QMC Calculations of Nuclei and Neutron Drops

Steven C. Pieper

Physics Division, Argonne National Laboratory

Work with

Ralph Butler (Middle Tennessee State)
Joseph Carlson (Los Alamos)
Stefano Gandolfi (Los Alamos)
E. L. (Rusty) Lusk (Argonne)
Ivan Brida (Argonne)
Kenneth M. Nollett (Argonne)
Saori Pastore (Argonne)
Robert B. Wiringa (Argonne)

- Hamiltonian and QMC methods
- GFMC ^{12}C progress
- GFMC for nuclear overlaps (Brida)
- GFMC for ^{10}C Fermi Beta decay
- Deliverables and plans

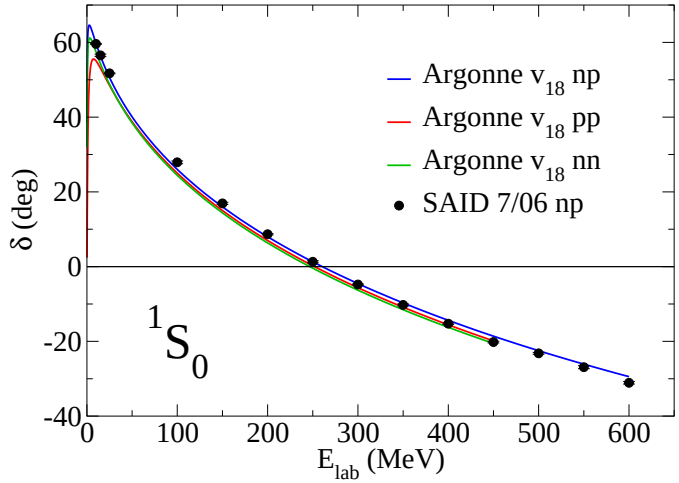
NUCLEAR HAMILTONIAN

$$H = \sum_i K_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

K_i: Non-relativistic kinetic energy, m_n-m_p effects included

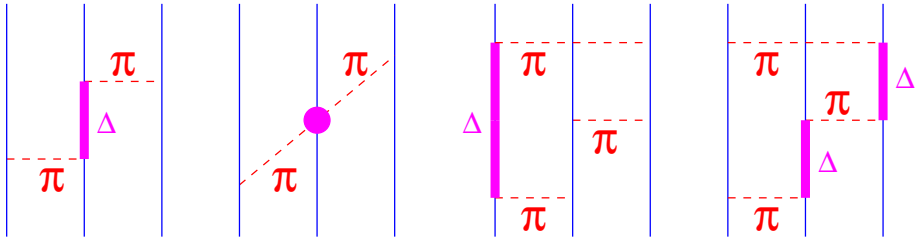
Argonne v$_{18}$: $v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{I} + v_{ij}^{S} = \sum v_p(r_{ij}) O_{ij}^{p}$

- predominantly local operator structure – good for QMC
- EM and strong CD and CSB terms included
- fits Nijmegen PWA93 data base with χ^2/d.o.f.=1.1
- qualitatively good to ~1 GeV



Wiringa, Stoks, & Schiavilla, PRC **51**, (1995)

Urbana & Illinois: $V_{ijk} = V_{ijk}^{2\pi} + V_{ijk}^{3\pi} + V_{ijk}^{R}$



- Urbana has standard 2π P-wave + short-range repulsion for matter saturation
- Illinois adds 2π S-wave + 3π rings to provide extra T=3/2 interaction
- Illinois-7 has four parameters fit to 23 levels in $A \leq 10$ nuclei

Pieper, Pandharipande, Wiringa, & Carlson, PRC **64**, 014001 (2001)
Pieper, AIP CP **1011**, 143 (2008)

QUANTUM MONTE CARLO

Variational Monte Carlo (VMC): construct Ψ_V that

- Are fully antisymmetric and translationally invariant
- Have cluster structure and correct asymptotic form
- Contain non-commuting 2- & 3-body operator correlations from v_{ij} & V_{ijk}
- Are orthogonal for multiple J^π states
- Minimize $E_V = \langle \Psi_V | H | \Psi_V \rangle \geq E$

These are $\sim 2^A \binom{A}{Z}$ component (270,336 for ^{12}C) spin-isospin vectors in $3A$ dimensions

Green's function Monte Carlo (GFMC): project out the exact eigenfunction

- $\Psi(\tau) = \exp[-(H - E_0)\tau]\Psi_V = \sum_n \exp[-(E_n - E_0)\tau] a_n \Psi_n \Rightarrow \Psi_0$ at large τ
- Propagation done stochastically in small time slices $\Delta\tau$
- Exact $\langle H \rangle$ for local potentials; mixed estimates for other $\langle O \rangle$
- Constrained-path propagation controls fermion sign problem for $A \geq 5$
- Multiple excited states for same J^π stay orthogonal

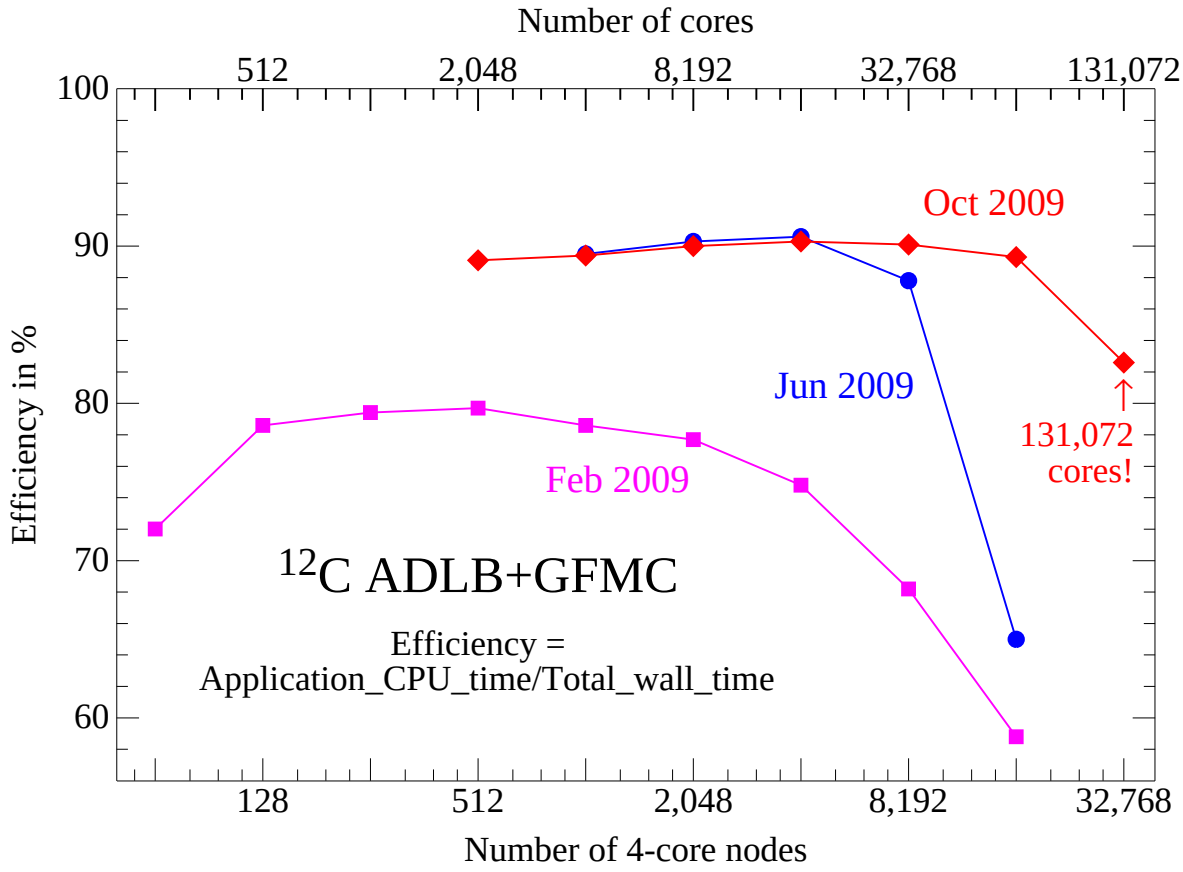
Many tests demonstrate 1–2% accuracy for realistic $\langle H \rangle$

Wiringa, Pieper, Carlson, & Pandharipande, PRC **62**, 014001 (2000)
Pieper, Varga, & Wiringa, PRC **66**, 044310 (2002)
Pieper, Wiringa, & Carlson, PRC **70**, 054325 (2004)
Pieper, NPA **751**, 516c (2005)

MAKING GFMC WORK ON 131,072 PROCESSORS AND ^{12}C

Work with Mathematics & Computer Science Division under UNEDF SciDAC

- General purpose load balancing library (ADLB) developed to run under MPI
  - GFMC code is driver and testbed
  - Achieves 82% efficiency on 32,768 nodes of Argonne's IBM Blue Gene/P
- Open MP used for 4 cores on each node = 131,072 processors total



2010: Attempted new ADLB using one-sided puts & gets; could not achieve above performance

^{12}C(0^+) Trial Wave Functions

The Jastrow part of Ψ_V for J=0^+ states is a major part of the entire calculation.

There are 5 LS-basis J=0^+ states in ^{12}C in the $0P$ shell:
^{1}S[444], ^{3}P[4431], ^{1}S[4422], ^{5}D[4422], ^{3}P[4332]

Only the ^{1}S[444] can be directly constructed in reasonable computer time. Carlson found a way to construct all 5 states by projection from a closed $(p3/2)^8$ state.

^{12}C states have strong triple-alpha structure; Pandharipande made a subroutine that explicitly makes triple-alpha states with one α in the $0S$ shell and two in the $0P$ shell.

Last year we reported results for the ground state using both the AV18 and AV18+IL7 Hamiltonians – the latter in excellent agreement with experiment for energy and density.

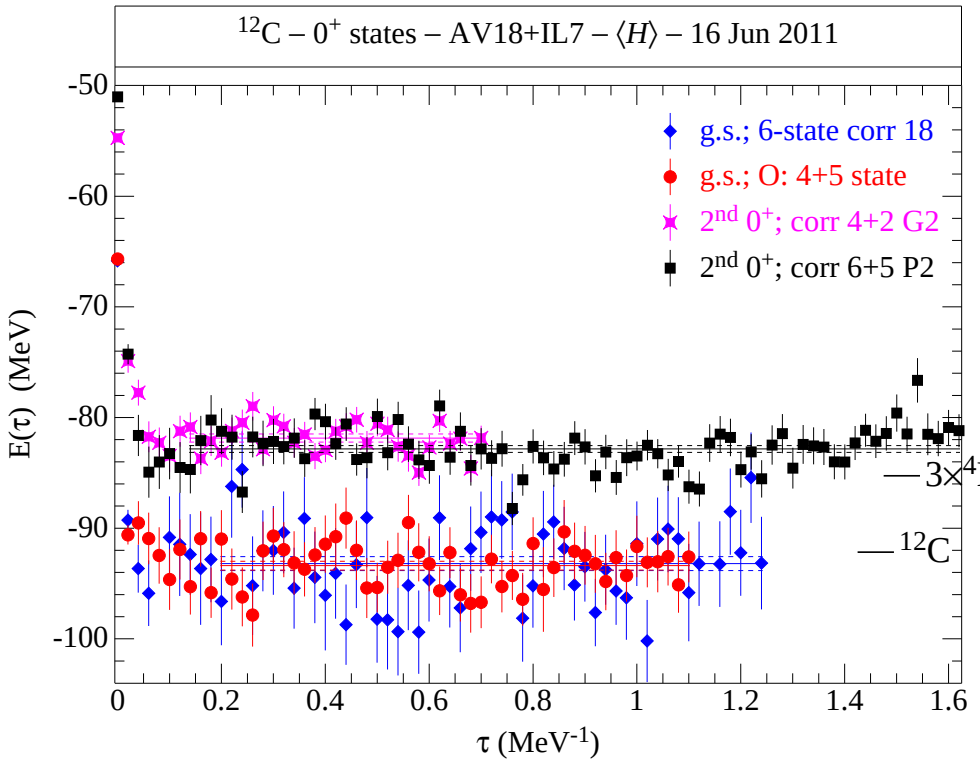
SECOND 0^+ (HOYLE) STATE OF ^{12}C

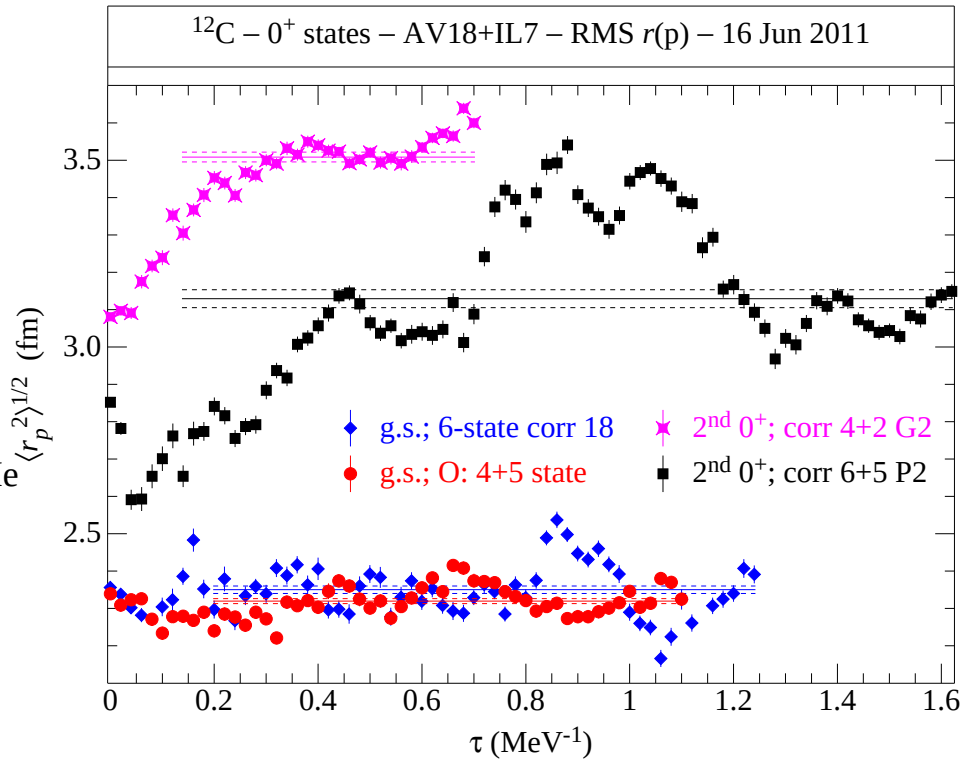
The second 0^+ state of ^{12}C is the famous triple-alpha burning or Hoyle state

- Resonance only 0.38 MeV above 3α breakup threshold
- Doorway state postulated by Fred Hoyle for $3\alpha \rightarrow {}^{12}$C in stars
- Shell model calculations show it to be 4-particle 4-hole excitation
- Not yet converged in *ab initio* no-core shell model.
- We add Pandharipande triple-α component to Ψ_V with α's in $0S$ shell, $0P$ shell, and $1S$-$0D$ shell
- We also try only a pair in $1S$-$0D$ shell, i.e., an α made of $0P^2 0D^2$ or $0P^2 1S^2$
- Total of 11 states to be diagonalized in Ψ_V
- The $1S$-$0D$ shell one-body $\phi(r)$ are given a large RMS radius
- Suggestion of Kevin Schmidt:
- We make an initial diagonalization to get the g.s. Ψ_V
- Then compute overlaps of the GFMC g.s. propagation with the 11 components of Ψ_V
- Diagonalize these overlaps (rank 10) to get the next 0^+ state

SECOND 0^+ (HOYLE) STATE OF ^{12}C – PRELIMINARY

Convergence as a function of imaginary time (τ)

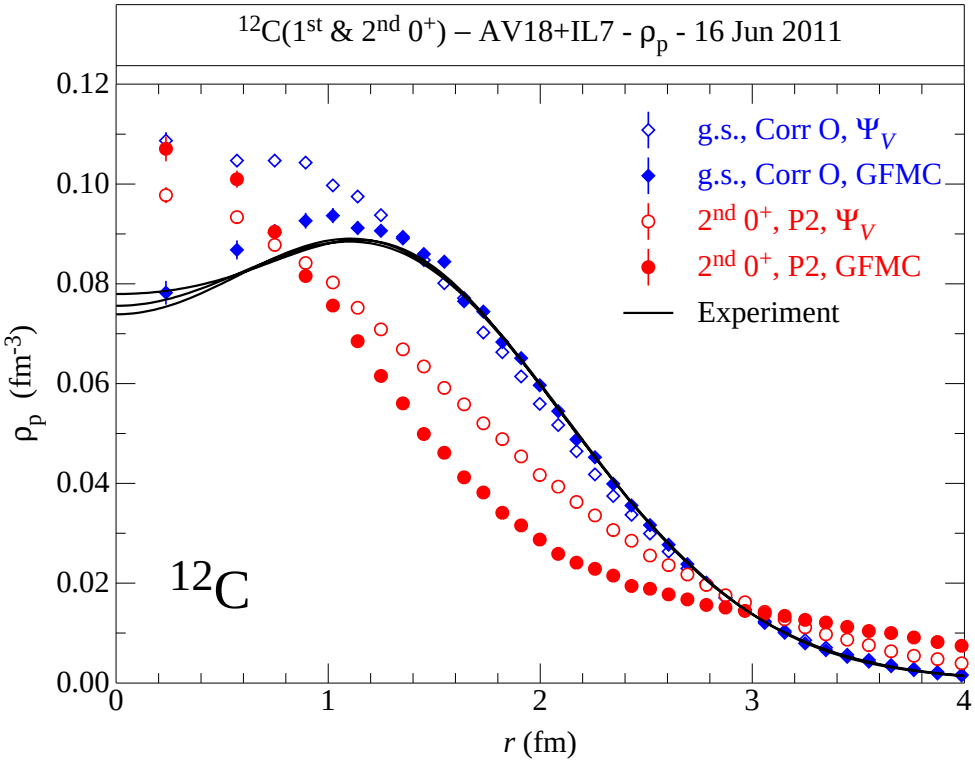


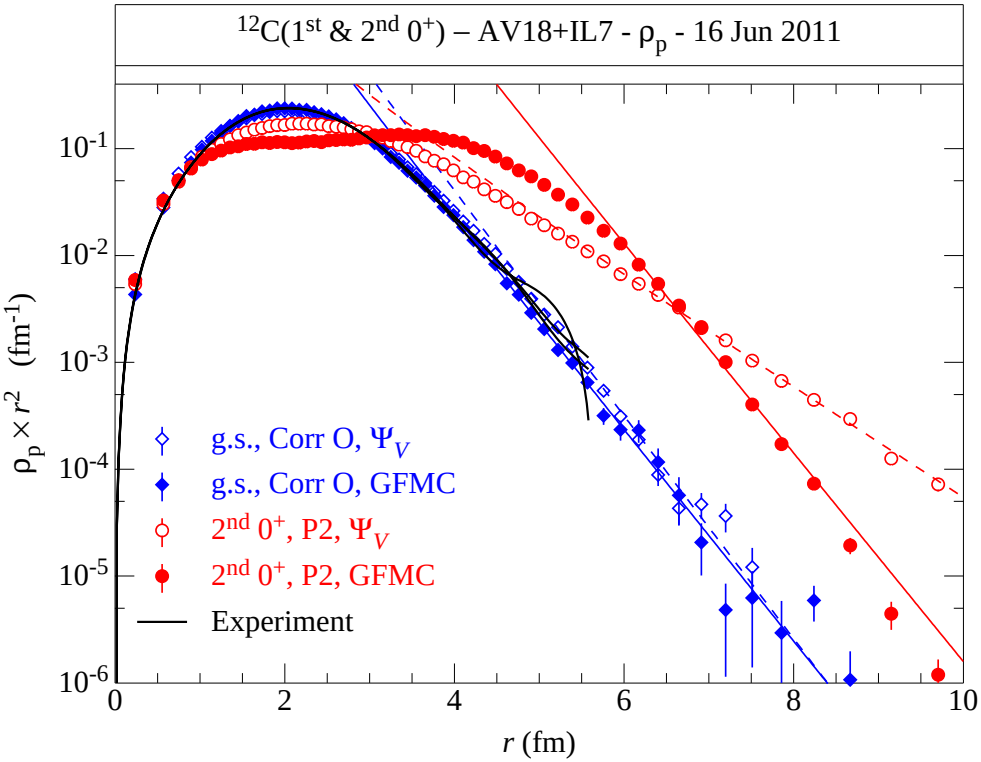


	g.s. energy			2^{nd} 0^+ E^*		
	VMC	GFMC	Expt.	VMC	GFMC	Expt.
AV18	–44.9(2)	–73.2(5)		10.0(3)	7.9(6)	
AV18+IL7	–65.7(2)	–93.3(4)	–92.16	14.7(2)	10.4(5)	7.65

SECOND 0^+ (HOYLE) STATE OF ^{12}C – PRELIMINARY

One-body density





- Ground-state $\rho(r)$ has dip at $r = 0$ – suggests(?) equilateral triangle of 3 α's
- $2^{\rm nd}$ 0^+ $\rho(r)$ has no dip at $r = 0$ – suggests(?) $\sim$ line of 3 α's
- Ground-state $\rho(r)$ falls asymptotically at correct single-nucleon removal E_{sep} rate
- GFMC makes $2^{\rm nd}$ 0^+ $\rho(r)$ fall much too rapidly

ONE-NUCLEON OVERLAPS IN VMC/GFMC

For antisymmetric and translationally invariant parent $\Psi_A(\alpha)$ and daughter $\Psi_{A-1}(\gamma)$ wave functions, with $\alpha \equiv [J^\pi_A, T_A, T_{z_A}]$, $\gamma \equiv [J^\pi_{A-1}, T_{A-1}, T_{z_{A-1}}]$, and single-nucleon quantum numbers $\nu \equiv [l, s, j, t, t_z]$, the translationally invariant overlap function is:

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

where $\mathcal{Y}(\nu)(\hat{r}') = [Y_l(\hat{r}') \otimes \chi_s]_j \, \chi_t$ and $|\Psi_{A-1}(\gamma)|^2 = 1$, $|\Psi_A(\alpha)|^2 = 1$.

The corresponding spectroscopic factor is the norm of the overlap:

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

Overlap functions R satisfy a one-body Schrödinger equation with appropriate source terms. Asymptotically, at $r \to \infty$, these source terms contain core-valence Coulomb interaction at most, and hence for parent states below core-valence separation thresholds:

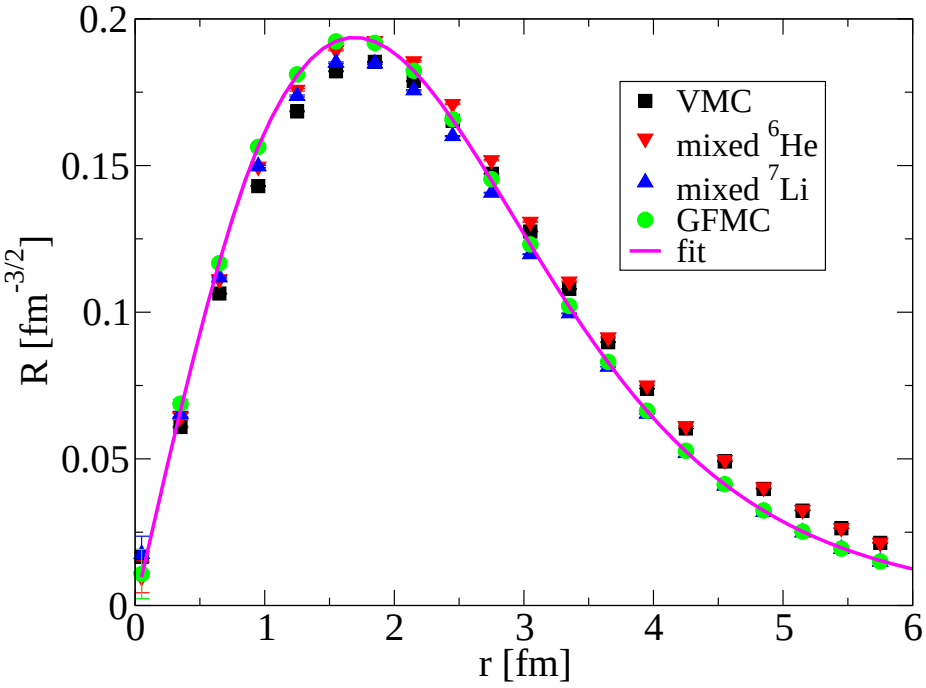
$$R(\alpha, \gamma, \nu; r) \to r \to \infty C(\alpha, \gamma, \nu) \frac{W_{-\eta, l+1/2}(2kr)}{r},$$

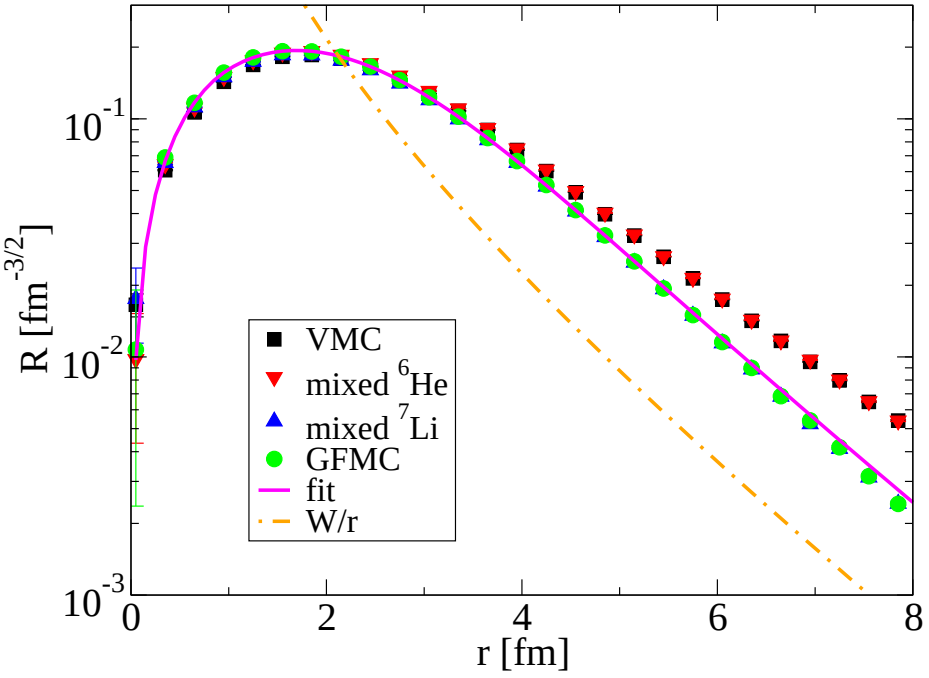
where $W_{-\eta, l+1/2}(2kr)$ is a Whitakker function with $k = \sqrt{2\mu B}/\hbar$, B is the separation energy, and $C(\alpha, \gamma, \nu)$ is the asymptotic normalization coefficient or ANC.

GFMC evaluation of R is by extrapolation requiring two mixed estimates minus the VMC result:

$$R(\alpha,\gamma,\nu;r;\tau) \approx \langle R(\alpha,\gamma,\nu;r;\tau)\rangle_{M_A} + \langle R(\alpha,\gamma,\nu;r;\tau)\rangle_{M_{A-1}} - \langle R(\alpha,\gamma,\nu;r)\rangle_V ,$$

where M_A denotes a mixed estimate where parent $\Psi_A(\alpha;\tau)$ has been propagated in GFMC and M_{A-1} is a mixed estimate where daughter $\Psi_{A-1}(\gamma;\tau)$ has been propagated.





Imaginary time evolution of overlaps in the $p_{3/2}$ channel of the overlap $\langle {}^6\mathrm{He} + p | {}^7\mathrm{Li}\rangle$

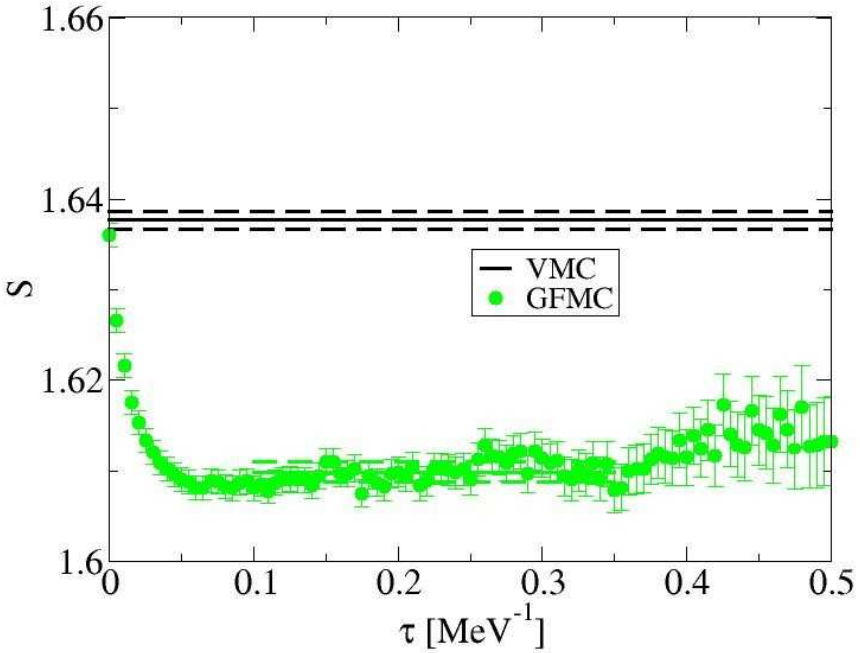
A convenient parametrization for input to PTOLEMY or other direct reaction code is provided by fitting a single-particle potential to reproduce the overlap R:

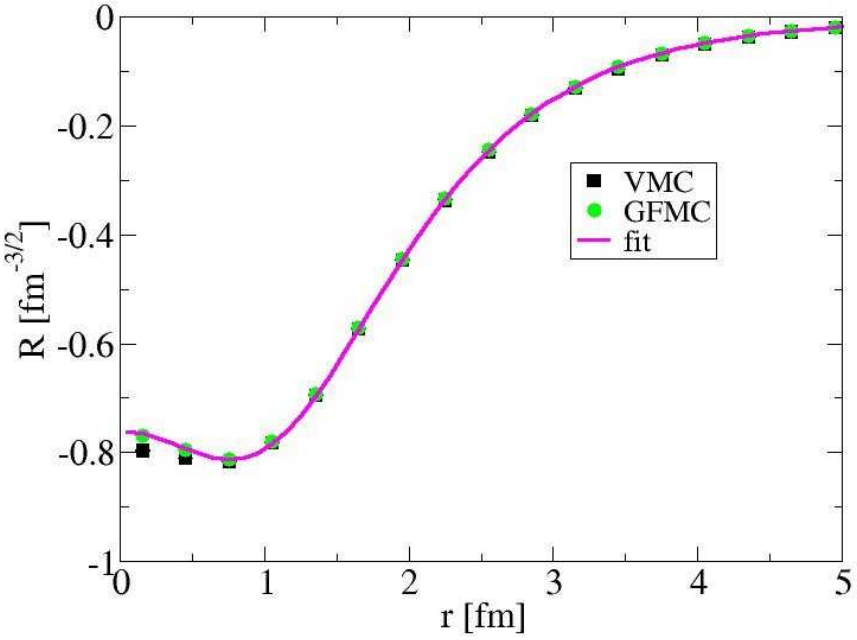
$$V(r) = V_{WS}\left[\frac{1}{1+\exp((r-R_{WS})/a_{WS})} - \beta\exp(-(r/\rho)^2)\right] + \left(4\vec{l}\cdot\vec{s}\right)\frac{V_{so}}{r}\frac{d}{dr}\left[\frac{1}{1+\exp((r-R_{so})/a_{so})}\right] + V_{Coul}$$

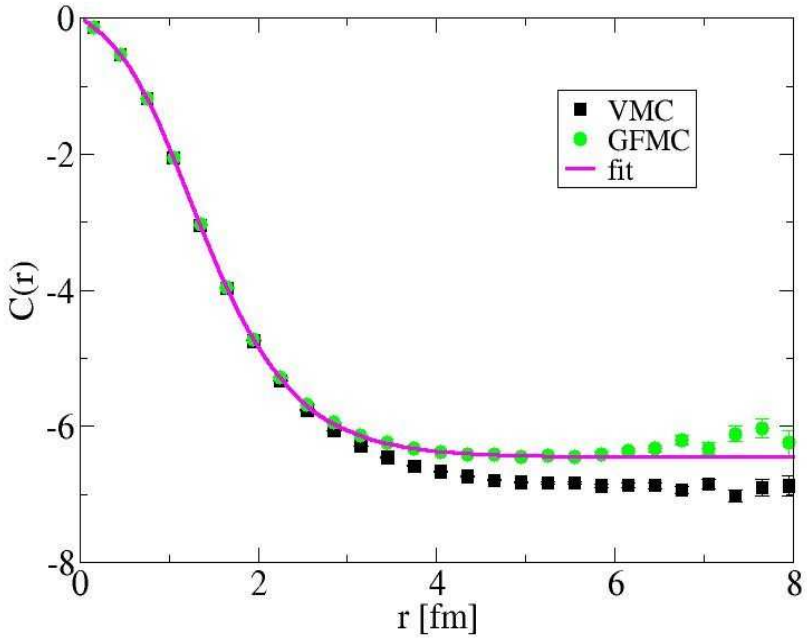
The potential parameters are adjusted to minimize χ^2 under the constraint that the overlap tail falls off with the correct core-valence separation energy B. This helps in extraction of the ANCs.

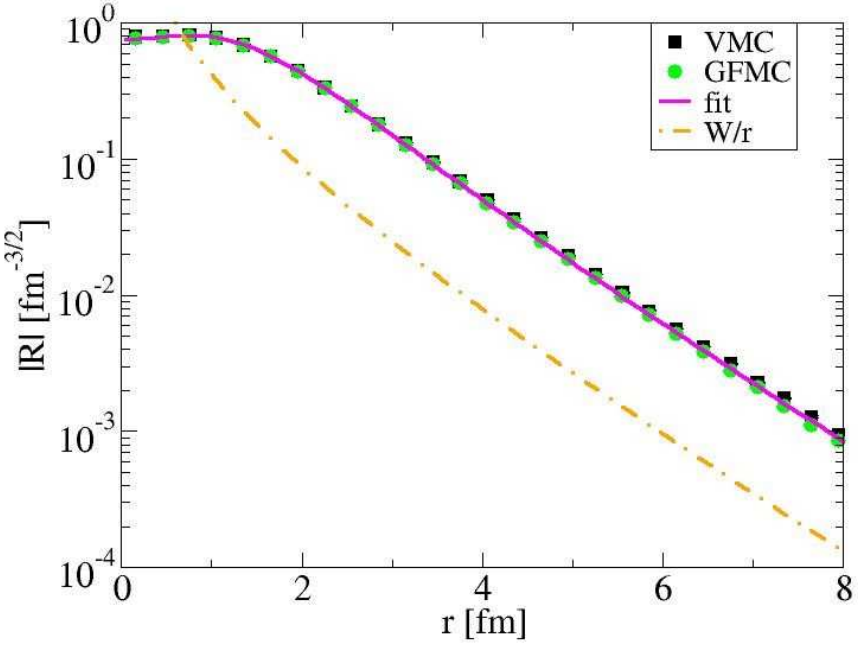
Brida, Pieper, & Wiringa, http://arxiv.org/abs/1106.3121

Example: (^{3}H,^{4}He), $s_{1/2}$ overlap

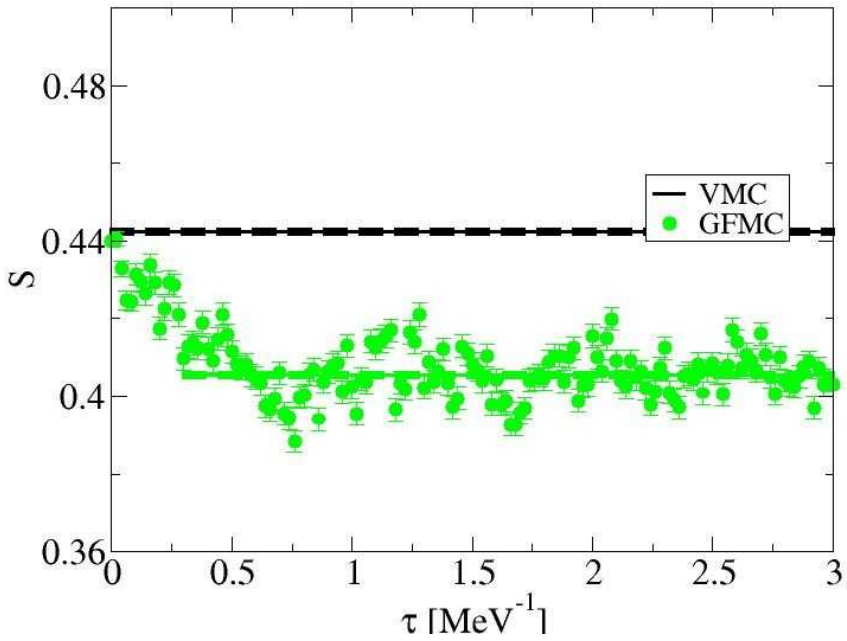


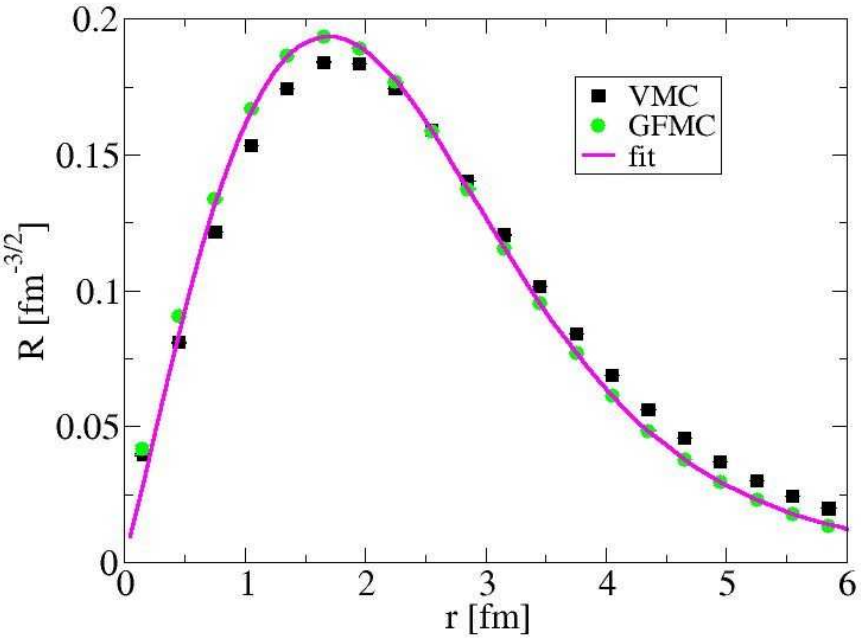


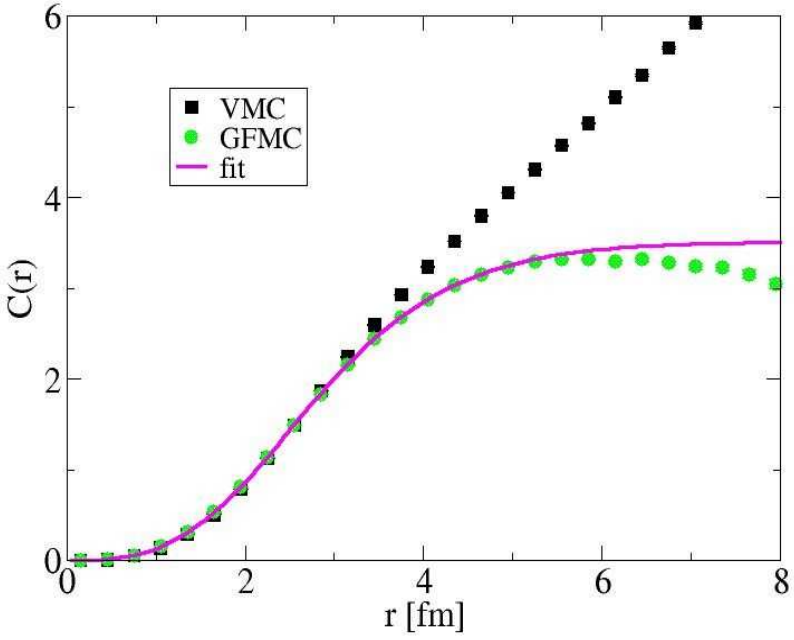


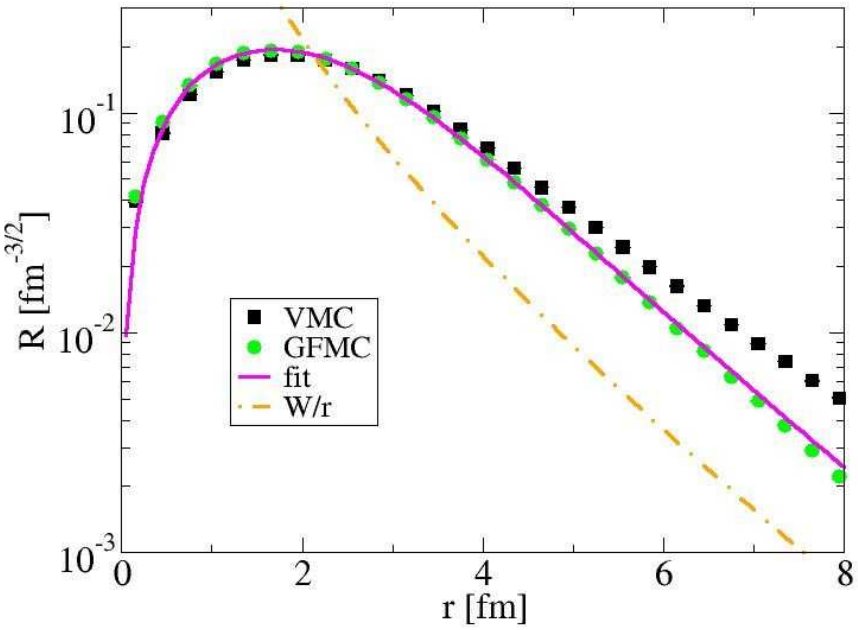


Example: (^{6}He,^{7}Li), $p_{3/2}$ overlap









GFMC separation energies

A	A-1	*B* [MeV]	
		GFMC	exp
^{3}H	^{2}H	6.24	6.26
^{3}He	^{2}H	5.49	5.49
^{4}He	^{3}H	19.96	19.81
	^{3}He	20.71	20.58
^{7}Li(g.s.)	^{6}He(g.s)	9.88	9.98
	^{6}Li(g.s)	7.15	7.25
	^{6}Li(3+)	9.49	9.44
	^{6}Li(0+)	10.65	10.81
^{7}Li(1/2-)	^{6}Li(g.s)	6.95	6.77
^{7}Be(g.s.)	^{6}Li(g.s)	5.69	5.61
	^{6}Li(3+)	8.03	7.79
	^{6}Li(0+)	9.18	9.17

- total energies are within 1% around exp. values
- sep. energies are within 3% around exp. values
- use exp. sep. energies for ANCs accounting for uncertainties

s-shell: spectroscopic factors

A	A-1	channel	S	
			GFMC	exp
^{3}H	^{2}H	$s_{1/2}$	1.30	
		$d_{3/2}$	0.0224	
^{3}He	^{2}H	$s_{1/2}$	1.31	
		$d_{3/2}$	0.0221	
^{4}He	^{3}H	$s_{1/2}$	1.61	1.4-1.6
	^{3}He	$s_{1/2}$	1.60	

GFMC systematic uncertainties are 2-3% or less

exp. values: Pandharipande et al, RMP 69 (1997) 981

s-shell: ANCs

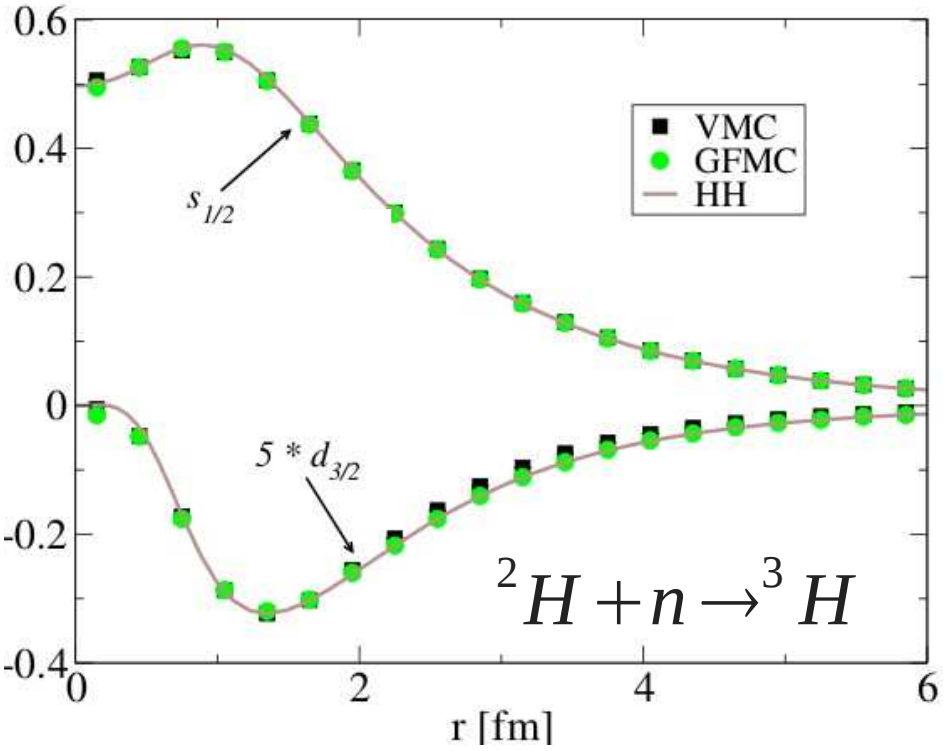
A	A-1	channel	*ANC* [fm$^{-1/2}$]	
			GFMC	exp
^{3}H	^{2}H	$s_{1/2}$	2.14	2.11(3), 2.07(2), 1.87(14)
		$d_{3/2}$	-0.0848	
		$d_{3/2}/s_{1/2}$	-0.0396	-0.0418(15)
^{3}He	^{2}H	$s_{1/2}$	2.10	2.10(16), 1.76(11)
		$d_{3/2}$	-0.0762	
		$d_{3/2}/s_{1/2}$	-0.0363	-0.0389(42)
^{4}He	^{3}H	$s_{1/2}$	6.45	7.36(19), 6.70(50), 5.44(15)
	^{3}He	$s_{1/2}$	6.45	6.77(51), 6.52(49)

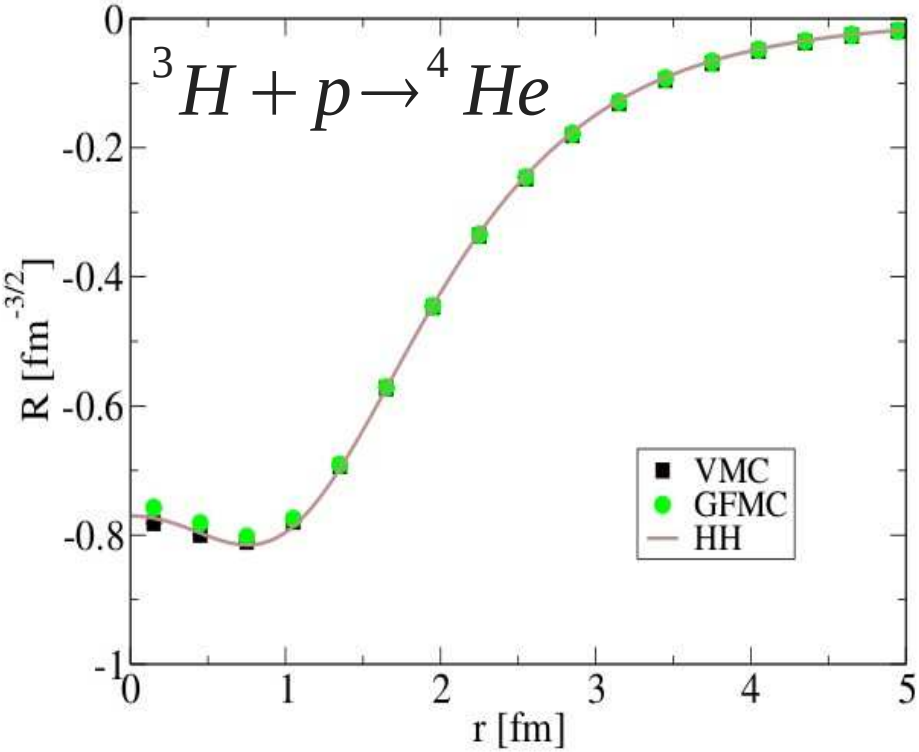
GFMC systematic uncertainties are 5% or less

exp. values: Timofeyuk (2010), Girard (1979), Locher (1978, Purcell (2010), Blimov (1985, Blokhintsev (1977)

s-shell: comparing with HH

potential: Av18+UIX





	channel	GFMC	HH
S	$s_{1/2}$	1.30	1.30
	$d_{3/2}$	0.0223	0.0225
ANC	$s_{1/2}$	2.14	~2.12
	$d_{3/2}$	-0.0842	

	channel	GFMC	HH
S	$s_{1/2}$	1.61	1.60
ANC	$s_{1/2}$	6.49	~6.48

p-shell: spectroscopic factors

A	A-1	channel	S	
			GFMC	exp
^{7}Li(g.s.)	^{6}He(g.s)	$p_{3/2}$	0.406	0.44(6), 0.42(4)
	^{6}Li(g.s)	$p_{1/2}$	0.230	
		$p_{3/2}$	0.438	
		$\sum S$	0.668	0.74(11), 073(5)
	^{6}Li(3+)	$p_{3/2}$	0.435	0.72(14), 0.58(13)
	^{6}Li(0+)	$p_{3/2}$	0.203	0.19(3)
^{7}Li(1/2-)	^{6}Li(g.s)	$p_{1/2}$	0.060	
		$p_{3/2}$	0.759	
		$\sum S$	0.819	1.15, 0.90(9)

SFs for overlaps with ^{7}Be(g.s) are close to ^{7}Li(g.s)
Shell-model SFs quenched by as much as 40%.

GFMC systematic uncertainties are 2-3% or less

exp. values: Wuosmaa (2008), Lapikas (1999), Ju (2010),
Li (1969), Towner (1969), Schiffer (1967)

p-shell: ANCs

A	A-1	channel	ANC [fm$^{-1/2}$]	
			GFMC	*exp*
^{7}Li(g.s.)	^{6}He(g.s)	$p_{3/2}$	3.52	2.48
	^{6}Li(g.s)	$p_{1/2}$	1.73	
		$p_{3/2}$	2.29	
		$\sqrt{\sum ANC^2}$	2.87	1.26-2.82
	^{6}Li(3+)	$p_{3/2}$	3.50	2.06-3.00
	^{6}Li(0+)	$p_{3/2}$	2.39	1.71-2.62
^{7}Li(1/2-)	^{6}Li(g.s)	$p_{1/2}$	0.57	
		$p_{3/2}$	2.85	
		$\sqrt{\sum ANC^2}$	2.91	

ANCs for overlaps with ^{7}Be(g.s) are close to ^{7}Li(g.s)

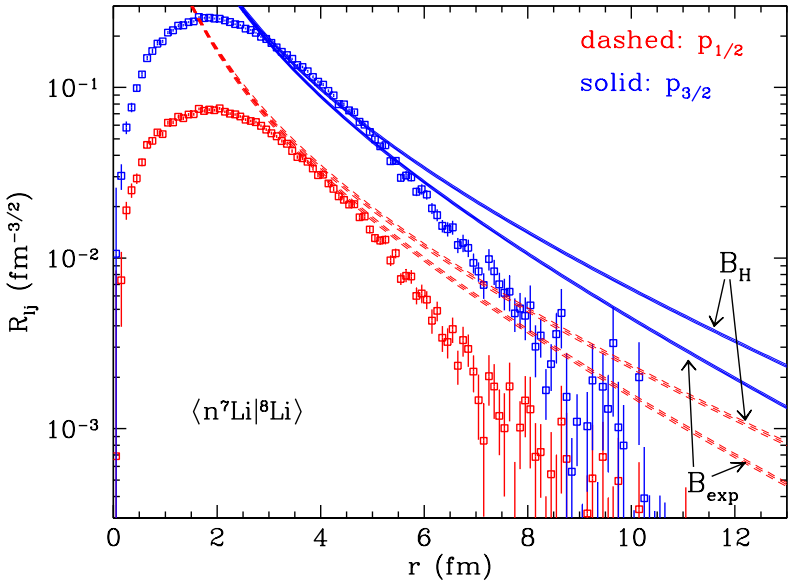
GFMC systematic uncertainties are 5% or less

exp. values: Gulamov (1995), Bekbaev (1991)

A Better Method for ANCs

$$\Phi(r \to \infty) = \langle \Psi_{A-1} | a_{\ell j}(r \to \infty) | \Psi_A \rangle = C_{\ell j} W_{-\eta, \ell+\frac{1}{2}}(2kr)/r$$

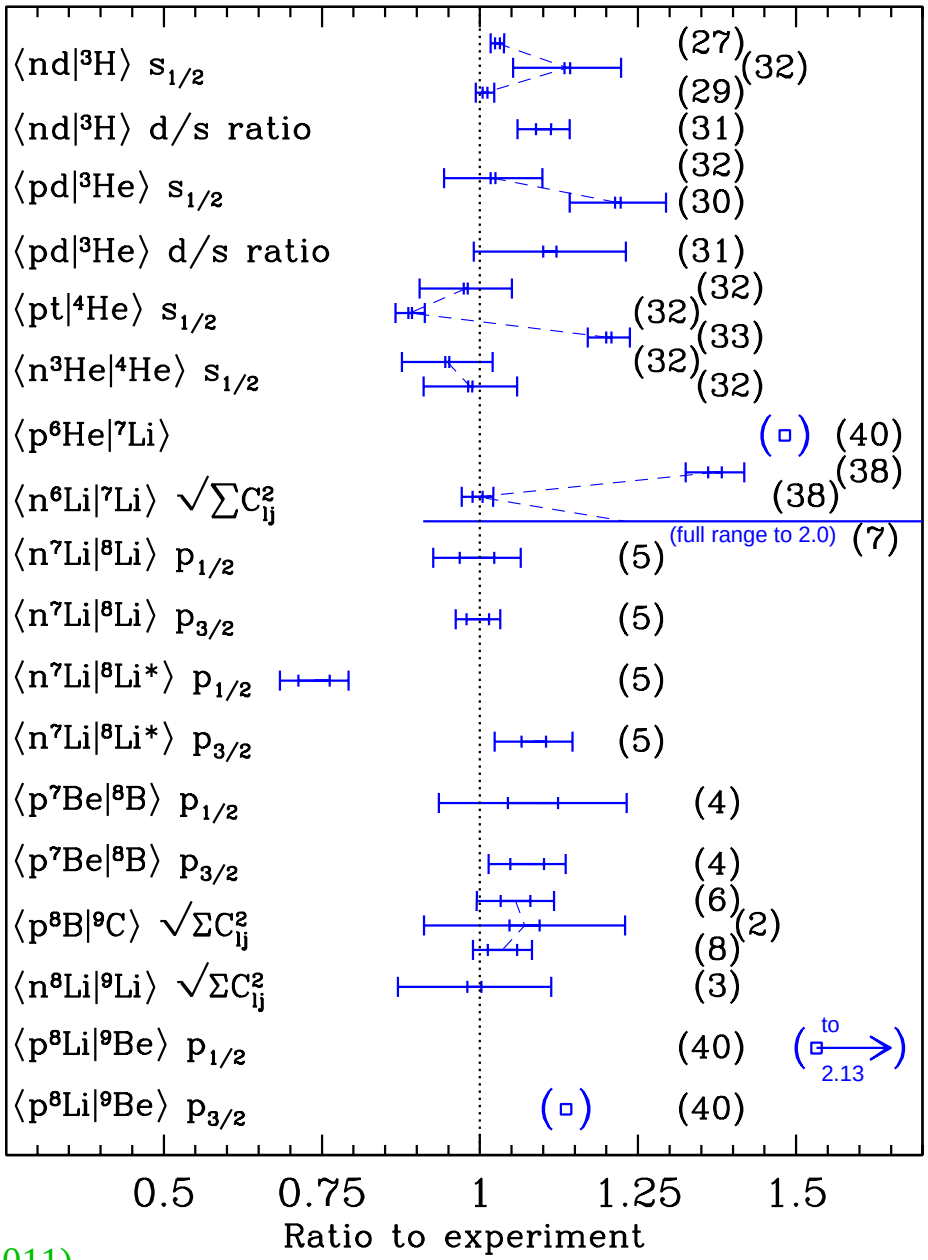
- Best laboratory handle on many astrophysical reactions
- Much recent expt. interest
- Normalization to overlap tails is difficult



- Can be recast into a short-ranged integral

$$C_{\ell j} \sim \mathcal{A} \int M_{-\eta\, \ell+\frac{1}{2}}(2kr)/r \times \Psi^{\dagger}_{A-1} \chi^{\dagger} Y^{\dagger}_{lm}(\hat{\mathbf{r}}) \left(U_{\rm rel} - V_C\right) \Psi_A d\mathbf{R}$$

- This integral is ideal for QMC evaluation



K.M. Nollett and R. B. Wiringa, Phys. Rev. C **83**, 041001(R) (2011).

^{10}C $\rightarrow$ ^{10}B Fermi Beta Decay

- One of the Fermi Beta decays being used to determine the v_{ud} CKM matrix element
- Extracting v_{ud} requires a reliable value of the nuclear matrix element
- If ^{10}C & ^{10}B wave functions are isospin symmetric, $\langle {}^{10}\text{B} \mid \text{F} \mid {}^{10}\text{C} \rangle / \sqrt{2} = 1$
- Up to now, GFMC calculations have assumed isospin conservation to save time
- Can still have non-isospin symmetric ^{10}C & ^{10}B w.f., both with good T=1, by propagating each with different Z
- AV18 contains charge-independence breaking (CIB) terms: strong & E.M.
- These could be important for determining the small departure of $\langle {}^{10}\text{B} \mid \text{F} \mid {}^{10}\text{C} \rangle / \sqrt{2}$ from unity
- Have enhanced GFMC to work in pn total charge basis
  – GFMC wave function has components for all allowed total isospins
  – A=10 w.f. have $\sim$2.5$\times$ more components

Wave function times on one Blue Gene/P node using 4 OMP cores

	^{10}C			^{10}B		
	Components	milli sec	MFLOPS	Components	milli sec	MFLOPS
Good isospin	46,080	218	1201	46,080	218	1201
Charge basis	107,520	164	1930	129,024	251	1636

Time does not scale with number of components

- $\tau \cdot \tau$ operation is much simpler for charge basis
- CPU more efficient with longer inner loops

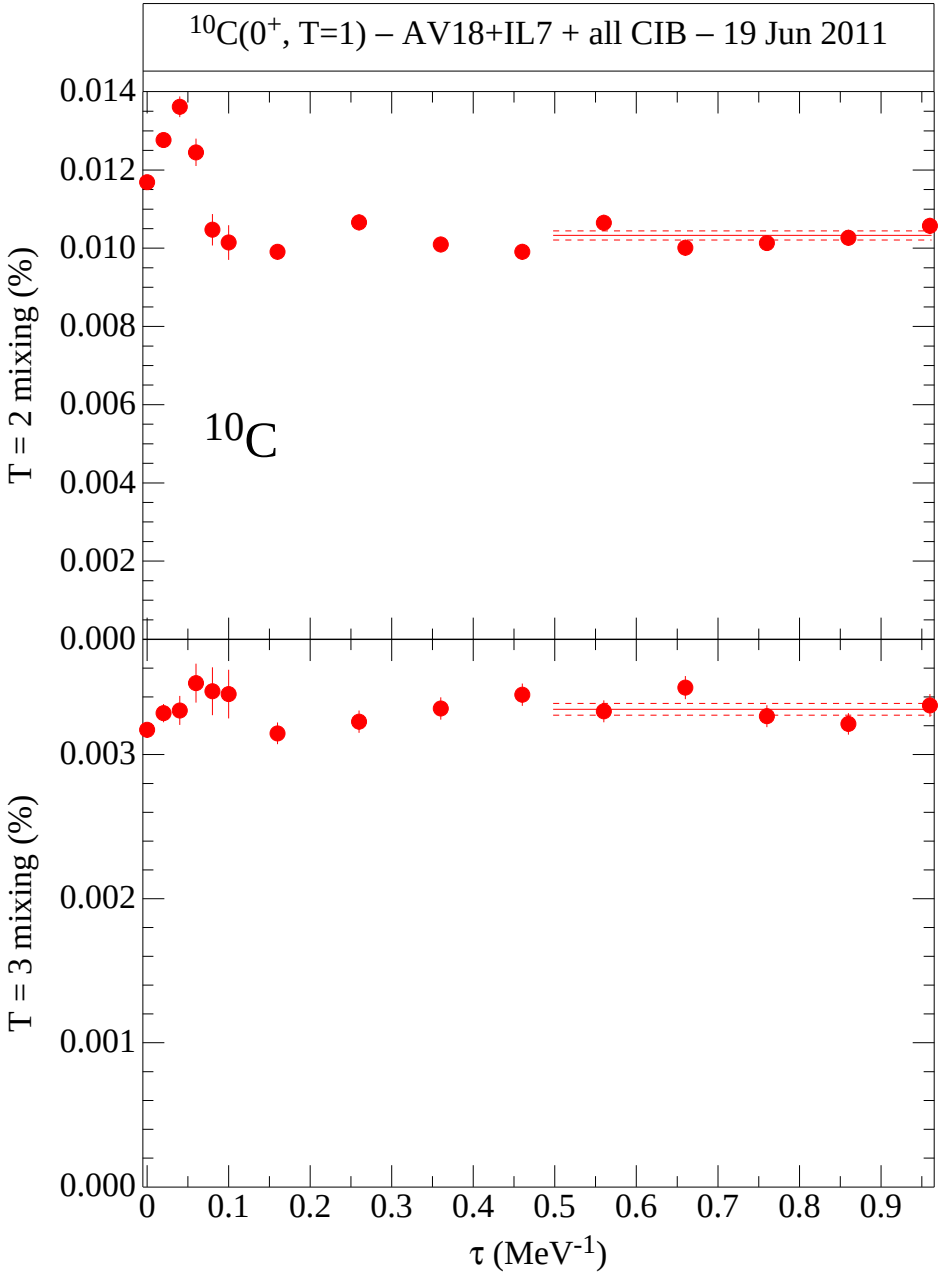
^{10}C & ^{10}B WITH CHARGE-INDEPENDENCE BREAKING

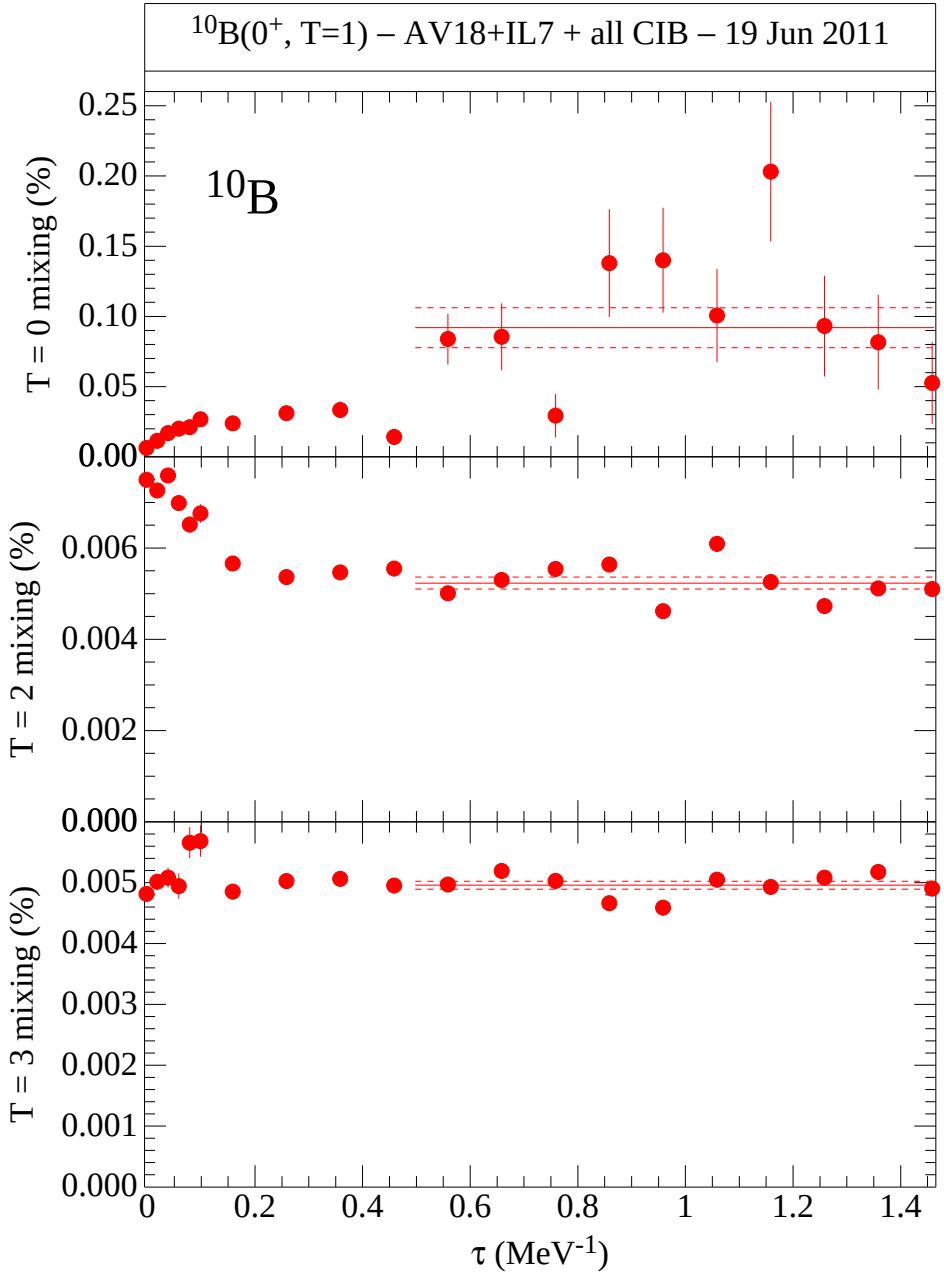
PRELIMINARY

	^{10}C		^{10}B	
	Good T basis	pn basis	Good T basis	pn basis
Energies (Mev)				
Total	-59.99(19)	-60.15(16)	-62.91(16)	-62.77(13)
CIB	0.148(6)	0.045(4)	-0.118(9)	-0.219 8)
E & M	7.890(31)	7.877(24)	5.506(20)	5.452(18)
$r_p - r_n$	0.28(1)	0.28(1)	0.	-0.03(1)
% T=0	-	–	-	0.077%
% T=2	-	0.010%	-	0.0053%
% T=3	-	0.0033%	-	0.0050%

- Total energies not accurate enough to see improvement from charge basis
- Can see clear improvement in NN CIB terms
- Some signal of improvement in E&M terms
- Non T=1 components are very small

^{10}C & ^{10}B WITH CIB – PRELIMINARY





What is happening with ^{10}B T=0?

$^{10}C \rightarrow {}^{10}B$ Fermi Beta Decay

Sorry, it's still too preliminary

STATUS OF DELIVERABLES FOR THIS YEAR

- Continue improvements to ADLB resulting in community usable code
  – Approach based on puts & gets not competitive on IBM Blue Gene/P
- Calculate the Hoyle state with GFMC
  – Much progress made
- Further calculate homogeneous neutron matter and neutron drops in external fields using GFMC and AFDMC to create pseudo-data for constraining energy density functionals
  – PRL published; full paper being written; results being used

Following should have been in the list

- GFMC calculations of nuclear overlaps and spectroscopic factors
  – Large paper on overlaps up to A=7 posted and submitted

PLANS – REMAINDER OF THIS YEAR

- Finish ^{10}C $\rightarrow$ ^{10}B Fermi Beta Decay
- Continue ADLB work aimed at next generation machines
- Continue work on ^{12}C(0_2^+) Hoyle state
- More ^{12}C calculations, including 2^+ state and $E2$ transition
- VMC (GFMC?) computation of density matrix

PLANS – AFTER THIS YEAR