Ab initio Calculations of Light-ion Reactions
No-core shell model & Resonating group method

- **Combine** the *ab initio* no-core shell model (NCSM) with the resonating group method (RGM)

- **The NCSM**: An approach to the solution of the $A$-nucleon bound-state problem
  - Accurate nuclear Hamiltonian
  - Finite harmonic oscillator (HO) basis
  - Complete $N_{\text{max}} f_{\Omega}$ model space
    - Relative or single-particle coordinates
  - Effective interaction due to the model space truncation
    - Similarity-Renormalization-Group evolved NN(+NNN) potential
  - Short & medium range correlations, no continuum
  - Description of single-particle degrees of freedom

- **The RGM**: A microscopic approach to the $A$-nucleon scattering of clusters
  - Nuclear Hamiltonian may be simplistic
  - Cluster wave functions may be simplified and inconsistent with the nuclear Hamiltonian
  - Long range correlations
  - Description of clusters and their relative motion

*Ab initio NCSM/RGM*: Combines the best of both approaches
- Accurate nuclear Hamiltonian, consistent cluster wave functions
- Coupling to continuum, Pauli principle and translational invariance
The \textit{ab initio} NCSM/RGM in a snapshot

- Ansatz: \[ \Psi^{(A)} = \sum_v \int d\vec{r} \varphi_v(\vec{r}) \hat{A} \Phi^{(A-a,a)}_{\nu\vec{r}} \]

- Many-body Schrödinger equation:

\[ H \Psi^{(A)} = E \Psi^{(A)} \]

\[ \sum_v \int d\vec{r} \left[ \mathcal{H}_{\mu\nu}^{(A-a,a)}(\vec{r}', \vec{r}) - E \mathcal{N}_{\mu\nu}^{(A-a,a)}(\vec{r}', \vec{r}) \right] \varphi_v(\vec{r}) = 0 \]

- Hamiltonian kernel: \( \langle \Phi^{(A-a,a)}_{\mu\vec{r}} | \hat{A} H \hat{A} | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle \)

- Norm kernel: \( \langle \Phi^{(A-a,a)}_{\mu\vec{r}} | \hat{A}^2 | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle \)

- Non-local integro-differential coupled-channel equations:

\[ \left[ \hat{T}_{\text{rel}}(r) + \hat{V}_C(r) - (E - E_V) \right] u_{\nu}(r) + \sum_v \int d\vec{r}' r' W_{\nu\nu'}(r, r') u_{\nu'}(r') = 0 \]

NCSM/RGM: NCSM microscopic wave functions for the clusters involved, and realistic (bare or derived NCSM effective) interactions among nucleons. Proper boundary conditions for scattering and/or bound states.

eigenstates of \( H^{(A-a)} \) and \( H^{(a)} \) in the \textit{ab initio} NCSM basis

realistic nuclear Hamiltonian

N = 1, J = \frac{1}{2} (^1S_{1/2})

N^3LO

\( n + \alpha(g.s.) \)

\[ W_{\nu\nu'}(r, r') \text{ [MeV fm}^3\text{]} \]
\( n + ^4\text{He} \) differential cross section and analyzing power

- NCSM/RGM calculations with
  - \( N + ^4\text{He}(\text{g.s., } 0^+0) \)
  - SRG-N^3LO NN potential with \( \Lambda=2.02 \text{ fm}^{-1} \)

- Differential cross section and analyzing power @17 MeV neutron energy
  - Polarized neutron experiment at Karlsruhe

NNN missing: Good agreement only for energies beyond low-lying 3/2^- resonance
$p+^{4}\text{He}$ differential cross section and analyzing power
Neutron-triton elastic scattering at 14 MeV

- Important for the NIF physics
  - deuteron-triton fusion generates 14 MeV neutrons
- Experimental situation confusing
- Good data for $p^+\,^3\text{He}$ elastic scattering

Use NCSM/RGM calculation to relate the two reactions and predict $n^+\,^3\text{H}$ cross section

Supported by PEM
**$p + ^7Be$ scattering**

- $N_{\text{max}} = 12$ NCSM/RGM calculation with $p + ^7Be(g.s.,1/2^-, 7/2^-)$
  - SRG-N$^3$LO NN potential with $\Lambda = 2.02$ fm$^{-1}$
  - $^8B$ $2^+$ state unbound by 200 keV (experimentally bound by 137 keV)

- Predict: $0^+, 1^+, 2^+$ resonances
  - No evidence for $2^-$ resonance

- Scattering length:
  - Expt: $a_{02} = -7(3)$ fm
  - Calc: $a_{02} = -10.2$ fm

- Excellent prospects for calculating $^7Be(p,\gamma)^8B$
What is the ground state of $^{9}$He?

- NCSM/RGM calculation of $n^+\ ^{8}$He
  - SRG-$N^3$LO NN potential with $\Lambda = 2.02$ fm$^{-1}$
  - $^8$He $0^+$ g.s. and $2^+$, $1^+$ excited states included
  - Up to $N_{\text{max}} = 10$

![Diagram](image-url)
What is the structure of $^{10}$Li?

- NCSM/RGM calculation of $n^{+9}$Li
  - SRG-$N^3$LO NN potential with $\Lambda = 2.02$ fm$^{-1}$
  - $^9$Li $3/2^-$ g.s. and $1/2^-, 5/2^-$ excited states included
  - Up to $N_{\text{max}}=6$

**Preliminary results:**
- No bound states
- $2^-$, $1^-$ S-waves closer to threshold
- $P$-waves ordering: $1^+, 0^+, 2^+$
Toward the first \textit{ab initio} calculation of the Deuterium-Tritium fusion

\[\int dr \ r^2 \left( \langle r' \alpha_n | \hat{\mathbf{A}}_1 (H - E) \hat{\mathbf{A}}_1 | \alpha_n r \rangle + \langle r' \alpha_n | \hat{\mathbf{A}}_2 (H - E) \hat{\mathbf{A}}_2 | 3^\text{H} d \rangle \right) = 0\]

- \(d + 3^\text{H} \rightarrow d + 3^\text{H}\) \textit{exchange} part of norm kern
  - S-wave channel: \(J=3/2^+, J=1/2^+\)

\[d(\uparrow) + 3^\text{H}(\uparrow)\]

\[d(\uparrow) + 3^\text{H}(\downarrow)\]
$d^+{^3}H$ and $n^+{^4}He$ elastic scattering: phase shifts

- **$d^+{^3}H$ elastic phase shifts:**
  - Resonance in the $^4S_{3/2}$ channel
  - Repulsive behavior in the $^2S_{1/2}$ channel → Pauli principle

- **$n^+{^4}He$ elastic phase shifts:**
  - $d^+{^3}H$ channels produces slight increase of the $P$ phase shifts
  - Appearance of resonance in the $3/2^+ D$-wave, just above $d^+{^3}H$ threshold

The D-T fusion takes place through a transition of $d^+{^3}H$ is S-wave to $n^+{^4}He$ in $D$-wave
The first results, still preliminary:
- \( N_{\text{max}} = 11 \) (d-T), 13 (d-\(^3\)He)
- SRG-N\(^3\)LO NN (\( \Lambda = 1.5 \text{ fm}^{-1} \)) potential
- NNN interaction interaction effects for \( A = 3, 4, 5 \) partly included by the choice of \( \Lambda \)
- Only g.s. of \( d, \ 3\)H, \( 4\)He included above

\[
S(E) = E\sigma(E)\exp\left( \frac{2\pi Z_1 Z_2 e^2}{\hbar \sqrt{2mE}} \right)
\]

Supported by PEM, LDRD
The cross section improves with the inclusion of virtual breakup of the deuteron

- Deuteron weakly bound: easily gets polarized and easily breaks
- These effects included below the breakup threshold with continuum discretized by excited deuteron pseudo-states

First *ab initio* results for *d*-T and *d*-³He fusion:
Very promising, correct physics, becoming competitive with fitted evaluations …
NCSM/RGM \textit{ab initio} calculation of $d$-$^{4}\text{He}$ scattering

- NCSM/RGM calculation with $d + ^{4}\text{He}(\text{g.s.})$ up to $N_{\text{max}} = 10$
  - SRG-N$^3$LO potential with $\Lambda = 1.5$ fm$^{-1}$
  - Deuteron breakup effects included by continuum discretized by pseudo states in $^3S_1$-$^3D_1$, $^3D_2$ and $^3D_3$-$^3G_3$ channels

The $1^+0$ ground state bound by 1.9 MeV (expt. 1.47 MeV)
- Calculated $T=0$ resonances: $3^+$, $2^+$ and $1^+$ in correct order close to expt. energies

*Supported by LDRD*
FY10 accomplishments

- Development of *ab initio* many-body reaction theory by merging the NCSM and the RGM (P. Navratil and S. Quaglioni)
  - Results with NN potentials used by UNEDF collaboration
    - $p$-$^7$Be with SRG-$N^3$LO using the importance-truncated NCSM
    - $n$-$^8$He with SRG-$N^3$LO
    - $n$-$^9$Li with SRG-$N^3$LO
    - Collaboration with R. Roth (TU Darmstadt)
  - Deuteron-nucleus scattering: $d$+$^4$He
    - $^3$H($d,n$)$^4$He and $^3$He($d,p$)$^4$He fusion cross section calculations
    - Development of $^3$H & $^3$He projectile formalism

- Development of the TRDENS transition density code
  - three-body density for $A$=3,4 nuclei

- SRG evolution of NN+NNN interactions in the p-shell
  - Collaboration with E. Jurgenson (LLNL) and R. Furnstahl (OSU)

- $A$=14 nuclei with chiral EFT NN+NNN up to $N_{\text{max}}$=8
  - Transformation of NNN to SD basis up to $N_{\text{max}}$=8
  - Collaboration with J. Vary, P. Maris, H. Nam, E. Ormand and D. Dean
Publications relevant to UNEDF in 2009/2010

- P. Navratil, R. Roth, and S. Quaglioni, “Ab initio many-body calculations of nucleon scattering on $^4$He, $^7$Li, $^7$Be, $^{12}$C and $^{16}$O”, in preparation, (2010).


- Lisetskiy, AF; Kruse, MKG; Barrett, BR; Navratil, P; Stetcu, I; Vary, JP. "Effective operators from exact many-body renormalization", Phys. Rev. C 80, 024315 (2009).

Future plan

- The rest of Year 4 and Year 5
  - $n^{-8}$He, $n^{-9}$Li calculations
  - Continue work on $d^{-3}$H fusion (supported by PEM, LDRD)
  - Development of $^3$H and $^3$He – nucleus formalism (supported by LDRD)
  - Development of the coupling of NCSM/RGM and NCSM $\rightarrow$ NCSMC
  - Similarity-renormalization-group evolution of NN+NNN interactions
    - Application to $p$-shell nuclei (supported by DOE/SC/NP)
  - Further development of importance-truncation NCSM scheme
  - High profile science: Capture reactions
    - $^7$Be$(p,\gamma)^8$B
    - $^3$He$(\alpha,\gamma)^7$Be

- Computational challenges:
  - $n$-body density ($n>2$) calculations
    - Distribution of structure allocation, parallelization