for all nuclei: Size Extensivity !



Nucleus	E/A	V/A	Q	$\Delta E/A$	$\langle r^2 \rangle_{ch}^{1/2}$	$\langle r^2 \rangle_{ch}^{1/2} (Exp)$
^4He	-5.99	-22.75	0.90	1.08		1.673(1)
^{16}O	-6.72	-30.69	1.08	1.25	2.72(5)	2.737(8)
^{40}Ca	-7.72	-36.40	1.18	0.84	3.25(9)	3.4764
^{48}Ca	-7.40	-37.97	1.21	1.27	3.24(9)	3.4738
^{48}Ni	-6.02	-36.04	1.20	1.21	3.52(15)	?

3. ^{48}Ca and ^{48}Ni CCSD ground state densities



Summary: Two-year plan on track !

Proposed:

- Benchmarking
- CC calculations for Ca, Ni isotopes
- Densities
- Response to external fields (densities and binding energies)
- Currents in odd-mass nuclei ($A\pm 1$)
- Progress on parallelization
- CC – DFT interface

Status:

- ✓ done
- ✓ done
- ✓ done
- ✓ can now be done
- ✓ in progress
- ✓ in progress
- ✓ not done

Proposed work was supposed to be done with 1.5 post-doc
Actual work was done with < 0.5 post-doc due to programmatic alignments

Personnel status

Staff:

Hagen (ORNL); Papenbrock (UT/ORNL); Dean (ORNL)

Students:

Oivind Jensen (Bergen)

Post-doc joining in October 2008:

Maxim Kartamyshev (Oslo)

ORNL R&D Staff:

Hai Ah Nam (from UCSF)

Changes in Year 2:

October 2007 --> Dean moves to Director's Office; research at 20% time for 2 years.

January 2008 --> Hagen becomes R&D staff member

Present work

Physics Problems:

- Interface with DME (with S. Bogner and R. Furnstahl)
- Spectroscopic factors, overlap functions with applications to reactions (with O. Jensen)
- Density dependent part of three-nucleon force (with S. Bacca and A. Schwenk)

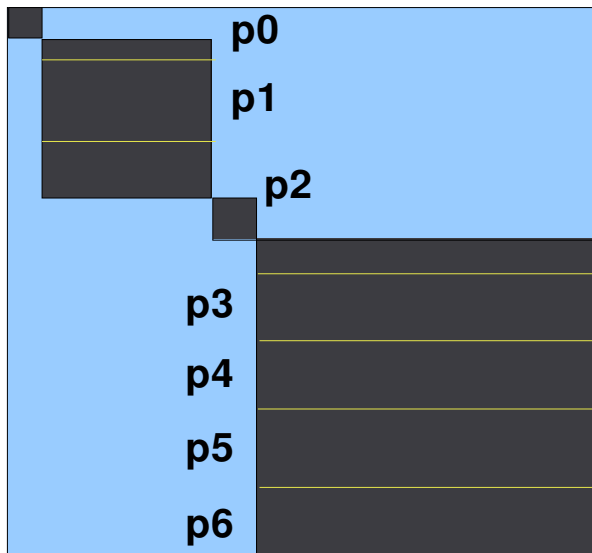
Computational Issues:

- Parallelization of spherical CC code (optimization and load balancing) (with B. Velamuri Asokan)
- Tensor multiplies (with K. Roche)
- Inclusion of approximate and full triples correction (with M. Kartamyshev)

Parallelization of spherical CCSD code

1. Scaling of non-uniformly block-structured matrix operations
2. Load balancing algorithms
 1. Computational efficiency \sim matrix-matrix operations
 2. Parallel decomposition of matrix to maximize processor work
3. Processor topologies
 1. Creating processor groups based on symmetry
4. Memory management
 1. Classic trade-off “memory vs speed”
5. Interfacing with existing parallel, nonlinear, approximate Newton solvers

Parallelization of spherical CCSD code - Issues



Load balancing

- Memory per processor scales with number of matrix elements stored
- Computation per processor scales with square of number of matrix elements stored

Load trade-off

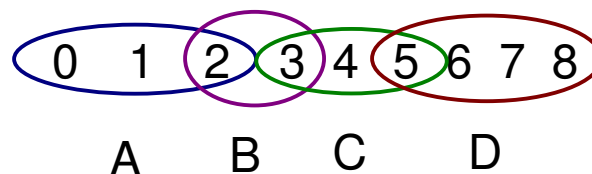
- Memory vs computation
- Distribute X elements per processor that solves $\max \{ AX^2 + BX; A+B=1; 0 \leq A, B \leq 1 \}$

Symmetry issues

- Enforcing symmetry is sequential, processors are grouped with overlap
- Idle time increases (when one group performs computations other groups idle)

Exclusion mapping – an elegant solution

- Parallelizing symmetry based operations
- Exclude intersecting proc. groups, perform computations, refresh



- Groups A and C can perform computations simultaneously (procs 6, 7, 8 idle)
- Groups B and D can perform computations simultaneously (procs 0, 1, 4 idle)
- No easy way to avoid the sequential part here

Future work (year 2 and 3)

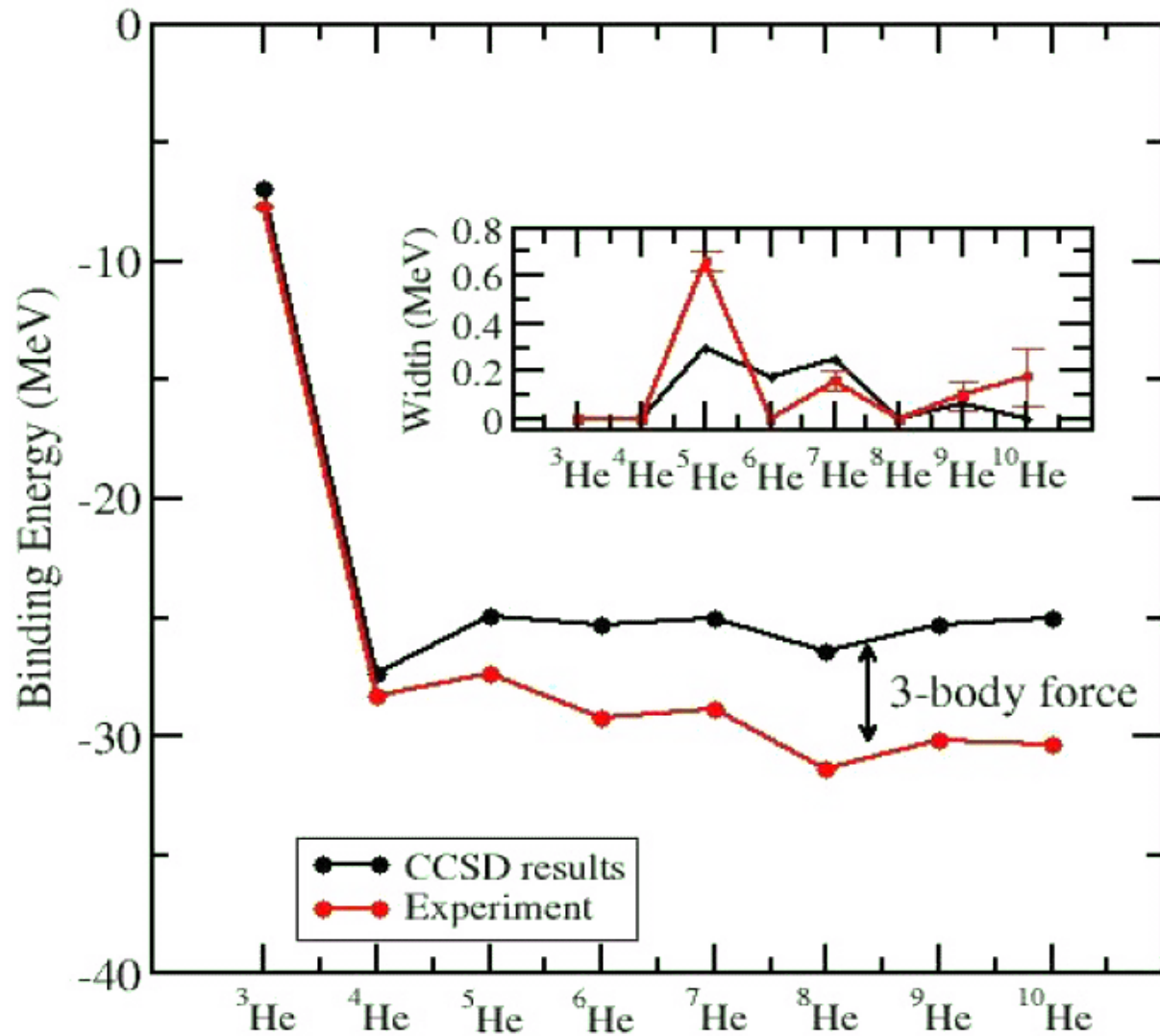
1. Particle attached/removed EOMCCSD for A +/-1 nuclei
 1. For computation of currents
 2. Diagrammatics and implementation of energy and one-body observables using spherical symmetry
 3. Interface with DFT
 4. Spectroscopic factors and overlap functions for transfer reactions (see year 4 and 5)
2. Inclusion of approximate triples correction for energy and observables
 1. For error estimates and higher precision
 2. Derive, implement and test various iterative and non-iterative triples corrections schemes.
3. Scalable and load balanced parallel version of spherical CCSD code
 1. For heavier nuclei and inclusion of full triples (“gold” standard), ^{100}Sn and ^{208}Pb within reach
 2. Issues: load balancing and scaling
4. Coupled-Cluster approach to nuclear matter for interface with DFT
 1. Within spherical scheme (trade spherical symmetry for translational invariance)
 2. Needs parallel code due to large number of orbitals

Future work (year 4 and 5)

Ab-Initio reactions in medium mass nuclei Tie reactions in selected nuclei to microscopic physics

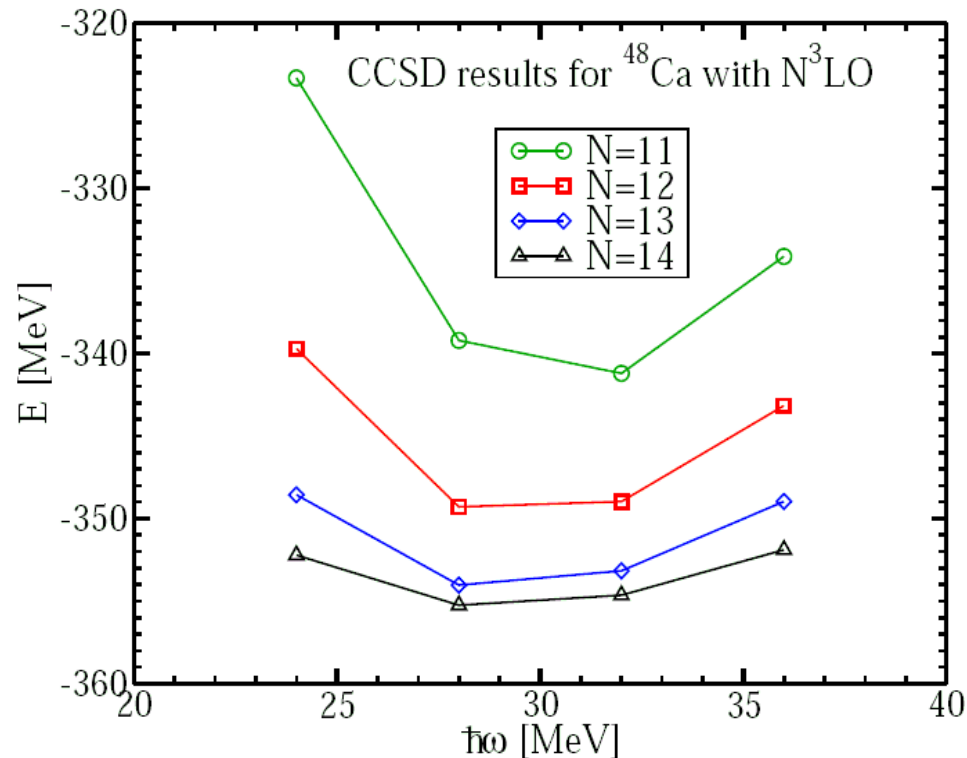
1. Ab-initio description of weakly bound and unbound nuclear states; unification of nuclear structure and reactions
2. Reaction cross sections via Lorentz integral transform (implement Spherical EOMCCSD for excited states)
 1. Need excited states and transition densities
3. Realistic densities for optical potentials (need two-body observables for CoM-corrected densities)
 1. Based on the Jeukenne, Lejeune and Mauhaux (JLM) approach
4. Spectroscopic factors and one-body overlap functions for neutron transfer reactions
 1. in progress already now (graduate student)

Weakly bound and unbound He isotopes with the Coupled Cluster Method



Possible showcase:

fully converged ^{48}Ca with triples correction and three-body forces



Requires full parallelization of spherical code

Full triples require peta-scale computing

CCSDT for ^{48}Ca in 25 major shells requires 10,000 times more cycles

FIG. 4: (Color online) CCSD results for ^{48}Ca from the chiral NN potential at order $N^3\text{LO}$ as a function of the oscillator spacing $\hbar\omega$ and the size of the model space.

Budget

- Papenbrock/Dean/Hagen (and Nam) covered by other sources
- Post-doctoral support through UT; same as last year: 1.5 Post-docs
 - 1.0 Post-doc/year for CC developments (M. Kartamyshev)
 - 0.5 Post-doc/year for CC/DFT interface
- Total cost (science application part): approximately \$120k/year
- Continuing support of Roche (computer science)

This year we missed hiring a Post-Doc due to UNEDF delay