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

Presented by

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Nuclear Coupled-cluster Collaboration:
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SC07

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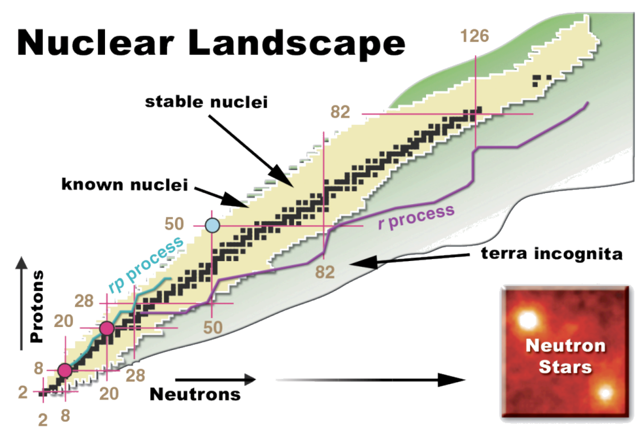
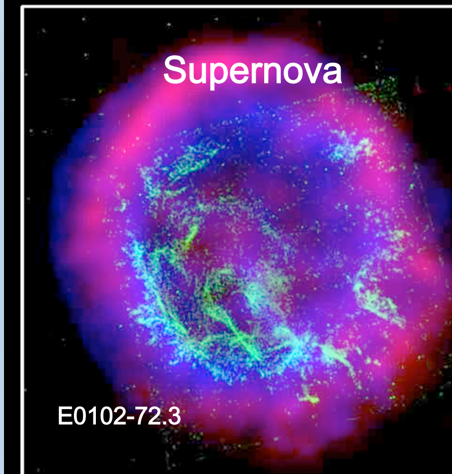
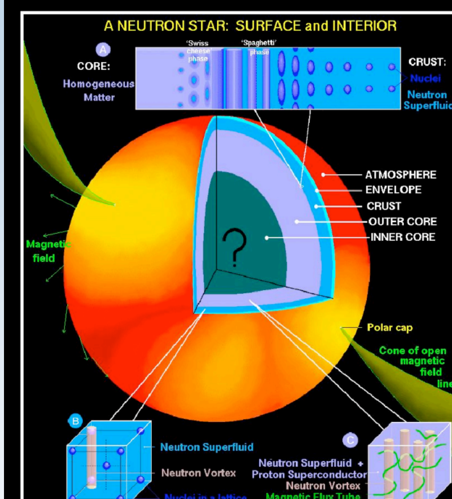
"Given a lump of nuclear material, what are its properties, and how does it interact?"

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.







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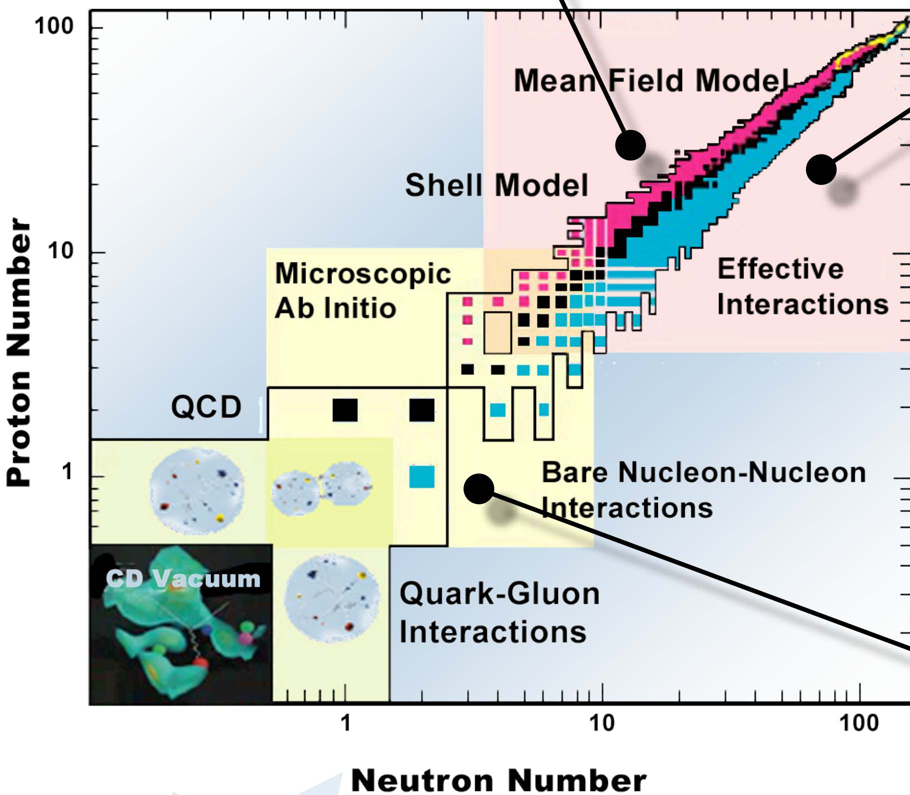
Pushing the nuclear boundaries

Thermal properties regions

Nuclear DFT effort



The Leadership Computing Facility effort will

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

Nuclear Coupled Cluster effort

All Regions: Nuclear cross-section efforts (NNSA, SC/NP, Nuclear Energy)

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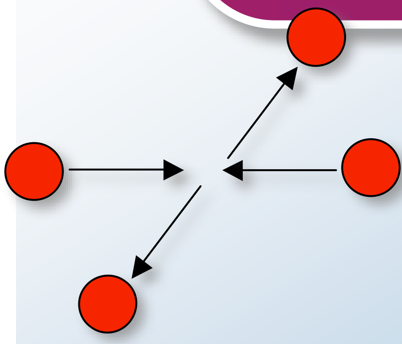
Nuclear interactions: Cornerstone of the entire theoretical edifice

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



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

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

$$\mathrm{H}|\Psi\rangle = \mathrm{E}|\Psi\rangle$$

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

Correlation operator

Reference Slater determinant

$$T = T_1 + T_2 + T_3 + \cdots$$

$$T_1 = \sum_{\substack{i<\varepsilon_f \\ a>\varepsilon_f}} t_{ai} a_a^+ a_i$$

$$T_2 = \sum_{\substack{ij<\varepsilon_f \\ ab>\varepsilon_f}} t_{abij} a_a^+ a_b^+ a_j a_i$$

Energy

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

Amplitude equations

$$\langle\Phi_{ij\ldots}^{ab\ldots}|\exp(-T) H \exp(T)|\Phi\rangle = \langle\Phi_{ij\ldots}^{ab\ldots}|\overline{H}|\Phi\rangle = 0$$

- 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}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

$$|\Psi\rangle = \exp(T)|\Phi\rangle$$

$$T = T_1 + T_2 + T_3 + \ldots$$

$$E = \langle\Phi|\overline{H}|\Phi\rangle = \langle\Phi|e^{-T}He^{T}|\Phi\rangle$$

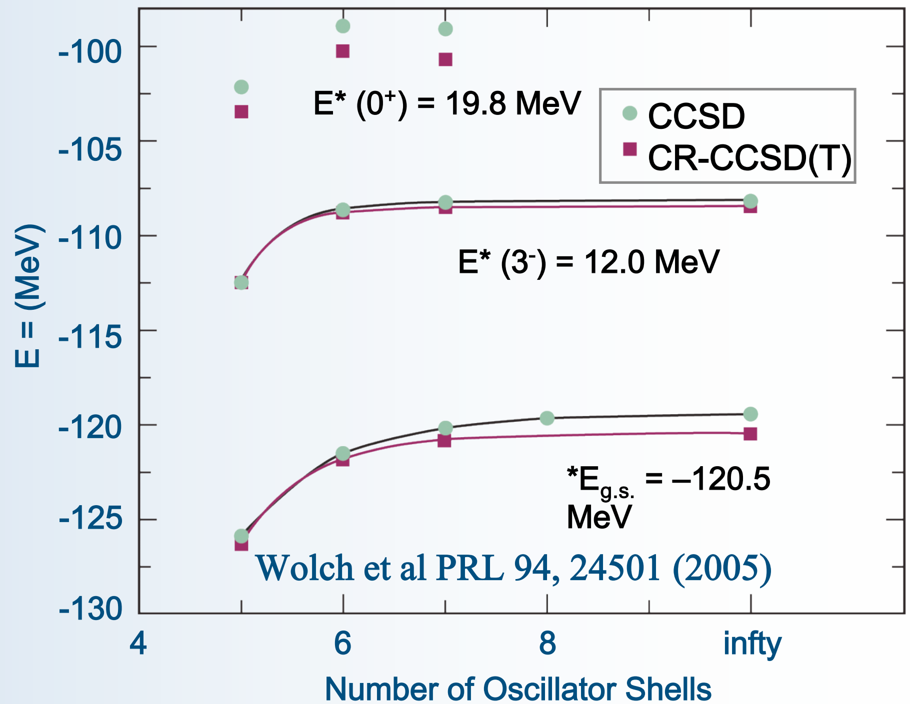
$$\langle\Phi^{ab\ldots}_{ij\ldots}|\overline{H}|\Phi\rangle = 0$$

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

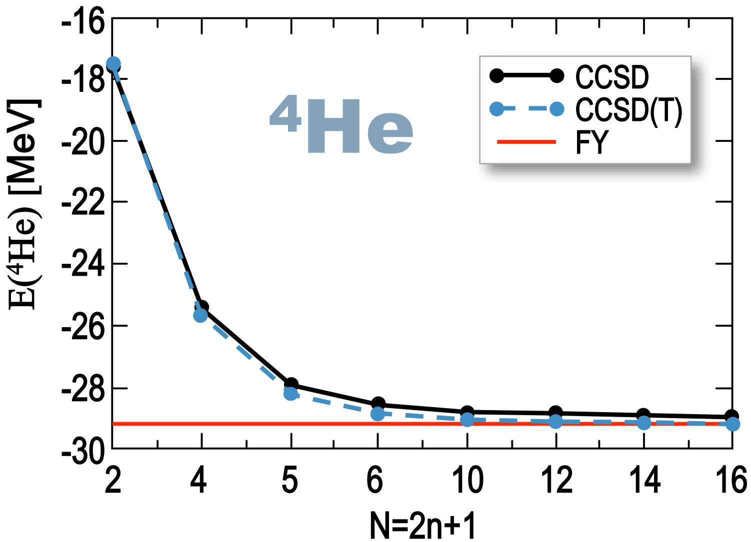
R = excitation operator

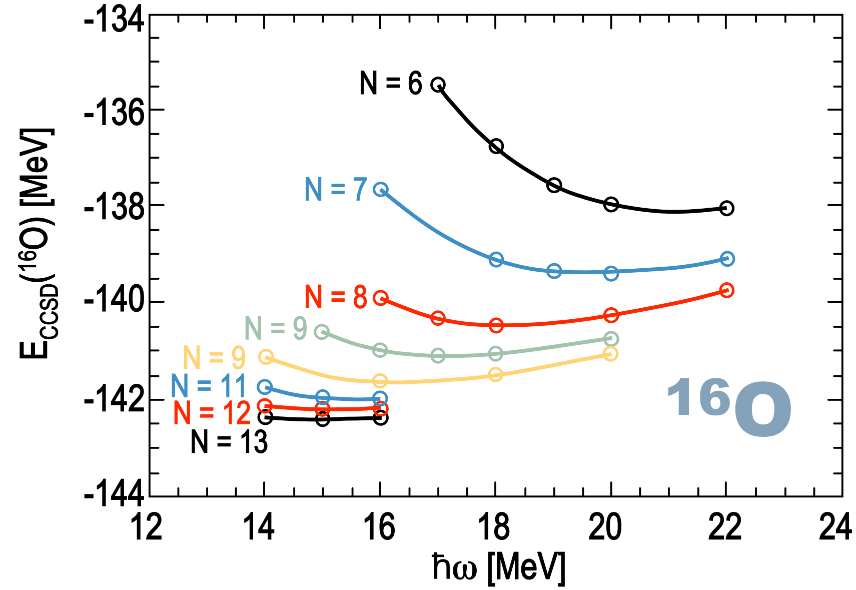
POLYNOMIAL SCALING!! *(good)*

Early results

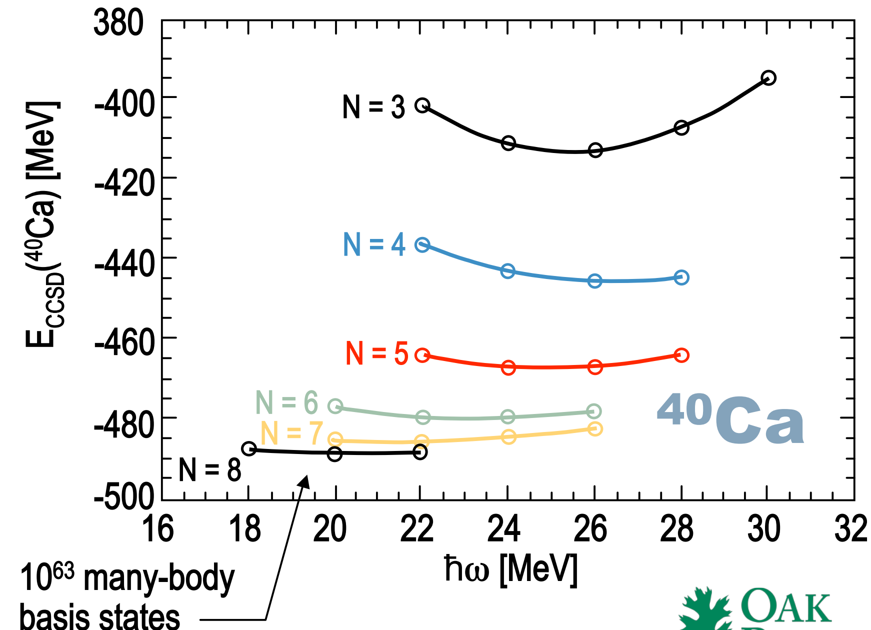


Ab initio in medium mass nuclei





Hagen et al., *Phys. Rev. C* **76**, 044305 (2007)

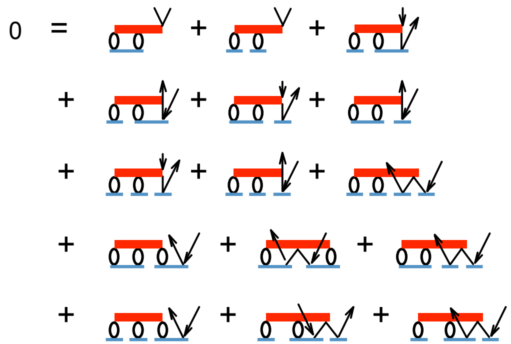


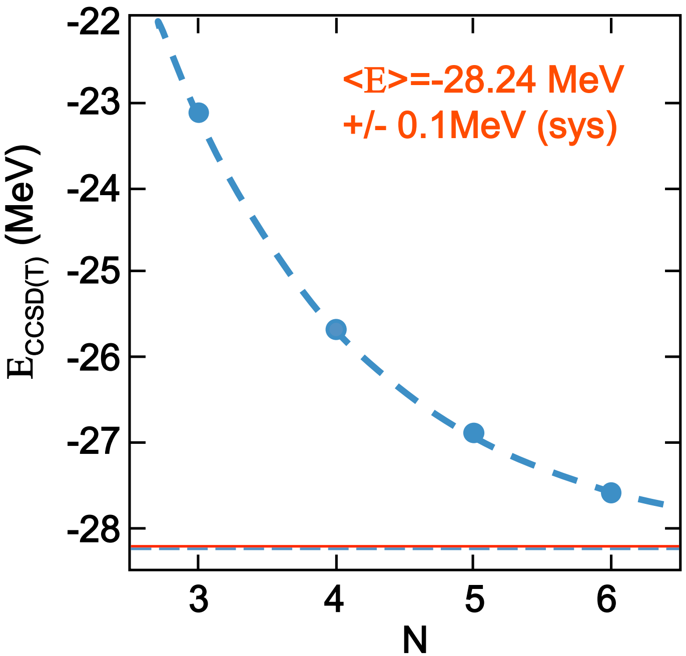
Error estimate:	<< 1%	< 1%	1%
	^{4}He	^{16}O	^{40}Ca
E0	-11.8	-60.2	-347.5
ΔE_{CCSD}	-17.1	-82.6	-143.7
$\Delta E_{CCSD(T)}$	-0.3	-5.4	-11.7
$\Delta E_{CCSD(T)}$	-29.2	-148.2	-502.9
Exact (FY)	-29.19(5)		

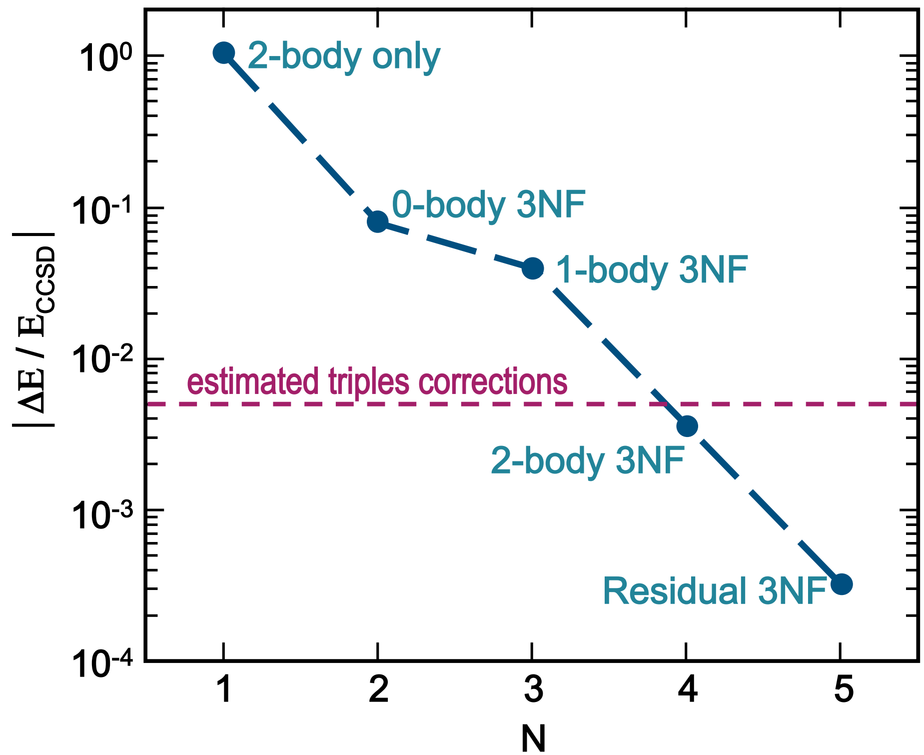
Fast convergence with cluster rank

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

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



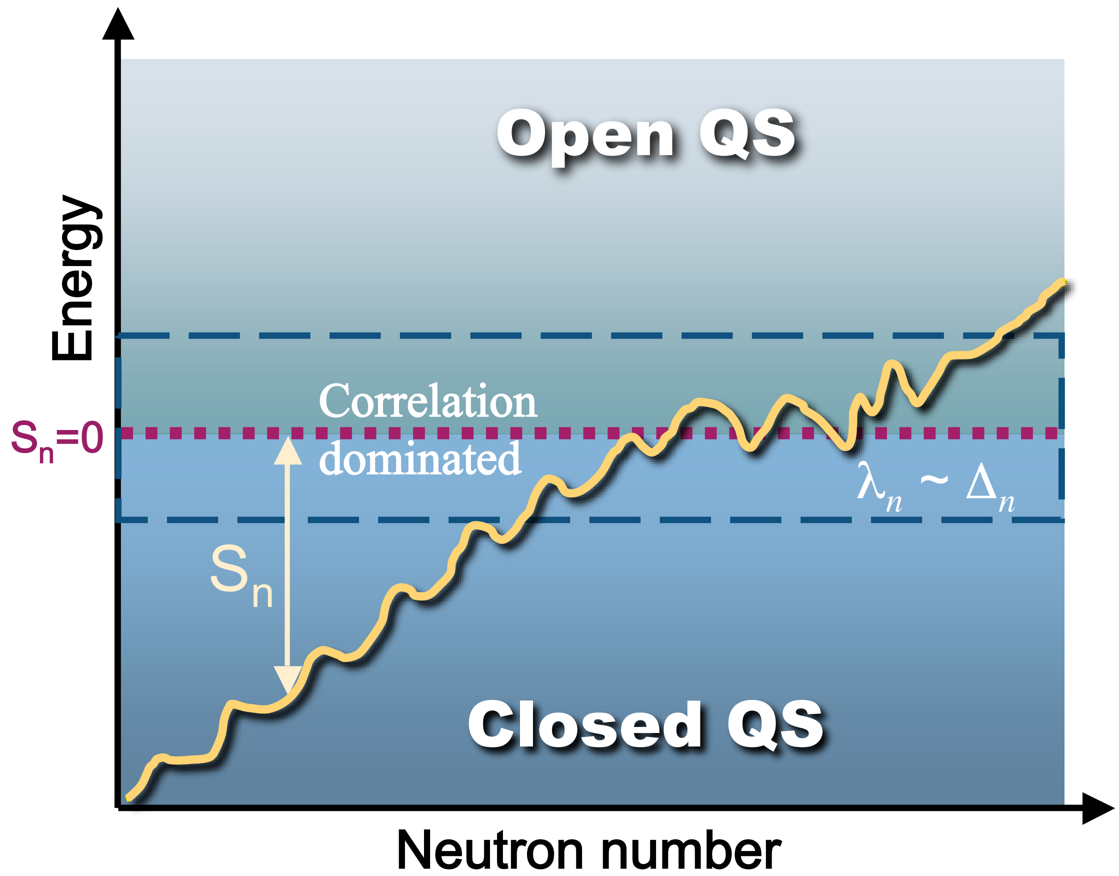


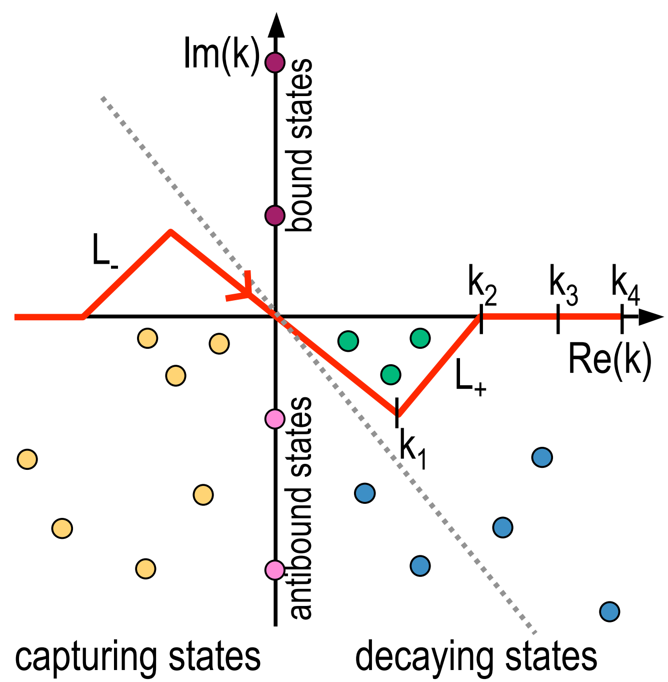


Challenge: Do we really need the full 3-body force, or just its density dependent terms?

Hagen, Papenbrock, Dean, Schwenk, Nogga, Wloch, Piecuch, *Phys. Rev. C* **76**, 034302 (2007)

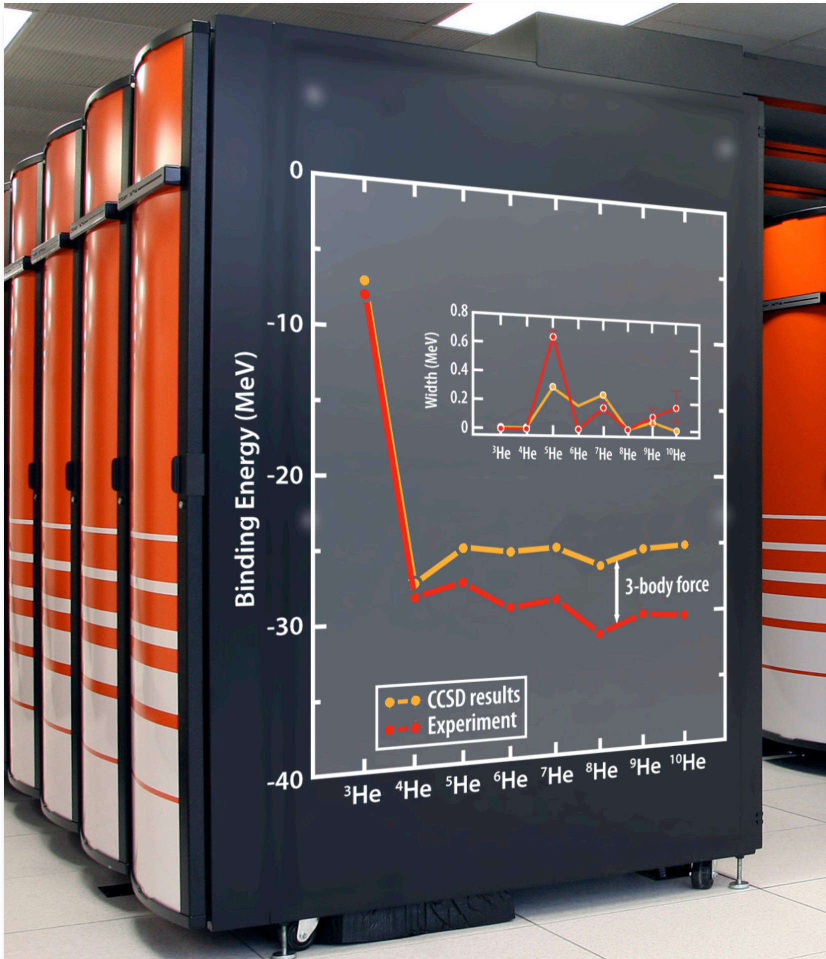
Coupling of nuclear structure and reaction theory (microscopic treatment of open channels)





Introduction of
continuum basis states (Gamow, Berggren)

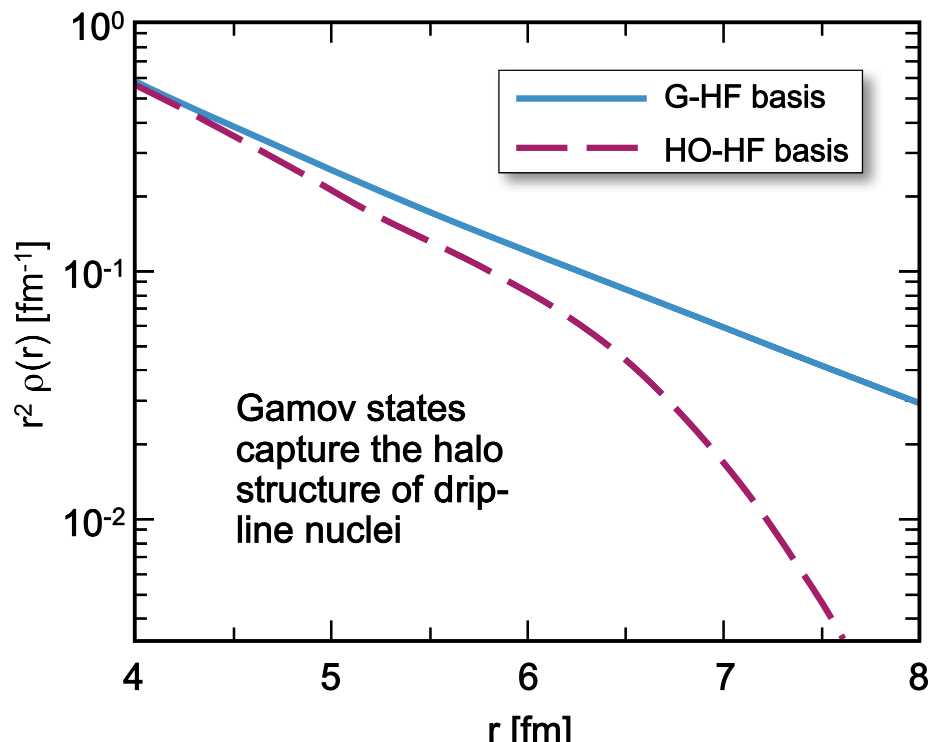
Ab initio weakly bound and unbound nuclei



[feature article in *Physics Today* (November 2007)]

Challenge: Include 3-body force

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}He



Solution of coupled-cluster equation

Basic numerical operation:

$$t_{new}(ab, ij) = \sum_{\substack{k,l=1,n \\ c,d=n+1,N}} V(kl, cd)\, t_{old}(cd, ij)\, t_{old}(ab, kl)$$

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

- **Many such terms exist.**
- **Cast into a matrix-matrix multiply algorithm.**
- **Parallel issue: block sizes of V and t.**

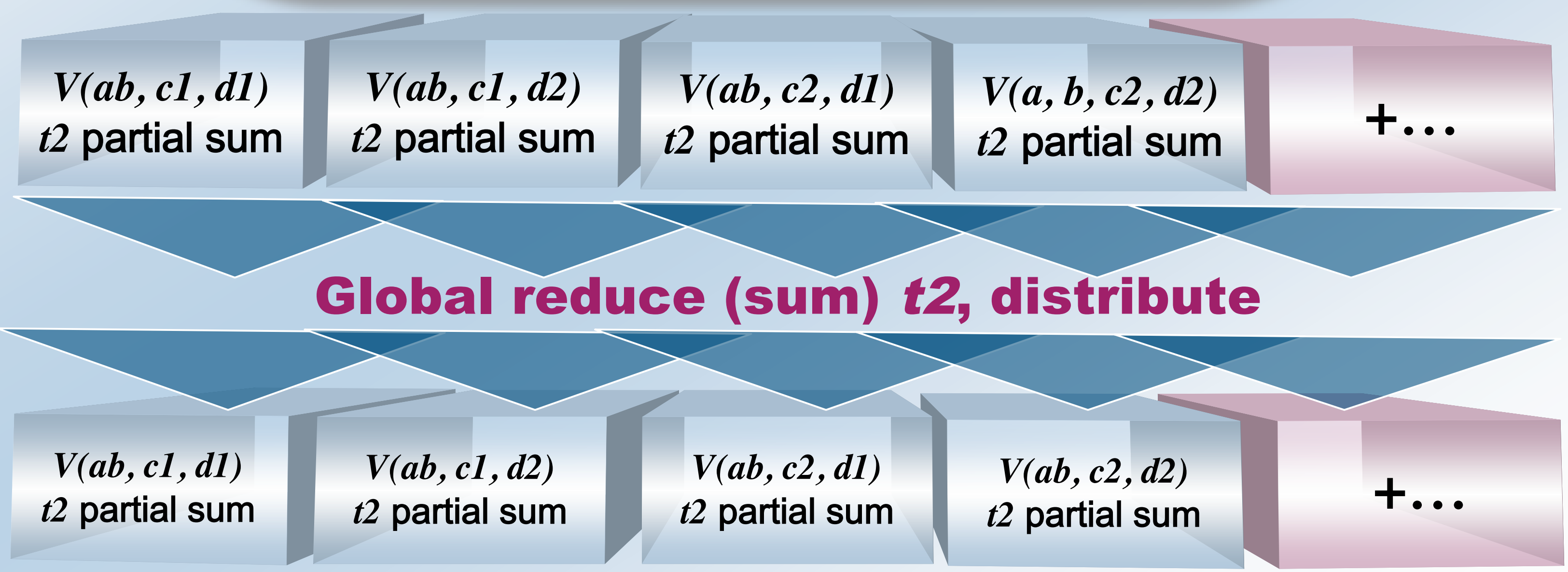
Code parallelism

Memory distribution across processors

$$t_2(ab,ij) = \sum_{\substack{kl<\varepsilon_f \\ cd>\varepsilon_f}} V(kl,cd)\, t_{ij}^{cd}\, t_{kl}^{ab}$$

Partial sum

t2 reside on each processor



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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

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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)