

# Lawrence Livermore National Laboratory

## *Ab initio Nuclear Reactions*



Team:

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**Physical and Life Sciences/Physics**

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# Ab initio Reactions: NCSM/RGM

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- Team:
  - Sofia Quaglioni (Early career award)
  - Petr Navratil (TRIUMF, LLNL-LOA)
- LLNL effort:
  - UNEDF – Year 5:
    - Benchmark n-<sup>8</sup>He, and n-<sup>9</sup>Li scattering.
    - ✓ – Investigate p-<sup>7</sup>Be scattering and capture reactions.
    - Investigate <sup>3</sup>He-<sup>4</sup>He scattering and capture reactions.
    - Use two-, three-, and four-body transition densities for A=3,4 nuclei.
    - Development of three-body transition density calculation for A>4.
  - LDRD
    - Develop formalism for a=2,3,4 clusters in the RGM formalism
    - Code Hamiltonian and Norm kernels for a=2,3,4 clusters with NN
    - Primary goal is to get to <sup>12</sup>C(α,γ)<sup>16</sup>O
    - Ambitious goal, will get to a=3 clusters this year



# Ab initio Reactions: NCSM/RGM

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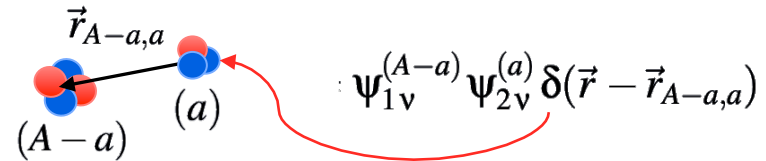
- FY11 UNEDF DOE/NP budget decreased by 50%
  - Effort on ab initio reactions was decreased to zero on UNEDF
    - Due to commitment to post-doctoral employees in other efforts
- Reduction will be restored, and deliverables will be rethought
- Still operating under CR rules
  - Funding received in pro-rated amounts quarterly
  - Currently, only 42% of the reduced budget has been received
    - Affects subcontract to SDSU



# Ab initio NCSM/RGM Formalism

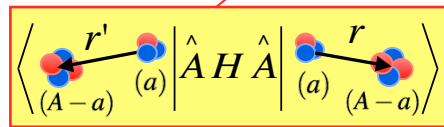
S. Quaglioni & P. Navrátil, Phys. Rev. Lett. 101, 092501 (2008); Phys. Rev. C 79, 044606 (2009)

- *Ab initio* calculations for reactions and clustering in nuclei
- Constructs integration kernels ( $\approx$  projectile-target potentials) starting from
  - NCSM wave functions
  - NN(+NNN) interactions

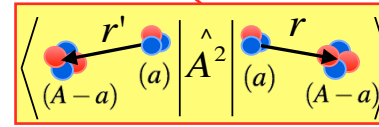


- Solves:

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



**Hamiltonian kernel**

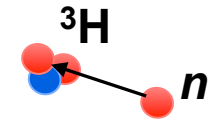


**Norm kernel**

The Resonating Group Method correctly accounts for:  
 1) the interaction (Hamiltonian kernel) and the Pauli principle (Norm kernel) between clusters and 2) all the available channels

Ultimate Goal:  $3\alpha \rightarrow {}^{12}\text{C}$  and  ${}^{12}\text{C}(\alpha, \gamma){}^{16}\text{O}$

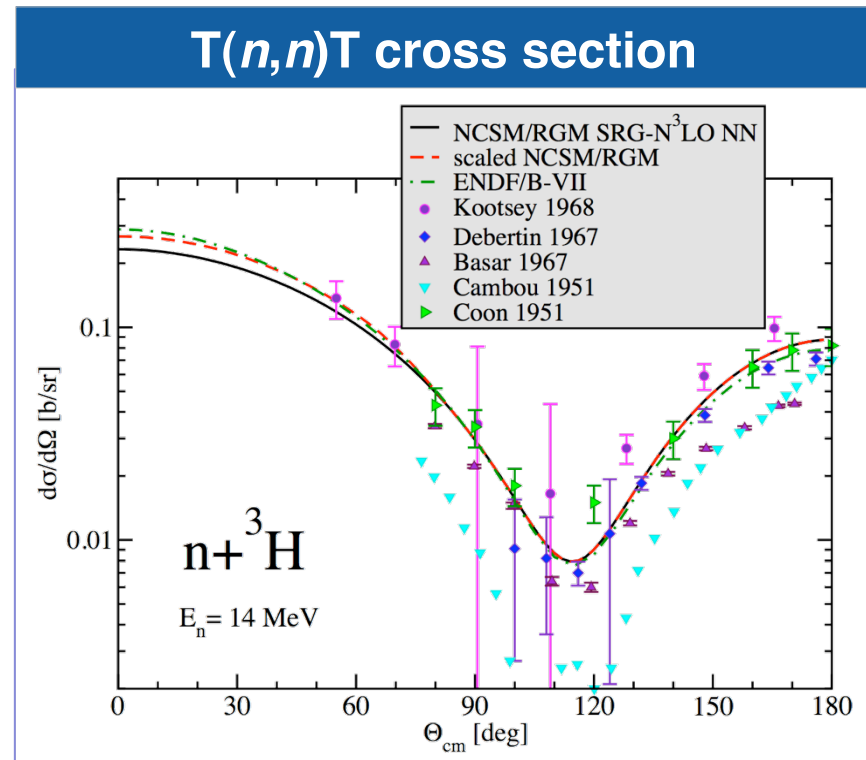
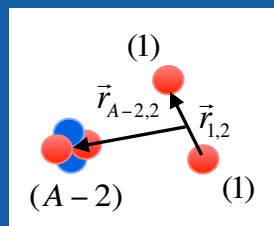
# Accurate evaluations and uncertainties for nuclear astrophysics and fusion diagnostic



- The elastic  $n$ - $^3\text{H}$  cross section for 14 MeV neutrons, important for understanding how the fuel is assembled in an implosion at NIF, was not known precisely enough
- Nuclear theory was asked to help
- Delivered evaluated data with required 5% uncertainty and successfully compared to measurements using an Inertial Confinement Facility

- $T(T,2n)^4\text{He}$  also important

- ⇒ Requires 3-body cluster states



*Ab initio* theory reduces uncertainty due to conflicting data (•, ♦, ▲, ▼, ►)

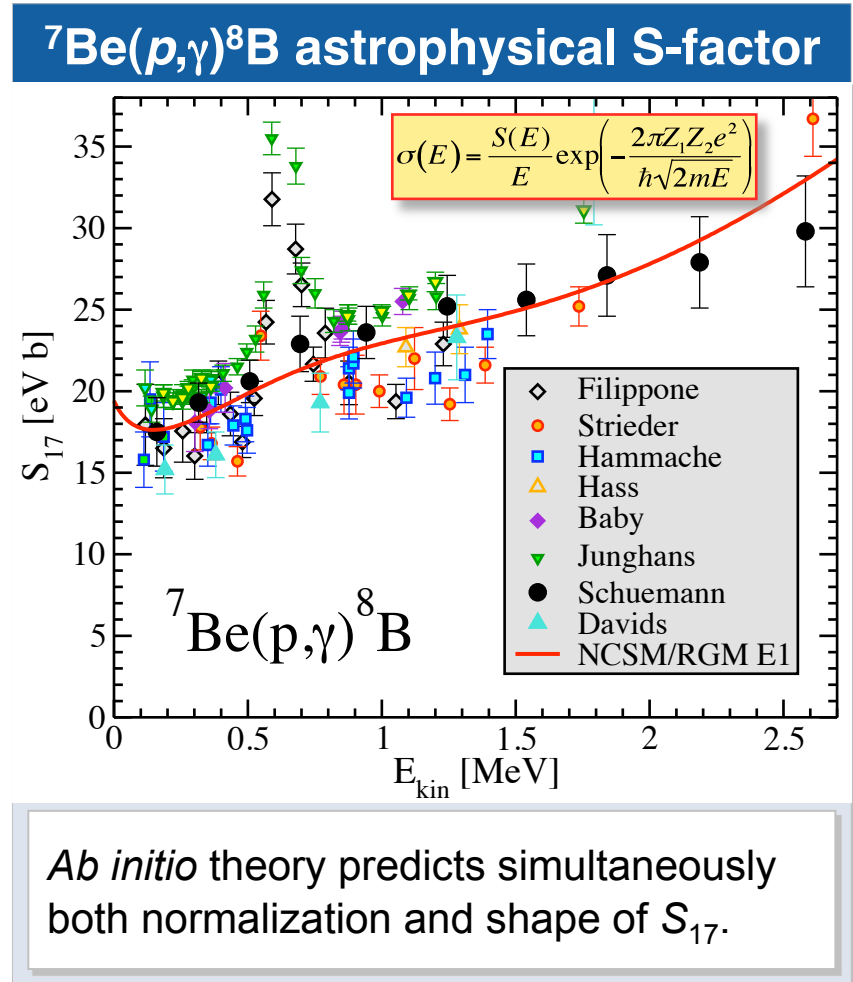
Navrátil *et al.*, LLNL-TR-423504, LLNL-TR-435981, arXiv.1009.3965



# Reactions important for solar astrophysics

P. Navrátil, R. Roth and S. Quaglioni, submitted to Phys. Rev. Lett., arXiv:1105.5977

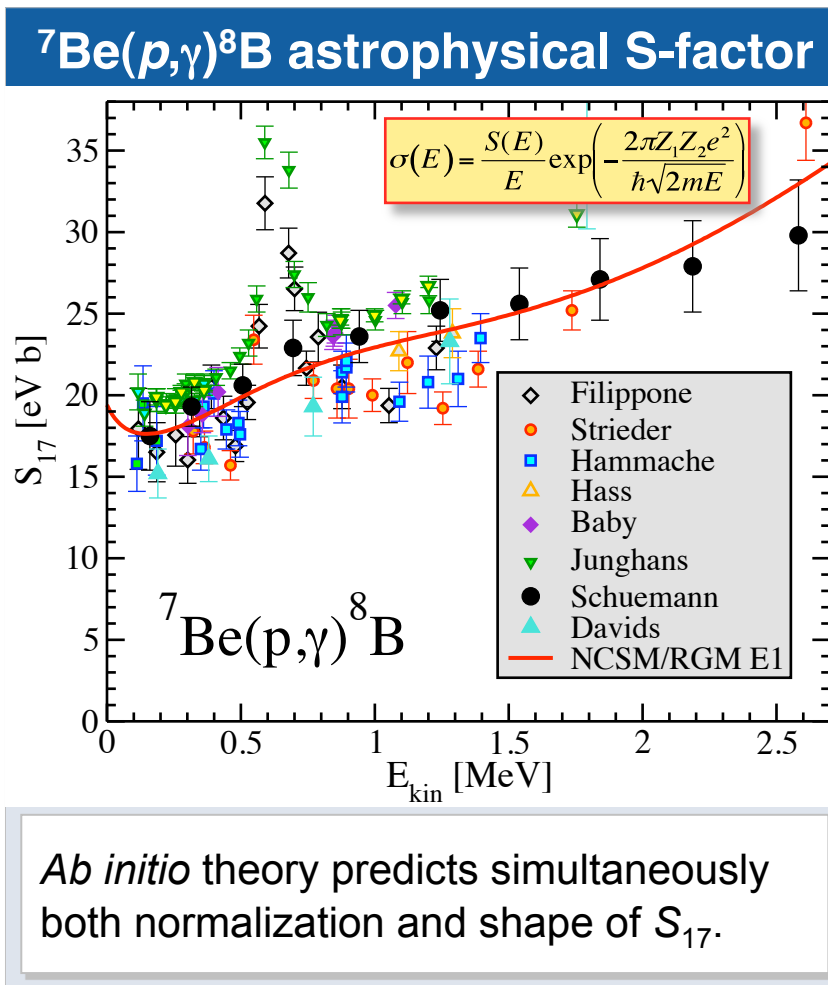
- The  ${}^7\text{Be}(p,\gamma){}^8\text{B}$  is the final step in the nucleosynthetic chain leading to  ${}^8\text{B}$
- $\sim 10\%$  error in latest  $S_{17}(0)$ : dominated by uncertainty in theoretical models
- NCSM/RGM results with largest realistic model space
  - SRG- $\text{N}^3\text{LO}$  NN potential ( $\lambda = 1.86 \text{ fm}^{-1}$ )
  - $N_{\text{max}} = 10$
  - $p+{}^7\text{Be}(\text{g.s.}, 1/2^-, 7/2^-, 5/2_1^-, 5/2_2^-)$
- Sep. energy: 136 keV (Expt. 137 keV)
- $S_{17}(0) = 19.4 \text{ eV b}$  on the lower side of, but consistent with latest evaluation
- Run time:  $\sim 150,000 \text{ CPU hrs}$



# Reactions important for solar astrophysics

P. Navrátil, R. Roth and S. Quaglioni, submitted to Phys. Rev. Lett., arXiv:1105.5977

- Remaining uncertainties
- Larger  $N_{\max}$ 
  - $N_{\max} = 10, 12$  calculations with 3 lowest  ${}^7\text{Be}$  eigenstates very close
  - ➔  $N_{\max} = 10$  reasonable HO model space
- Higher  ${}^7\text{Be}$  eigenstates
  - $N_{\max} = 8$  with 8 lowest  ${}^7\text{Be}$  eigenstates
  - ➔ Influence of  $7/2_2^-$  could be significant
  - **But:**  $N_{\max} = 8$  is not sufficient!
  - $N_{\max} = 10$ , with 8  ${}^7\text{Be}$  eigenstates presently out of reach
- $\pm 0.7$  eV b uncertainty on  $S_{17}(0)$
- **NNN force (SRG-induce + “real”) still missing**

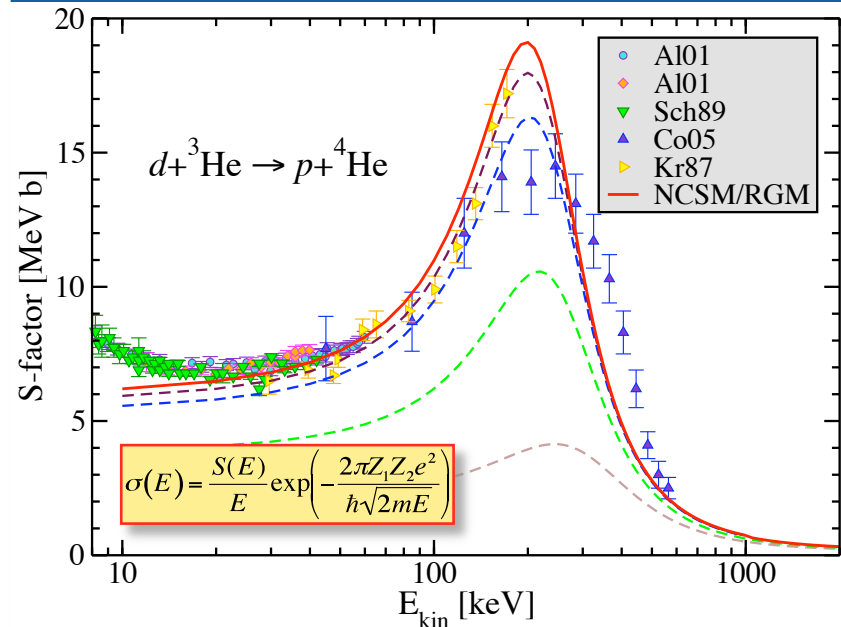


# Reactions with clusters – LDRD -> SciDAC-3

P. Navrátil, S. Quaglioni & R. Roth, Proceedings of INPC 2010, arXiv.1009.3965

- NCSM/RGM results for  $d(^3\text{He},p)^4\text{He}$ 
  - SRG-N<sup>3</sup>LO NN potential ( $\lambda = 1.5 \text{ fm}^{-1}$ )
  - Approx. treatment of virtual breakup:  
Include multiple excited deuteron pseudo-states
- Data curve up and deviate from theoretical results at low energy due to laboratory electron-screening.
- Run time:  $\sim 100,000$  CPU hrs

## $^3\text{He}(d,p)^4\text{He}$ astrophysical S-factor



- $d(\text{g.s.}) + 7$
  - $d(\text{g.s.}) + 5$
  - $d(\text{g.s.}) + 3$
  - $d(\text{g.s.}) + 1$
  - $d(\text{g.s.})$
- } Excited  $d$  pseudo-states in both  $^3S_1$ - $^3D_1$  and  $^3D_2$  channels

Fundamental description still requires:

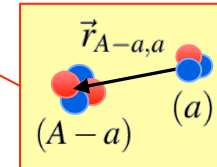
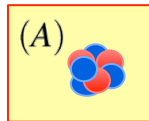
- 1) NNN force (SRG-induced + “real”)
- 2) 3-body cluster states & solution of 3-body scattering problem



# NCSM/RGM in the future

- Couple NCSM/RGM ( $A$ - $\underline{a}$ , $a$ ) basis with NCSM  $A$ -body eigenstates (NCSMC)

$$\Psi_{NCSMC}^{(A)} = \sum_{\lambda} c_{\lambda}^{(A)} |A \lambda J^{\pi} T\rangle + \sum_{a,v} \int d\vec{r} \varphi_v^{(A-a,a)}(\vec{r}) \hat{A}^{(A-a,a)} |\Phi_{v\vec{r}}^{(A-a,a)}\rangle$$



- Solve:

$$\begin{pmatrix} H & h \\ h & \mathcal{H} \end{pmatrix} \begin{pmatrix} c \\ \varphi \end{pmatrix} = E \begin{pmatrix} 1 & g \\ g & \mathcal{N} \end{pmatrix} \begin{pmatrix} c \\ \varphi \end{pmatrix}$$

- First step,  $A + (A-1, 1)$  formalism, under development by S. Baroni & P. Navratil
- Develop the NCSMC formalism with  $a > 1$
- Consistent treatment of bound and continuum states
- Three-body final states  $T(T, 2n)^4\text{He}$



# Activities with restoration

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- Benchmark n-<sup>8</sup>He, and n-<sup>9</sup>Li scattering.
- ✓ ■ Investigate p-<sup>7</sup>Be scattering and capture reactions.
- ✓ ■ Investigate <sup>3</sup>He-<sup>4</sup>He scattering and capture reactions.
- Use two-, three-, and four-body transition densities for A=3,4 nuclei.
- Development of three-body transition density calculation for A>4.
- ✓ ■ Include NNN interaction for n+A and p+A systems

