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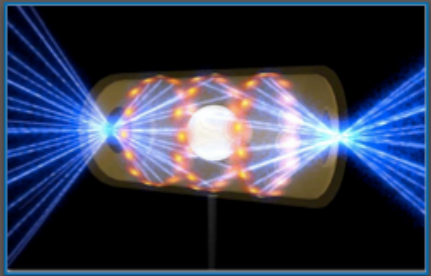
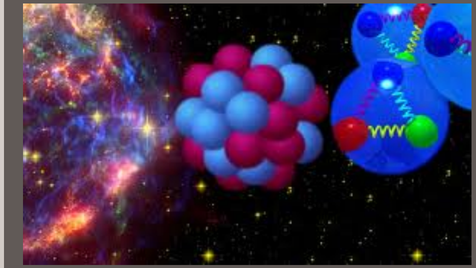
Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucléaire et en physique des particules

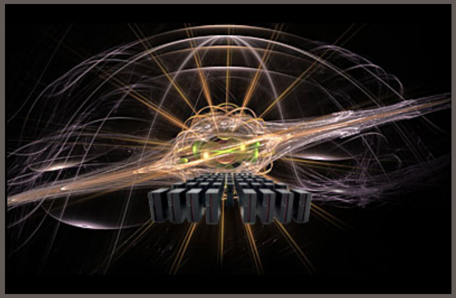
Ab initio approaches to nuclear reactions





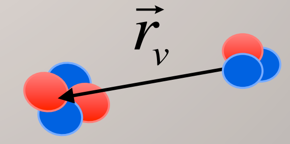
International Conference on Nuclear Theory in the Supercomputing Era - 2013
Iowa State University, Ames, Iowa
15th May 2013

Petr Navratil | TRIUMF



Outline

- *Ab initio* and microscopic nuclear reaction methods
  - Exact few-body calculations
  - GFMC
  - FMD
  - CCM
- No-core shell model
- Including the continuum with the resonating group method
  - NCSM/RGM
  - NCSMC
- Outlook



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Ab initio Nuclear Reaction approaches

Microscopic
- ✧ All nucleons are active
- ✧ Exact Pauli principle

Ab initio
- ✧ All nucleons are active
- ✧ Exact Pauli principle
- ✧ Realistic inter-nucleon interactions
- ✧ Controllable approximations

- Few-nucleon techniques using realistic NN (+ NNN) interactions
  - Faddeev (Witala *et al.*), AGS (Deltuva *et al.*), FY (Lazauskas *et al.*), HH (Viviani *et al.*), LIT/EIHH (Bacca *et al.*), LIT/NCSM, RGM (Hoffman *et al.*), …
- Many-body techniques using realistic NN (+ NNN) interactions
  - GFMC (Nollett *et al.*), NCSM/RGM, NCSMC (Quaglioni, PN), CCM with Gamow HF basis (Hagen *et al.*) …
- Microscopic cluster techniques using semi-realistic NN interactions
  - RGM, GCM (Descouvemont *et al.*), FMD (Neff *et al.*), AMD, …

Chiral Effective Field Theory

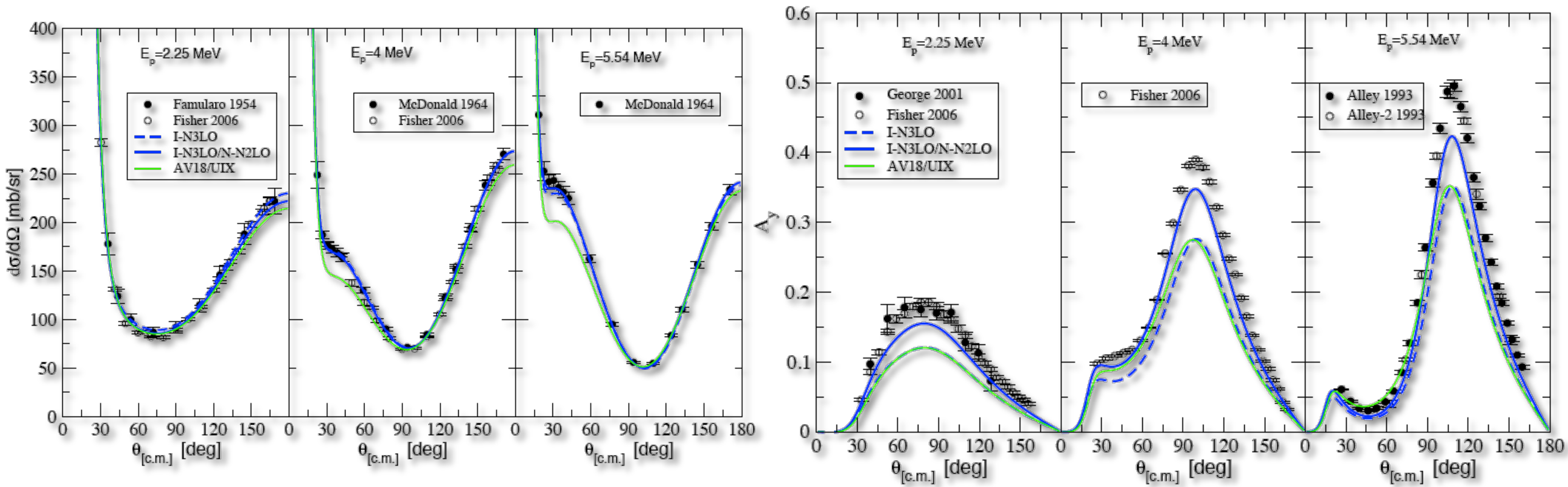
- **First principles for Nuclear Physics:**
  QCD
  - Non-perturbative at low energies
  - Lattice QCD in the future
- ***For now a good place to start*:**
- Inter-nucleon forces from chiral effective field theory
  - Based on the symmetries of QCD
    - Chiral symmetry of QCD ($m_u \approx m_d \approx 0$), spontaneously broken with pion as the Goldstone boson
    - Degrees of freedom: nucleons + pions
  - Systematic low-momentum expansion to a given order (Q/Λ_χ)
  - Hierarchy
  - Consistency
  - Low energy constants (LEC)
    - Fitted to data
    - Can be calculated by lattice QCD

Λ_χ~1 GeV :
Chiral symmetry breaking scale

Proton-^{3}He elastic scattering with χEFT NN+NNN

- Hypherspherical-harmonics variational calculations
  - M. Viviani, L. Girlanda, A. Kievski, L. E. Marcucci, and S. Rosati, arXiv:1004.1306
- **A_y puzzle resolved** with the chiral N^{3}LO NN plus **local chiral N^{2}LO NNN**
  - *used with the NCSM and other methods*

A=3 binding energy constraint, c_D=+1, c_E=-0.029, Λ=500 MeV



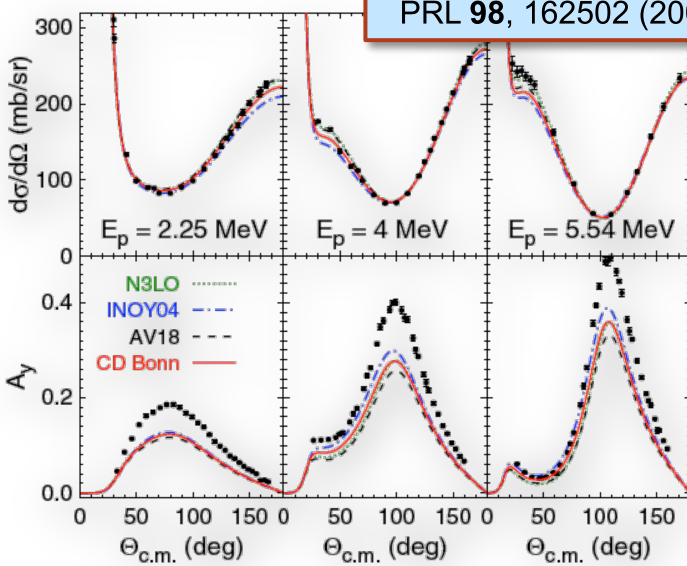
Chiral NN+NNN Hamiltonian provides the best agreement with the cross section and analyzing power data and with the new TUNL PSA analysis

Ab initio calculations of N-^{3}H, N-^{3}He scattering

Four-Body Calculation of Proton-^{3}He Scattering

A. Deltuva and A. C. Fonseca

PRL **98**, 162502 (2007)

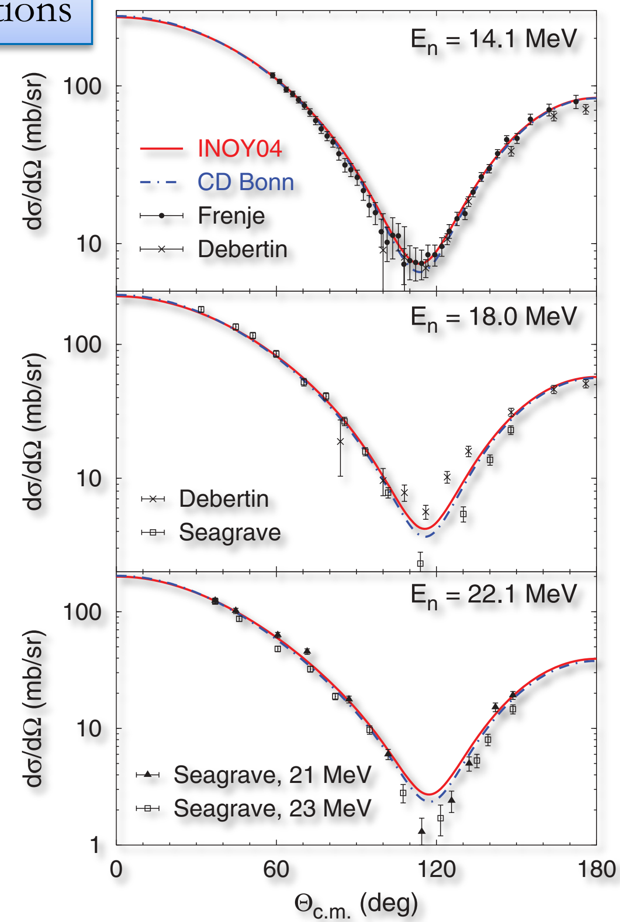


AGS equations

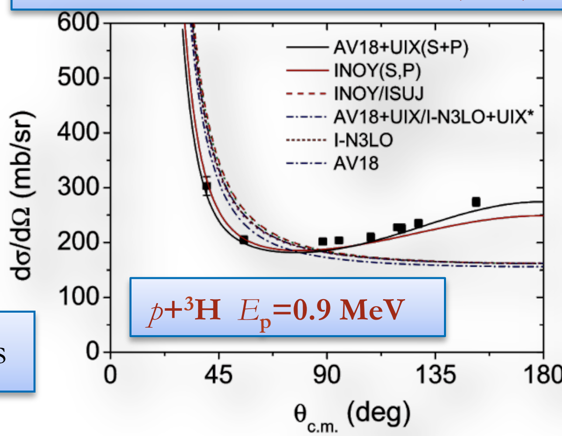
PHYSICAL REVIEW C **86**, 011001(R) (2012)

Neutron-^{3}H scattering above the four-nucleon breakup threshold

A. Deltuva and A. C. Fonseca



A. Lazauskas, PRC 79, 054007 (2009)



p+^{3}H E_p=0.9 MeV

FY equations

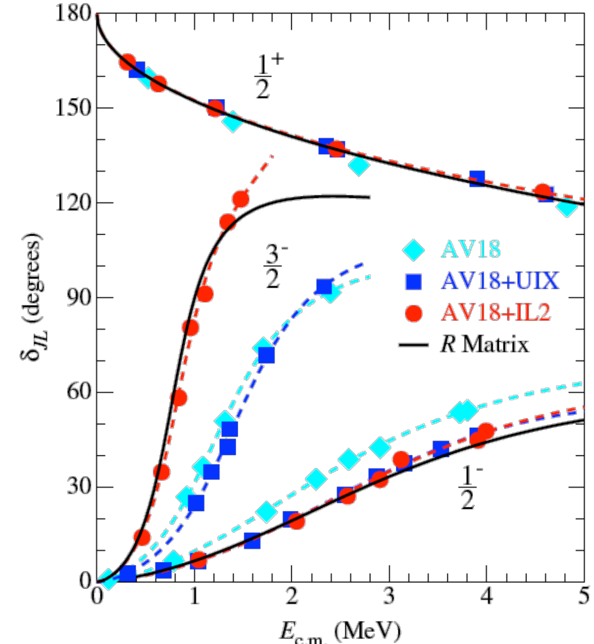
Quantum Monte Carlo Calculations of Neutron-^{4}He Scattering

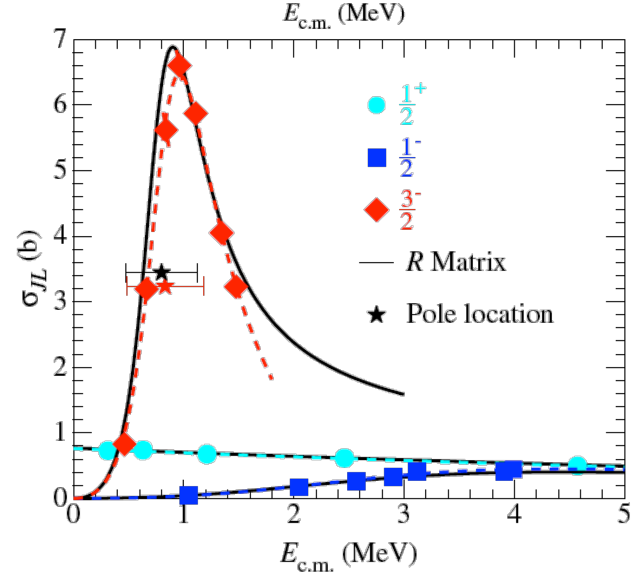
- GFMC method generalized for scattering
  - Similar to GFMC for bound states
    - Essential difference: **boundary conditions**
- Realistic NN plus NNN interactions
  - Importance of the three-body force for *P*-waves

Method

- Pick a log derivative χ at the boundary (R >7 fm)
- Starting w.f.: VMC with scattering boundary χ
- Special method for propagation to preserve χ
- Finds E(R, χ)
- Repeat for many χ until δ(E) is mapped out

K. Nollett et al., PRL99, 022502 (2007)





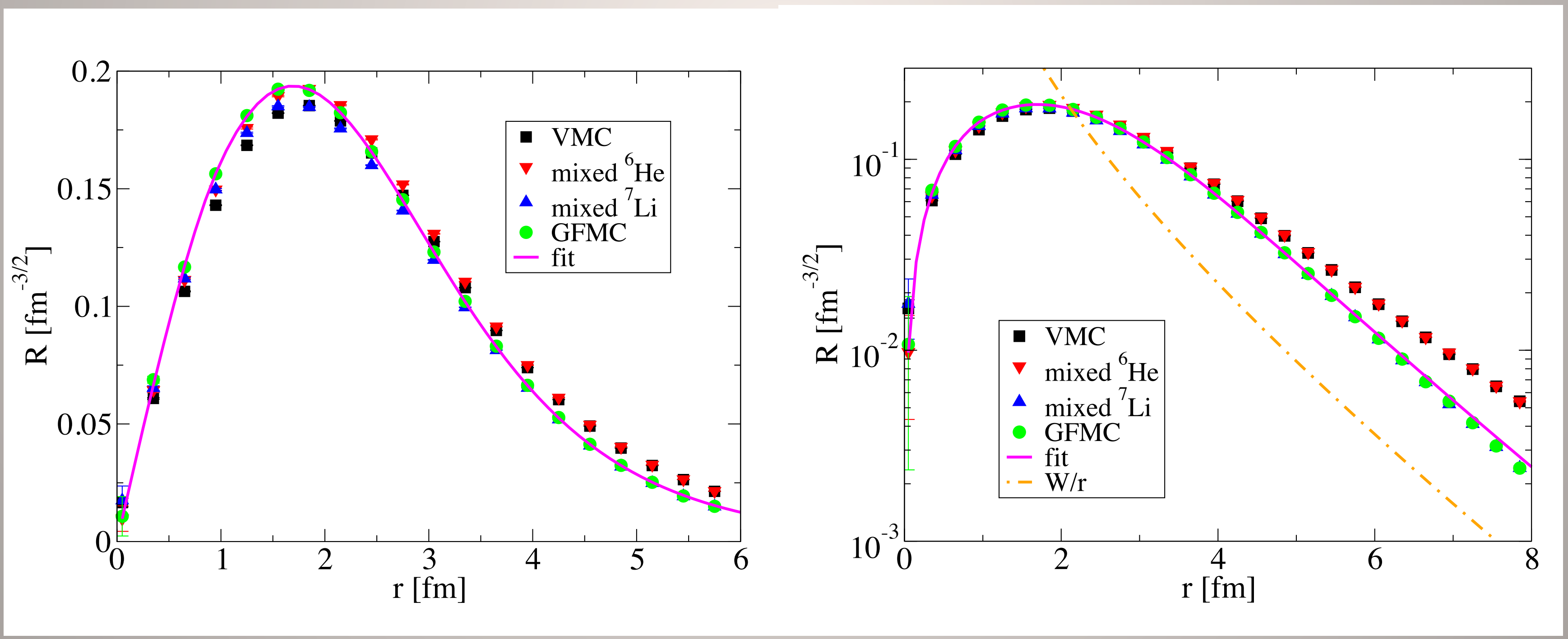
GFMC evaluation of spectroscopic overlaps

Overlap: $R(\alpha,\gamma,\nu;r) = \sqrt{A}\left\langle [\Psi_{A-1}(\gamma)\otimes\mathcal{Y}(\nu)(\hat{r}')]_{J_A,T_A}\left|\frac{\delta(r-r')}{r^2}\right|\Psi_A(\alpha)\right\rangle$

Spectroscopic factor: $S(\alpha,\gamma,\nu) = \int |R(\alpha,\gamma,\nu;r)|^2 r^2 dr$

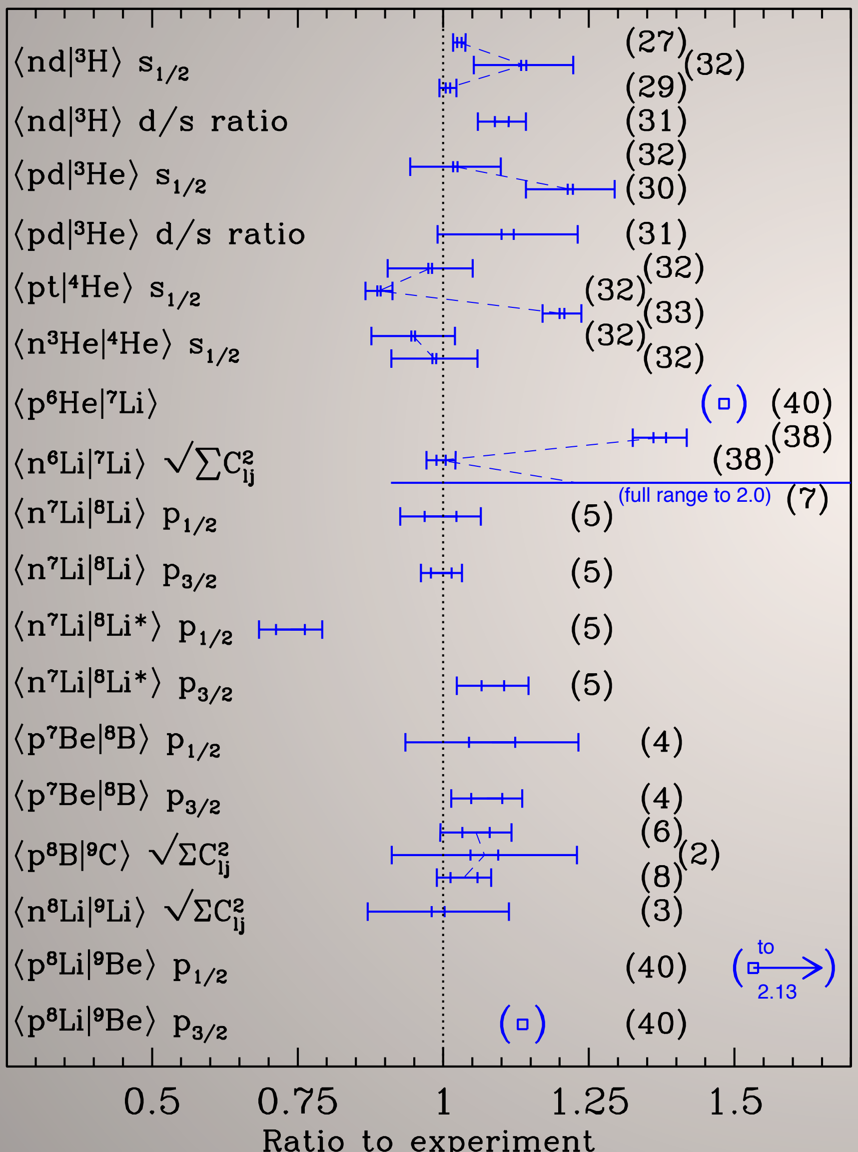
Asymptotic normalization constant (ANC): $R(\alpha,\gamma,\nu;r) \xrightarrow{r\to\infty} C(\alpha,\gamma,\nu)\frac{W_{-\eta,l+1/2}(2kr)}{r}$

$$\langle\, {}^6\mathrm{He}(0^+) + p\,|{}^7\mathrm{Li}({}^3/{}_2^-)\,\rangle$$



Brida, Pieper, & Wiringa, PRC **84**, 024319 (2011)

ANCs by integral relations with VMC wave functions



$$C_{lj}(\alpha,\gamma,\nu) = \frac{2\mu}{k\hbar^2 w}\mathcal{A}\int \frac{M_{-\eta,l+\frac{1}{2}}(2kr_{cc})}{r_{cc}}$$

$$\Psi^\dagger_{A-1}(\gamma)\chi^\dagger(\nu)Y^\dagger_{lm}(\hat{\mathbf{r}}_{cc})(U_{\rm rel} - V_C)\Psi_A(\alpha)\, d\mathbf{R}$$

$M_{-\eta,l+\frac{1}{2}}(2kr)$ is the "other" Whittaker function irregular at $r \to \infty$, and

$U_{\rm rel} = \sum_{i<A} v_{iA} + \sum_{i<j<A} V_{ijA}$.

At large separation of the last nucleon, $U_{\rm rel} \to V_C$, so $(U_{\rm rel} - V_C) \to 0$.

Results for one-nucleon removal $3 \leq A \leq 9$

- Small error bars are VMC statistics
- Large ones are "experimental"
- With a few exceptions, these are the first *ab initio* ANCs in $A > 4$

Nollett and Wiringa, PRC **83**, 041001(R) (2011)

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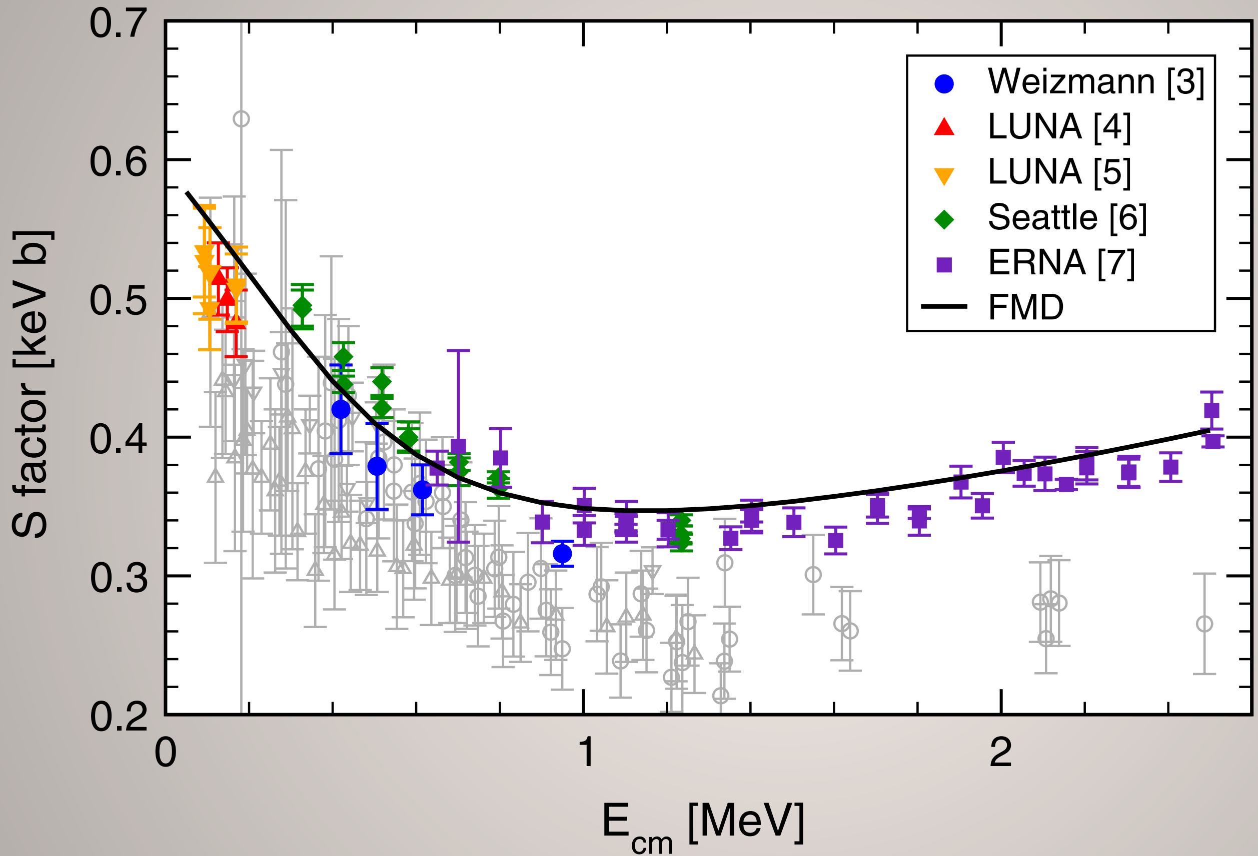
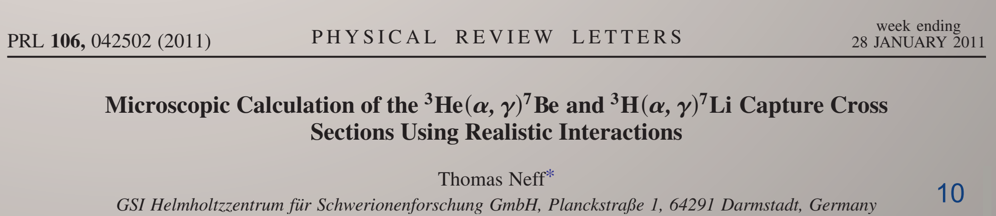
Microscopic Fermionic Molecular Dynamics calculation of $^3He(\alpha,\gamma)^7Be$ capture



The most realistic calculation of $^3He(\alpha,\gamma)^7Be$ capture so far



PRL 106, 042502 (2011) PHYSICAL REVIEW LETTERS week ending 28 JANUARY 2011

Microscopic Calculation of the $^3He(\alpha,\gamma)^7Be$ and $^3H(\alpha,\gamma)^7Li$ Capture Cross Sections Using Realistic Interactions

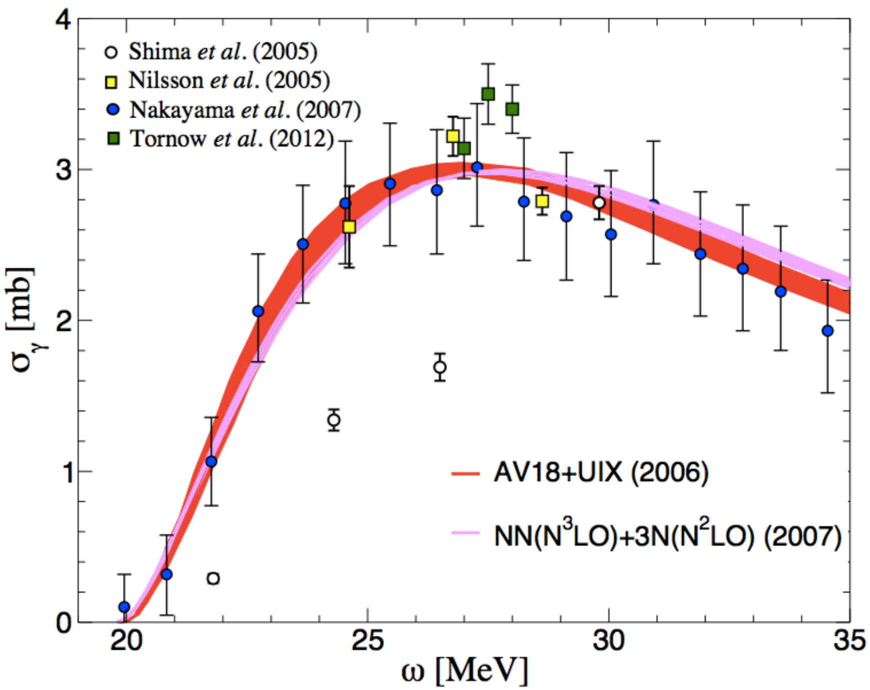
Thomas Neff*

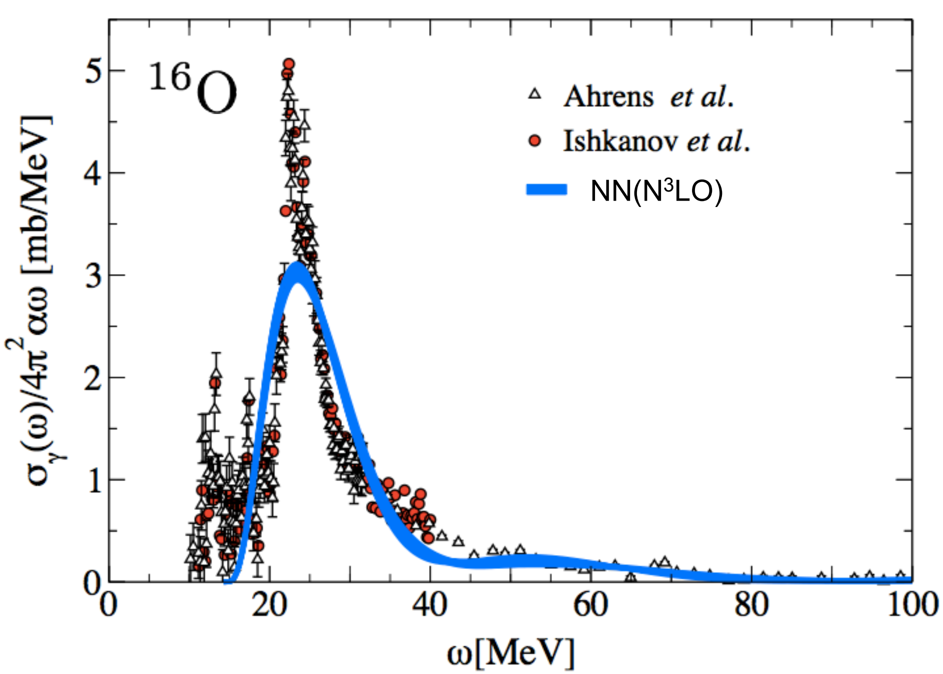
GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, 64291 Darmstadt, Germany

Photo-disintegration reactions

Photo-disintegration reactions can break the nucleus into many different clusters:
two-body clusters, three-body clusters, ..., A-nucleons ➡ terribly complicated many-body continuum state

Ab initio approach: Lorentz Integral Transform Method ➡ reduces the continuum problem to the solution of a bound-state equation which can be solved with any good bound-state technique





Hyperspherical Harmonics: Gazit, et al. PRL 96 112301 (2006)

NCSM: Quaglioni and Navratil PLB 652 (2007)

Coupled-Cluster Theory: Bacca et al., **arXiv:1303.7446**

Elastic proton/neutron scattering on ^{40}Ca

G. Hagen and N. Michel Phys. Rev. C **86**, 021602(R) (2012).

Elastic scattering of a nucleon on a target nucleus can be computed from the one-nucleon overlap function.

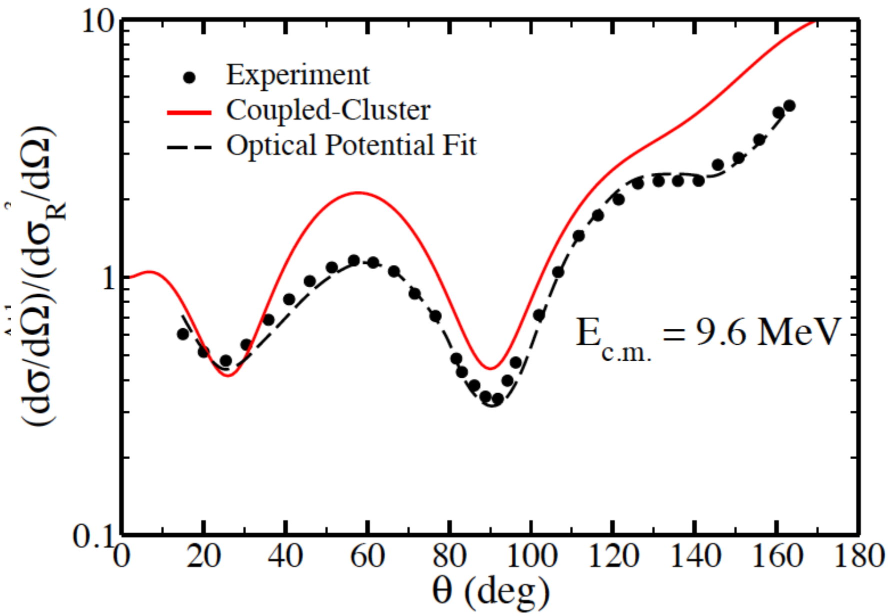
$$O_A^{A+1}(lj;kr) = \sum_n \left\langle A+1 \left\| \tilde{a}^\dagger_{nlj} \right\| A \right\rangle \phi_{nlj}(r).$$

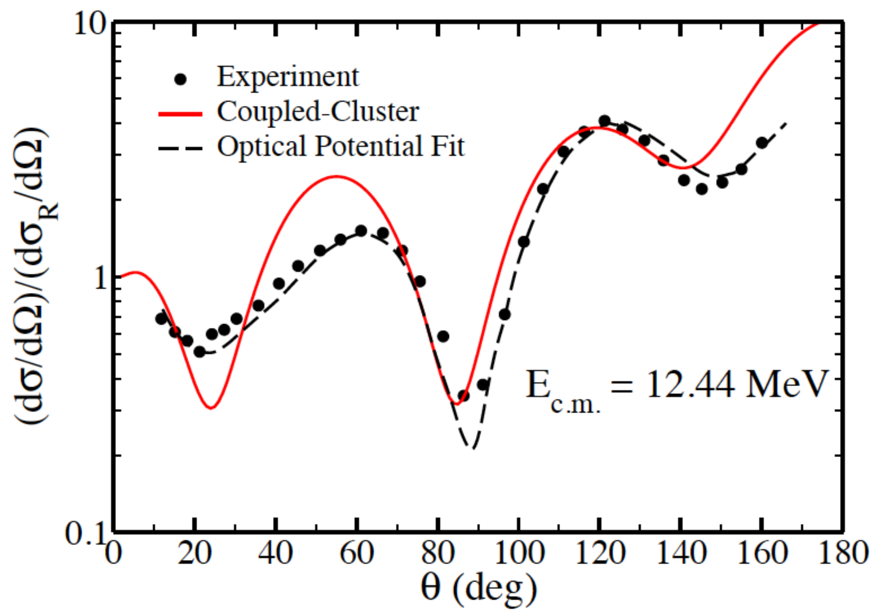
Beyond the range of the potential they are given by:

$$O_A^{A+1}(lj;kr) = C_{lj} \frac{W_{-\eta,l+1/2}(kr)}{r}, \quad k = i\kappa$$

$$O_A^{A+1}(lj;kr) = C_{lj} \left[F_{\ell,\eta}(kr) - \tan\delta_l(k) G_{\ell,\eta}(kr)\right]$$

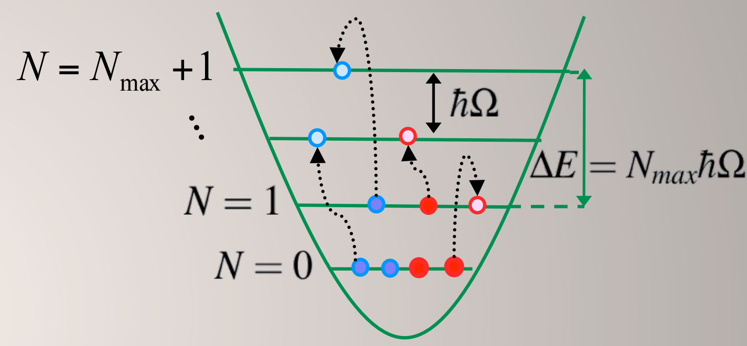
Using coupled-cluster theory to compute overlap functions we obtained cross sections at low-energy for elastic proton scattering on ^{40}Ca in fair agreement with experiment.



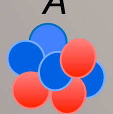


The *ab initio* no-core shell model (NCSM)

- The NCSM is a technique for the solution of the *A*-nucleon bound-state problem
- Realistic nuclear Hamiltonian
  - High-precision nucleon-nucleon potentials
  - Three-nucleon interactions
- Finite harmonic oscillator (HO) basis
  - *A*-nucleon HO basis states
  - complete $N_{max}\hbar\Omega$ model space
- ***Effective interaction tailored to model-space truncation*** for NN(+NNN) potentials
  - Okubo-Lee-Suzuki unitary transformation
- Or a **sequence of unitary transformations in momentum space**:
  - Similarity-Renormalization-Group (SRG) evolved NN(+NNN) potential



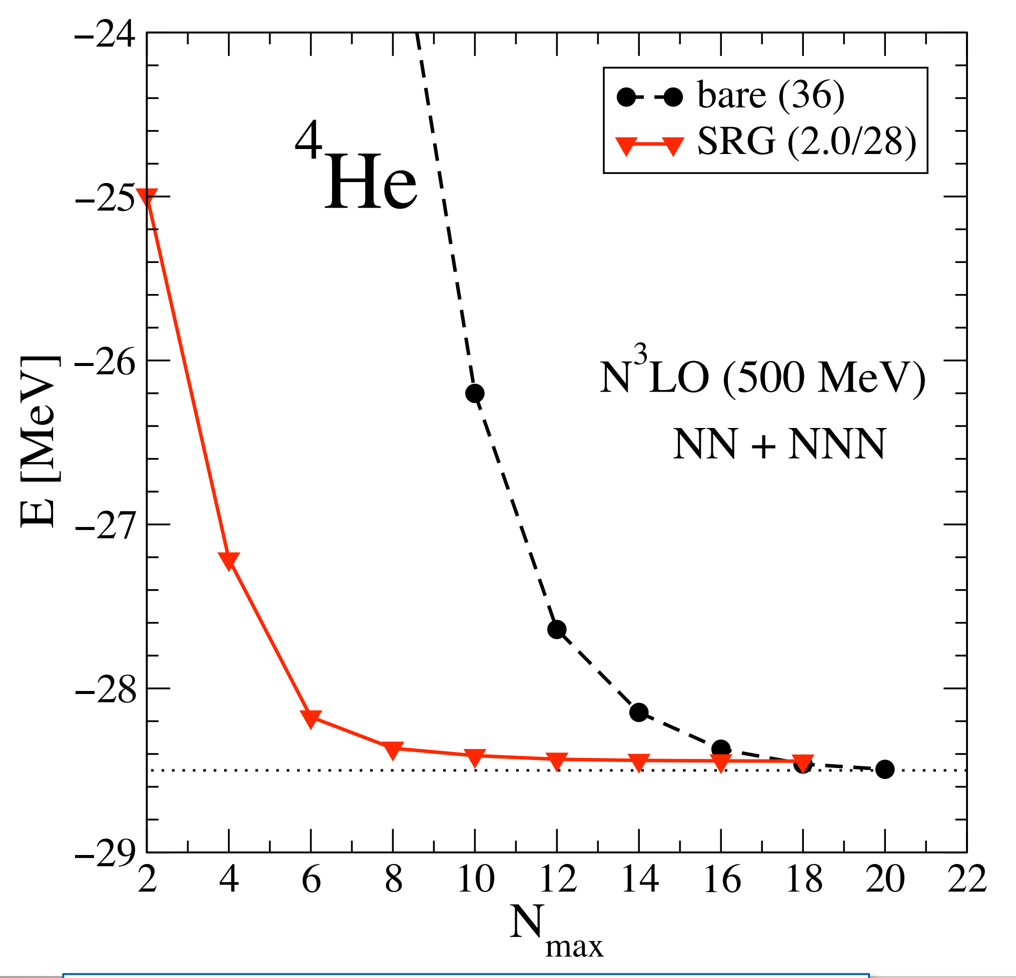
A

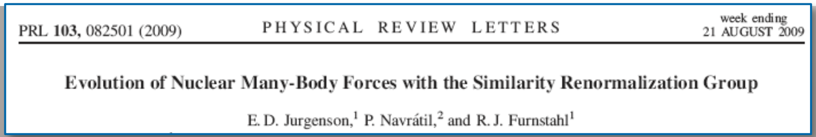


$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

Convergence to exact solution with increasing N_{max} for bound states. No coupling to continuum.

^{4}He from chiral EFT interactions: g.s. energy convergence




PRL 103, 082501 (2009) PHYSICAL REVIEW LETTERS week ending 21 AUGUST 2009

Evolution of Nuclear Many-Body Forces with the Similarity Renormalization Group

E. D. Jurgenson,[1] P. Navrátil,[2] and R. J. Furnstahl[1]

A=3 binding energy and half life constraint
c_D=-0.2, c_E=-0.205, Λ=500 MeV

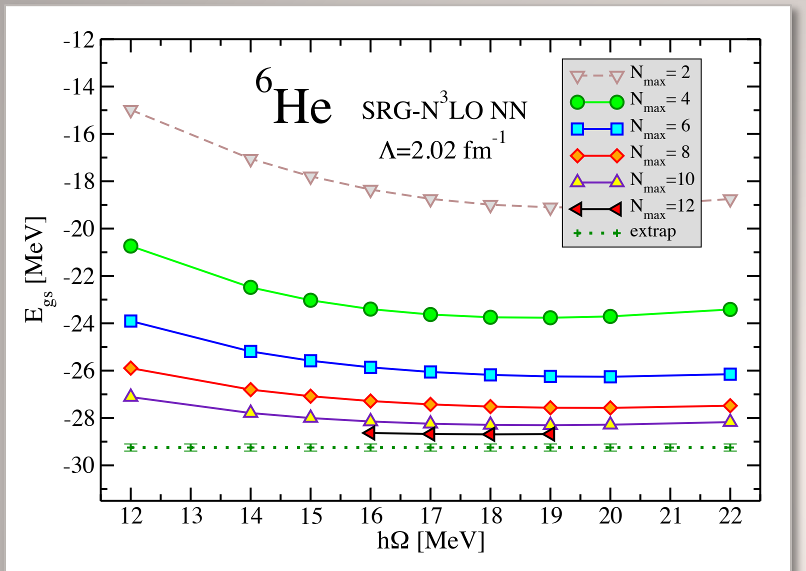
Chiral N^{3}LO NN plus N^{2}LO NNN potential

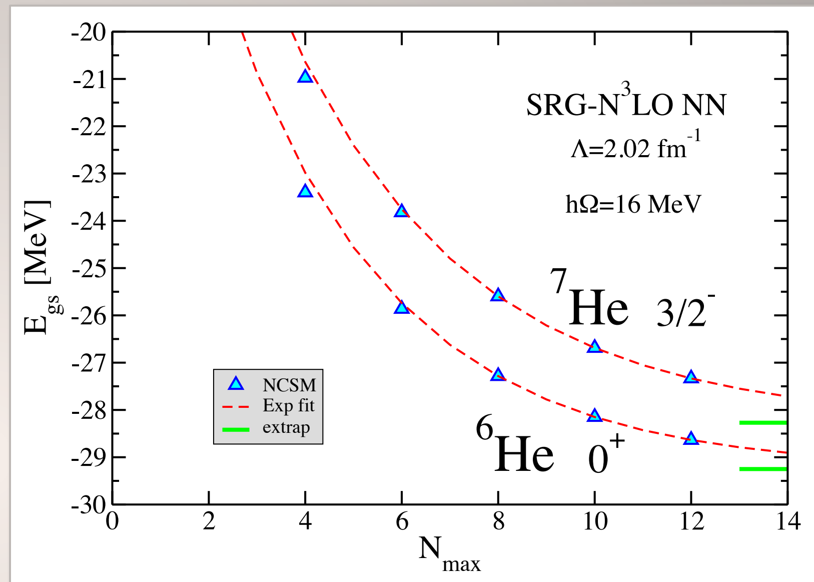
– Bare interaction (black line)
  - Strong short-range correlations
    - Large basis needed
– SRG evolved effective interaction (red line)
  - Unitary transformation

$$\boxed{H_\alpha = U_\alpha H U_\alpha^+ \Rightarrow \frac{dH_\alpha}{d\alpha} = [[T, H_\alpha], H_\alpha]} \quad \left(\alpha = 1/\lambda^4\right)$$

  - Two- plus *three*-body components, *four*-body omitted
  - Softens the interaction
    - Smaller basis sufficient

NCSM calculations of ^{6}He and ^{7}He g.s. energies

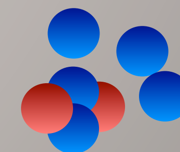




$E_{g.s.}$ [MeV]	^{4}He	^{6}He	^{7}He
NCSM N_{max}=12	-28.05	-28.63	-27.33
NCSM extrap.	-28.22(1)	-29.25(15)	-28.27(25)
Expt.	-28.30	-29.27	-28.84

- ✓ N_{max} convergence OK
- ✓ Extrapolation feasible
  - ^{6}He: E_{gs}=-29.25(15) MeV (Expt. -29.269 MeV)
  - ^{7}He: E_{gs}=-28.27(25) MeV (Expt. -28.84(30) MeV)
- ^{7}He unbound (+0.430(3) MeV), width 0.182(5) MeV
  - **NCSM: no information about the width**

^{7}He

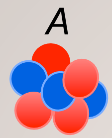


unbound

Extending no-core shell model beyond bound states

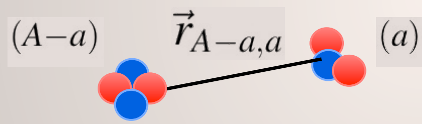
Include more many nucleon correlations…

NCSM



$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

+



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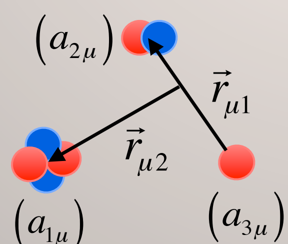


$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

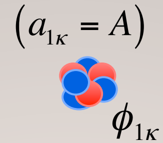
+

…

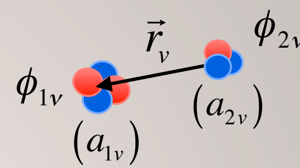
…using the Resonating Group Method (RGM) ideas

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



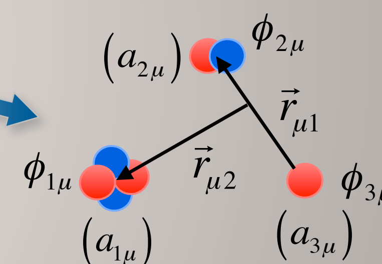
$$+ \sum_{\nu} \hat{A}_{\nu} \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



$$a_{1\nu} + a_{2\nu} = A$$

$$+ \sum_{\mu} \hat{A}_{\mu} \phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right) \phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right) \phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_{\mu}(\vec{r}_{\mu 1}, \vec{r}_{\mu 2})$$

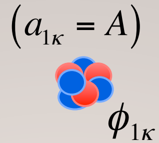
$$+ \cdots$$



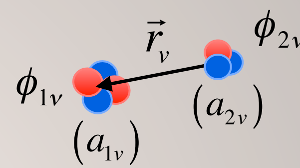
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \boxed{\phi_{1\kappa}}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



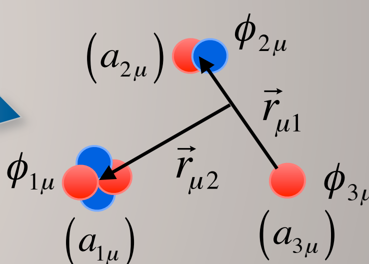
$$+ \sum_{\nu} \hat{A}_{\nu} \boxed{\phi_{1\nu}}\left(\left\{\vec{\xi}_{1\nu}\right\}\right) \boxed{\phi_{2\nu}}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_{\nu}(\vec{r}_{\nu})$$



$$a_{1\nu} + a_{2\nu} = A$$

$$+ \sum_{\mu} \hat{A}_{\mu} \boxed{\phi_{1\mu}}\left(\left\{\vec{\xi}_{1\mu}\right\}\right) \boxed{\phi_{2\mu}}\left(\left\{\vec{\xi}_{2\mu}\right\}\right) \boxed{\phi_{3\mu}}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_{\mu}(\vec{r}_{\mu 1}, \vec{r}_{\mu 2})$$

$$+ \cdots$$



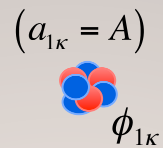
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

- ϕ : antisymmetric cluster wave functions
  - $\{\xi\}$: Translationally invariant internal coordinates

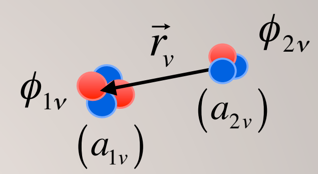
    (Jacobi relative coordinates)
  - These are known, they are an input

Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_\kappa \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



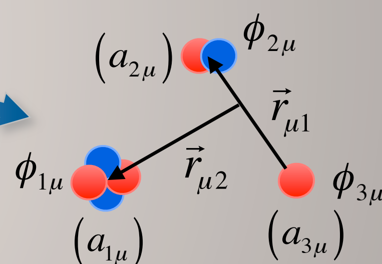
$$+ \sum_{\nu} \boxed{\hat{A}_\nu} \phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right) g_\nu(\vec{r}_\nu)$$



$$a_{1\nu} + a_{2\nu} = A$$

$$+ \sum_{\mu} \boxed{\hat{A}_\mu} \phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right) G_\mu(\vec{R}_{\mu 1}, \vec{R}_{\mu 2})$$

$$+ \cdots$$



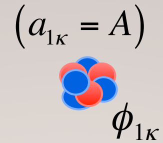
$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$

- $\boldsymbol{A_\nu}$, $\boldsymbol{A_\mu}$: intercluster antisymmetrizers
  - Antisymmetrize the wave function for exchanges of nucleons between clusters
  - Example:

$$a_{1\nu} = A-1,\ a_{2\nu} = 1 \quad \Rightarrow \quad \hat{A}_\nu = \frac{1}{\sqrt{A}}\left[1 - \sum_{i=1}^{A-1} \hat{P}_{iA}\right]$$

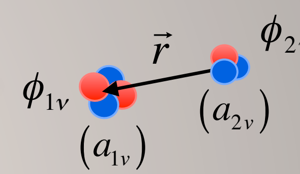
Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} \boxed{c_{\kappa}} \phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)$$



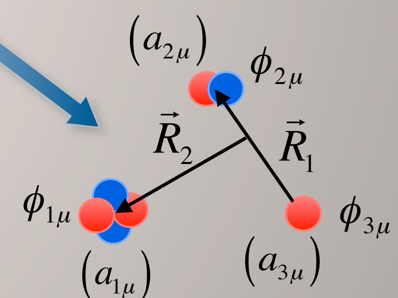
$$+ \sum_{\nu} \int \boxed{g_{\nu}(\vec{r})}\, \hat{A}_{\nu}\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_{\nu})\right] d\vec{r}$$

$a_{1\nu} + a_{2\nu} = A$



$$+ \sum_{\mu} \iint \boxed{G_{\mu}(\vec{R}_1, \vec{R}_2)}\, \hat{A}_{\mu}\left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1 - \vec{R}_{\mu 1})\delta(\vec{R}_2 - \vec{R}_{\mu 2})\right] d\vec{R}_1 d\vec{R}_2$$

$$+ \cdots$$

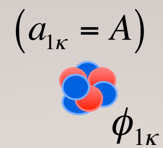


$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$

- ***c***, ***g*** and ***G***: discrete and continuous linear variational amplitudes
  - Unknowns to be determined

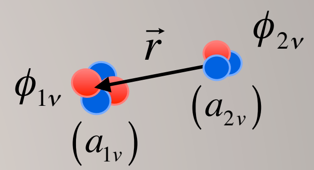
Trial function: generalized cluster wave function

$$\psi^{(A)} = \sum_{\kappa} c_{\kappa} \boxed{\phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)}$$



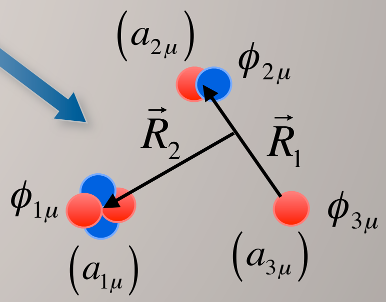
$$+ \sum_{\nu} \int g_{\nu}(\vec{r}\,)\ \hat{A}_{\nu} \boxed{\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r} - \vec{r}_{\nu})\right]} d\vec{r}$$

$a_{1\nu} + a_{2\nu} = A$



$$+ \sum_{\mu} \iint G_{\mu}(\vec{R}_1, \vec{R}_2)\ \hat{A}_{\mu} \boxed{\left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1 - \vec{R}_{\mu 1})\delta(\vec{R}_2 - \vec{R}_{\mu 2})\right]} d\vec{R}_1 d\vec{R}_2$$

$$+ \cdots$$



$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$

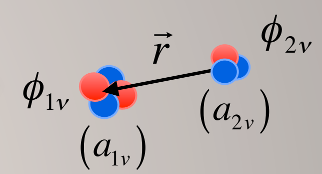
- Discrete and continuous set of basis functions
  - Non-orthogonal
  - Over-complete

Binary cluster wave function

$$\psi^{(A)} = \sum_{\kappa} \cancel{c_{\kappa}\phi_{1\kappa}\left(\left\{\vec{\xi}_{1\kappa}\right\}\right)}$$

$$a_{1\nu} + a_{2\nu} = A$$

$$+\sum_{\nu}\int g_{\nu}(\vec{r}\,)\ \hat{A}_{\nu}\left[\phi_{1\nu}\left(\left\{\vec{\xi}_{1\nu}\right\}\right)\phi_{2\nu}\left(\left\{\vec{\xi}_{2\nu}\right\}\right)\delta(\vec{r}-\vec{r}_{\nu})\right]d\vec{r}$$



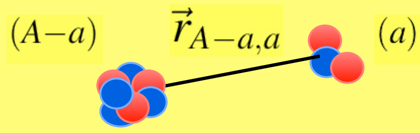
$$\cancel{+\sum_{\mu}\iint G_{\mu}(\vec{R}_1,\vec{R}_2)\ \hat{A}_{\mu}\left[\phi_{1\mu}\left(\left\{\vec{\xi}_{1\mu}\right\}\right)\phi_{2\mu}\left(\left\{\vec{\xi}_{2\mu}\right\}\right)\phi_{3\mu}\left(\left\{\vec{\xi}_{3\mu}\right\}\right)\delta(\vec{R}_1-\vec{R}_{\mu 1})\delta(\vec{R}_2-\vec{R}_{\mu 2})\right]d\vec{R}_1 d\vec{R}_2}$$

$$+\ \cdots$$

- In practice: function space limited by using relatively simple forms of Ψ chosen according to physical intuition and energetical arguments
  - Most common: expansion over binary-cluster basis

The *ab initio* NCSM/RGM in a snapshot

- Ansatz: $\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\, \varphi_\nu(\vec{r})\, \hat{\mathcal{A}}\, \Phi^{(A-a,a)}_{\nu\vec{r}}$



$$\psi^{(A-a)}_{1\nu}\, \psi^{(a)}_{2\nu}\, \delta(\vec{r} - \vec{r}_{A-a,a})$$

eigenstates of $H_{(A\text{-}a)}$ and $H_{(a)}$ in the *ab initio* NCSM basis

- Many-body Schrödinger equation:

$$H\Psi^{(A)} = E\Psi^{(A)}$$

$$T_{\mathrm{rel}}(r) + \mathcal{V}_{\mathrm{rel}} + \bar{V}_{\mathrm{Coul}}(r) + H_{(A-a)} + H_{(a)}$$

realistic nuclear Hamiltonian

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

$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}} H \hat{\mathcal{A}} | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$$

Hamiltonian kernel

$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}}^2 | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$$

Norm kernel

Norm kernel (Pauli principle)

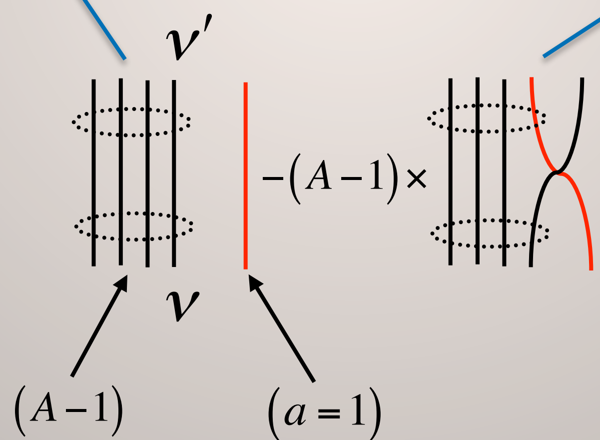
Single-nucleon projectile

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle \; (A-1) \;\; r' \;\; (a'=1) \; \middle| \; 1 - \sum_{i=1}^{A-1} \hat{P}_{iA} \; \middle| \; (a=1) \;\; r \;\; (A-1) \; \right\rangle$$

$$N^{J^\pi T}_{\nu' \nu}(r', r) = \underbrace{\delta_{\nu' \nu} \frac{\delta(r' - r)}{r' r}} - \underbrace{(A-1) \sum_{n' n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| \hat{P}_{A-1,A} \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle}$$

$${}_{SD}\left\langle \psi^{(A-1)}_{\mu_1} \middle| a^{+} a \middle| \psi^{(A-1)}_{\nu_1} \right\rangle_{SD}$$

Direct term:
Treated exactly!
(in the full space)

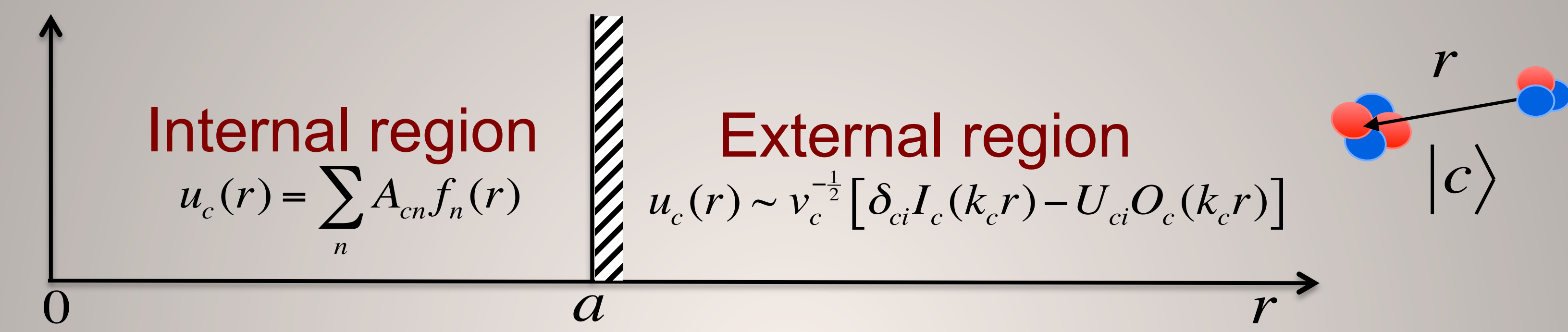


Exchange term:
Obtained in the model space!
(Many-body correction due to the exchange part of the inter-cluster antisymmetrizer)

$$\frac{\delta(r - r_{A-a,a})}{r \, r_{A-a,a}} = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

Microscopic *R*-matrix on a Lagrange mesh

Separation into "internal" and "external" regions at the channel radius a



- This is achieved through the Bloch operator: $L_c = \dfrac{\hbar^2}{2\mu_c} \delta(r-a) \left(\dfrac{d}{dr} - \dfrac{B_c}{r} \right)$
- System of Bloch-Schrödinger equations:

$$\left[\hat{T}_{rel}(r) + L_c + \overline{V}_{Coul}(r) - (E - E_c) \right] u_c(r) + \sum_{c'} \int dr' \, r' W_{cc'}(r,r') u_{c'}(r') = L_c u_c(r)$$

$$u_c(r) = \sum_n A_{cn} f_n(r)$$

- Internal region: expansion on square-integrable Lagrange mesh basis
- External region: asymptotic form for large r

$$\{ a x_n \in [0,a] \}$$

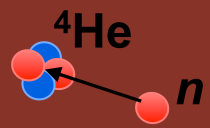
$$\int_0^1 g(x)dx \approx \sum_{n=1}^{N} \lambda_n g(x_n)$$

$$\int_0^a f_n(r) f_{n'}(r) dr \approx \delta_{nn'}$$

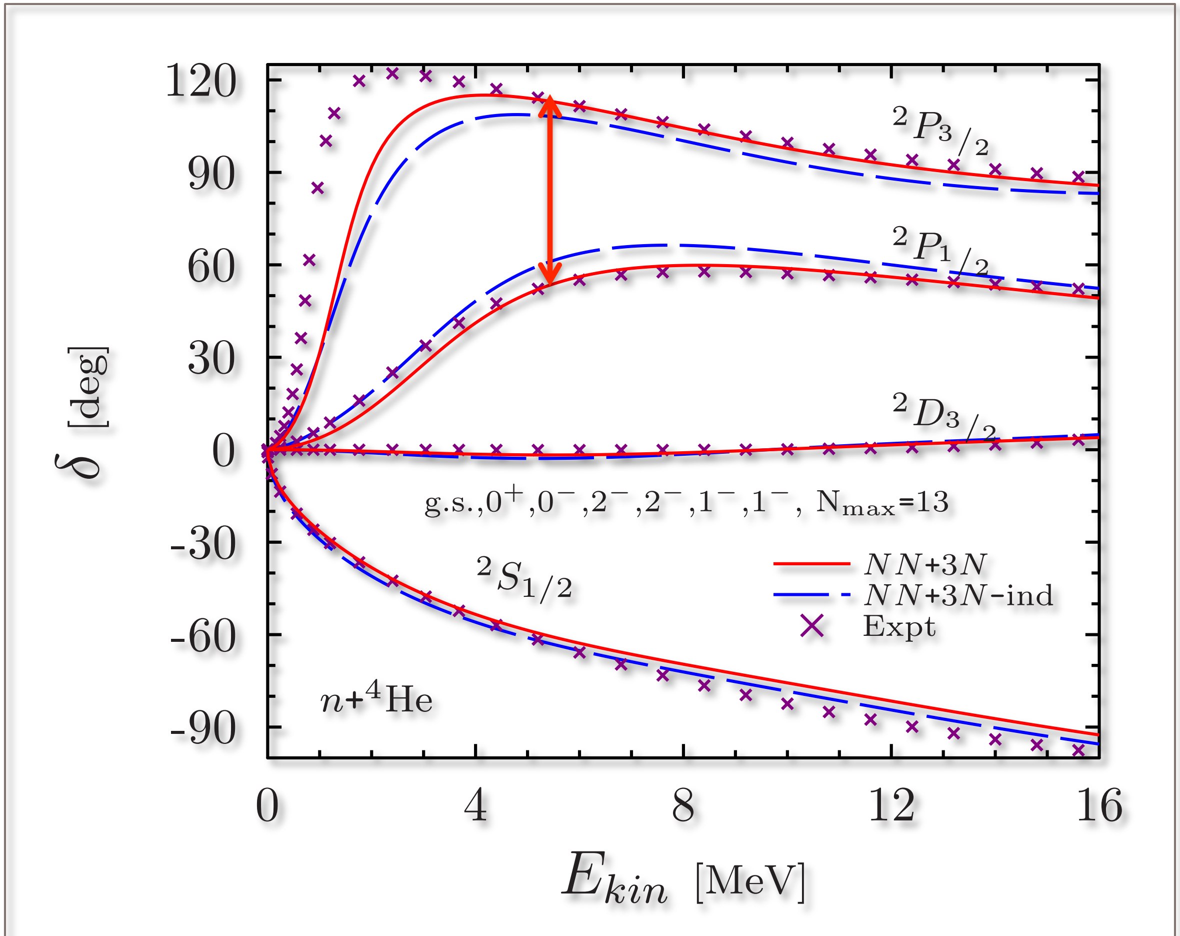
$$u_c(r) \sim C_c W(k_c r) \quad \text{or} \quad u_c(r) \sim v_c^{-\frac{1}{2}} \left[\delta_{ci} I_c(k_c r) - U_{ci} O_c(k_c r) \right]$$

Bound state | Scattering state | Scattering matrix

TRIUMF

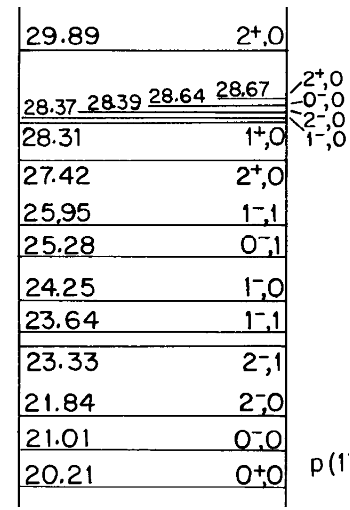


n-^{4}He scattering: NN vs. NN+NNN interactions



chiral NN+NNN(500)
chiral NN+NNN-induced
SRG λ=2 fm^{-1}
HO N_{max}=13, ħΩ=20 MeV

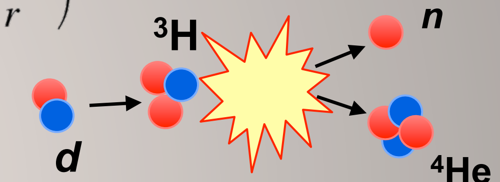
^{4}He g.s. and 6 excited states

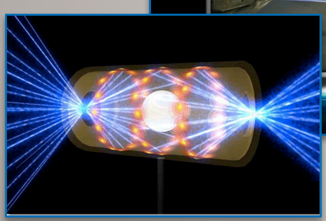


The largest splitting between the P-waves obtained with the chiral NN+NNN interaction

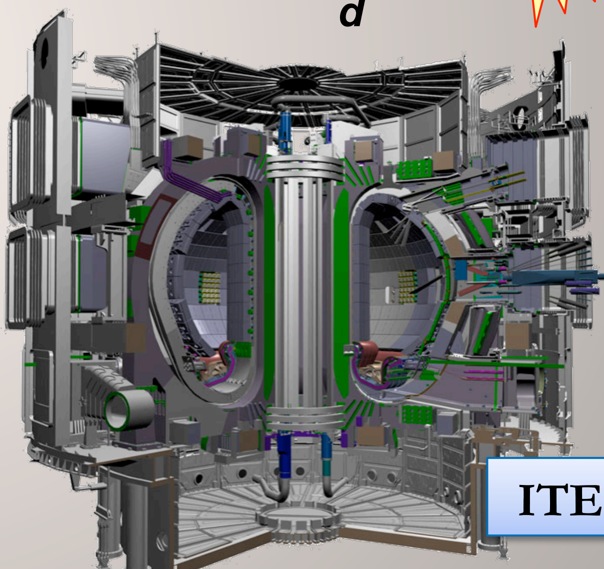
Ab initio calculation of the ^{3}H(*d*,*n*)^{4}He fusion

$$\int dr\, r^2 \begin{pmatrix} \left\langle {}_{n}^{r'}\alpha \right| \hat{A}_1 (H-E) \hat{A}_1 \left| \alpha\, {}_{n}^{r} \right\rangle & \left\langle {}_{n}^{r'}\alpha \right| \hat{A}_1 (H-E) \hat{A}_2 \left| {}^3\mathrm{H}\, {}_{d}^{r} \right\rangle \\ \left\langle {}_{d}^{r'}\,{}^3\mathrm{H} \right| \hat{A}_2 (H-E) \hat{A}_1 \left| \alpha\, {}_{n}^{r} \right\rangle & \left\langle {}_{d}^{r'}\,{}^3\mathrm{H} \right| \hat{A}_2 (H-E) \hat{A}_2 \left| {}^3\mathrm{H}\, {}_{d}^{r} \right\rangle \end{pmatrix} \begin{pmatrix} \frac{g_1(r)}{r} \\ \frac{g_2(r)}{r} \end{pmatrix} = 0$$





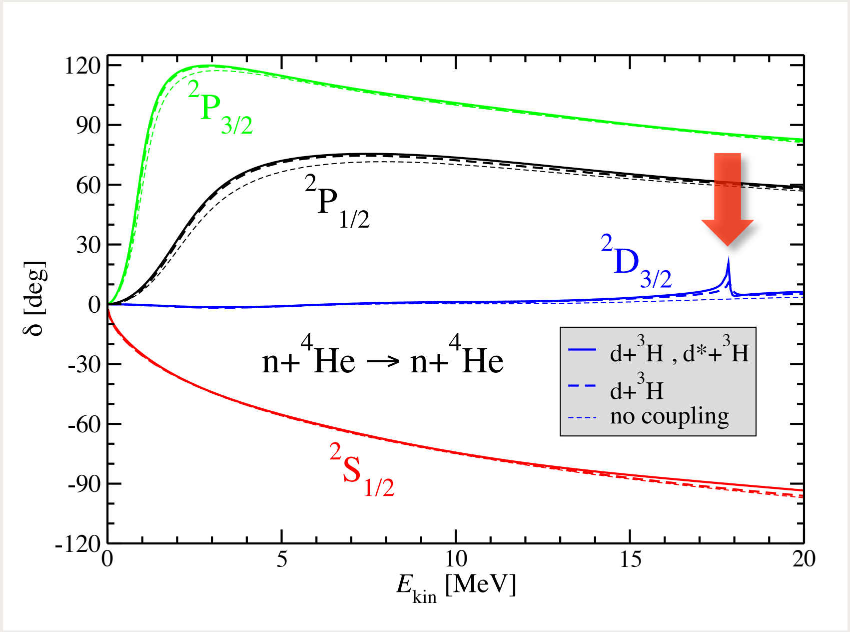
NIF

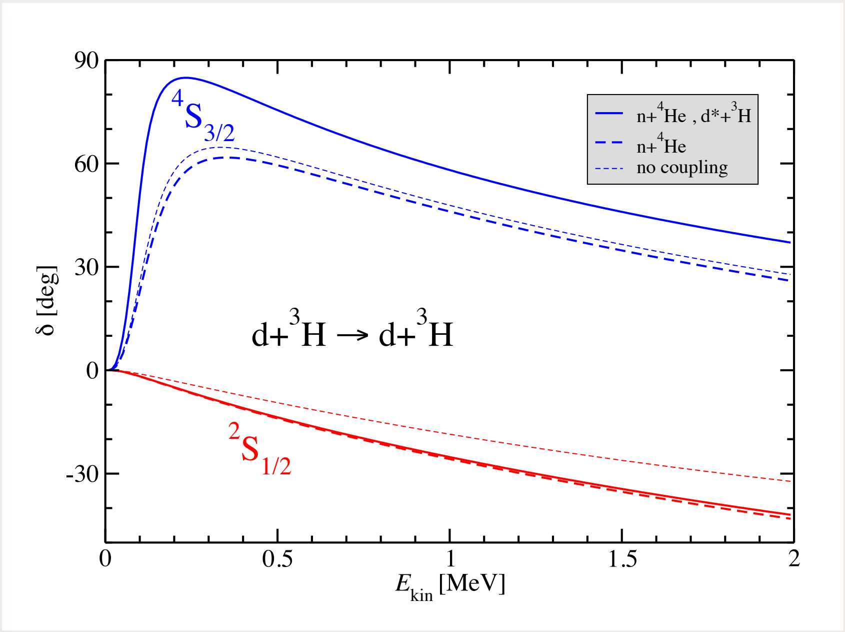


ITER

energy generation

d+^{3}H and n+^{4}He elastic scattering: phase shifts





- *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

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

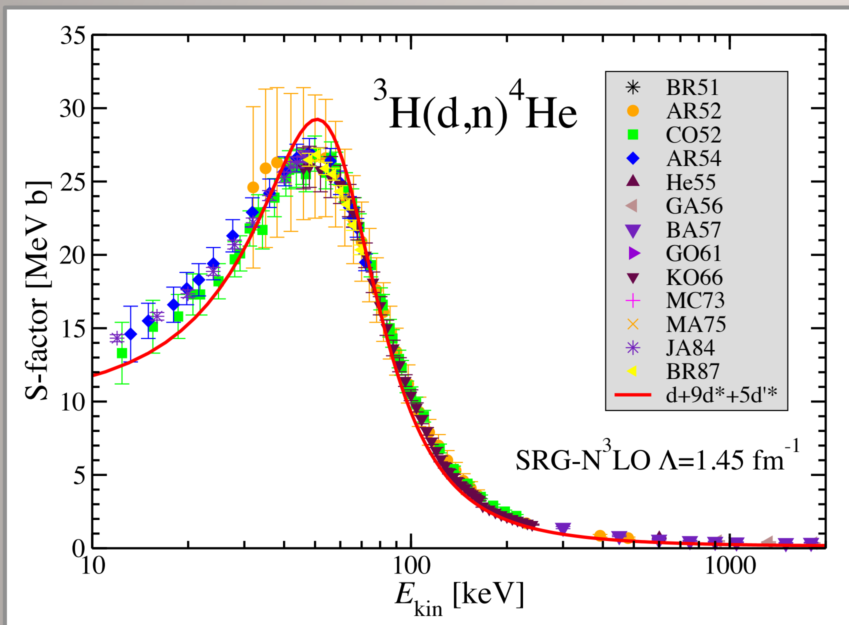
*d** deuteron pseudo state in $^3S_1$-$^3D_1$ channel: deuteron polarization, virtual breakup

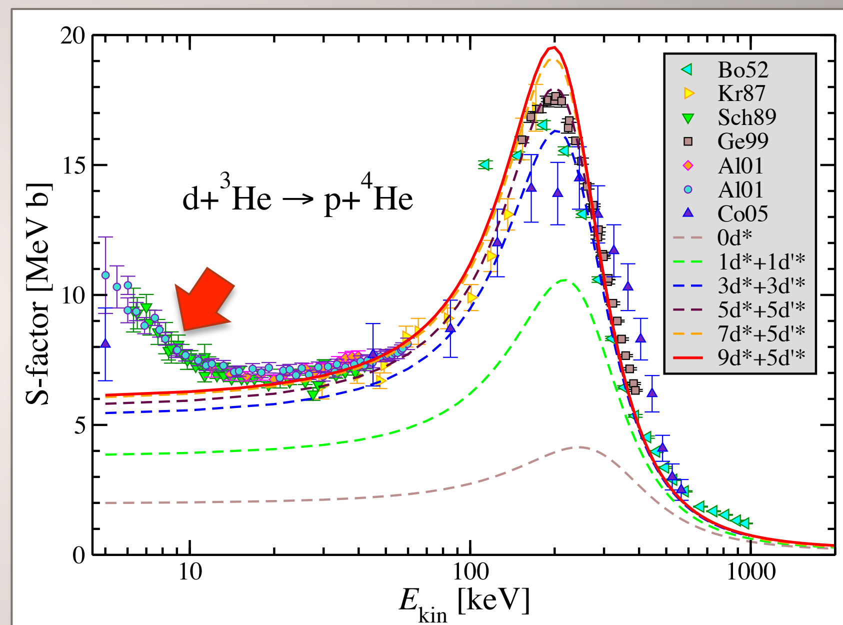
The *d*-^{3}H fusion takes place through a transition of *d*+^{3}H is *S*-wave to *n*+^{4}He in *D*-wave: Importance of the **tensor force**

TRIUMF

$^3H(d,n)^4He$ & $^3He(d,p)^4He$ fusion

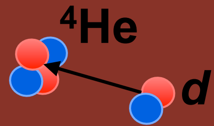
- NCSM/RGM with *SRG-N^{3}LO NN* potentials





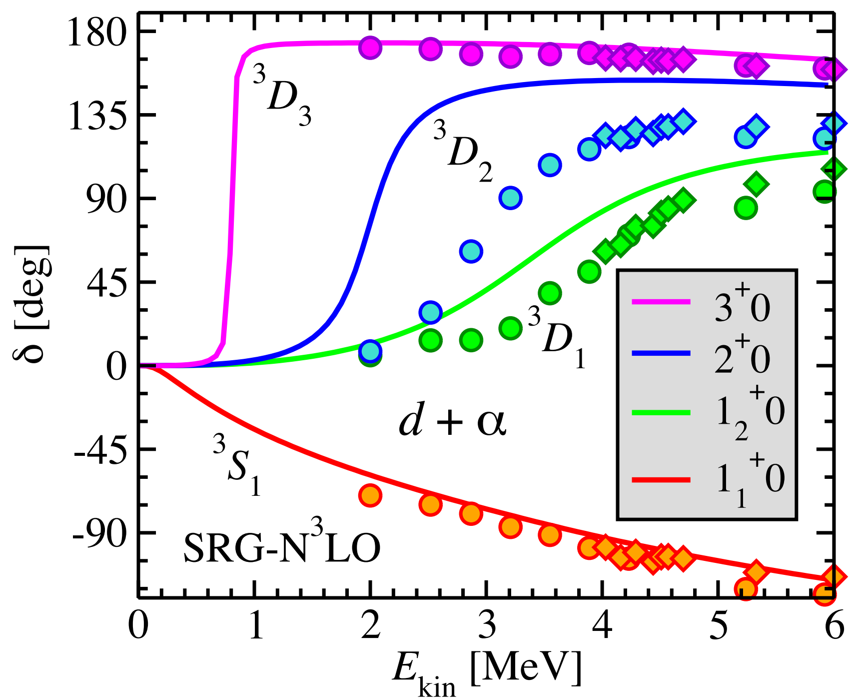
Potential to address unresolved fusion research related questions:
^{3}H(d,n)^{4}He fusion with polarized deuterium and/or tritium,
^{3}H(d,n γ)^{4}He bremsstrahlung,
Electron screening at very low energies …

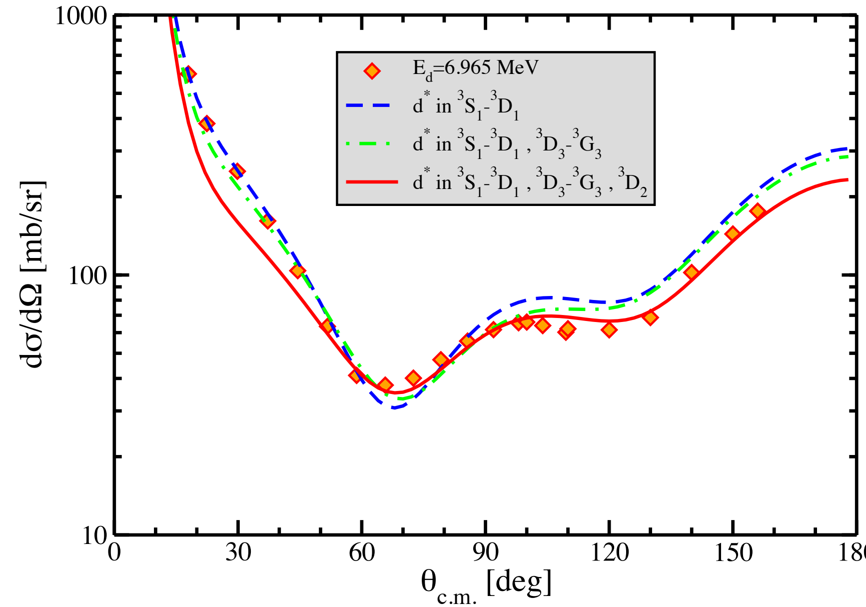
P.N., S. Quaglioni,
PRL **108**, 042503 (2012)

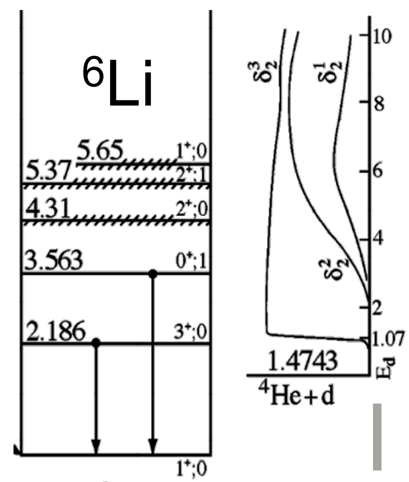


NCSM/RGM *ab initio* calculation of *d*-^{4}He scattering

PHYS. REV. C **83**, 044609 (2011)





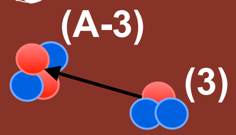


Scattering provides a strict test of NN and NNN forces

Important to include 6-nucleon correlations

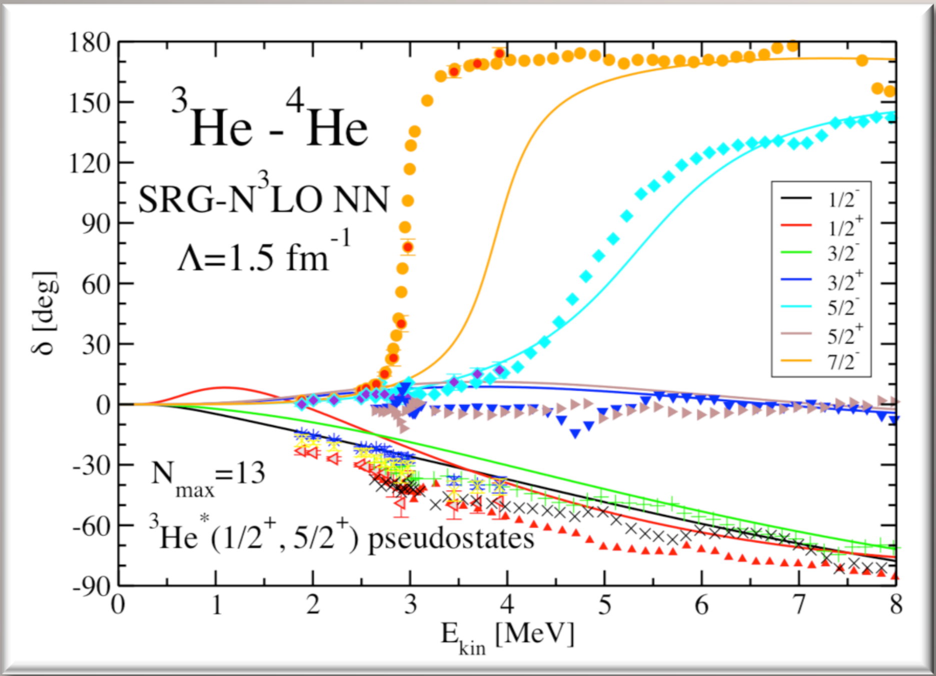
– deuteron (virtual) breakup …

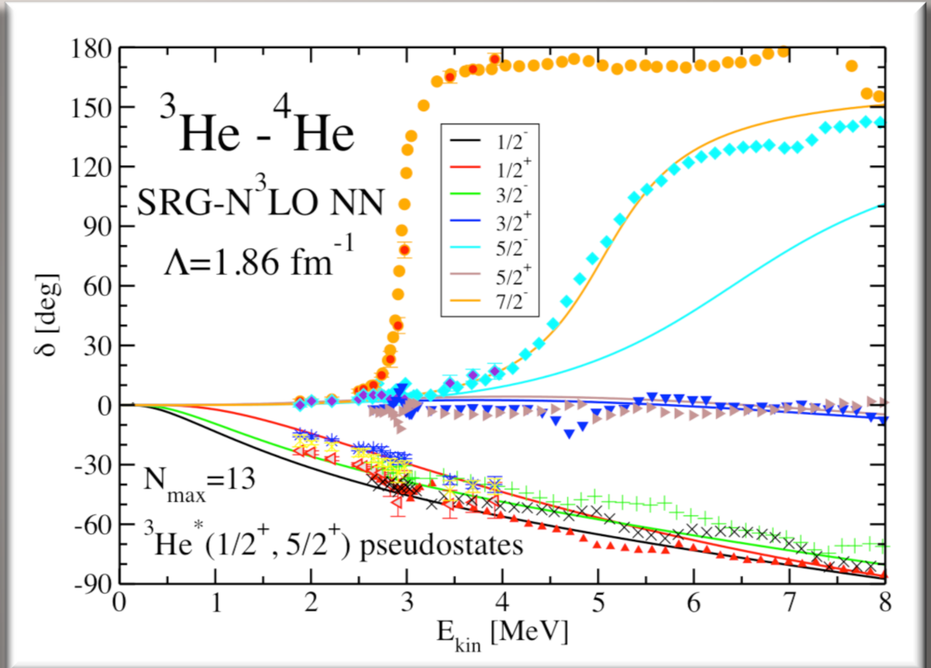
TRIUMF



NCSM/RGM calculations of ^{3}He+α scattering: (still preliminary)

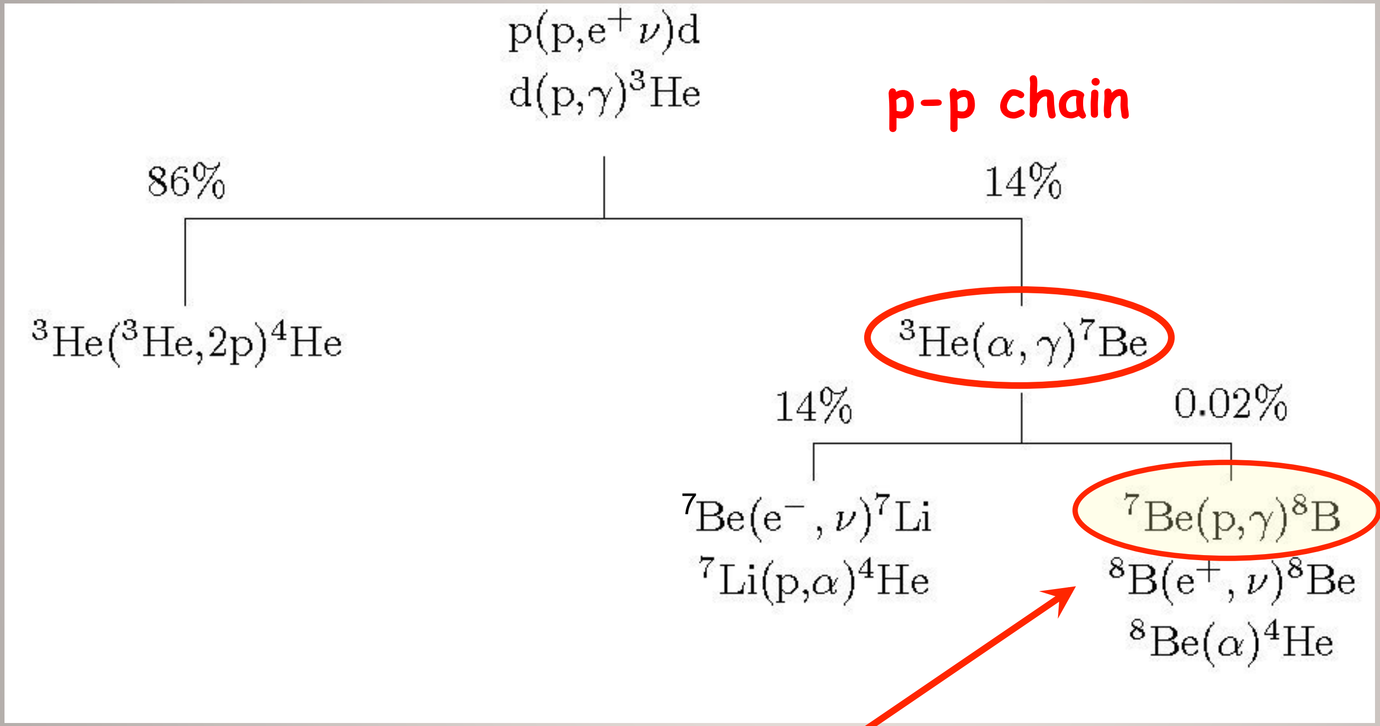
INCITE Award – James PI





Calculations for *a*=3 projectile under way:
Soft SRG interactions (Λ=1.5 fm^{-1}, Λ=1.86 fm^{-1})
Virtual breakup of ^{3}He included by pseudostates (in 1/2$^+$, 5/2$^+$ channels so far)
Large-scale computation, up to 98,304 cores used on *jaguar-xk6*

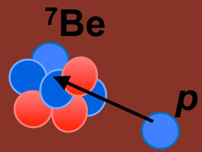
Solar *p-p* chain



Solar neutrinos

$E_\nu < 15$ MeV

TRIUMF



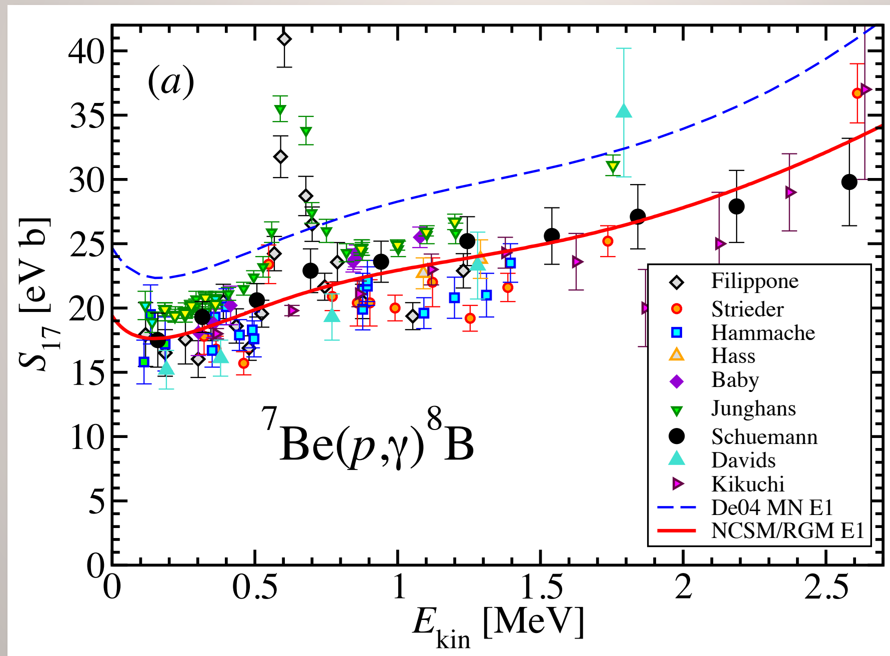
^{7}Be(p,γ)^{8}B radiative capture

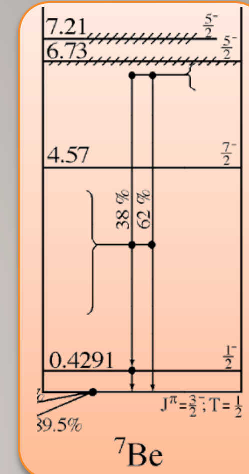
- NCSM/RGM calculation
  - ^{7}Be states $3/2^-$, $1/2^-$, $7/2^-$, $5/2^-_1$, $5/2^-_2$
  - Soft NN potential (chiral SRG-N^{3}LO with Λ = 1.86 fm^{-1})

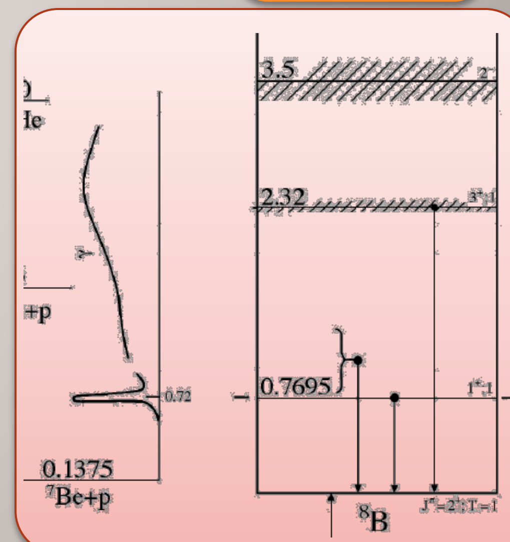
^{8}B 2$^+$ g.s. **bound** by 136 keV
(expt. 137 keV)

S(0) ~ 19.4(0.7) eV b

Data evaluation:
S(0)=20.8(2.1) eV b

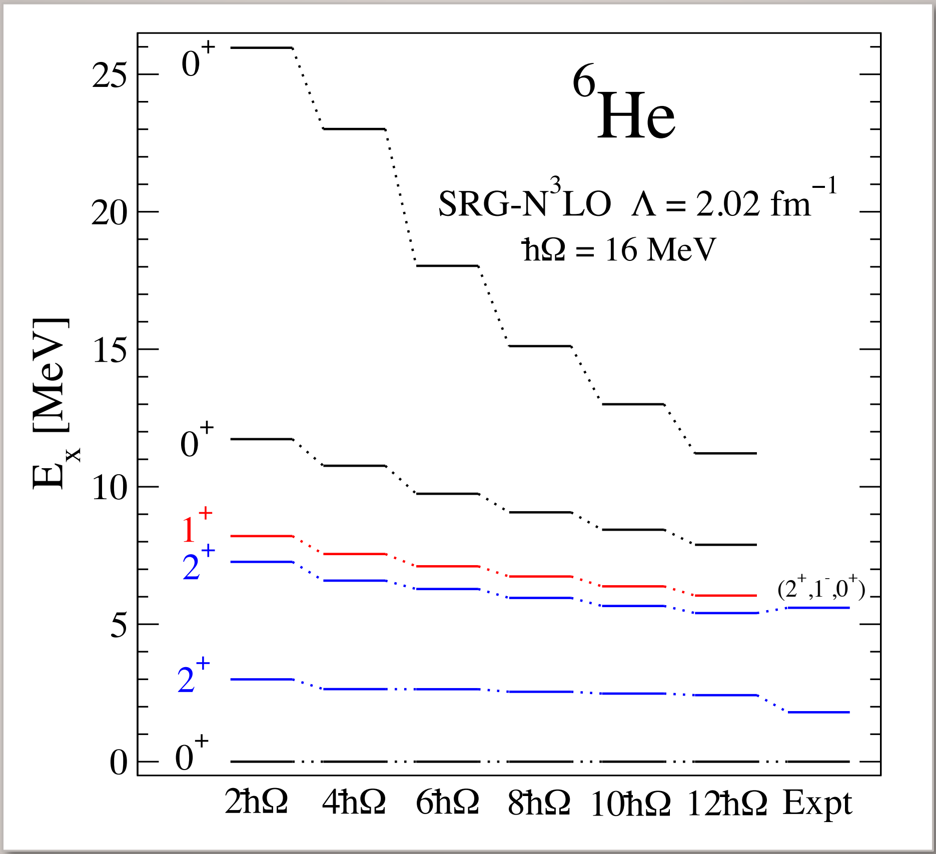






P.N., R. Roth, S. Quaglioni,
Physics Letters B 704 (2011) 379

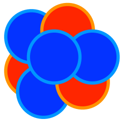
How about ^{7}He as n+^{6}He?



- All ^{6}He excited states above 2^+_1 broad resonances or states in continuum
- Convergence of the NCSM/RGM n+^{6}He calculation slow with number of ^{6}He states
  - Negative parity states also relevant
  - Technically not feasible to include more than ~ 5 states

New developments: NCSM with continuum

NCSM

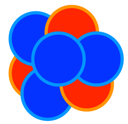


$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{Ni} c_{Ni} \left|ANiJ^\pi T\right\rangle$$

TRIUMF

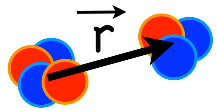
New developments: NCSM with continuum

NCSM



$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{Ni} c_{Ni} \left|ANiJ^\pi T\right\rangle$$

NCSM/RGM



$$|\Psi_A^{J^\pi T}\rangle = \sum_{\nu} \int d\vec{r} \chi_\nu(\vec{r}) \hat{A} \Phi_{\nu \vec{r}}^{J^\pi T (A-a,a)}$$

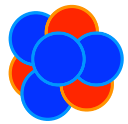
$$\mathcal{H}\chi = E\mathcal{N}\chi$$

$$\bar{\chi} = \mathcal{N}^{+\frac{1}{2}}\chi$$

$$\boxed{(\mathcal{N}^{-\frac{1}{2}}\mathcal{H}\mathcal{N}^{-\frac{1}{2}})\bar{\chi} = E\bar{\chi}}$$

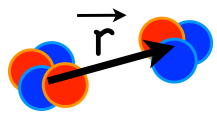
New developments: NCSM with continuum

NCSM



$$\left|\Psi_A^{J^\pi T}\right\rangle = \sum_{Ni} c_{Ni} \left|ANiJ^\pi T\right\rangle$$

NCSM/RGM



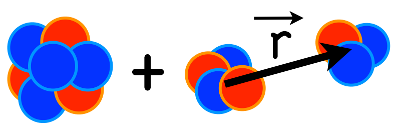
$$|\Psi_A^{J^\pi T}\rangle = \sum_\nu \int d\vec{r} \chi_\nu(\vec{r}) \hat{A} \Phi_{\nu\vec{r}}^{J^\pi T(A-a,a)}$$

$$\mathcal{H}\chi = E\mathcal{N}\chi$$

$$\bar{\chi} = \mathcal{N}^{+\frac{1}{2}}\chi$$

$$\boxed{(\mathcal{N}^{-\frac{1}{2}}\mathcal{H}\mathcal{N}^{-\frac{1}{2}})\bar{\chi} = E\bar{\chi}}$$

NCSMC

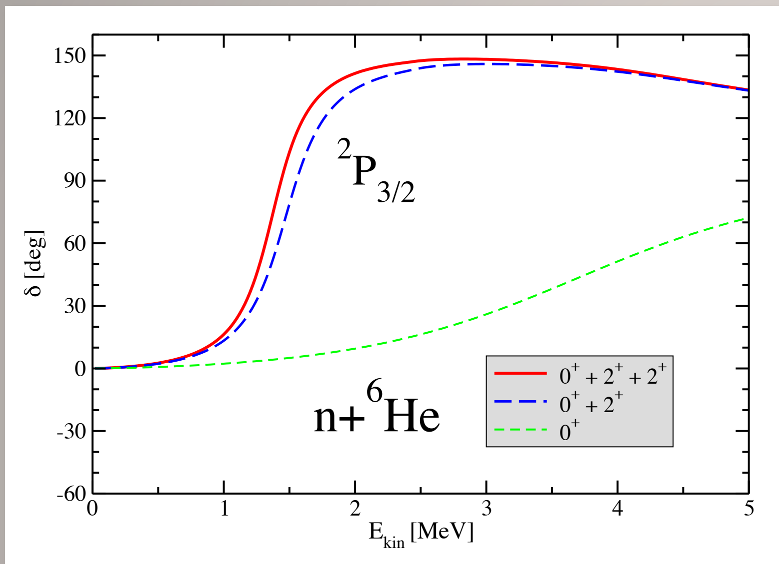


S. Baroni, P. N., and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

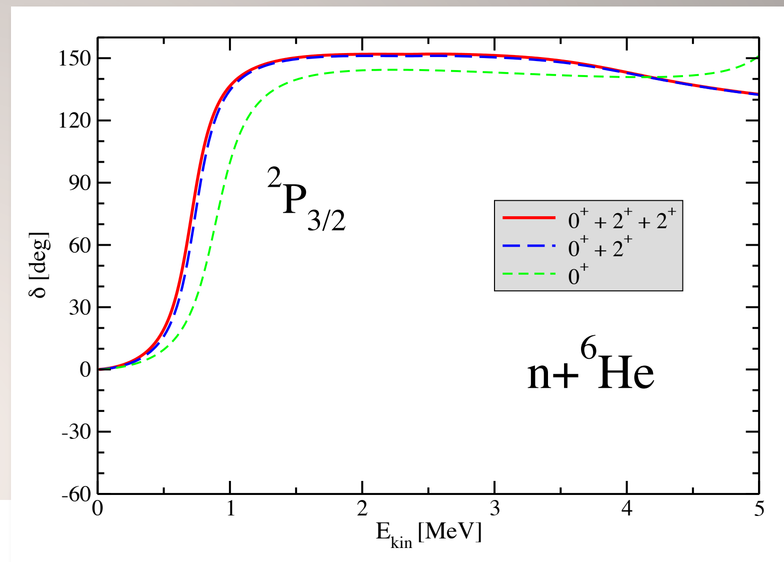
$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda |A\lambda J^\pi T\rangle + \sum_\nu \int d\vec{r} \left(\sum_{\nu'} \int d\vec{r}\,' \mathcal{N}_{\nu\nu'}^{-\frac{1}{2}}(\vec{r},\vec{r}\,')\bar{\chi}_{\nu'}(\vec{r}\,') \right) \hat{A}\Phi_{\nu\vec{r}}^{J^\pi T(A-a,a)}$$

$$\boxed{\begin{pmatrix} H_{NCSM} & \bar{h} \\ \bar{h} & \mathcal{N}^{-\frac{1}{2}}\mathcal{H}\mathcal{N}^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} c \\ \bar{\chi} \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ \bar{g} & 1 \end{pmatrix} \begin{pmatrix} c \\ \bar{\chi} \end{pmatrix}}$$

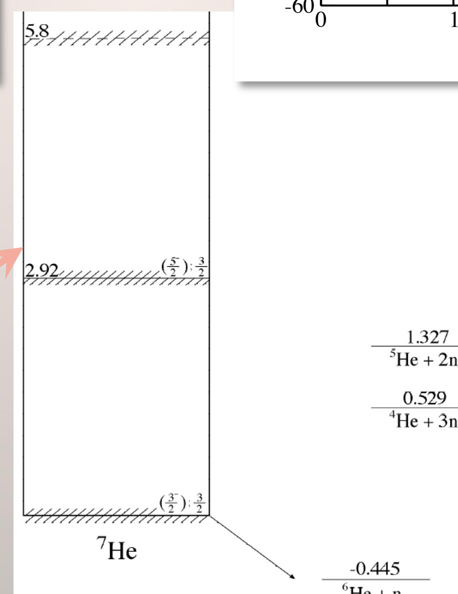
NCSM with continuum: ^{7}He $\leftrightarrow$ ^{6}He+n

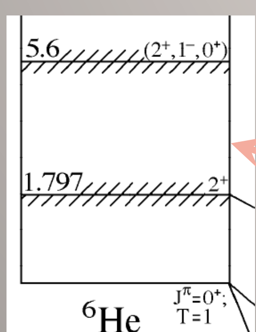


NCSM/RGM
with up to three ^{6}He states



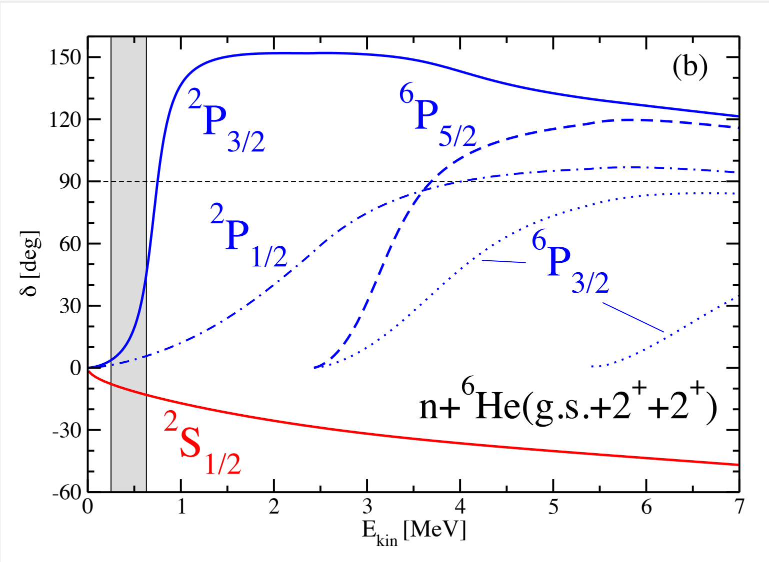
NCSMC
with up to three ^{6}He states
and four ^{7}He eigenstates
More **7-nucleon correlations**
Fewer target states needed



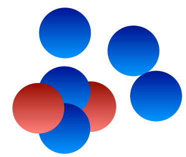


Expt.

NCSM with continuum: ^{7}He $\leftrightarrow$ ^{6}He+n



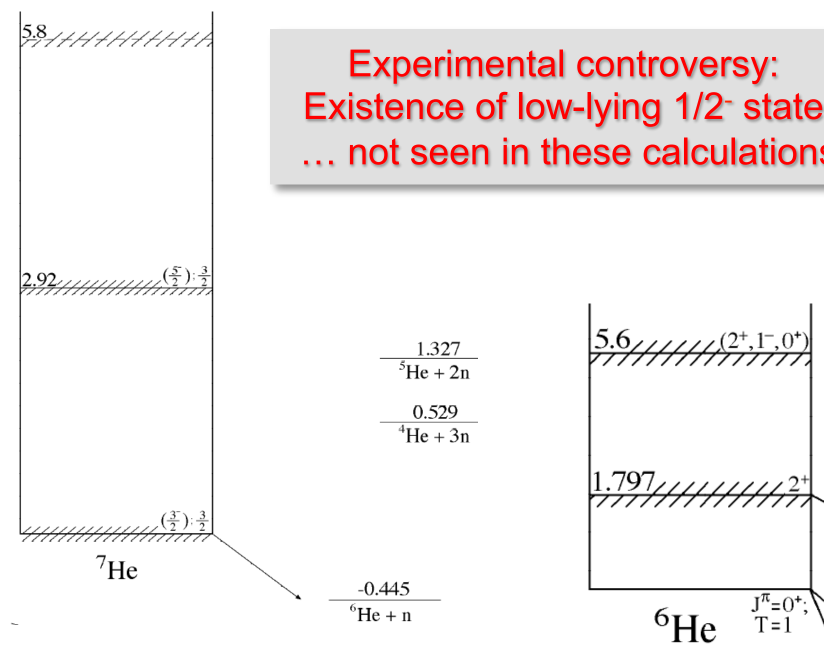
^{7}He



unbound

J^π	experiment			NCSMC	
	E_R	Γ	Ref.	E_R	Γ
$3/2^-$	0.430(3)	0.182(5)	[2]	0.71	0.30
$5/2^-$	3.35(10)	1.99(17)	[40]	3.13	1.07
$1/2^-$	3.03(10)	2	[11]	2.39	2.89
	3.53	10	[15]		
	1.0(1)	0.75(8)	[5]		

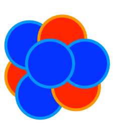
[11] A. H. Wuosmaa *et al.*, Phys. Rev. C **72**, 061301 (2005).



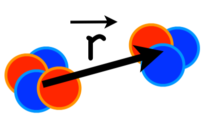
Experimental controversy:
Existence of low-lying 1/2$^-$ state
… not seen in these calculations

NCSMC
with three ^{6}He states
and ten ^{7}He eigenstates
More **7-nucleon correlations**
Fewer ^{6}He-core states needed

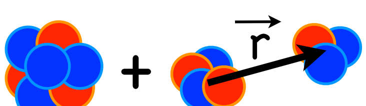
NCSM



NCSM/RGM



NCSMC



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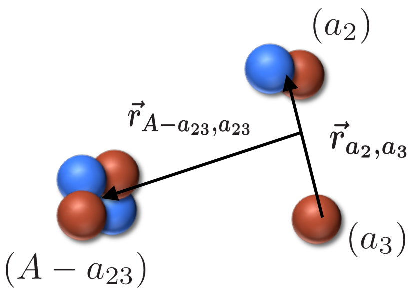
NCSM/RGM for three-body clusters

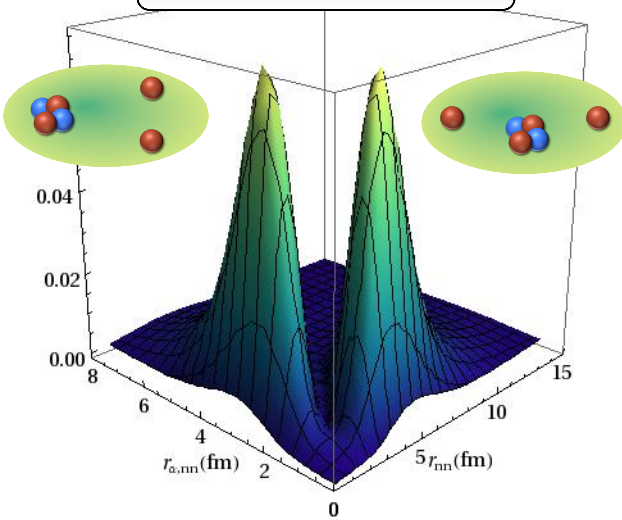


$$|\Phi^{J^\pi T}_{\nu r}\rangle \sim \underbrace{\Psi^{A-a_{23}}_{\alpha_1}\ \Psi^{a_2}_{\alpha_2}\ \Psi^{a_3}_{\alpha_3}}_{\text{NCSM}}$$

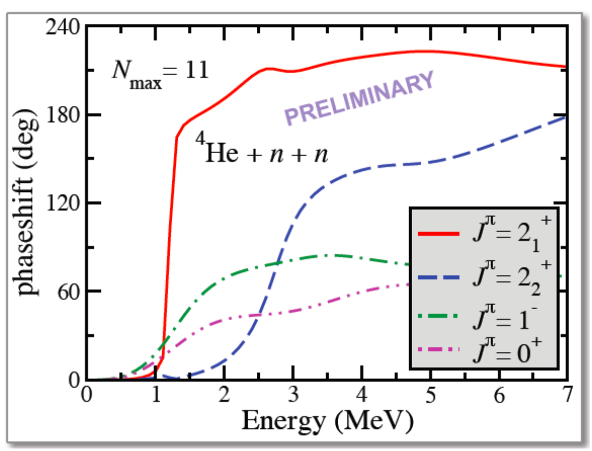
$$\boxed{|\Psi^{J^\pi T}\rangle = \sum_\nu \int dx\, x^2 \int dy\, y^2 G^{J^\pi T}_\nu(x,y)\hat{A}_\nu |\Phi^{J^\pi T}_{\nu x y}\rangle}$$

^{4}He(g.s.)+n+n

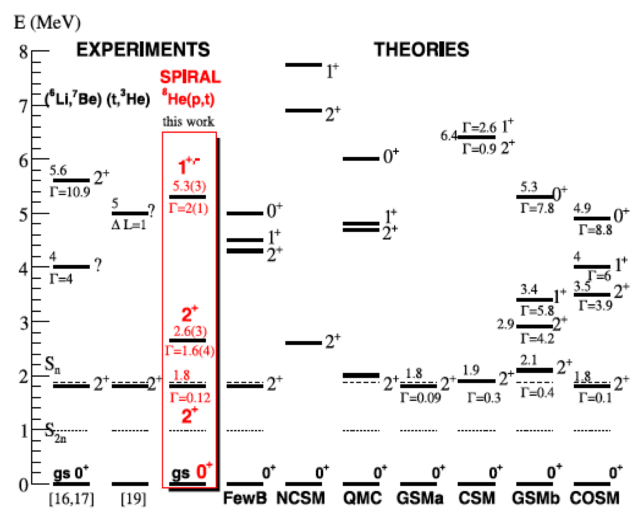
$\ell_x = \ell_y = L = S_{nn} = 0$



Phaseshifts (preliminary results)



Recent exp.: Phys. Lett. B 718 (2012) 441



INCITE Award – Titan

TRIUMF

Conclusions and Outlook

- *Ab initio* and microscopic calculations of nuclear reactions is a dynamic field with significant advances
- Several exact methods applicable to few-nucleon systems (*A*=3,4)
- Significant progress in *ab initio* approaches for *p*-shell nuclei an beyond
- GFMC
- We developed a new unified approach to nuclear bound and unbound states
  - Merging of the NCSM and the NCSM/RGM = **NCSMC**
- CCM with Berggren basis
- Outlook:
  - Inclusion of three-nucleon interactions in reaction calculations for *A*>5 systems
  - Extension to composite projectiles (deuteron, ^{3}H, ^{3}He, ^{4}He)
  - Extension to three-body clusters (^{6}He ~ ^{4}He+*n*+*n*)
  - Composite-projectile reactions on targets heavier than ^{4}He

TRIUMF

I met James for the first time in ~ 1998.
Soon after that we started a collaboration
and published

VOLUME 84, NUMBER 25 PHYSICAL REVIEW LETTERS 19 JUNE 2000

Properties of ^{12}C in the *Ab Initio* Nuclear Shell Model

P. Navrátil,[1,2] J.P. Vary,[3] and B.R. Barrett[1]

my most cited paper…

Happy birthday James!

TRIUMF

NCSMC and NCSM/RGM collaborators

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Guillaume Hupin, Michael Kruse (LLNL)

Simone Baroni (ULB)

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