GFMC Benchmarks and Scattering

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Work with

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- Benchmark results for $A = 4 – 10$ using just NN potentials
- Work on Automatic Dynamic Load-Balancing Library
- Neutron drops
- Transition matrix elements
- GFMC Scattering
- Plans for next year

Physics Division

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NN Benchmark Potentials

The 2001 ^{4}He benchmark paper* used AV8′ with no V_{ijk} as the Hamiltonian

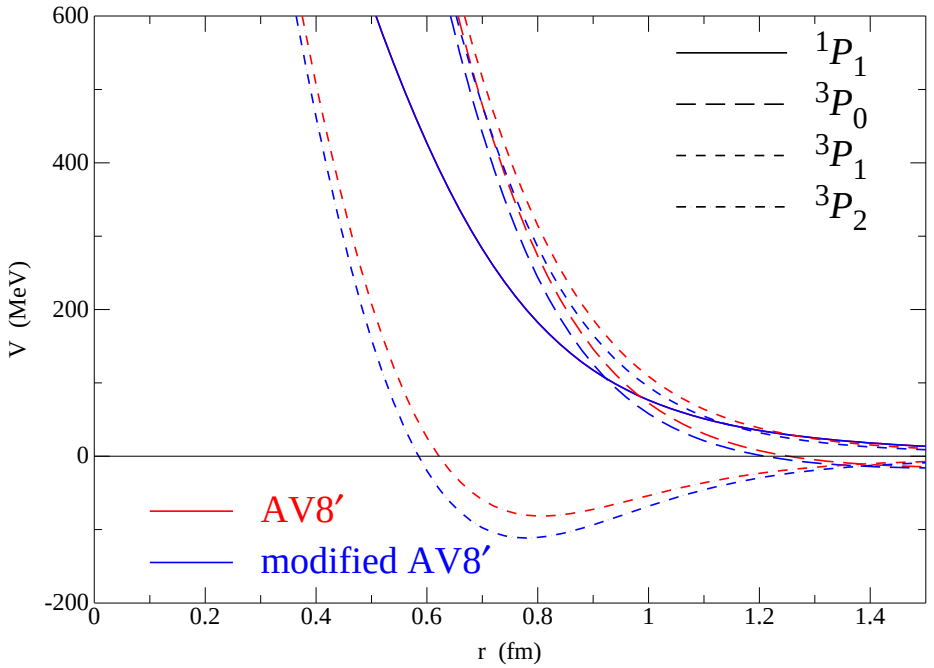
Ultimately we want a ^{12}C benchmark using AV8′ and AV8′ with some V_{ijk} (UIX or TM′).

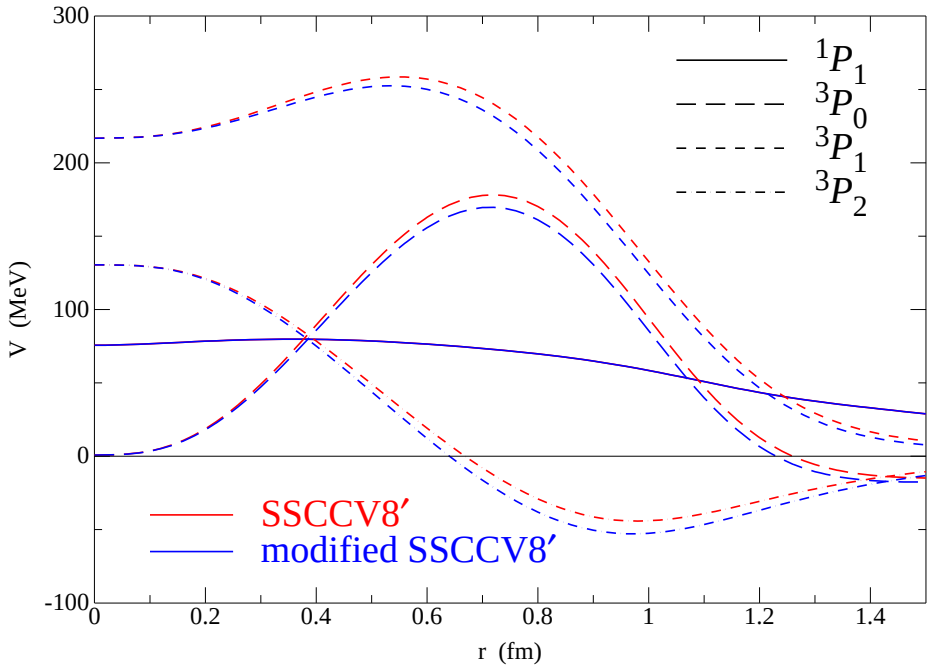
However it was felt that

1) There is a need for intermediate benchmarks (perhaps ^{6}Li, ^{6}He, ^{8}He).

2) A softer *NN* potential, such as SSCC, would also desirable.

The v_8' projection of the SSCC had to be modified to produce binding of A = 6 – 8 nuclei:

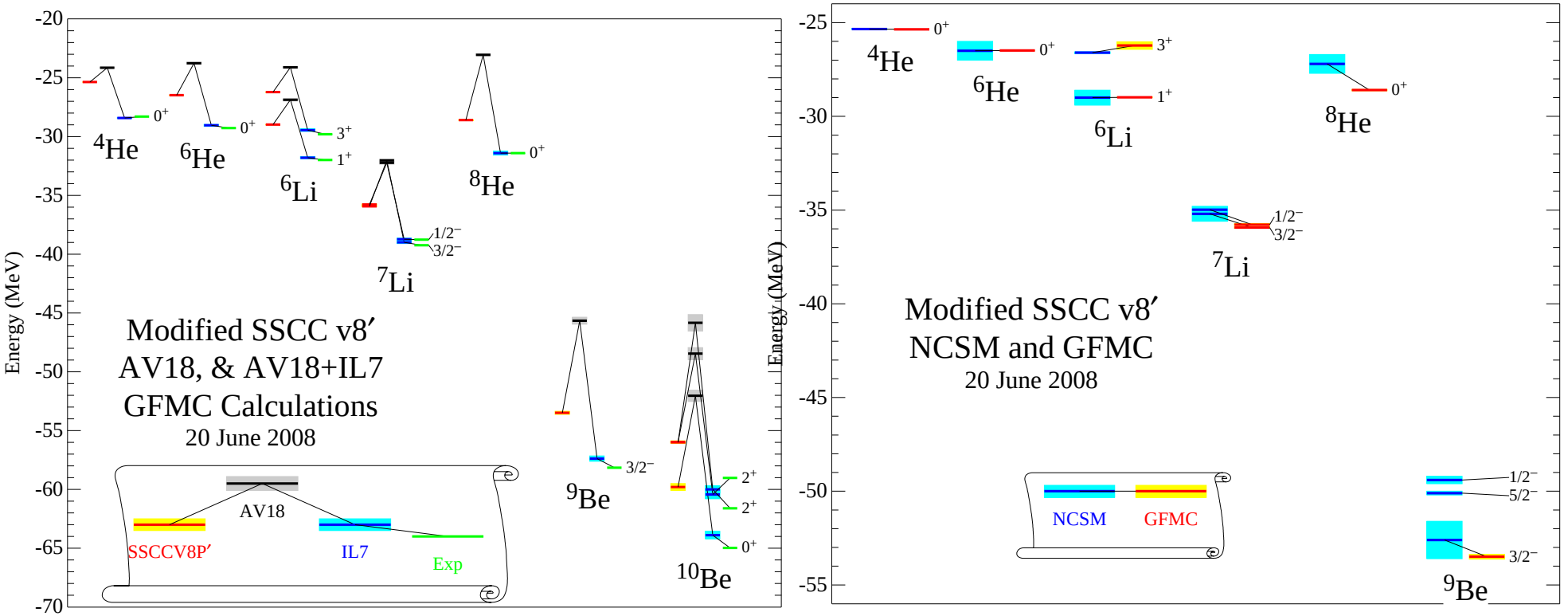




No changes in all even and singlet-odd partial waves

* H. Kamada *et al.*, Phys. Rev. C **64**, 044001 (2001)

NN Benchmark Potentials



- The modified SSCC v_8' qualitatively reproduces experimental binding energies
  – Spin-orbit splittings are too small
- NCSM and GFMC energies are in general agreement within the quoted error bars.

OTHER NCSM AND GFMC RESULTS USING MODIFIED SSCC V8′

	$\langle r_p^2 \rangle^{1/2}$		Quadrupole Moment		Magnetic Moment*	
	NCSM	GFMC	NCSM	GFMC	NCSM	GFMC
^{4}He	1.51(1)	1.51(2)				
^{6}Li	2.33(5)	2.55(4)	0.00(5)	+0.1(1)		
^{6}He	1.88(5)	1.96(4)				
^{7}Li	2.24(5)	2.42(4)	≤ -2.85	$-3.9(5)$	+3.01(3)	+2.879(3)
^{8}He	1.85(5)	1.83(5)				
^{9}Be	2.32(5)	2.46(5)				

*Exchange currents not included

AUTOMATIC DYNAMIC LOAD BALANCING (ADLB) LIBRARY

- A general-purpose library to help application codes dynamically share work
- Being developed by Rusty Lusk and Ralph Butler
- First application is enabling the GFMC program to use 10,000's processors
- Most of my UNEDF time has been converting the GFMC program and testing/learning
- Rusty will talk about its structure

GFMC needed to be redone for leadership class computers

- Old program did several Monte Carlo samples per processor
- Branching can kill samples – need enough not to fluctuate to zero
- ^{12}C will have 10,000 Monte Carlo samples
- Leadership class computers have 10,000's processors
- Need to split one sample over many processors

AUTOMATIC DYNAMIC LOAD BALANCING – CURRENT GFMC IMPLEMENTATION

Old GFMC

Each slave gets several configurations

Slave

propagates configurations

(few w.f. evaluations)

replicates or kills configs (branching)

$\longrightarrow$ periodic global redistribution

computes energies

(many w.f. evaluations)

Need $\sim$10 configs per slave

^{12}C will have only $\sim$10,000 configs.

Can't do on more than 2000 processors

Configurations cannot be unit of parallelization

With ADLB

A few "boss" slaves manage the propagation:

- Generate propagation work packages
  – Answers used to make 0,1,2,$\cdots$ new propagation packages (branching)
  – Number of prop. packages fluctuates
  – Global redistribution may be avoided
- Generate energy packages – No answers

When propagation done, become worker slaves

Most slaves ask ADLB for work packages:

- Propagation package
  – Makes w.f. and $3N$ potential packages
- Energy package
  – Makes many w.f. packages
  – Makes $3N$ potential packages
  – Result sent to Master for averaging
- Wave Function or $3N$ potential package
  – Result sent to requester

Wave function is parallelization unit

Can have many more processors than configs

AUTOMATIC DYNAMIC LOAD BALANCING – CALCULATIONS

Development is still continuing but VMC and GFMC calculations using ADLB are being made.

Calculations made principally to demonstrate ADLB

- 5,400-processor VMC for ^{7}Li – 95% efficency
- 16,384-processor GFMC for 14-neutron drop – 83% efficency

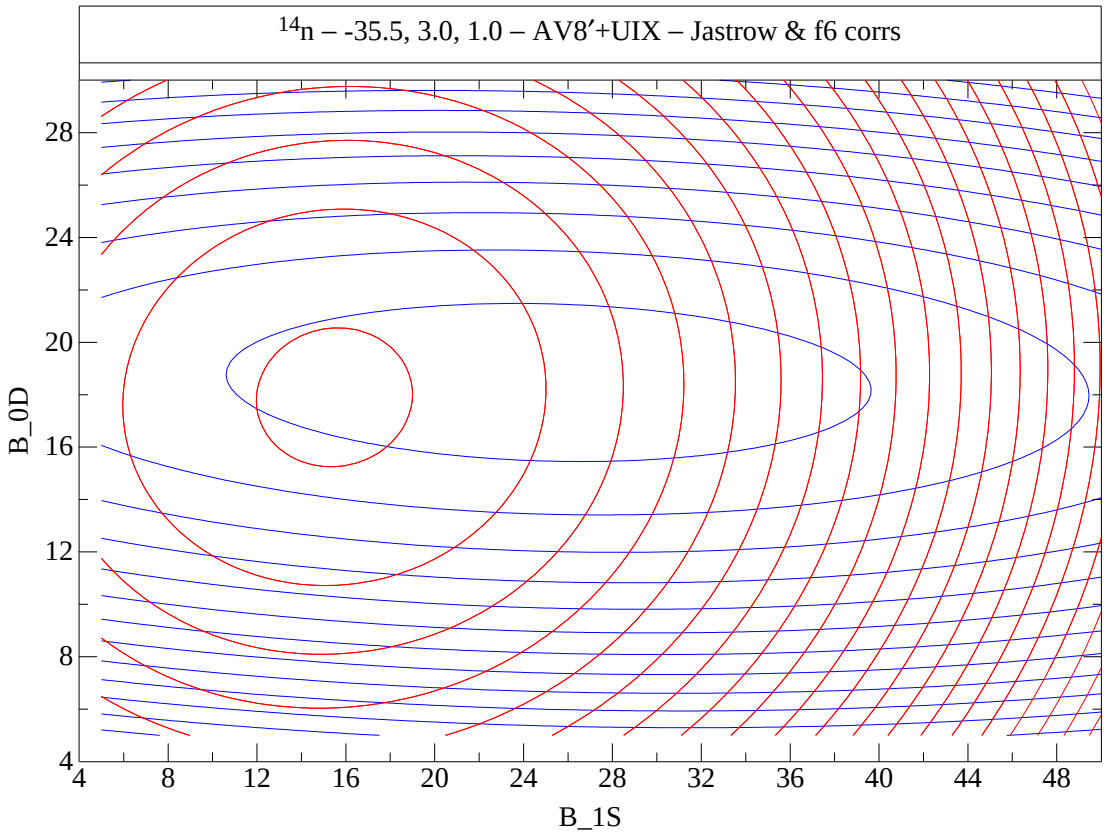
Calculations made for physics interest

- 2,000- to 8,192-processors: many 14-neutron drop with various H, Ψ_T, GFMC parameters
- 8,192-processor ^{9}Be with SSCC v_8'
- 4,096 – 8,192-processor ^{10}Be with SSCC v_8'
- up to 4,800 processors: nuclei up to ^{10}B with new Illinois V_{ijk}

NEUTRON DROPS

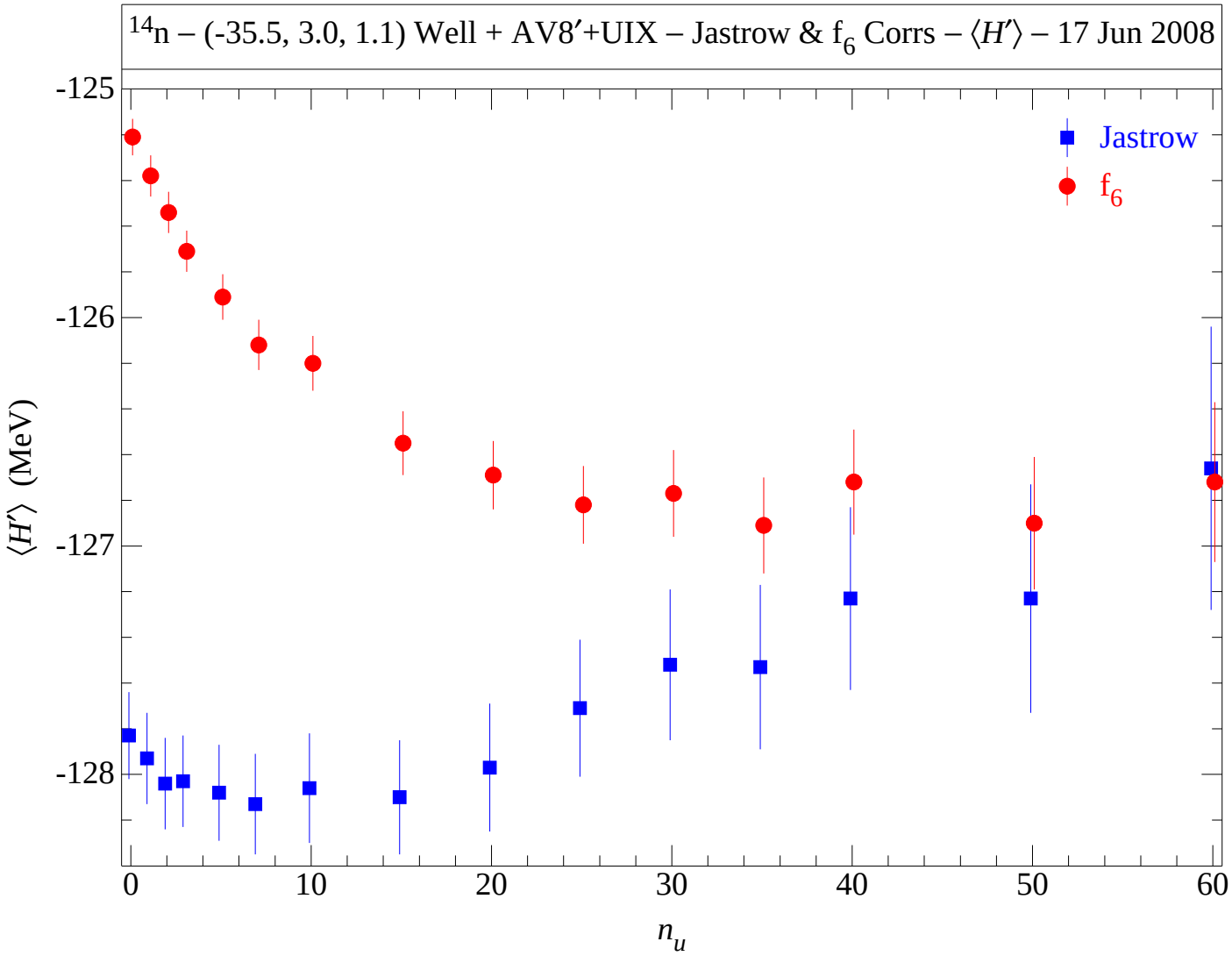
- Collection of neutrons interacting via standard NN and NNN Hamiltonian with added artificial external well
- Well can be adjusted to change density or surface thickness
- Well could be non-spherical
- If NN and NNN H is realistic, can provide input to EDF's
- GFMC can compute up to 16 neutrons (part-way through $S-D$ shell).

- Ψ_T has BCS one-body part with pairs of $0S, 0P, 1S, 0D$ neutrons
- $0S, 0P$ shells basically full; $1S, 0D$ occupations are variational parameters
- Ψ_T are pure Jastrow or Jastrow+f_6-pair correlations
- Contours show searches of $1S, 0D$ occupations: ^{14}n, AV8′+UIX
- blue contours for pure Jastrow Ψ_T
- red contours for Jastrow+f_6

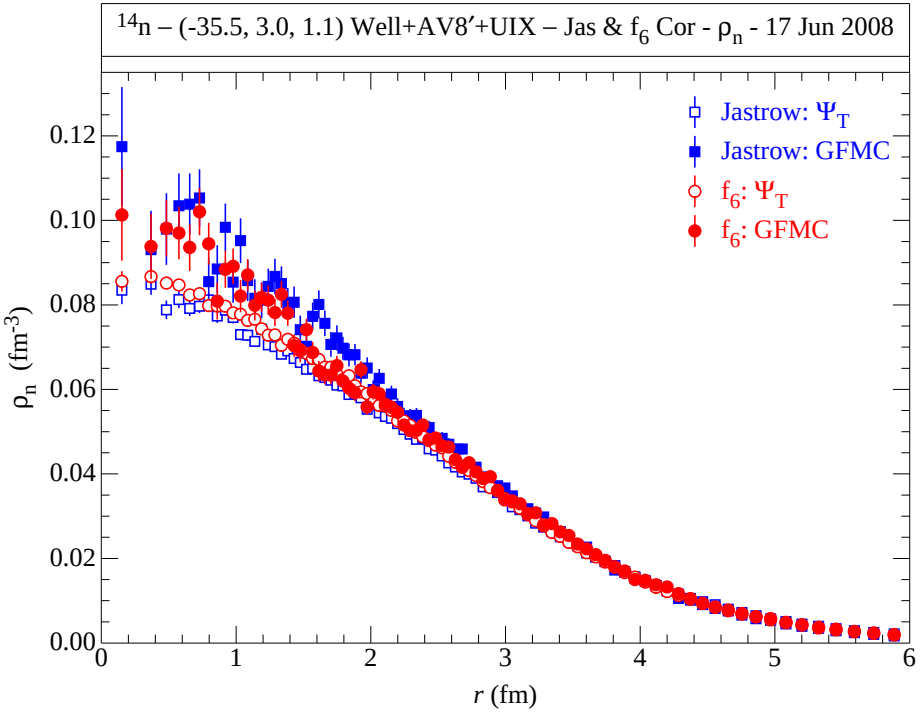


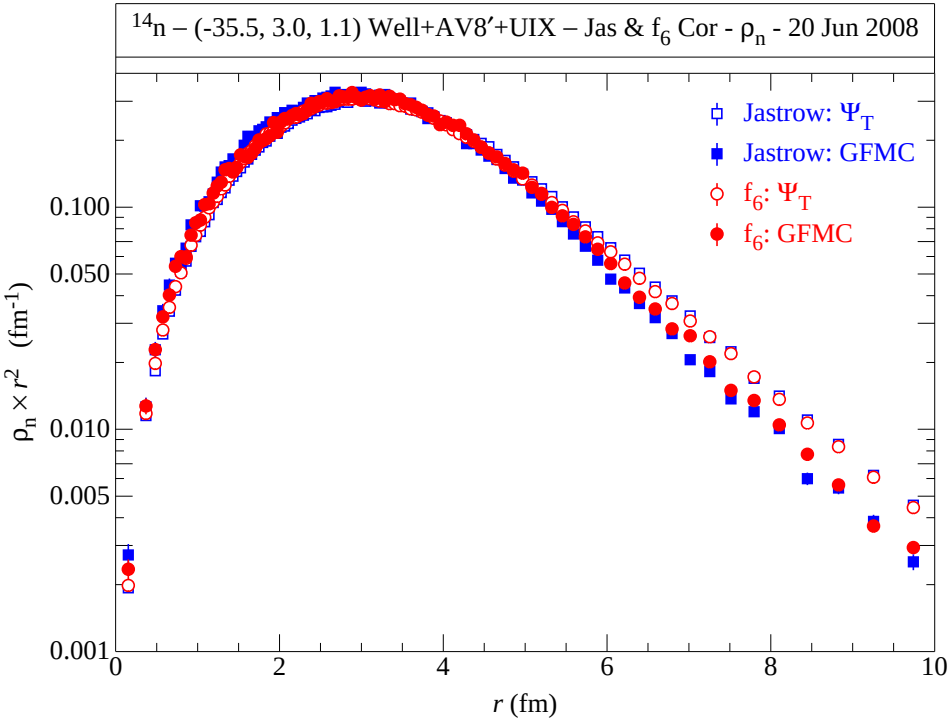
Neutron Drops - GFMC Constrained-path Convergence

- We use a number of unconstrained GFMC steps before computing energies
- Usually 10–20 unconstrained steps are adequate
- ^{8}He and neutron drops require more.

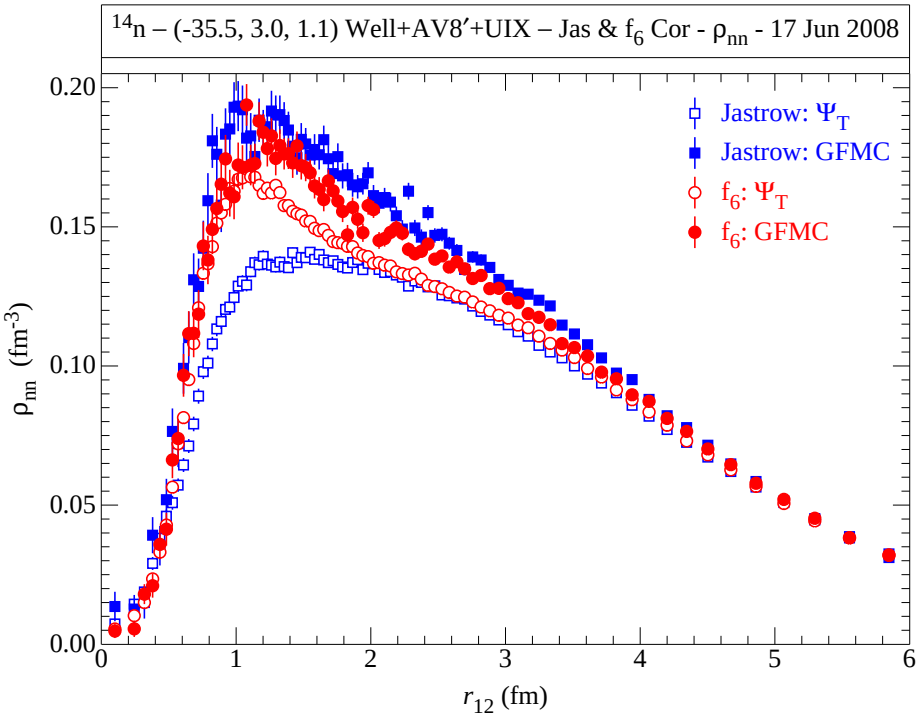


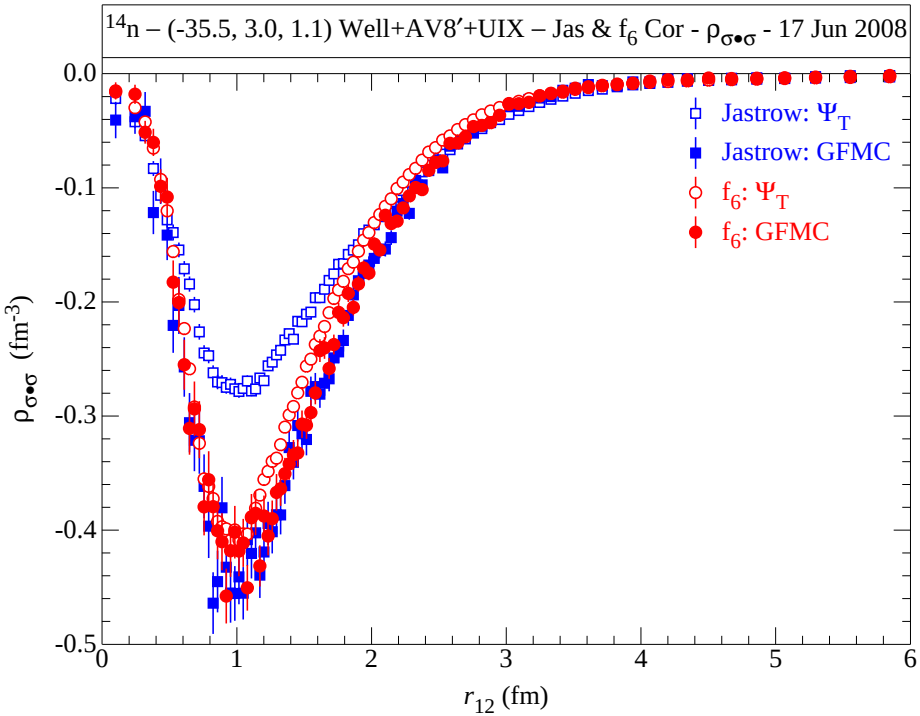
Neutron Drops – Single-neutron Density Distributions





Two-neutron Pair and $\sigma \cdot \sigma$ Density Distributions





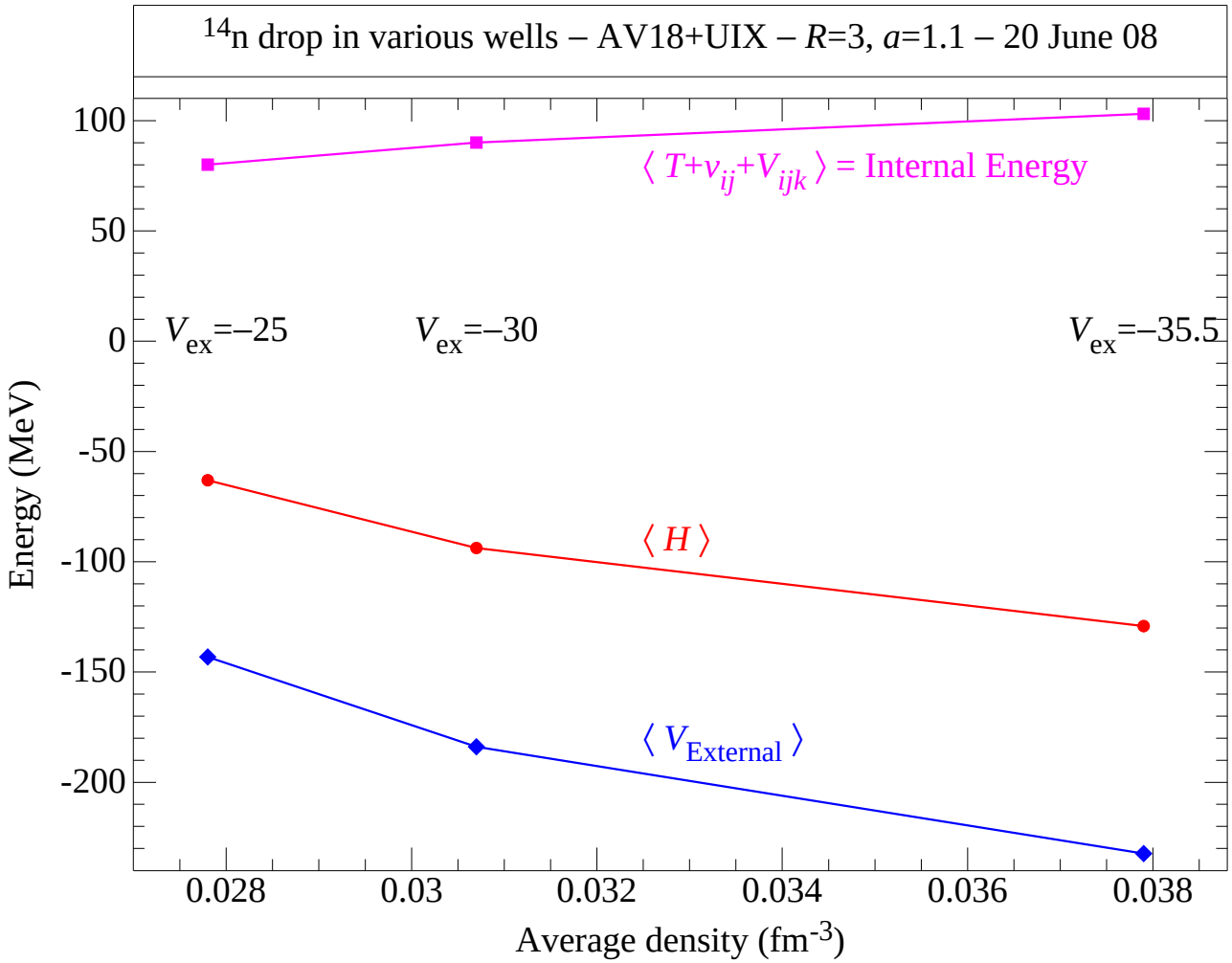
GFMC produces same final densities starting from very different Ψ_T densities

Neutron Drops – Dependence on External Well Depth

Calculations of 14 neutrons with AV18+UIX and three external wells:

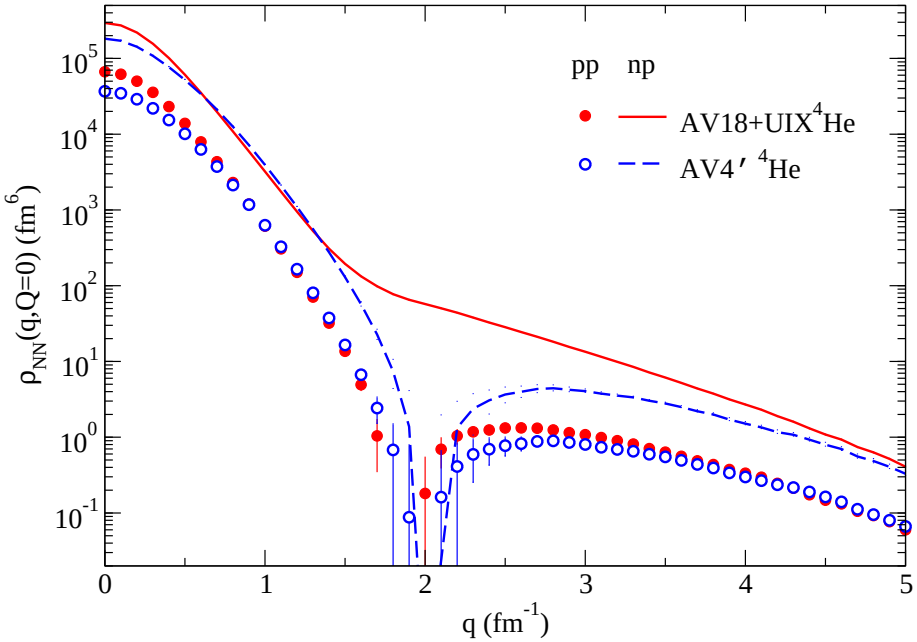
R = 3.0 fm; a = 1.1 fm; V_{ex} = 25, 30, & 35.5 MeV

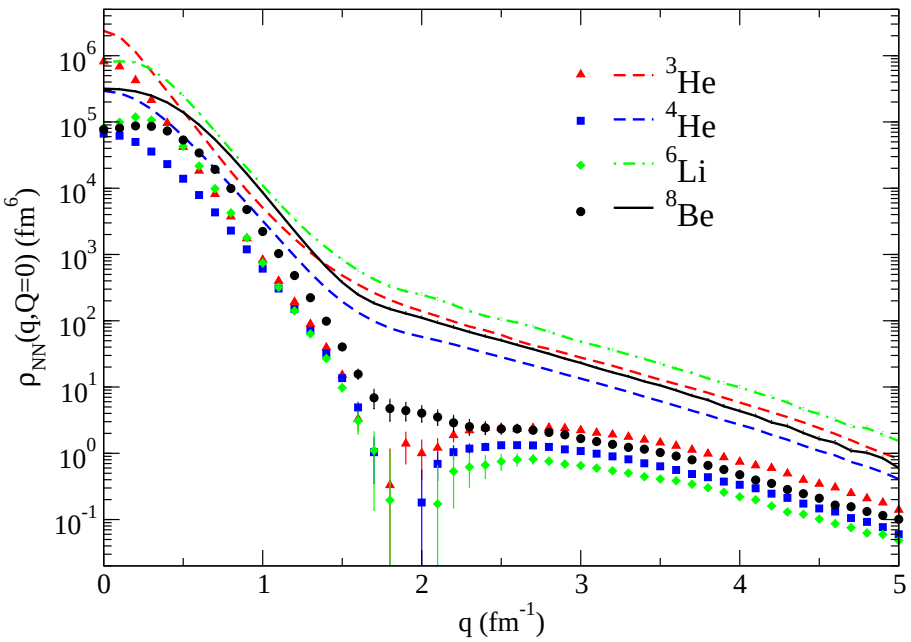
The computed energies have a (slightly) nonlinear dependence on the average density



Two-nucleon Knockout – $(e, e'pN)$

- Just published (Science) JLAB expt. for ^{12}C$(e, e'pN)$
- Measured back to back pp and np pairs of equal $|p_i|$; $Q_{\rm tot} = 0$
- Pairs with relative momentum 2–3 fm^{-1} show 10–20 $\times$ np enhancement (preliminary).



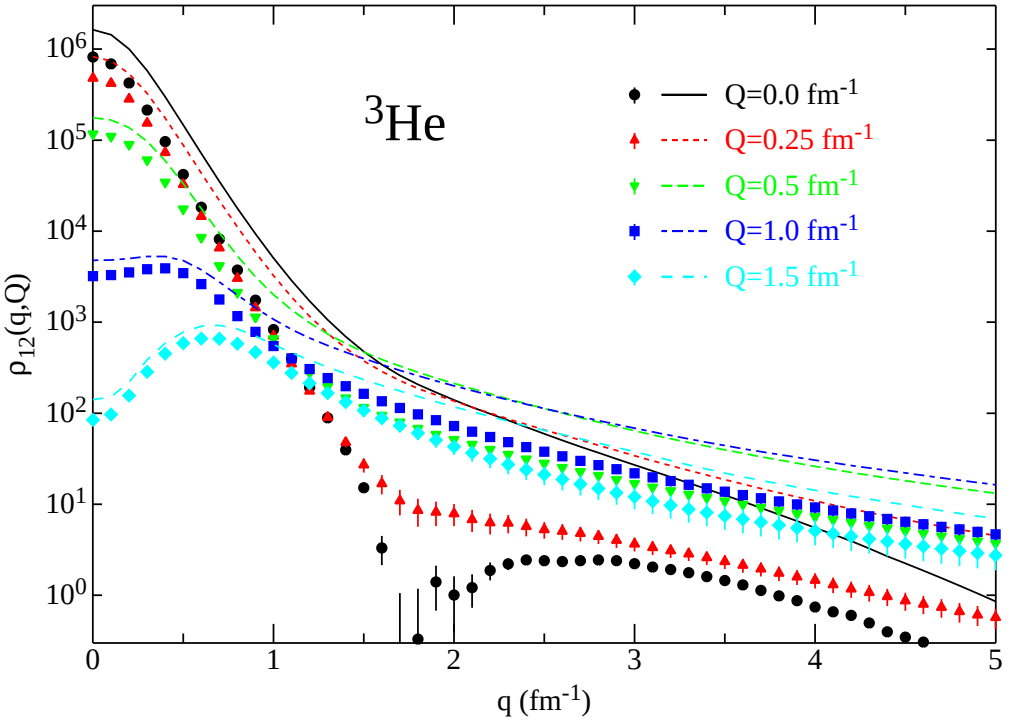


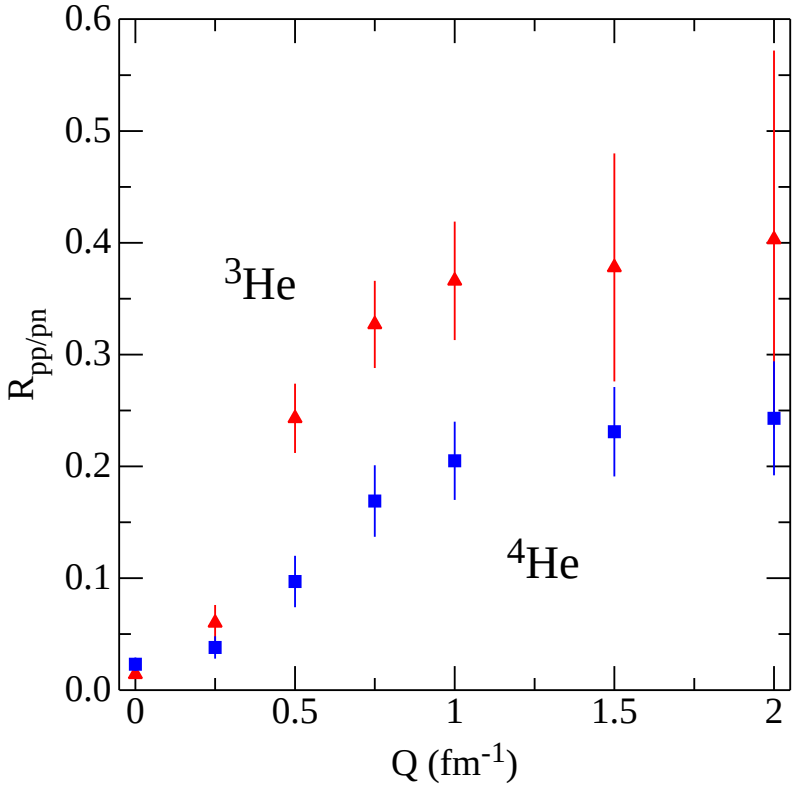
- VMC calculations for ^{3}He, ^{4}He, and ^{8}Be show this effect
- Effect disappears when tensor correlations are turned off
- Shows importance of tensor correlations to > 3 fm^{-1}.

R. Schiavilla, R. B. Wiringa, S. C. Pieper, and J. Carlson, Phys. Rev. Lett. **98**, 132501 (2007)

Two-nucleon Knockout – $(e, e'pN)$

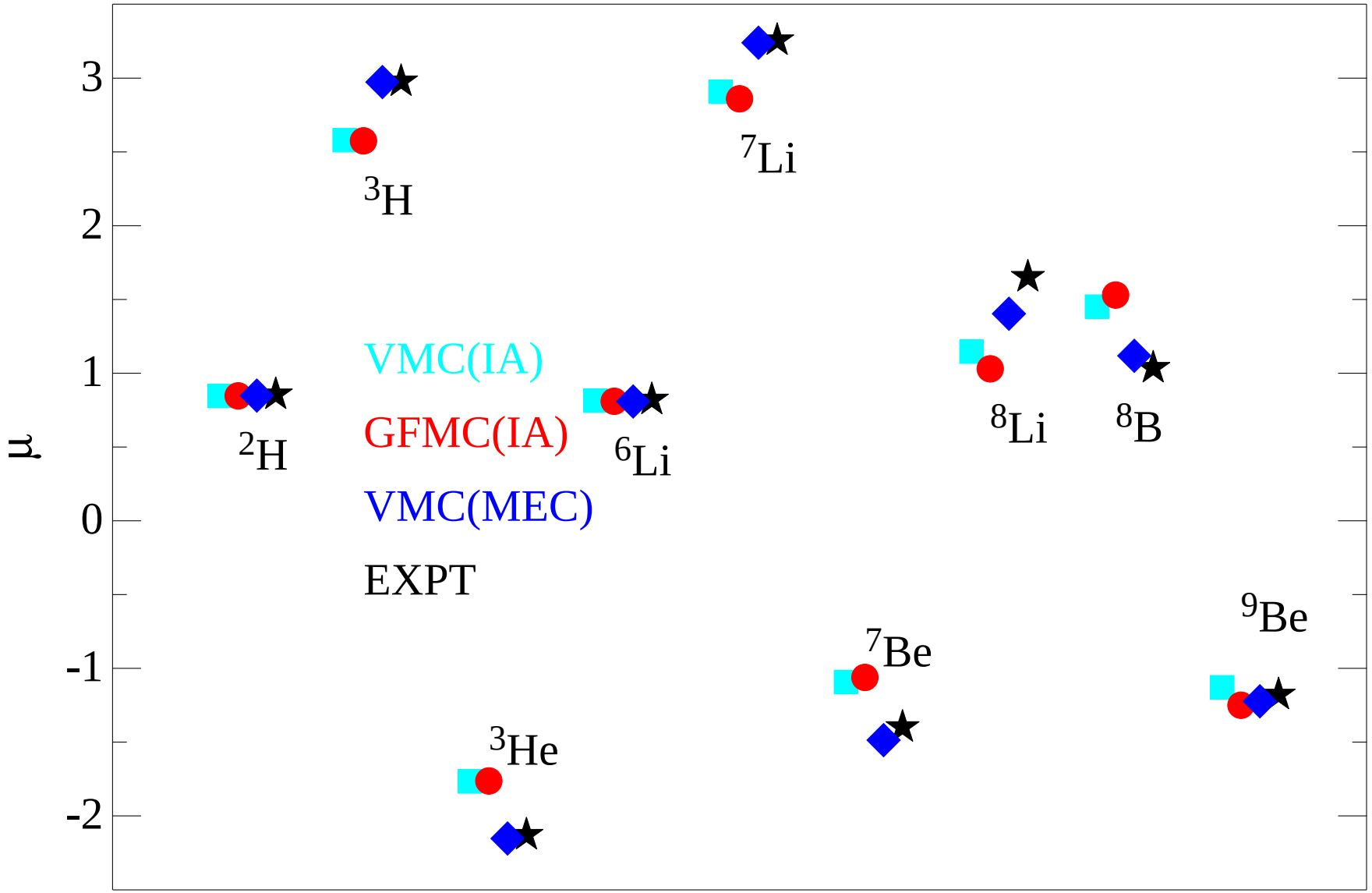
- New CLAS experiment for ^{3}He$(e, e'pp)n$ considers pairs with $Q_{\rm tot} \neq 0$
- For $Q_{\rm tot} > 0$, the minimum in pp distribution fills in
- Ratio of pp and pn pair cross sections integrated over $q_{\rm rel} = 300$–500 MeV/c
- Compares well with preliminary analysis of data
- Second JLAB experiment to demonstrate importance of tensor correlations at q ~ 2 fm^{-1}





Wiringa, Schiavilla, Pieper & Carlson, (arXiv:0806.1718)

Magnetic Moments



No effective charges or effective nucleon magnetic moments!

$M1$, $E2$, F, GT transitions

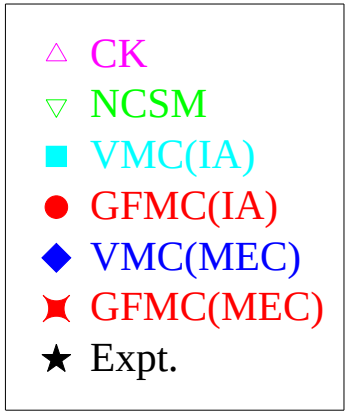
$$E2 = e\sum_k \tfrac{1}{2}\left[r_k^2 Y_2(\hat{r}_k)\right](1+\tau_{kz})$$

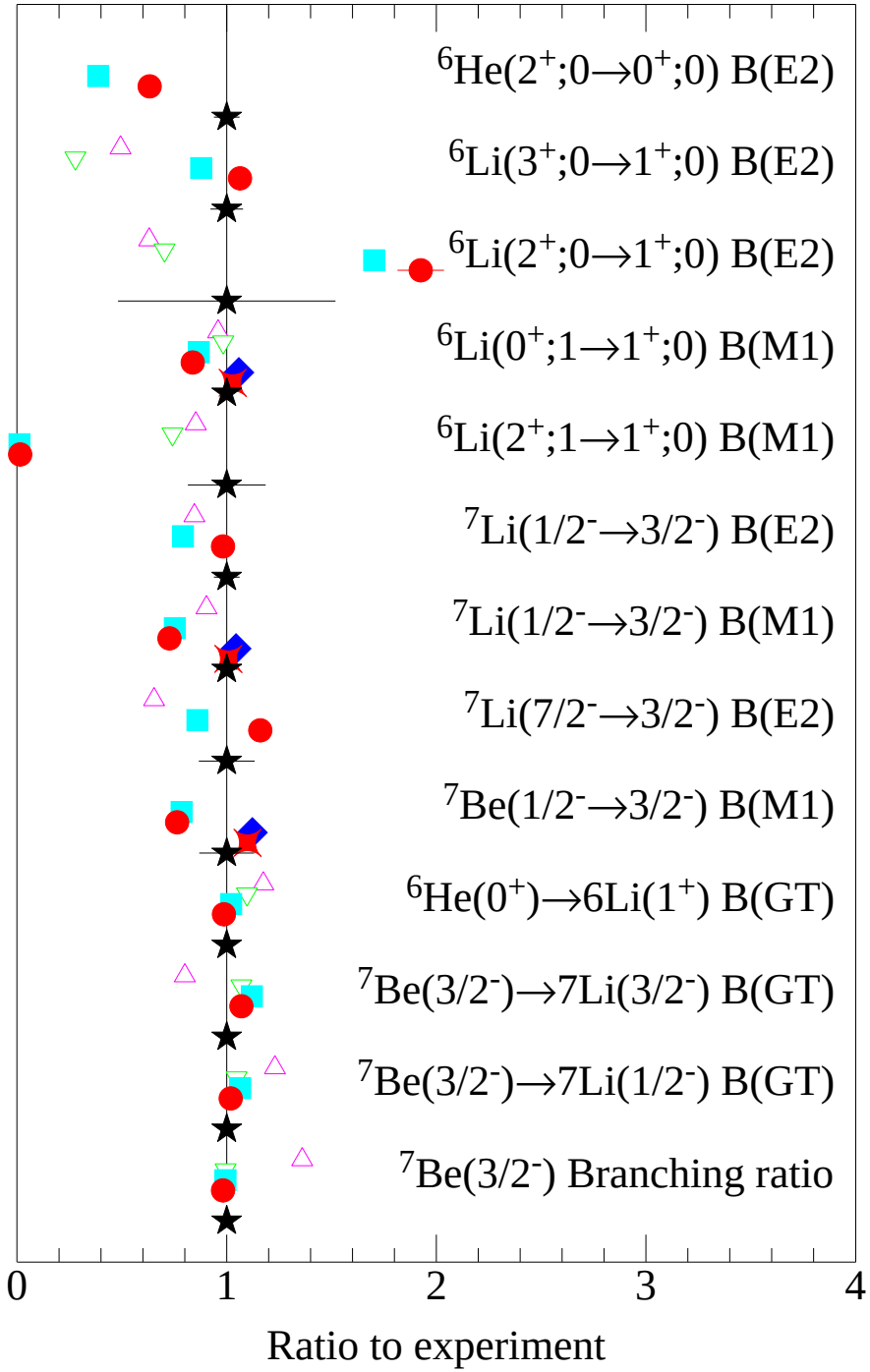
$$M1 = \mu_N \sum_k [(L_k + g_p S_k)(1+\tau_{kz})/2 + g_n S_k\ (1-\tau_{kz})/2]$$

$$\mathrm{F} = \sum_k \tau_{k\pm}\ ;\ \mathrm{GT} = \sum_k \sigma_k \tau_{k\pm}$$

No effective charges or
effective nucleon magnetic moments!

Pervin, Pieper & Wiringa, PRC **76**, 064319 (2007)





GFMC for Scattering States

GFMC treats nucleus as particle-stable system

– Should be good for narrow resonances

Many cases should be done as scattering states

– Wide resonances: ^{5,7}He, ^{6}Li(2^+), ^{8}Be(2^+,4^+), ...

– Will get widths of resonances

– Capture reactions: ^{4}He(d,γ)^{6}Li, ^{7}Be(p,γ)^{8}B, ...

1987 – early 1990's:

– Carlson *et al.* do ^{5}He states by VMC scattering

– Carlson also does preliminary ^{5}He GFMC scattering

Present:

– Joe Carlson doing ^{5}He for parity violation studies

– Ken Nollett has modified Argonne GFMC program for scattering and done ^{5}He

NCSM and CC are also computing resonance states

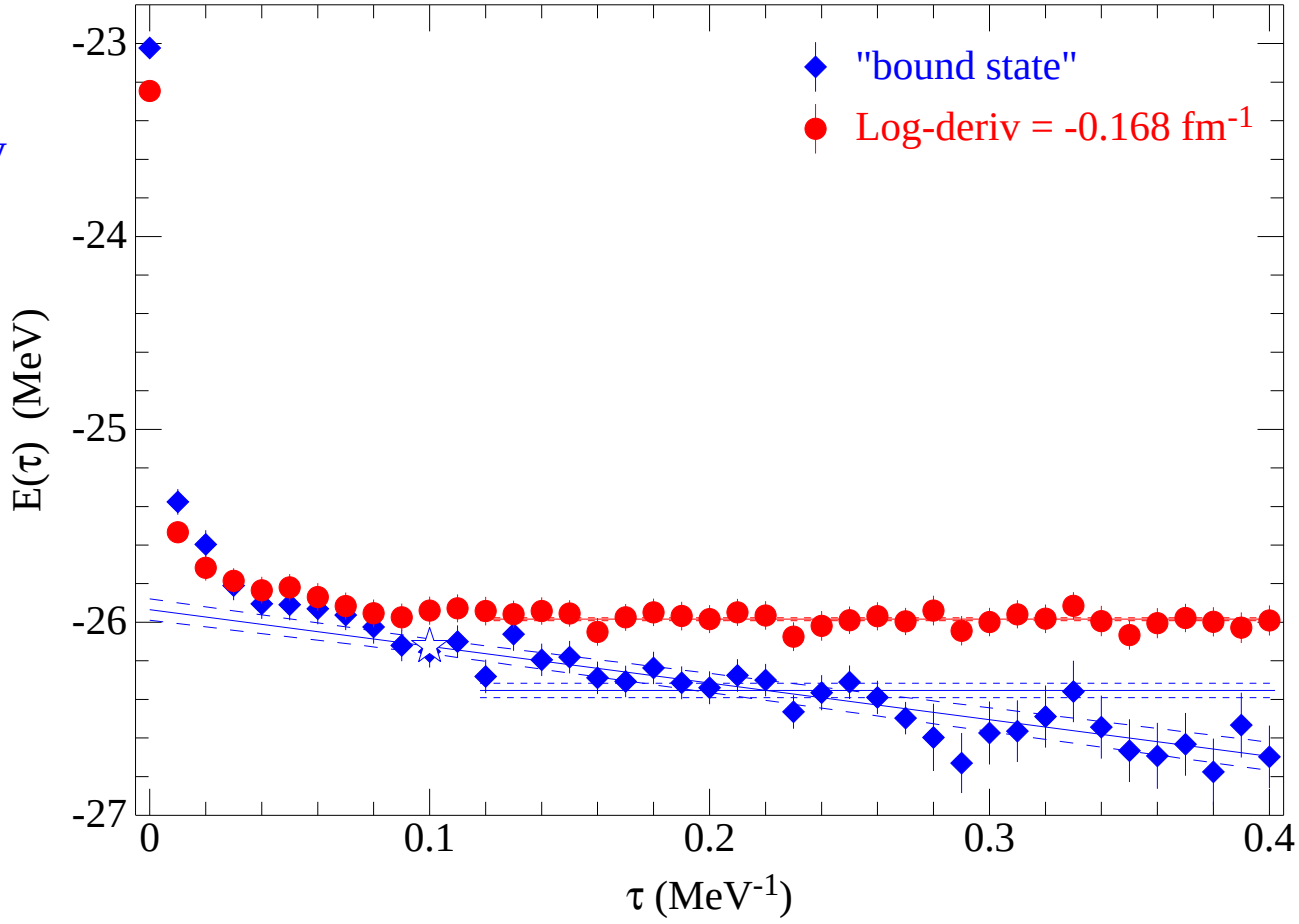
A benchmark comparison (^{5}He with SSCC v_8'?) would be useful

GFMC FOR SCATTERING STATES – METHOD

- Pick a logarithmic derivative, χ, at some large boundary radius ($R \geq 7$ fm)
- GFMC propagation, using method of images to preserve χ at R, finds $E(R, \chi)$
- Phase shift, $\delta(E)$, is function of R, χ, E
- Repeat for a number of χ until $\delta(E)$ is mapped out

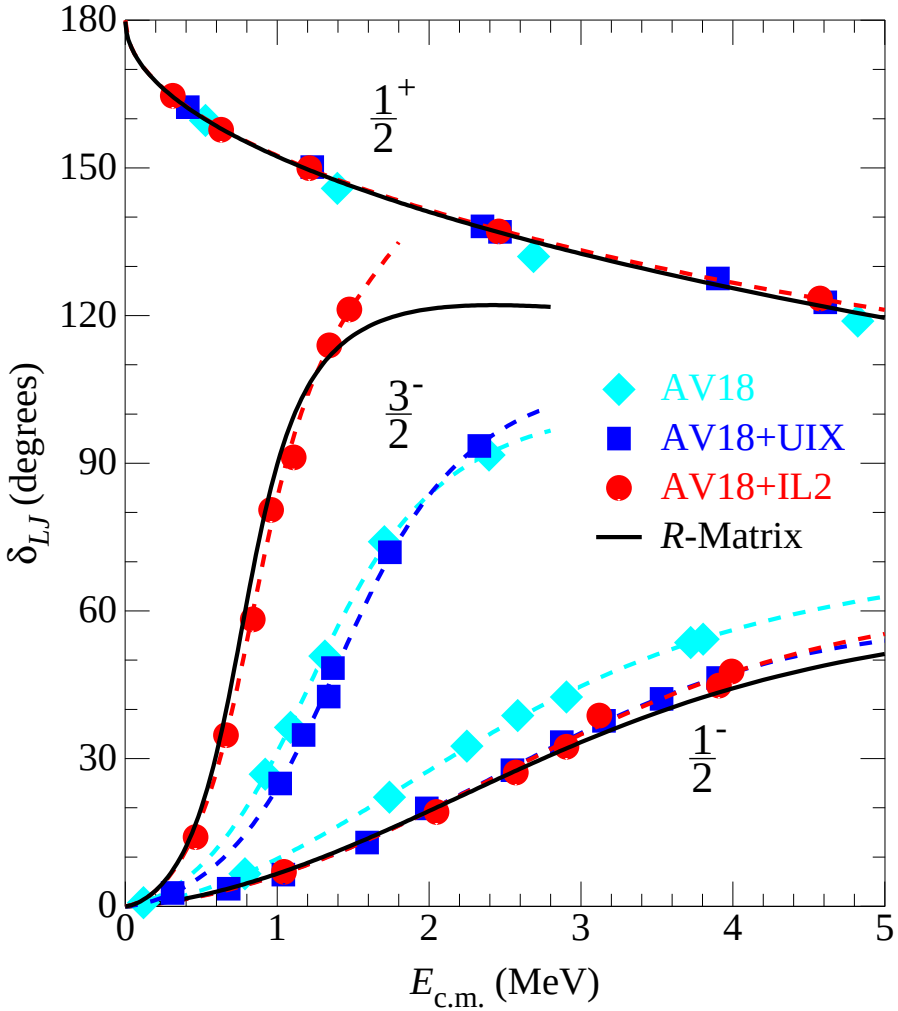
Example for $^5\mathrm{He}(\frac{1}{2}^-)$

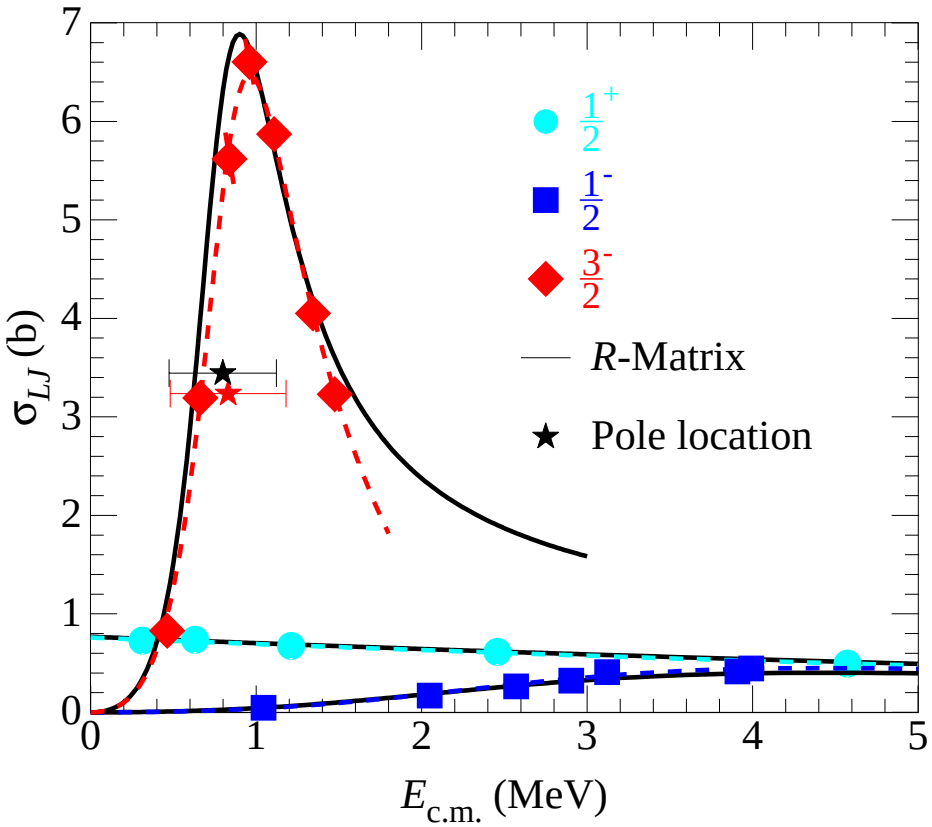
- "Bound-state" boundary condition does not give stable energy; Decaying to n+^{4}He threshold
- Scattering boundary condition produces stable energy.



GFMC FOR ^{5}HE AS n+^{4}HE SCATTERING STATES

- Black curves: Hale phase shifts from R-matrix analysis up to $J = \frac{9}{2}$ of data
- AV18 with no V_{ijk} underbinds ^{5}He($\frac{3}{2}^-$); overbinds ^{5}He($\frac{1}{2}^-$)
- AV18+IL2 was not fit to ^{5}He, reproduces locations and widths of both P-wave resonances
  – Spin-orbit splitting well reproduced by AV18+IL2





K.M. Nollett, S.C. Pieper, R.B. Wiringa, J. Carlson, G. M. Hale, Phys. Rev. Lett. **99**, 022502 (2007)

New Illinois potentials – Progress Report

- Illinois 1–5 parameters determined in 2000.
  - Fits made to $A \leq 8$ only
  - Preliminary nuclear matter calculations at Urbana (Morales, Pandharipande, Ravenhall) suggested at most IL2 is viable
  - Improved GFMC results in worse ^{8}He agreement
- Started new fitting up to $A = 10$
- Michele Viviani (Pisa) finds sign error in one piece of A_σ in $V_{ijk}^{3\pi}$
  - Formula was published correctly, but incorrectly programmed
  - Increased attraction for all nuclei
- New fit made with corrected A_σ: IL7
  - parameters weaker than for IL2 because of increased attraction
  - better quality reproduction of energies than IL2
  - so far have not found any significant difference in other observables
- Stefano Gandolfi (Trieste) doing Auxiliary Field Diffusion Monte Carlo (AFDMC) for neutron matter using AV8′+ILx.
  - IL2 and IL7 much too soft need much stronger short-ranged repulsion in V_{ijk}^{R}
  - Preliminary IL8 looks not unreasonable
  - For now AV18+UIX seems best for pure neutron systems

STATUS OF DELIVERABLES FOR THIS YEAR

- Finish first version of ADLB GFMC
  - Done: Several versions with one Monte Carlo sample sent to many processors
- Diagonal and off-diagonal (in VMC) densities of nuclei in external wells
  - Done: Diagonal densities of various neutron drops in various wells
  - Done: Two-body momentum distributions
- Improve ^{12}C VMC wave function
  - Still to be worked on

PLANS

Remainder of this year

- Continue ADLB work with aim of good efficiency on 30,000 processors
  – Global control of population growth or decay (being done locally now)
  – Not allowing too great a dispersion in time steps being processed
- Continue various neutron drop calculations
- Improved ^{12}C Ψ_T
- First ^{12}C calculations using ADLB version of GFMC (Benchmark NN potentials?)

Next year

- Continuing ADLB work and start multithreading of GFMC
- Many ^{12}C calculations
  – Full H for several states
  – Transitions and transition densities
- VMC (GFMC?) computation of density matrix
- Neutron drops with new Illinois potential
- Real nuclei in external wells
- Non-spherical external wells
- GFMC nucleon-nucleus scattering and comparison with other methods?

PLANS

Years 4 and 5

- Fully multithreaded version of GFMC
- Start changes of GFMC/ADLB for exoscale class computers (e.g. BG/Q)
- More ^{12}C calculations, specifically Hoyle state.
- $A > 12$ nuclei?