

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

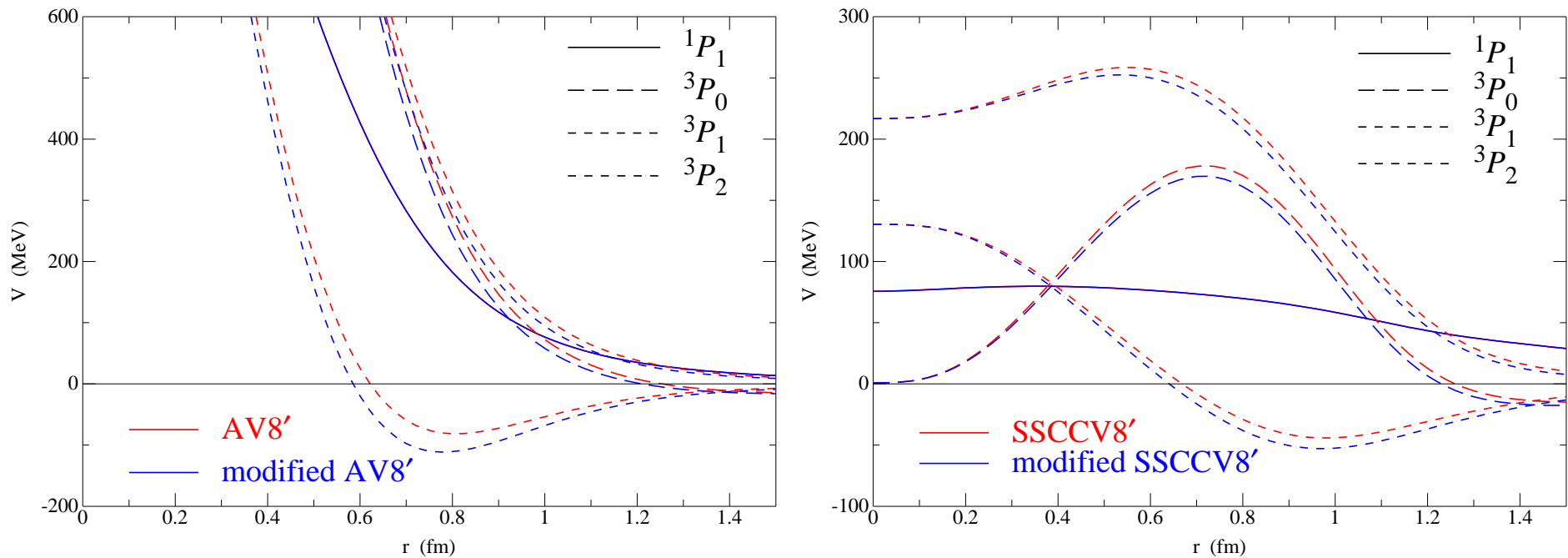
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NN BENCHMARK POTENTIALS

The 2001 ${}^4\text{He}$ benchmark paper* used AV8' with no V_{ijk} as the Hamiltonian
Ultimately we want a ${}^{12}\text{C}$ 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 ${}^6\text{Li}$, ${}^6\text{He}$, ${}^8\text{He}$).
- 2) A softer NN potential, such as SSCC, would also be desirable.

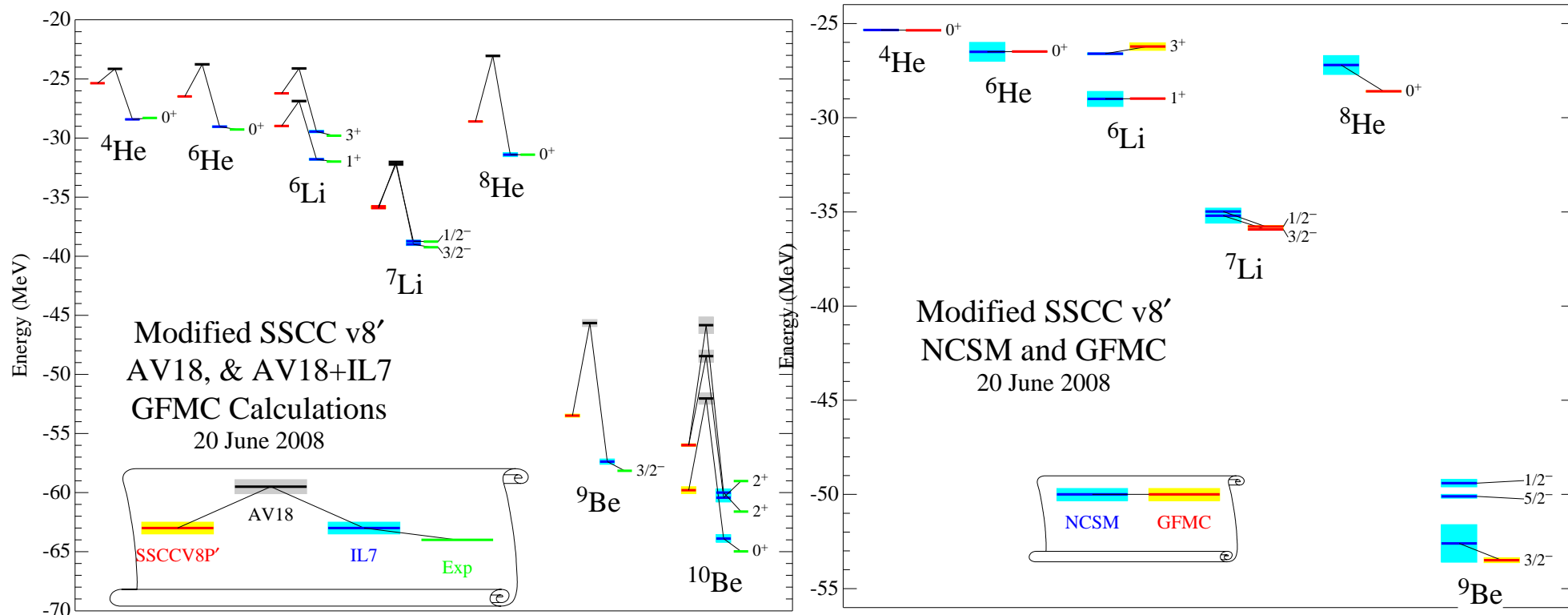
The v'_8 projection of the SSCC had to be modified to produce binding of $A = 6 - 8$ nuclei:



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 GFM 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
^4He	1.51(1)	1.51(2)				
^6Li	2.33(5)	2.55(4)	0.00(5)	+0.1(1)		
^6He	1.88(5)	1.96(4)				
^7Li	2.24(5)	2.42(4)	≤ -2.85	-3.9(5)	+3.01(3)	+2.879(3)
^8He	1.85(5)	1.83(5)				
^9Be	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)

→ periodic global redistribution

computes energies

(many w.f. evaluations)

Need ~ 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, ... 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

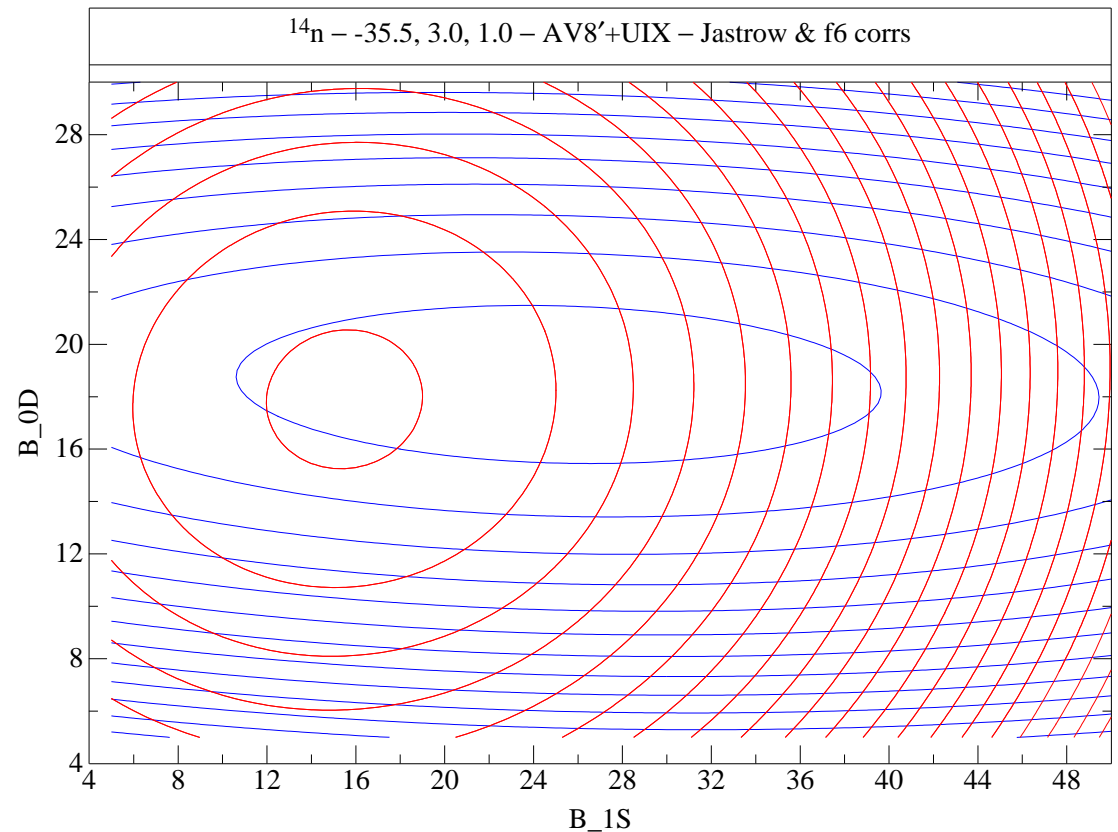
- 5,400-processor VMC for ${}^7\text{Li}$ – 95% efficiency
- 16,384-processor GFMC for 14-neutron drop – 83% efficiency

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 ${}^9\text{Be}$ with SSCC v'_8
- 4,096 – 8,192-processor ${}^{10}\text{Be}$ with SSCC v'_8
- up to 4,800 processors: nuclei up to ${}^{10}\text{B}$ with new Illinois V_{ijk}

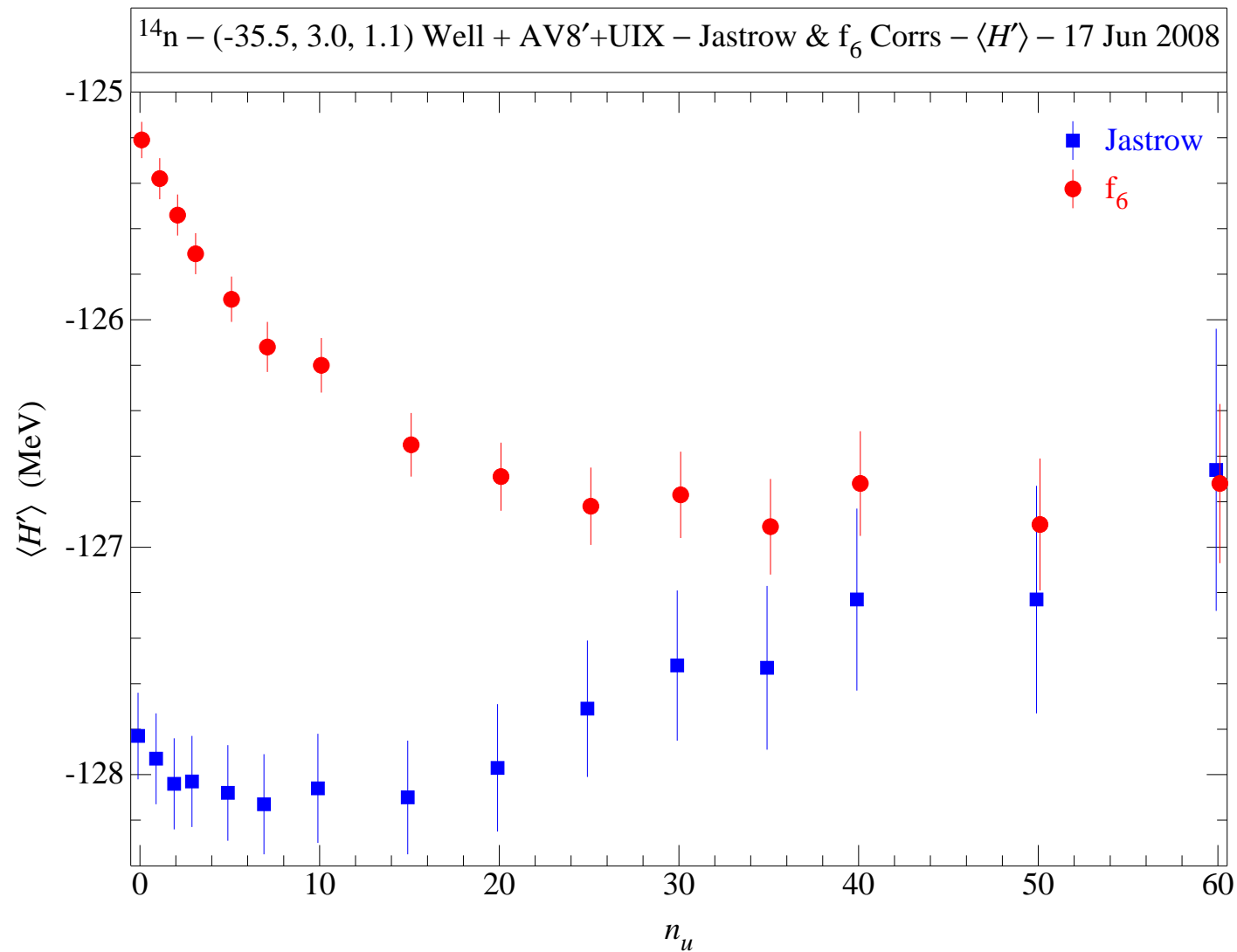
NEUTRON DROPS

- 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

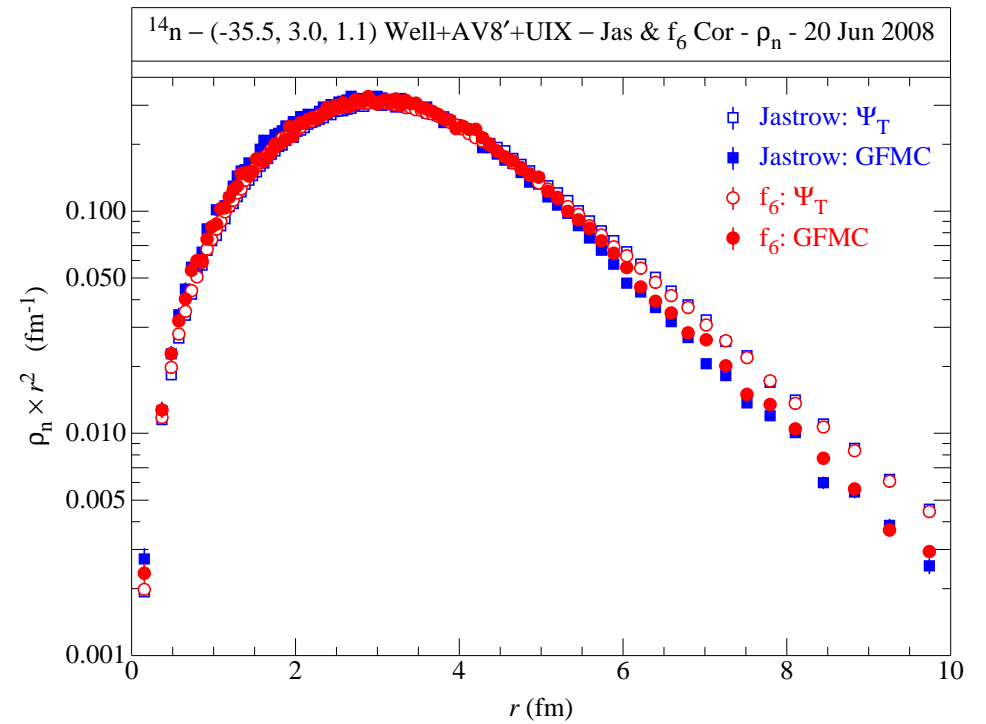
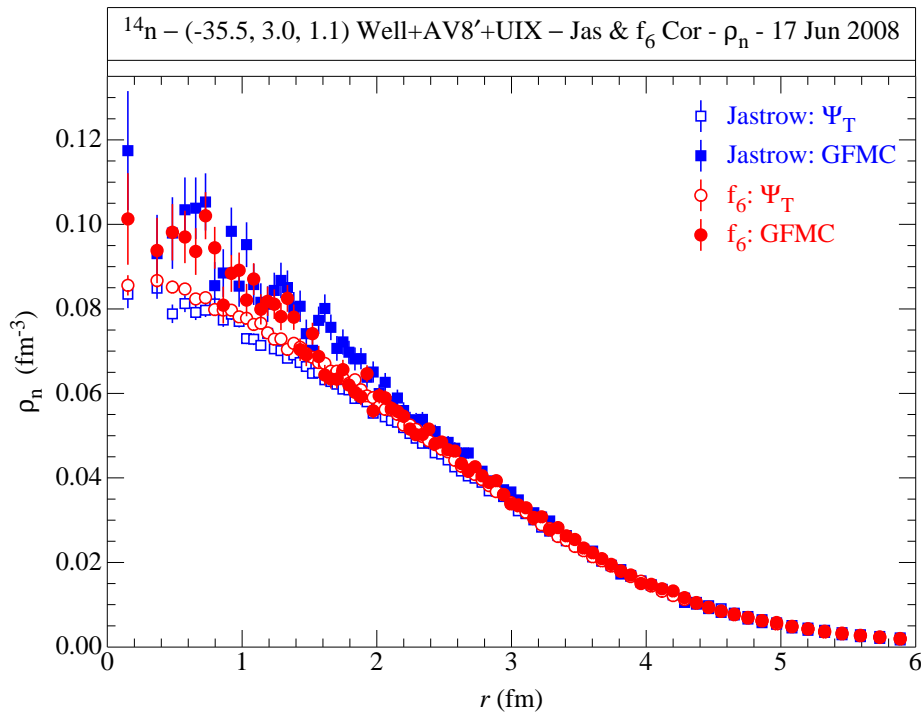


NEUTRON DROPS - GFMC CONSTRAINED-PATH CONVERGENCE

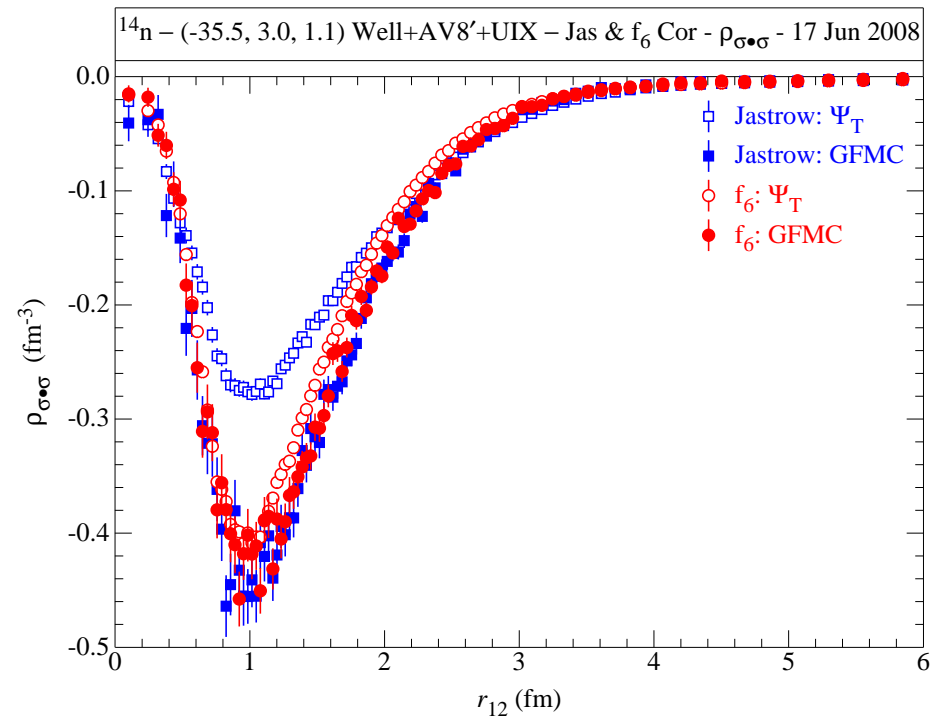
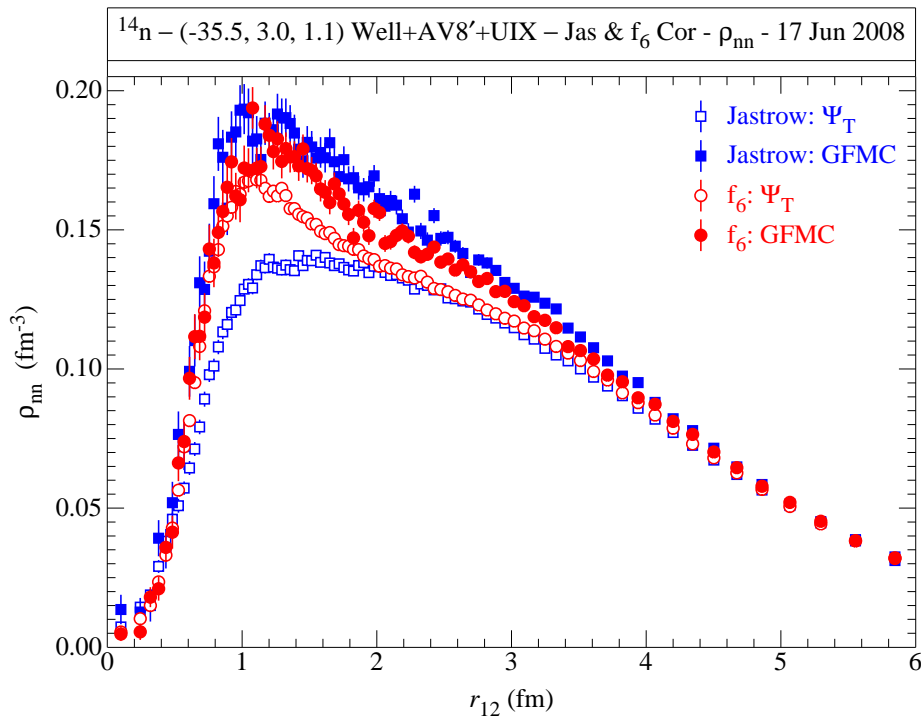
- We use a number of unconstrained GFMC steps before computing energies
- Usually 10–20 unconstrained steps are adequate
- ^8He and neutron drops require more.



NEUTRON DROPS – SINGLE-NEUTRON DENSITY DISTRIBUTIONS



TWO-NEUTRON PAIR AND $\sigma \cdot \sigma$ DENSITY DISTRIBUTIONS



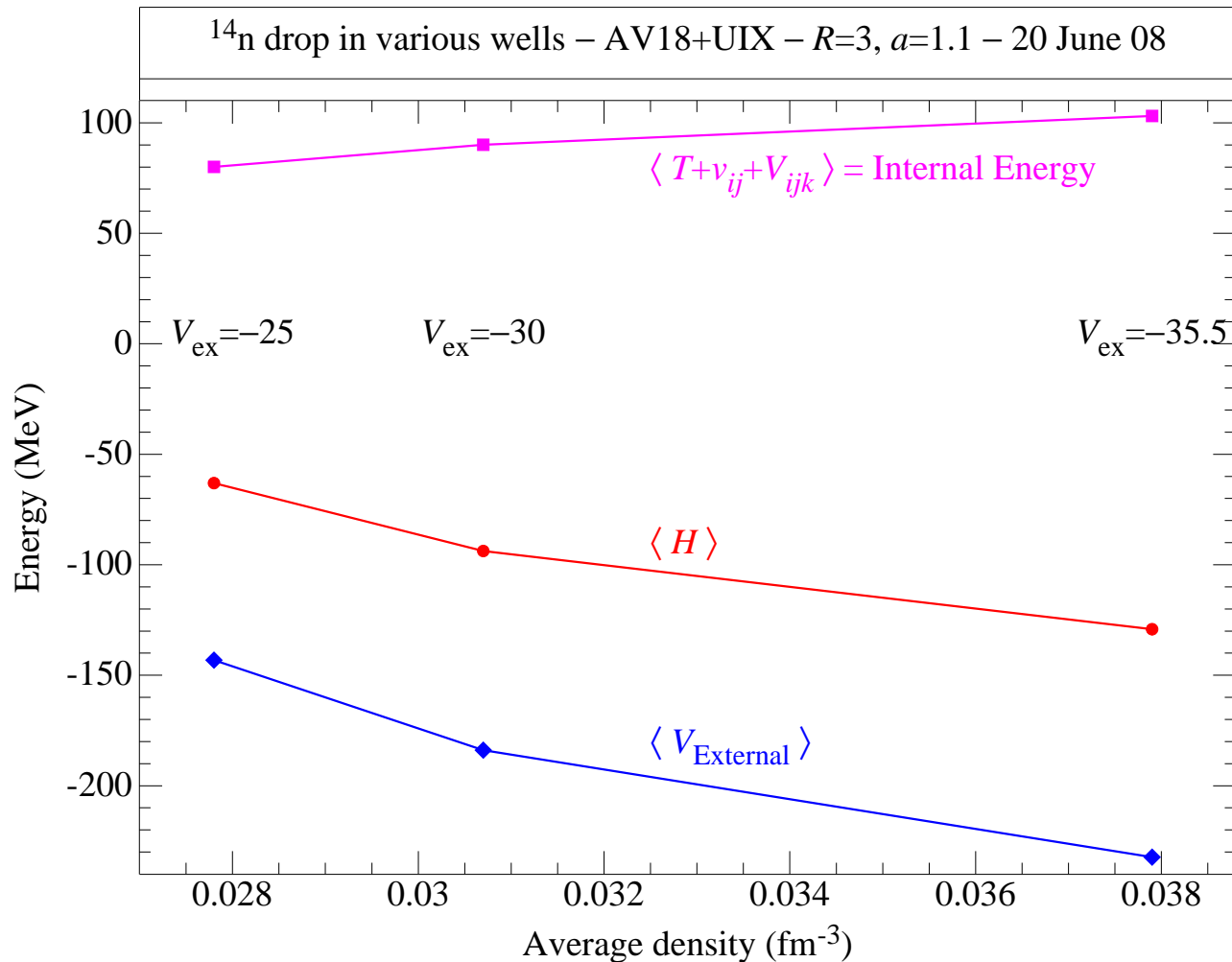
GFMC produces same final densities starting from very different Ψ_T densities

NEUTRON DROPS – DEPENDENCE ON EXTERNAL WELL DEPTH

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

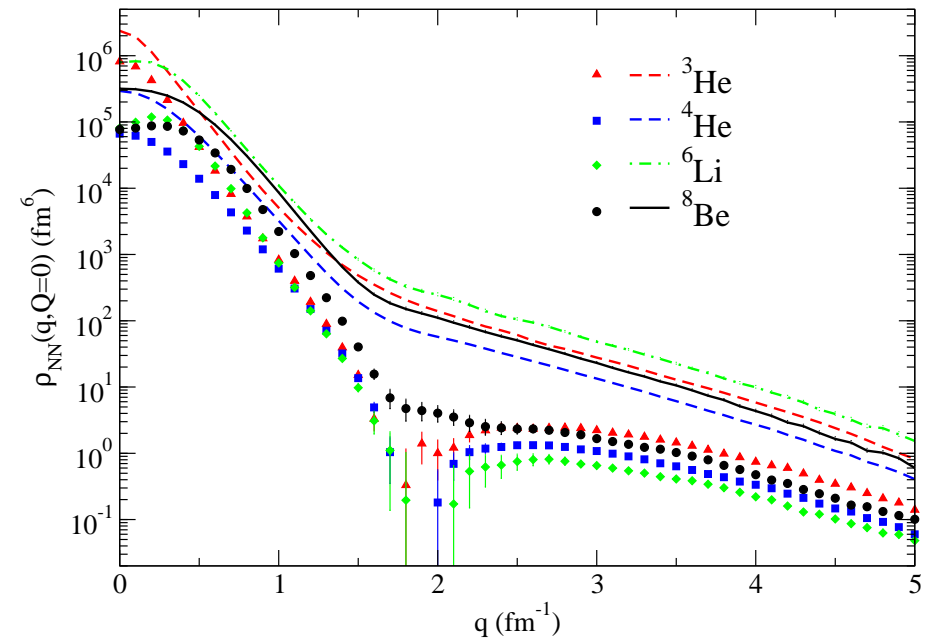
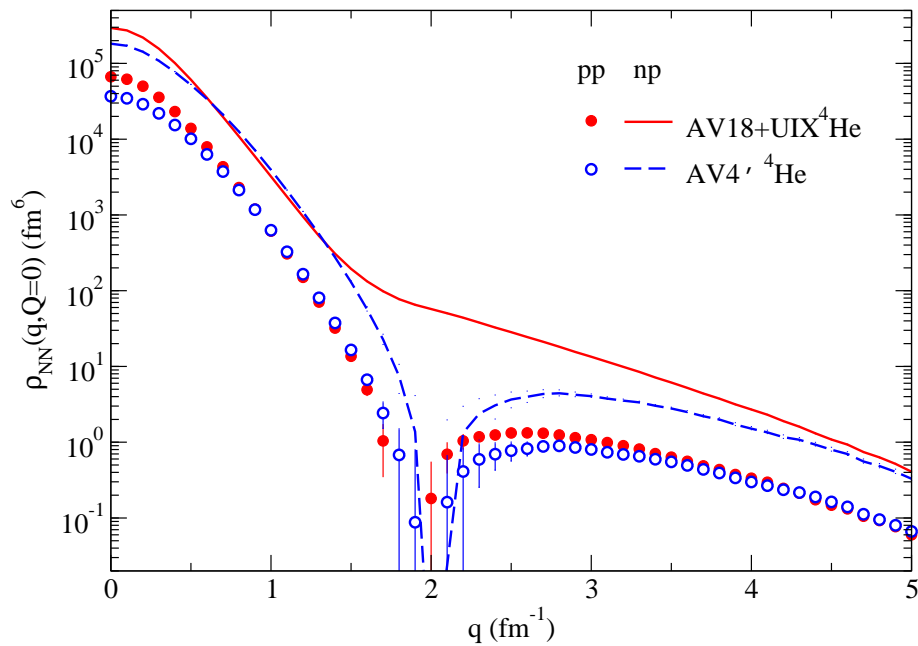
$R = 3.0$ fm; $a = 1.1$ fm; $V_{\text{ex}} = 25, 30, \& 35.5$ MeV

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



TWO-NUCLEON KNOCKOUT – $(e, e'pN)$

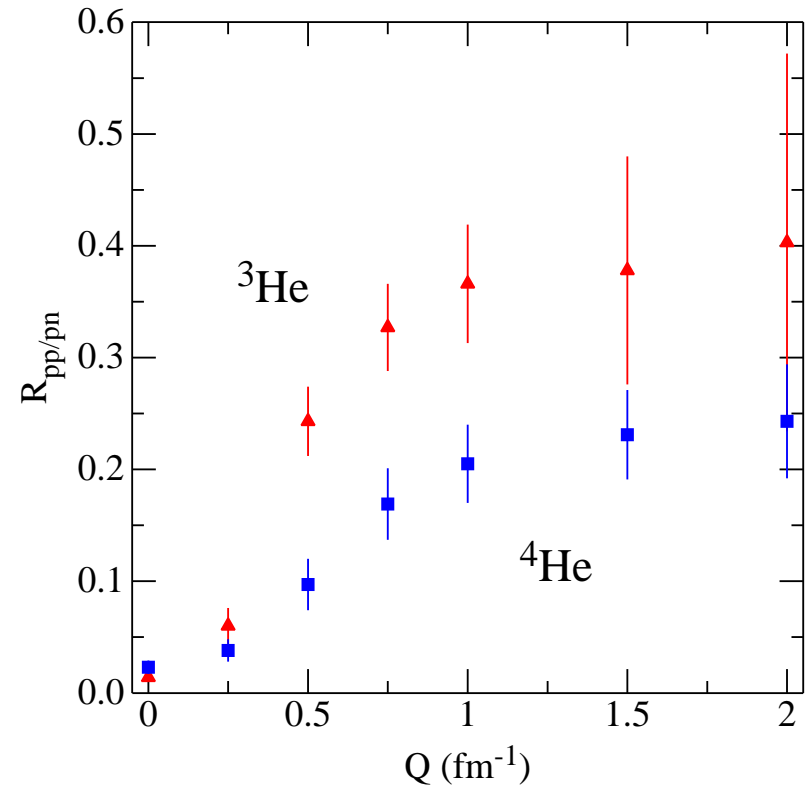
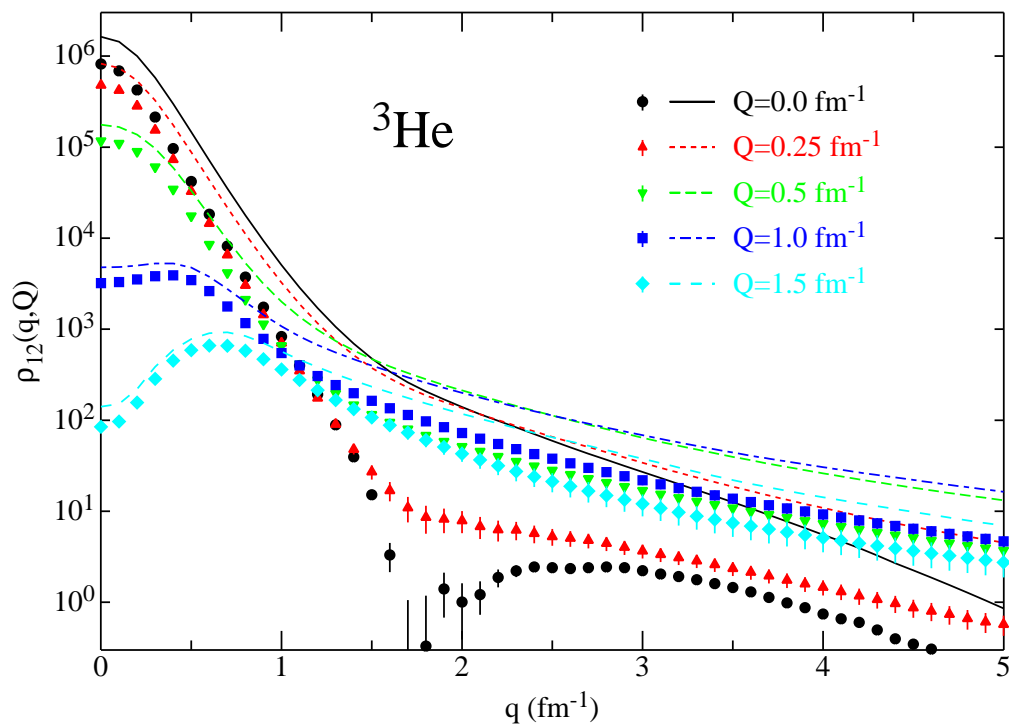
- Just published (Science) JLAB expt. for $^{12}\text{C}(e, e'pN)$
- Measured back to back pp and np pairs of equal $|p_i|$; $Q_{\text{tot}} = 0$
- Pairs with relative momentum $2\text{--}3 \text{ fm}^{-1}$ show $10\text{--}20 \times np$ enhancement (preliminary).



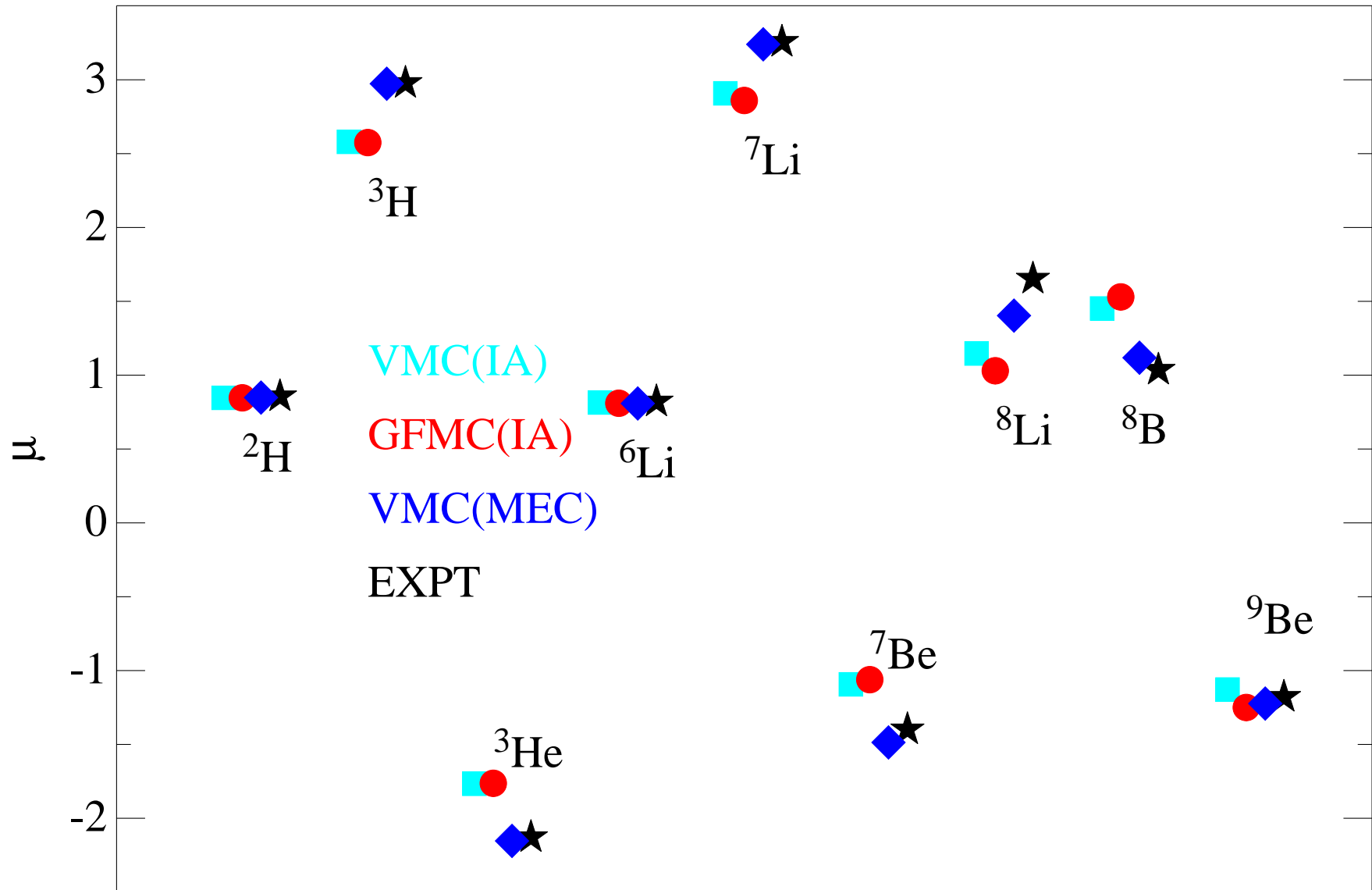
- VMC calculations for ^3He , ^4He , and ^8Be show this effect
- Effect disappears when tensor correlations are turned off
- Shows importance of tensor correlations to $> 3 \text{ fm}^{-1}$.

TWO-NUCLEON KNOCKOUT – $(e, e'pN)$

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



Magnetic Moments



No effective charges or effective nucleon magnetic moments!

M1, E2, F, GT transitions

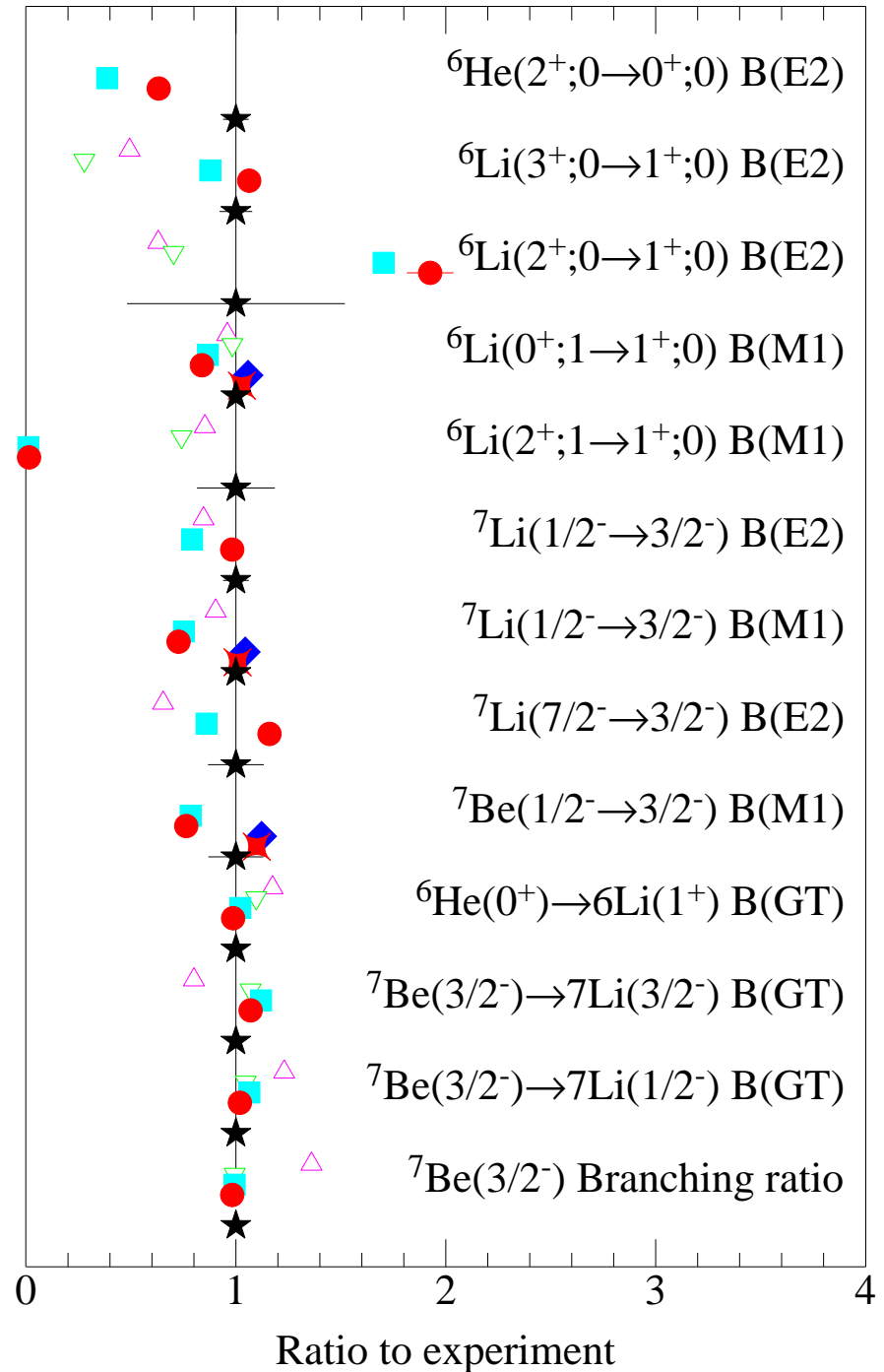
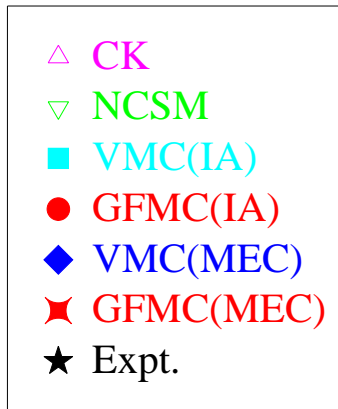
$$E2 = e \sum_k \frac{1}{2} [r_k^2 Y_2(\hat{r}_k)] (1 + \tau_{kz})$$

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

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

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: ${}^5,7\text{He}$, ${}^6\text{Li}(2^+)$, ${}^8\text{Be}(2^+,4^+)$, ...

– Will get widths of resonances

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

1987 – early 1990's:

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

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

Present:

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

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

NCSM and CC are also computing resonance states

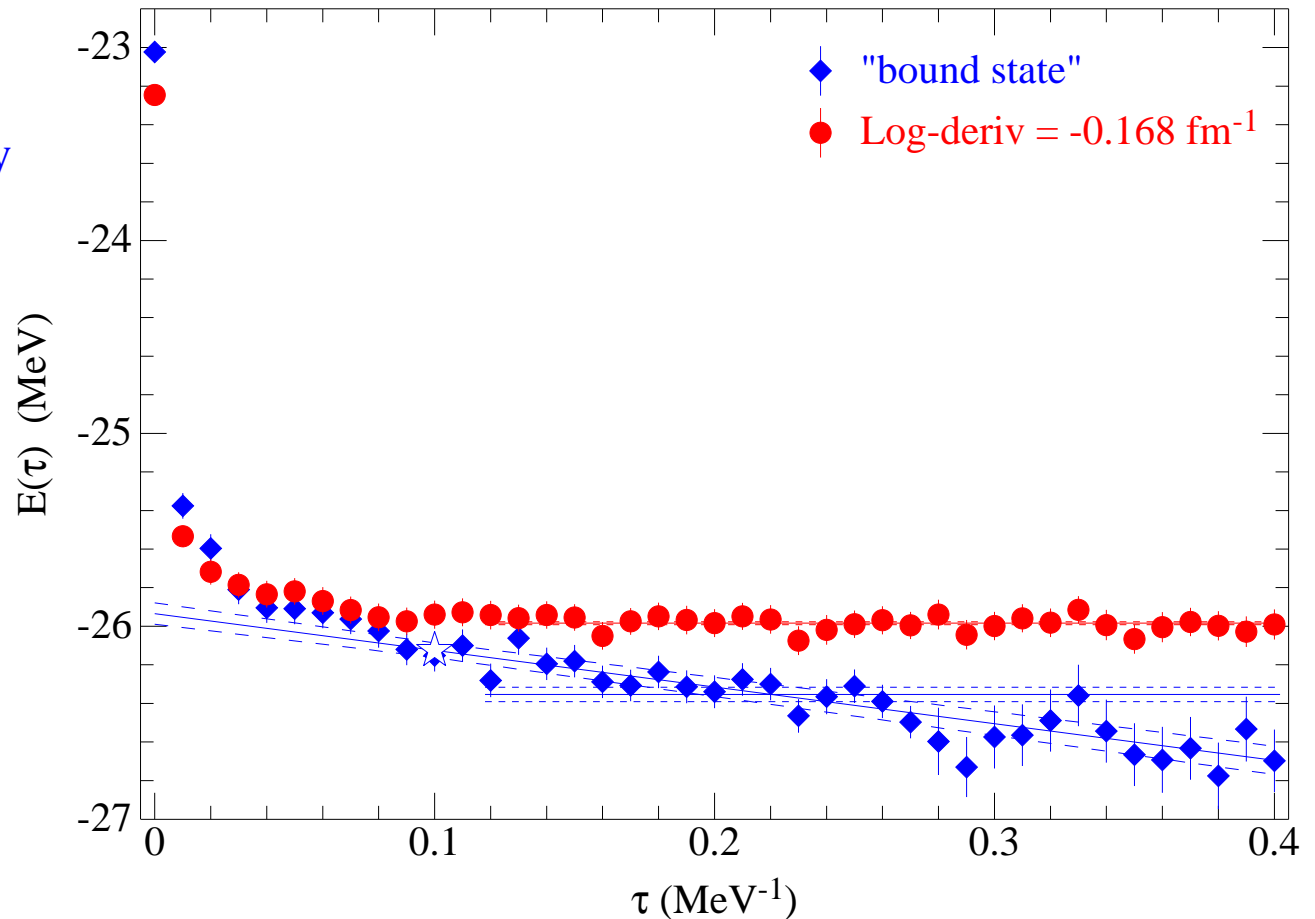
A benchmark comparison (${}^5\text{He}$ with SSCC v'_8 ?) would be useful

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

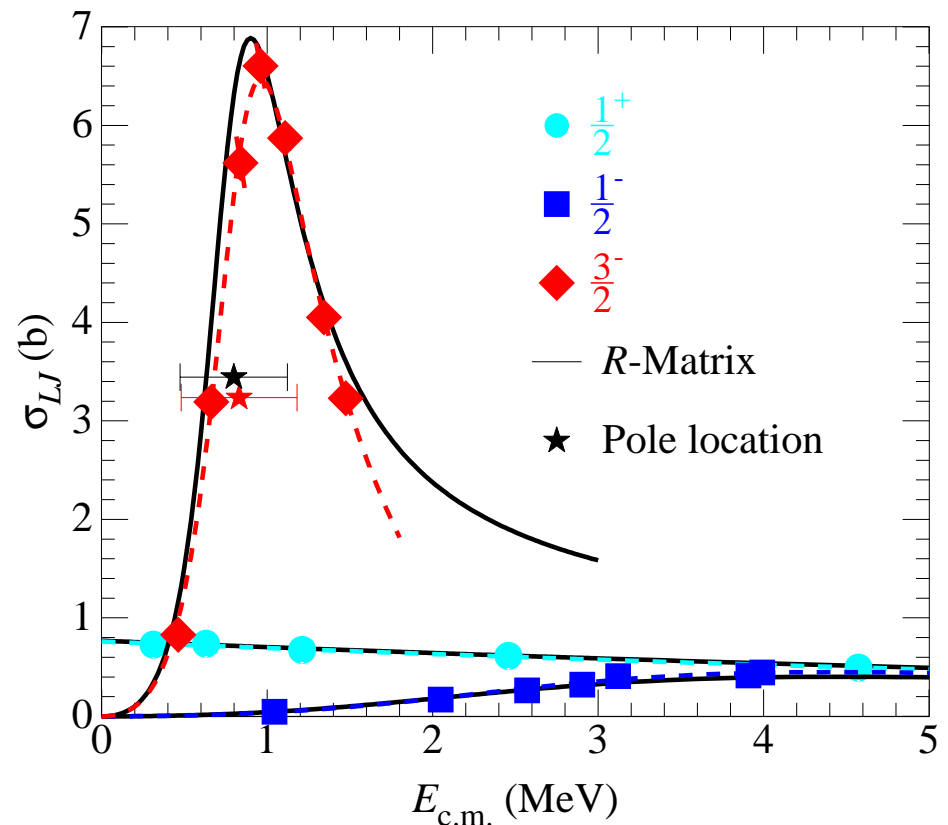
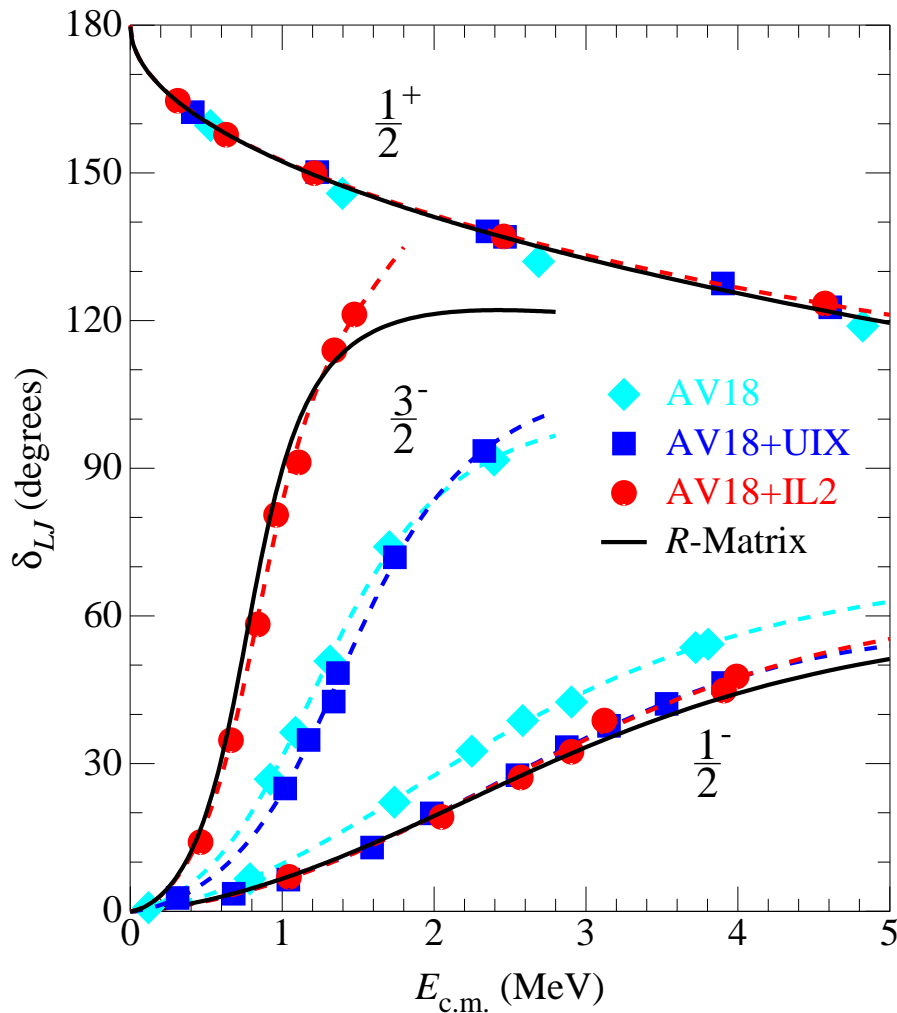
Example for ${}^5\text{He}(\frac{1}{2}^-)$

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



GFMC FOR ${}^5\text{He}$ AS $n+{}^4\text{He}$ 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 ${}^5\text{He}(\frac{3}{2}^-)$; overbinds ${}^5\text{He}(\frac{1}{2}^-)$
- AV18+IL2 was not fit to ${}^5\text{He}$, reproduces locations and widths of both P -wave resonances
 - Spin-orbit splitting well reproduced by AV18+IL2



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 ${}^8\text{He}$ 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?