GFMC Calculations

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Work with

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- Making GFMC work on 65,536 processors
- GFMC ^{12}C results
- Benchmark results for NN potentials
- Neutron drops
- GFMC for scattering
- Deliverables and plans

Argonne NATIONAL LABORATORY

Physics Division

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Making GFMC work on 65,536 processors

- Automatic Dynamic Load Balancing for sharing work between nodes
  - A general-purpose library to help application codes dynamically share work
  - Being developed by Rusty Lusk and Ralph Butler
  - Working very well on 8,192 nodes
  - Still trying to get good efficiency on 16,384 nodes
  - Rusty will talk about its structure

- OpenMP for work on one node
  - Individual nodes have multiple cores sharing a common memory (4 cores on BG/P)
  - Each core could be a separate MPI “node” but then each gets only 1/4 of memory
    This is too small on BG/P (512 Mbytes) for ^{12}C
  - OpenMP allows one copy of the Fortran program to use all 4 cores – (2 Gbyte available)

CHANGES FOR OPENMP

Generally these were minor

- Need to identify loops that can be run in parallel on the 4 cores
- Insert directive to tell OpenMP to run loop in parallel

```
!$OMP PARALLEL DO  PRIVATE( l, rcm, ... )
...
!$OMP END PARALLEL DO
```

- PRIVATE(l, rcm, ...) states that separate copies of these variables must be maintained for each thread
- Sometimes more extensive changes are needed

Original source

```
M = 0
do i = 1, ...
   do j = 1, function(i)
      M = M + 1
      x(M) = ...
   enddo
enddo
```

Modified for OMP

```
      M = 0
      do i = 1, ...
         MBASE(i) = M
         do j = 1, function(i)
            M = M + 1
         enddo
      enddo
...
!$OMP PARALLEL DO  PRIVATE( i, M, j, ...
      do i = 1, ...
         M = MBASE(i)
         do j = 1, function(i)
            M = M + 1
         enddo
      enddo
!$OMP END PARALLEL DO
```

Results so far

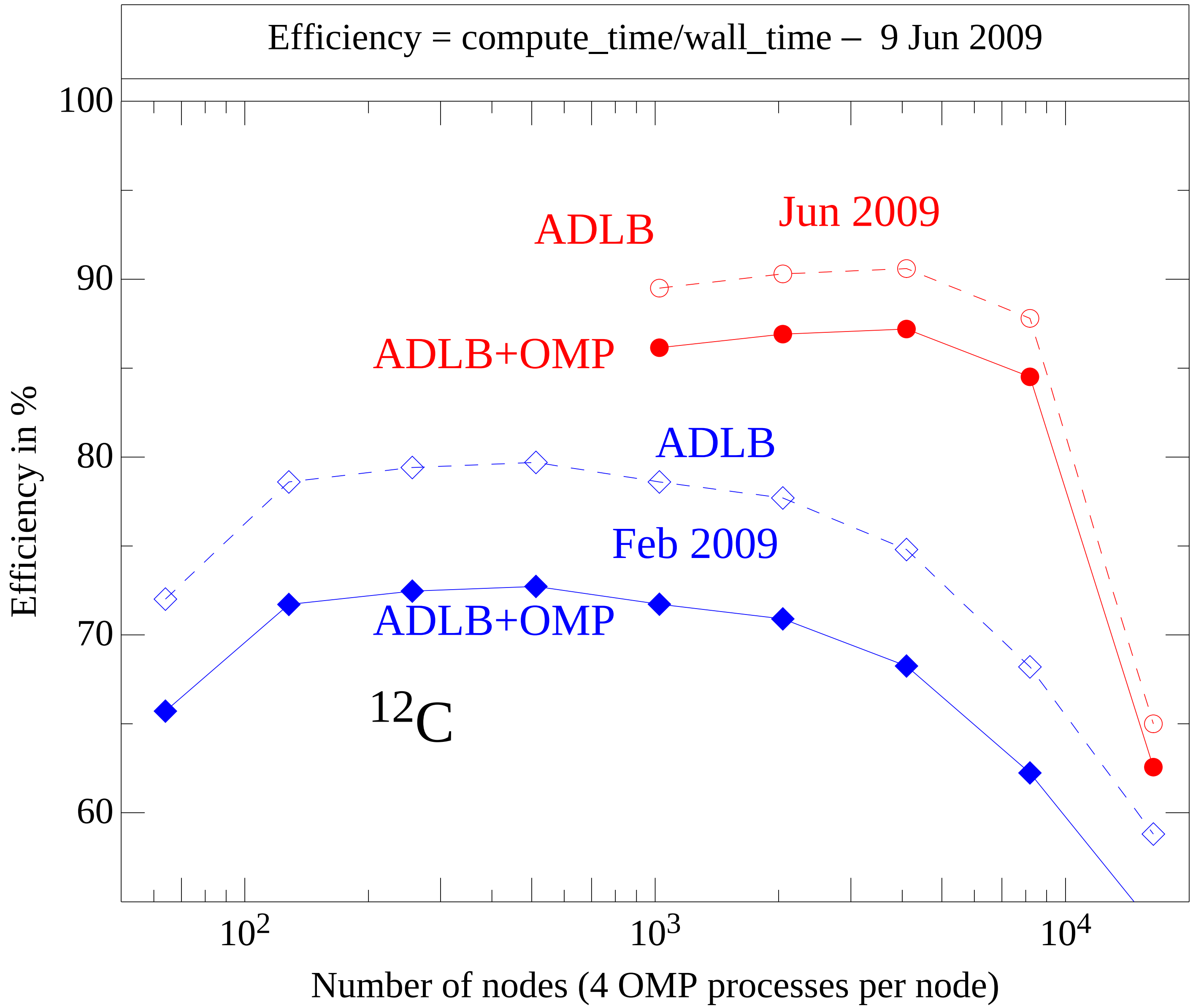
OpenMP is very successful, but the BG/P speeds are disappointing

^{12}C Speeds for two key subroutines

Subroutine	MFLOPS		speed up
	1 thread	4 threads	
Wave function	239	1022	4.0
V_{ijk}	319	1233	3.9

RESULTS SO FAR

ADLB performance is very good up to 8192 nodes (32,768 cores)



^{12}C RESULTS

In Dec. 2008 & Jan. 2009, the first ADLB+GFMC calculation of the ^{12}C(gs) was made.

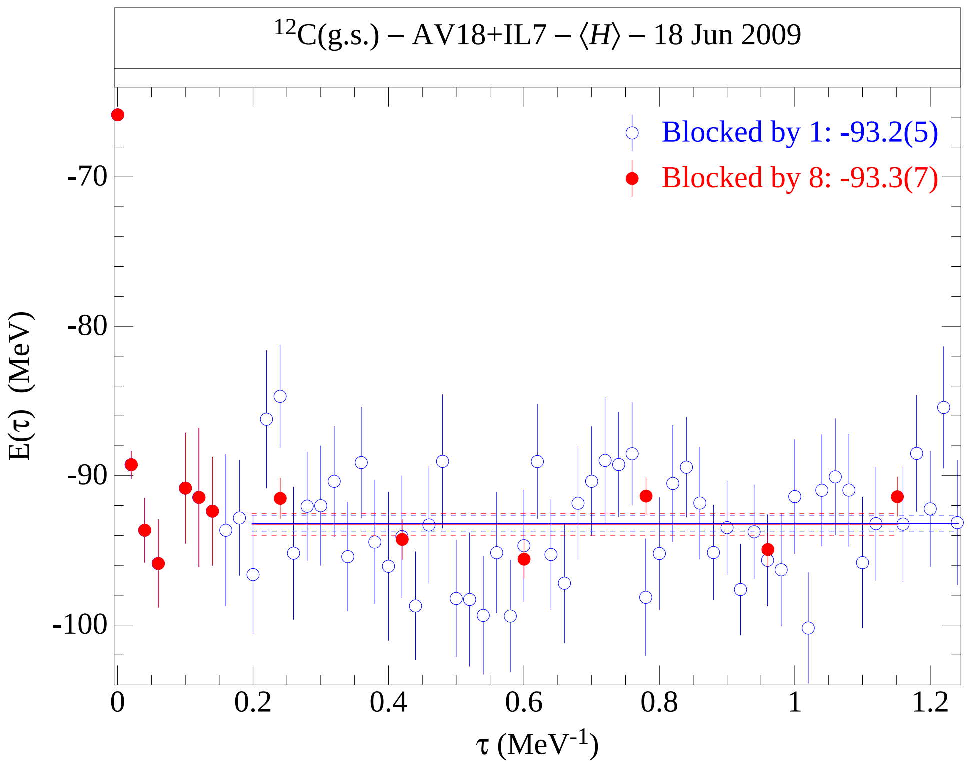
- AV18+IL7 Hamiltonian
- Improved (and slower) Ψ_T than in previous calculation
- GFMC result changed only a little
- 16,000 configurations propagated to $\tau = 1.24$ MeV^{-1} (2480 steps)
- 40 unconstrained time steps used before energy evaluations
- Used 8,192 nodes (32,768 cores) of BG/P
- 14 runs for total of 93 hours (first few very short)
- Speed of Ψ_T calculation significantly improved since
- Convergence is very good and shows that
  - smaller maximum τ can be used
  - fewer unconstrained time steps, and hence fewer configurations, can be used

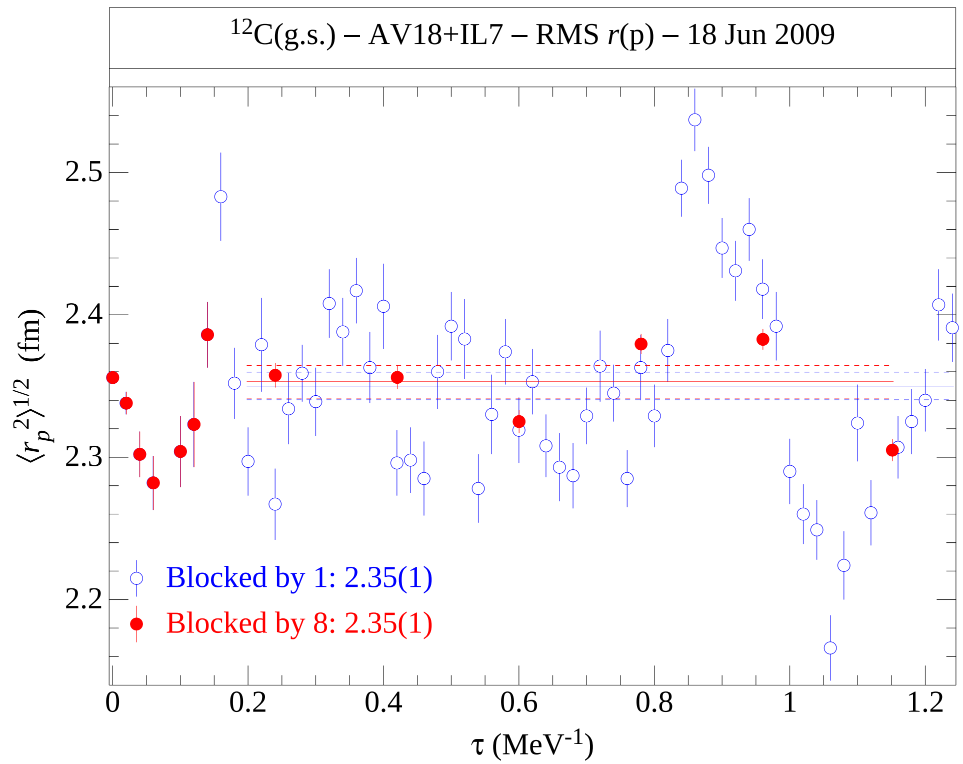
An ADLB+GFMC calculation using the benchmark modified SSCC v_8' NN potential was also made; this is much faster

- No L^2 terms in NN potential
- No NNN potential

^{12}C Convergence Studies

As a function of imaginary time (τ)

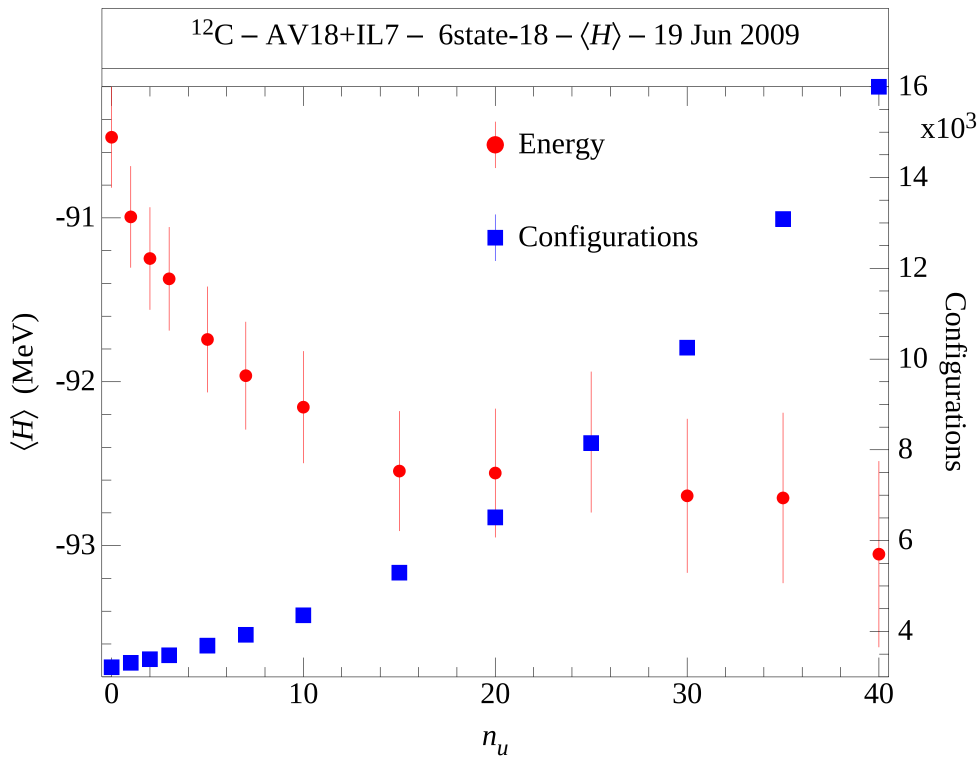


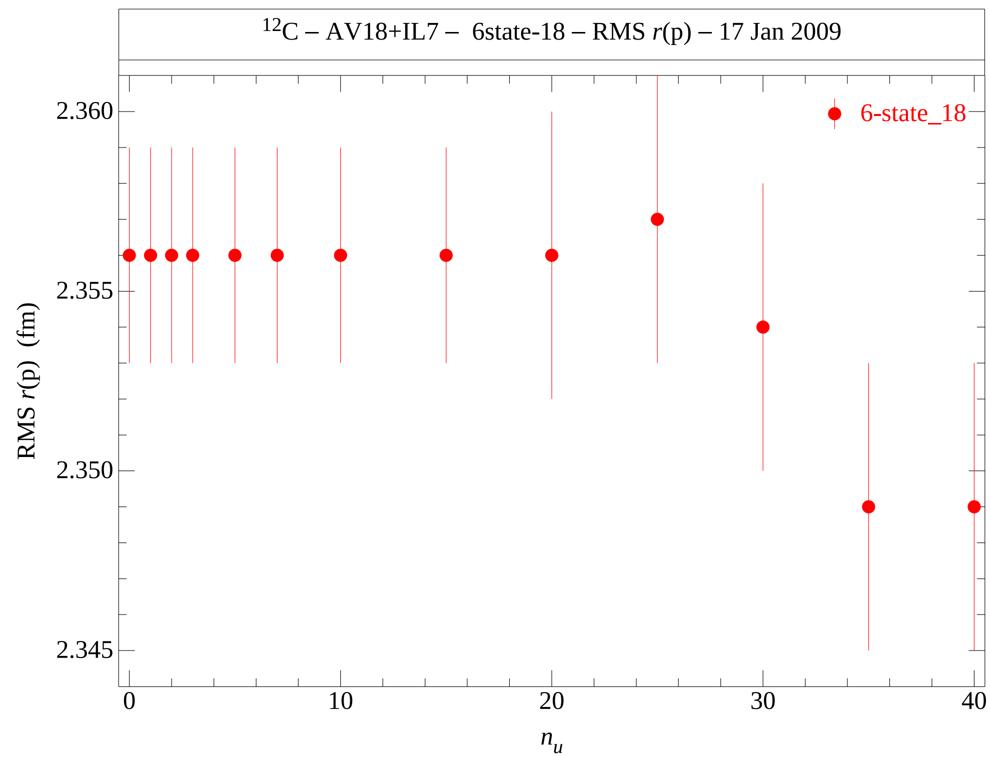


Modified SSCC v_8' convergence with τ is similar

^{12}C CONVERGENCE STUDIES

As a function of number of unconstrained steps (n_u)





$n_u = 20$ is converged, needs only half as many configurations

Modified SSCC v_8' convergence with n_u is better

^{12}C RESULTS – ENERGIES & RADII

	Energy			RMS radius		
	VMC	GFMC	Expt.	VMC	GFMC	Expt.
AV18+IL7	–65.8(2)	–93.2(6)	–92.16	2.36	2.35	2.33
Modified SSCC v_8'	–74.9(2)	–94.0(5)		2.21	2.24	

Modified SSCC v_8' gives reasonable energies at least up to A = 12

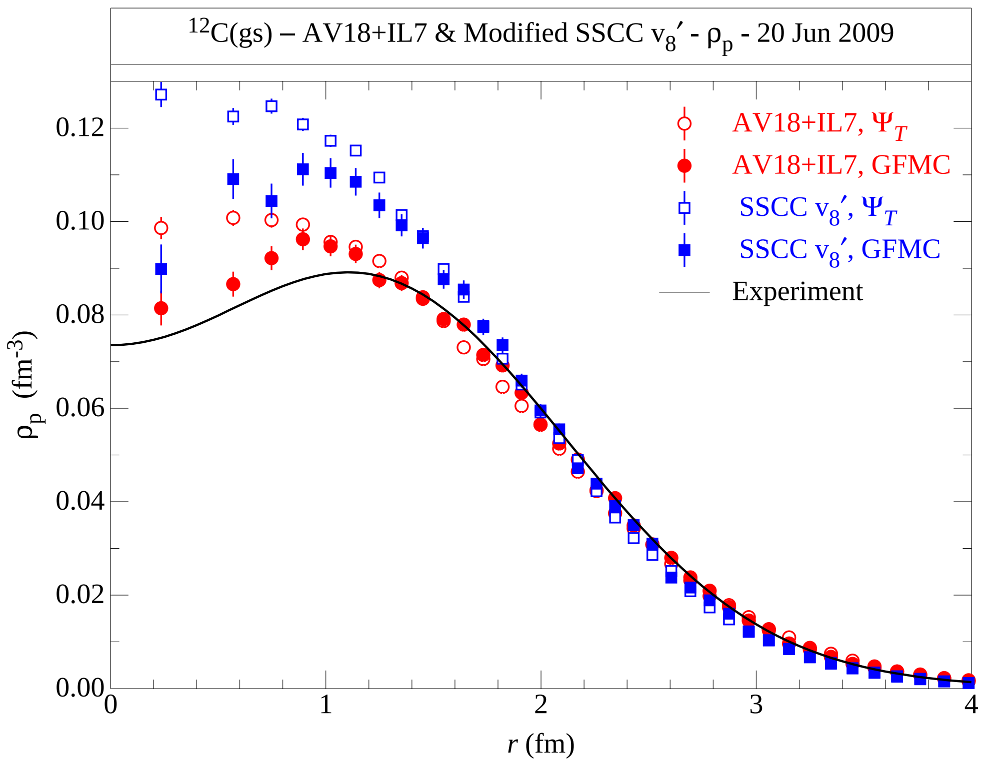
Remember that it does not accurately reproduce NN P-phase shifts

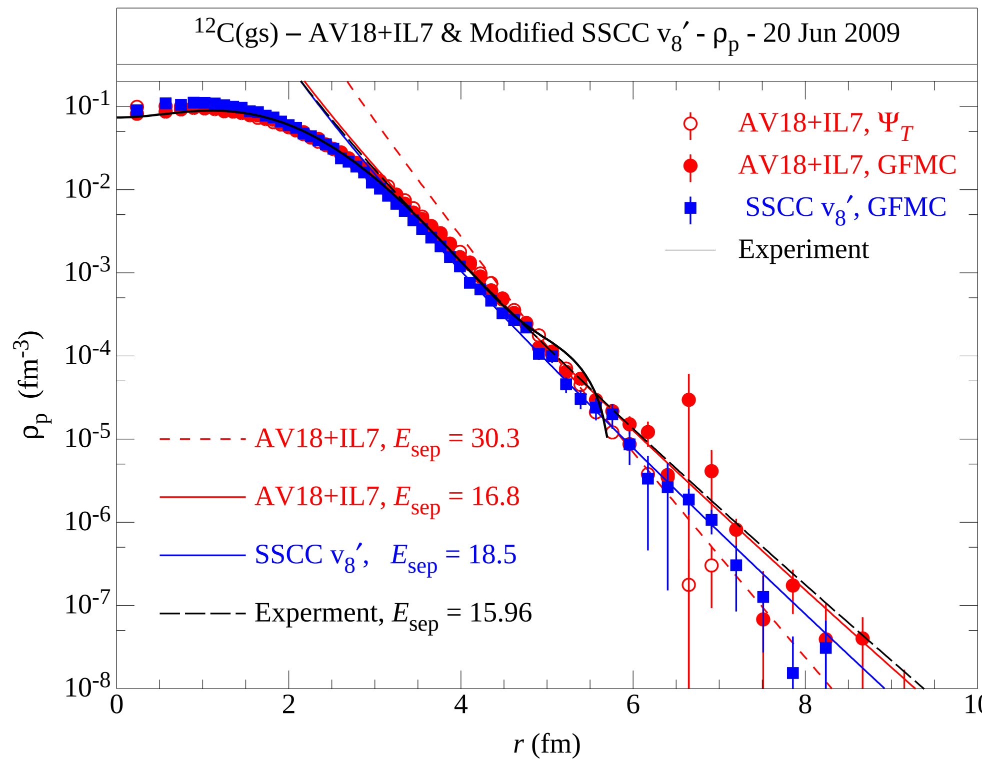
	K.E.	v_{1-4}'	$v_{t,t\tau}'$	$V_{ijk'}$
AV18+IL7	427.	–216.	–282.	–23.
Modified SSCC v_8'	350.	–220.	–223.	0.

K.E. of SSCC v_8' is not so small, despite much smaller central repulsion

Could be associated with the still large $v_{t,t\tau}'$

^{12}C RESULTS – ONE-BODY DENSITY





The Ψ_T density is significantly improved by GFMC

- Central dip is generated
- AV18+IL7 tail falls at rate dictated by $E_{\rm sep} = E(^{11}{\rm B}) - E(^{12}{\rm C})$ instead of twice as fast
- SSCC v_8' $E_{\rm sep}$ is also good

Benchmarks Results for Modified SSCC v_8'

	SSCC v_8'	Experiment
^{4}He(0^+)	$-25.36(1)$	$-28.30(0)$
^{6}He(0^+)	$-26.48(1)$	$-29.27(0)$
^{6}Li(1^+)	$-28.98(2)$	$-31.99(0)$
^{6}Li(3^+)	$-26.22(2)$	$-29.800(2)$
^{7}Li($\frac{3}{2}^-$)	$-35.93(4)$	$-39.24(0)$
^{7}Li($\frac{1}{2}^-$)	$-35.78(5)$	$-38.760(0)$
^{8}He(0^+)	$-28.60(3)$	$-31.41(1)$
^{9}Be($\frac{3}{2}^-$)	$-53.49(13)$	$-58.16(0)$
^{10}Be(0^+)	$-61.34(16)$	$-64.98(0)$
^{10}Be(2^+)	$-58.85(22)$	$-61.61(0)$
^{10}Be(2^+, 2^{nd})	$-57.13(17)$	$-59.02(0)$
^{12}C(0^+)	$-94.00(47)$	$-92.16(0)$

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

NEUTRON DROPS

- Last year we computed a series of drops confined in Woods-Saxon external wells
- A few small improvements to these results were made this year
- Most effort has been on drops confined in oscillator wells, $\hbar\omega = 5\&10$ MeV
- Comparisons with AFDMC results obtained by Stefano Gandolfi are generally good
  - Energies agree to $\leq 1\%$
  - For $\hbar\omega = 5$ MeV external well agreement gets worse for larger drops; may be due to insufficient pairing in AFDMC.

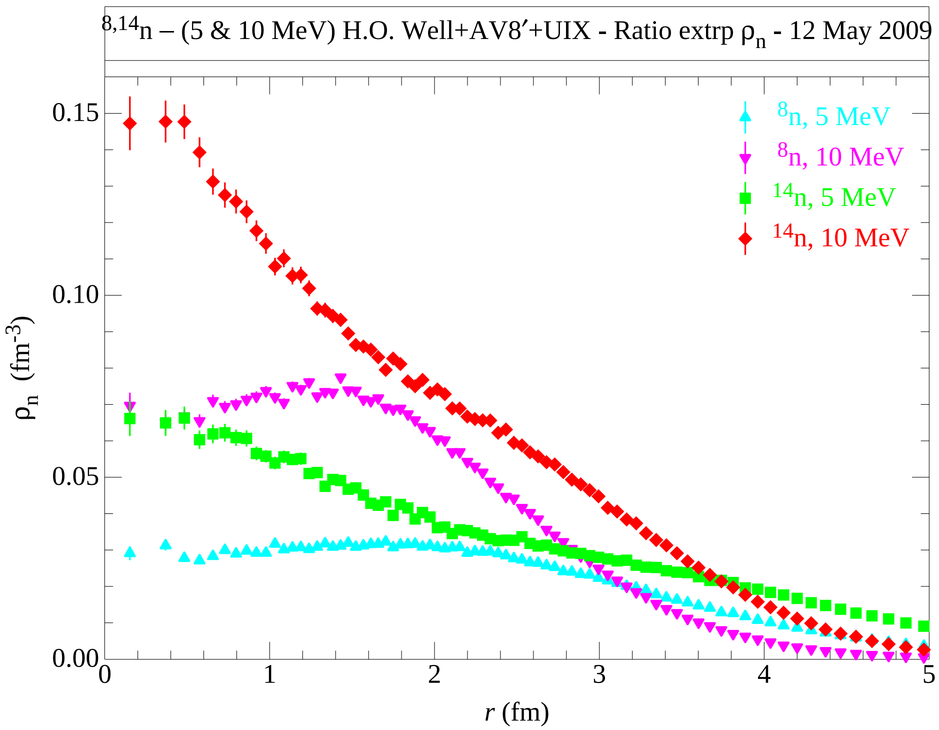
Neutron Drops – Energies

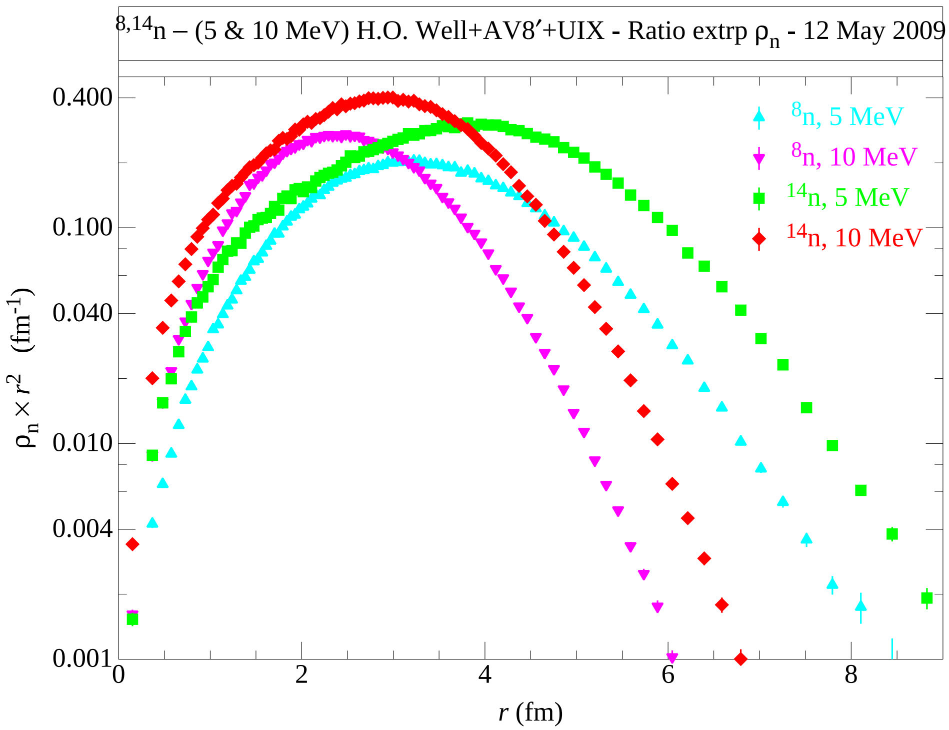
	Energy	Kinetic	V_{Extern}	v_{ij}	V_{ijk}	RMS r
$\hbar\omega = 5$ MeV external well + AV18 + UIX						
^{8}n(0^+)	67.09(2)	76.2(4)	32.00(3)	−45.79(37)	0.26(1)	3.642(2)
^{9}n($\frac{1}{2}^+$)	80.95(4)	86.2(2)	39.06(3)	−53.64(38)	0.43(1)	3.793(2)
^{9}n($\frac{5}{2}^+$)	81.24(4)	86.2(2)	38.94(3)	−52.67(35)	0.36(1)	3.787(2)
^{10}n(0^+)	92.22(8)	102.0(4)	45.44(5)	−65.41(61)	0.49(2)	3.881(2)
^{12}n(0^+)	118.26(15)	128.0(5)	58.68(7)	−82.26(80)	0.79(4)	4.026(2)
^{13}n($\frac{1}{2}^+$)	130.88(13)	141.(1)	65.31(12)	−90.74(89)	0.75(4)	4.081(4)
^{13}n($\frac{5}{2}^+$)	131.63(13)	138.(1)	65.65(13)	−87.55(89)	0.90(4)	4.092(4)
^{14}n(0^+)	142.33(16)	157.(1)	71.07(12)	−102.85(98)	1.08(4)	4.102(4)
$\hbar\omega = 10$ MeV external well + AV18 + UIX						
^{8}n(0^+)	136.04(5)	136.0(5)	71.41(9)	−76.93(47)	1.53(3)	2.720(2)
^{9}n($\frac{1}{2}^+$)	163.84(9)	154.0(4)	85.8(1)	−90.75(57)	2.34(4)	2.811(2)
^{9}n($\frac{5}{2}^+$)	163.35(8)	154.0(3)	84.92(10)	−89.66(55)	1.93(3)	2.797(2)
^{12}n(0^+)	242.12(58)	224(1)	131.69(32)	−138.24(2.10)	4.03(21)	3.016(4)
^{13}n($\frac{1}{2}^+$)	268.44(54)	248(2)	146.83(57)	−153.4(2.2)	4.11(22)	3.06(1)
^{13}n($\frac{5}{2}^+$)	267.94(60)	249(2)	147.18(53)	−156.34(2.26)	4.32(24)	3.063(6)
^{14}n(0^+)	292.51(22)	275(1)	159.97(42)	−175.1(1.4)	5.28(15)	3.077(4)

NEUTRON DROPS – SINGLE-NEUTRON DENSITY DISTRIBUTIONS

Oscillator well + AV18 + UIX

$\hbar\omega = 5\&10$ MeV





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

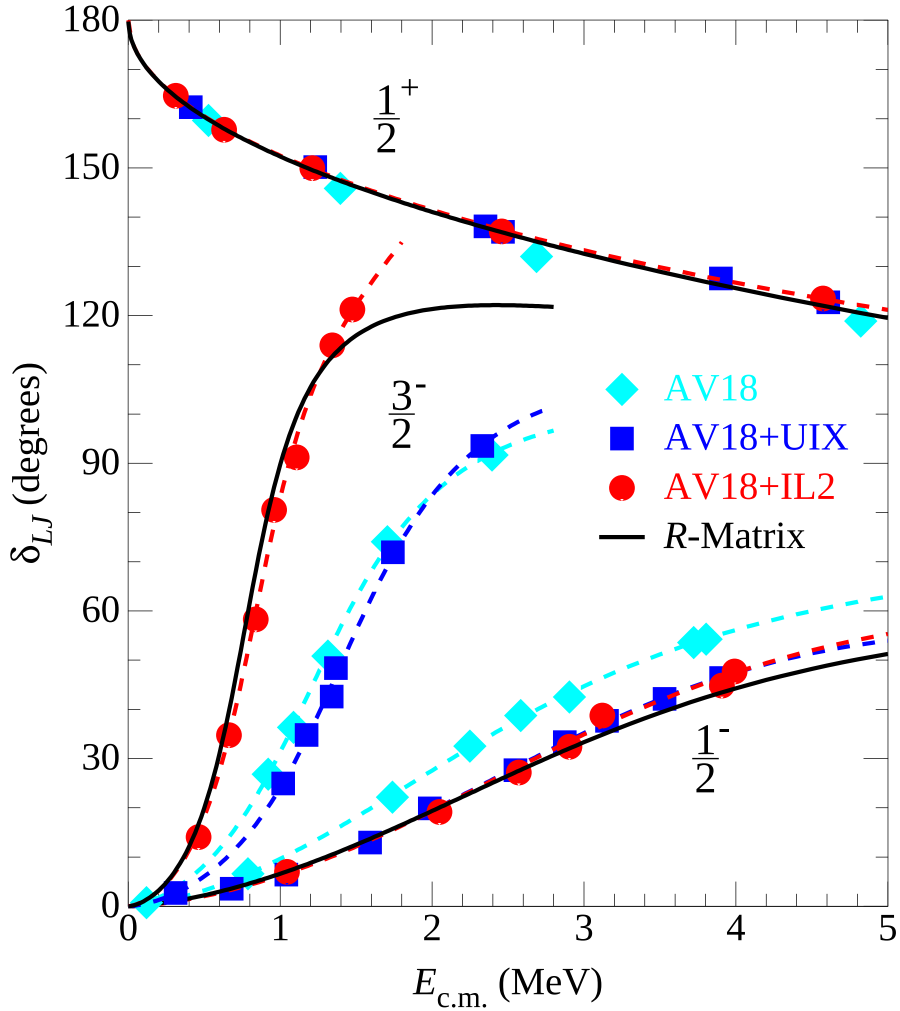
– Ken Nollett has modified Argonne GFMC program for scattering and done ^{5}He

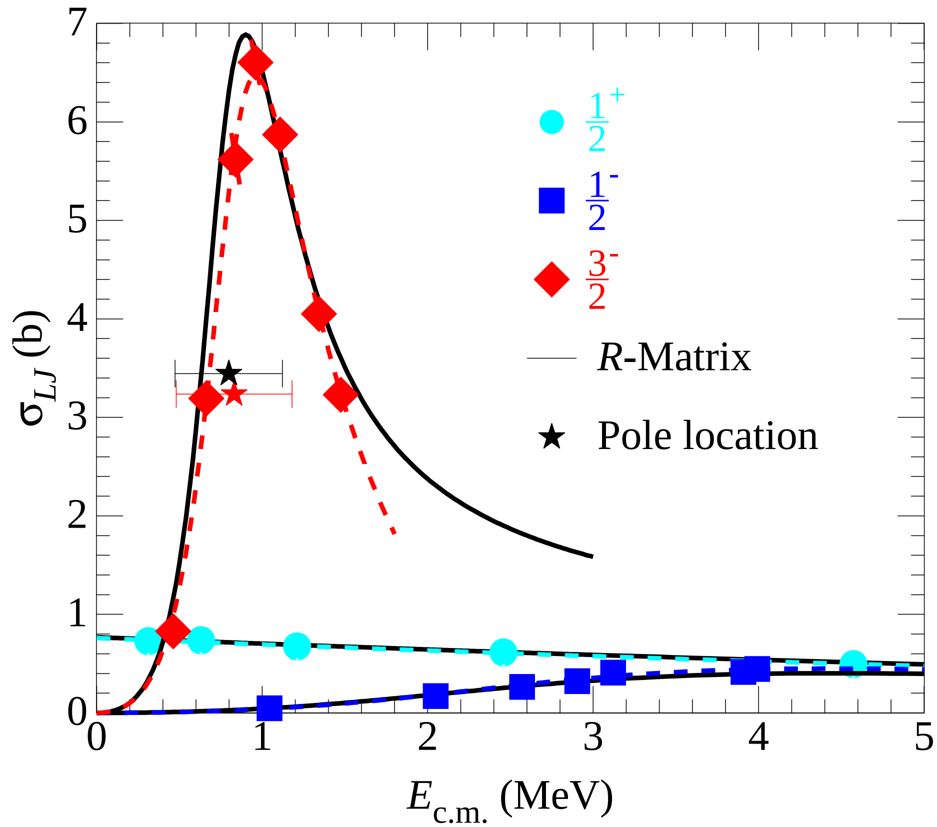
NCSM and CC are also computing resonance states

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

GFMC for ^{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

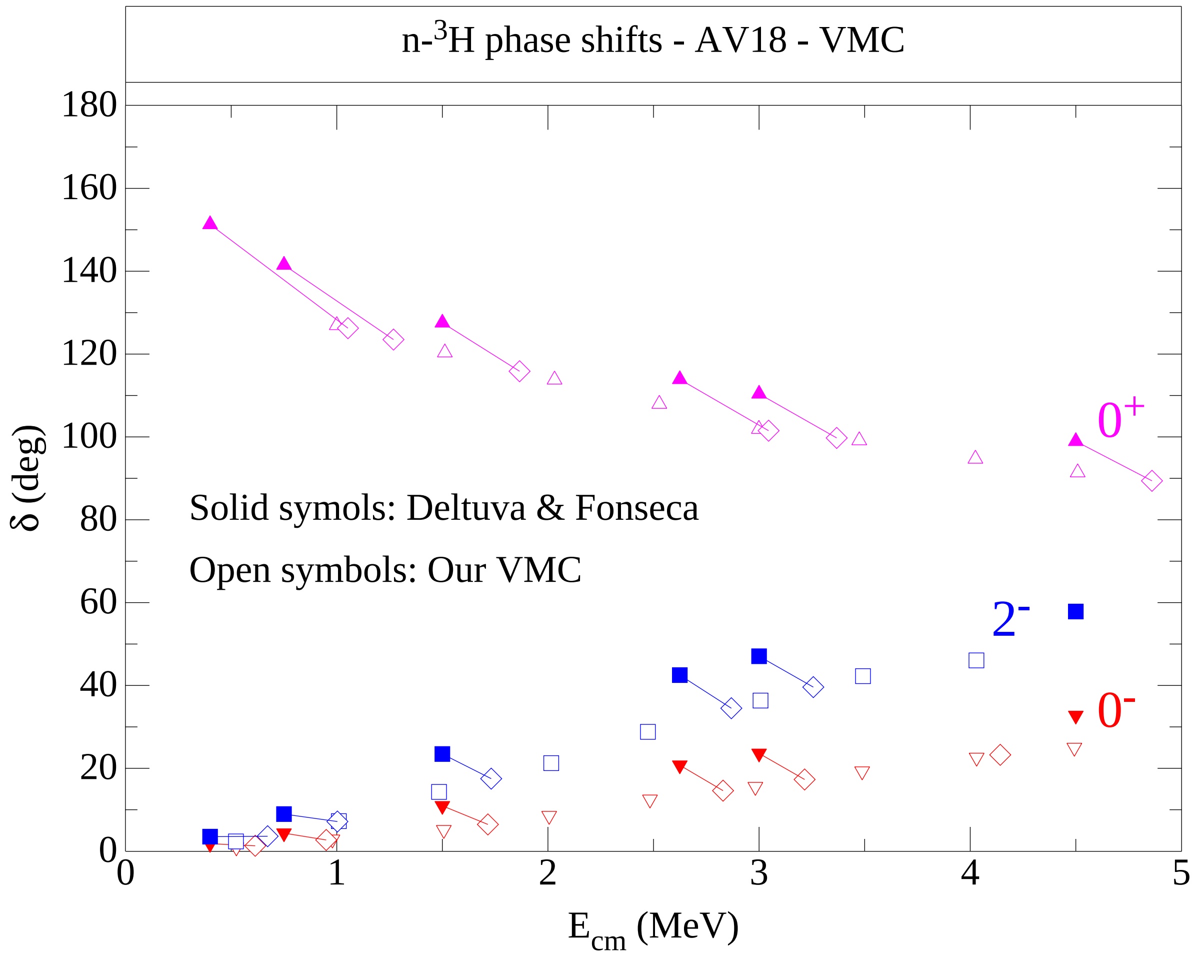




K.M. Nollett, S.C. Pieper, R.B. Wiringa, J. Carlson, G. M. Hale, Phys. Rev. Lett. **99**, 022502 (2007)

^{4}H as n–^{3}H Scattering

- We are starting to do n–^{3}H and p–^{3}He scattering
- Comparison with "exact" results of Deltuva & Fonseca will be a good test of our results
- So far have VMC results for several n–^{3}H partial waves



Status of Deliverables for this Year

- Ab-initio calculations for neutron drops and asymmetric nuclear matter, including the response to external potentials

  – Done for spherical drops in several harmonic oscillator wells

- Calculate ab initio one-body densities for spherical and deformed nuclei and use them to inform DFT

  – Done: Densities of spherical nuclei

- Asynchronous Dynamic Load-Balancing improvements (microparallelization, debugging) for ^{12}C in GFMC

  – OpenMP fully implemented, much progress on ADLB

  – production AV18+IL7 ^{12}C calculation done on 32,768 processors

  – Benchmark SSCC v_8' also done for ^{12}C

- Investigate reactions in light nuclei using ab initio methods: NCSM with RGM, and GFMC. Benchmark n–^{7}Li, n–^{8}He, and move towards nuclear projectiles

  – n–^{3}H scattering being done in VMC

Following should have been in the list

- Improve ^{12}C VMC wave function

  – Structure of Ψ_T significantly improved since full GFMC calculation above. Still in progress

PLANS

Remainder of this year

- Continue ADLB work with aim of good efficiency on 65,536 processors
  – Non synchronous control of population growth or decay (presently uses a barrier)
  – Not allowing too great a dispersion in time steps being processed
- Further improvements to ^{12}C Ψ_T
  – $J = 0^+$ basis states that allow Hoyle state to be represented
  – More than just one $J = 2^+$ basis state
- Deformed neutron-drop calculations if desired
- More ^{12}C(gs) calculations using ADLB version of GFMC (Benchmark NN potentials?)
- GFMC nucleon-nucleus scattering and comparison with other methods

Next year: Not all of the following will be possible in one year!

- Continuing ADLB work in GFMC – finer-grain parallelization for BG/Q
- Many ^{12}C calculations
  – Full H for several states (Hoyle state?)
  – Transitions and transition densities
- VMC (GFMC?) computation of density matrix if interesting
- 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

Year 5: Some of these could be in year 4 with and some year 4 ones in year 5

- More changes of GFMC/ADLB for exascale class computers (e.g. BG/Q)
- More ^{12}C calculations, specifically Hoyle state.
- other A = 11,12 nuclei
- $A > 12$ nuclei?
- ^{11}Li and densities in ^{9}Li-n-n space

ADDITIONAL MATERIAL FROM PREVIOUS TALKS

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.

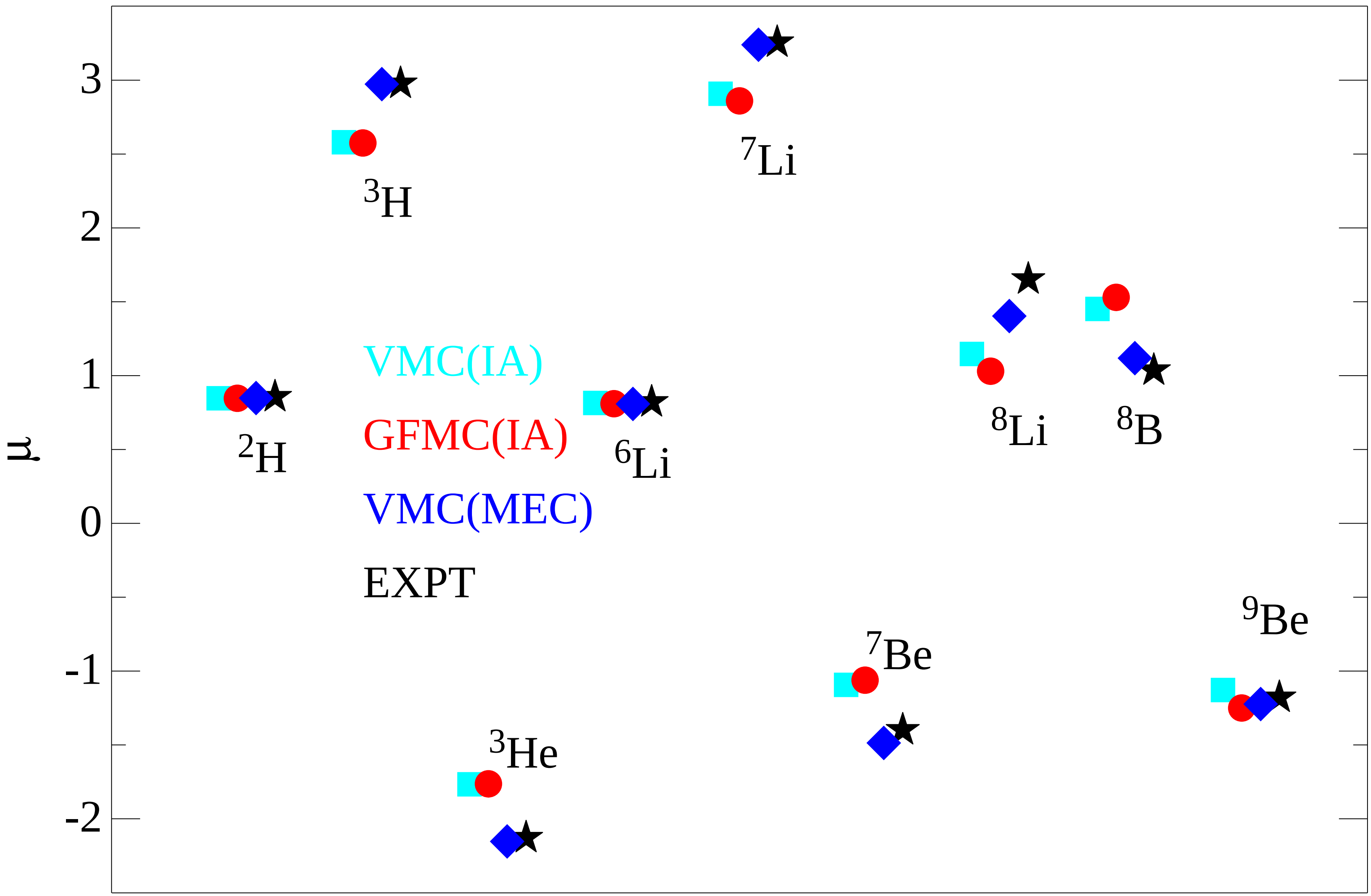
Calculations made principally to demonstrate ADLB

- 5,400-processor VMC for ^{7}Li – 95% 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}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}

Magnetic Moments



No effective charges or effective nucleon magnetic moments!

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

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

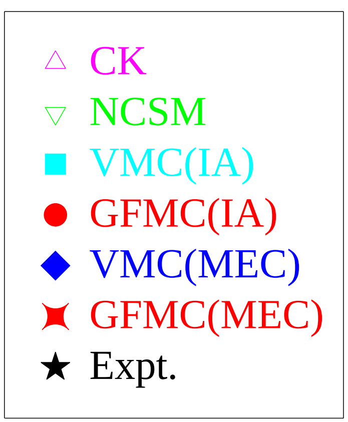
$$M1 = \mu_N \sum_k [(L_k \; + \; g_p S_k)(1+\tau_{kz})/2 \\ + g_n S_k \;\; (1-\tau_{kz})/2]$$

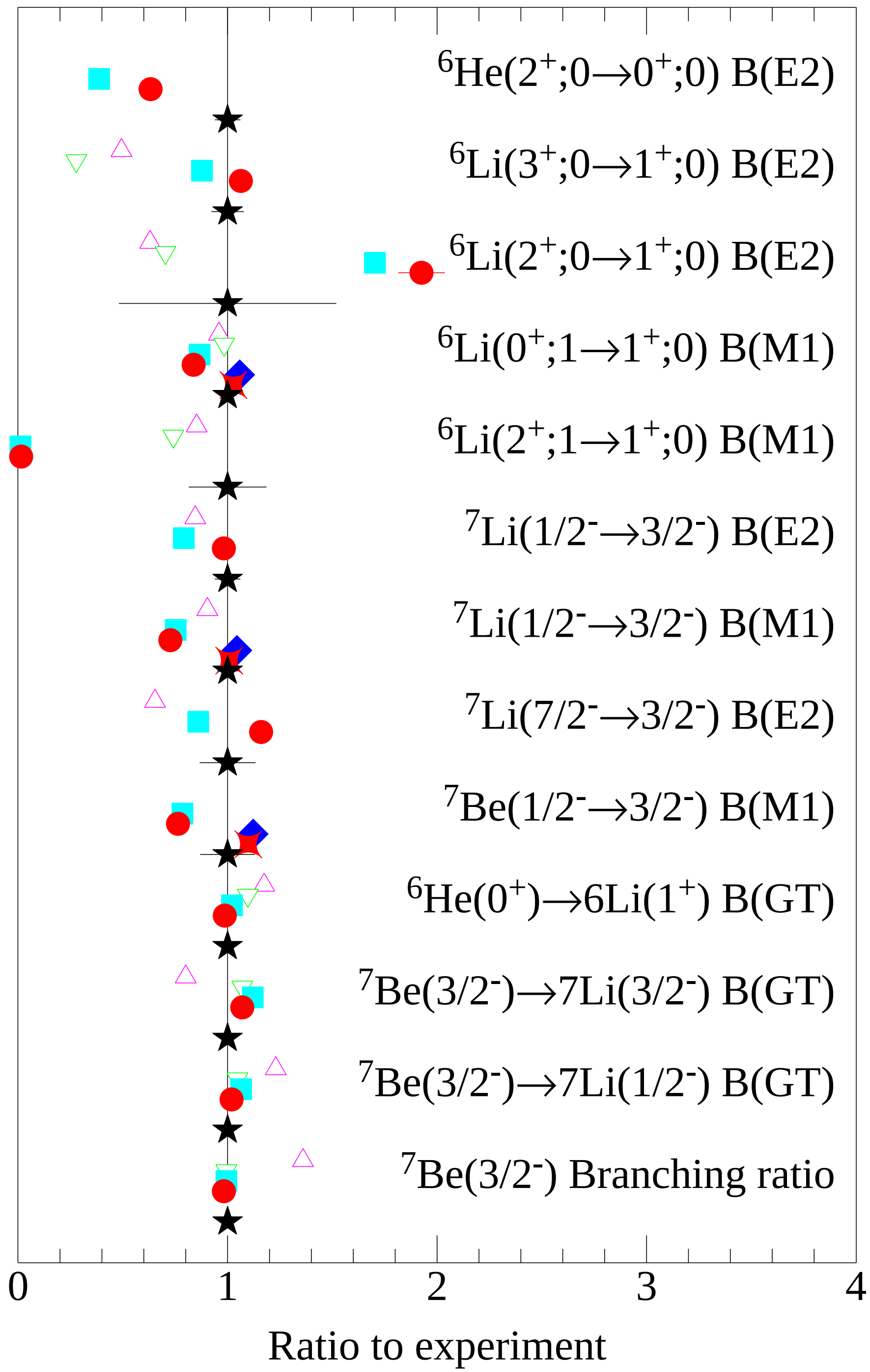
$$\mathrm{F} = \sum_k \tau_{k\pm} \;\; ; \;\; \mathrm{GT} = \sum_k \sigma_k \tau_{k\pm}$$

No effective charges or

effective nucleon magnetic moments!

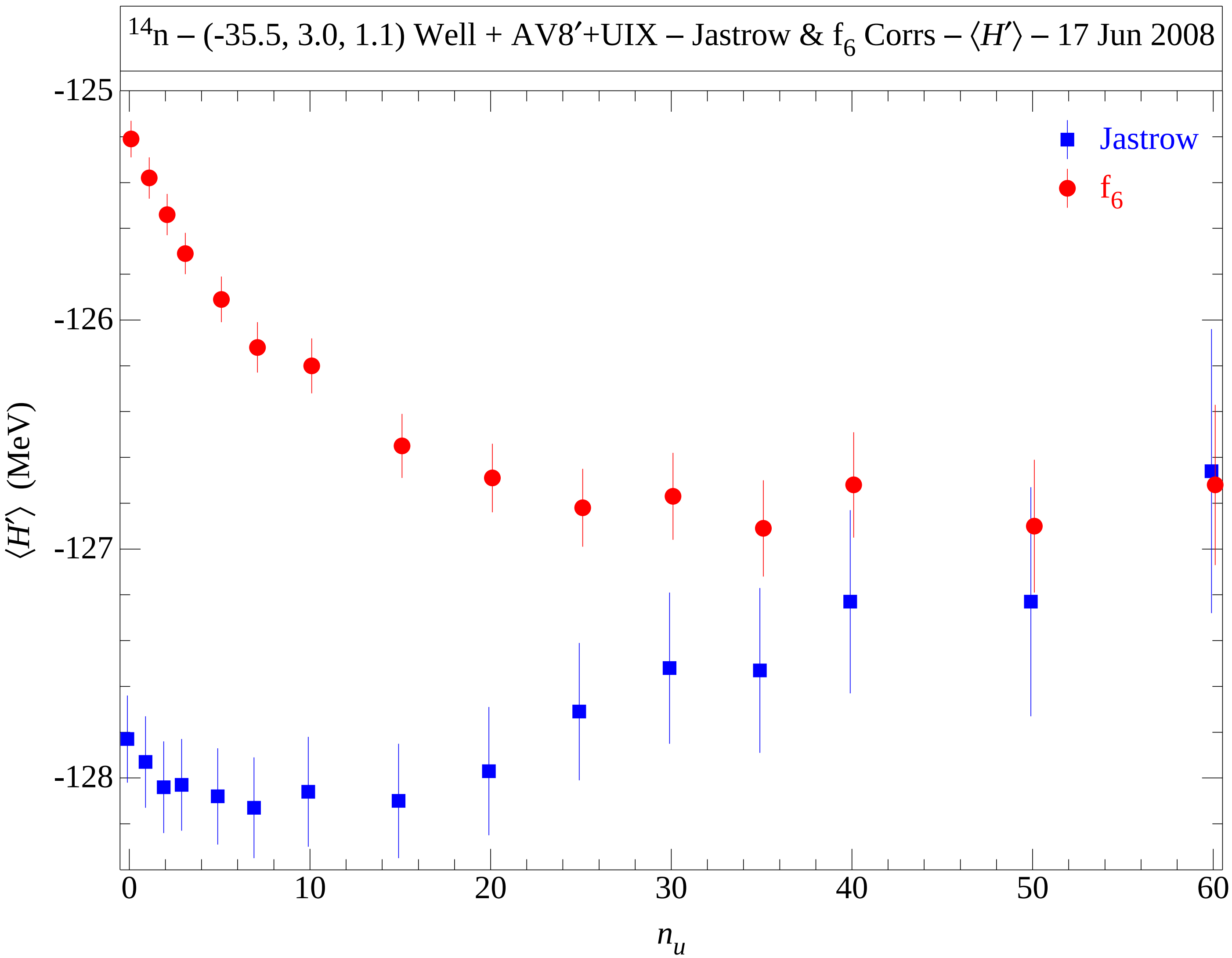
Pervin, Pieper & Wiringa, PRC **76**, 064319 (2007)



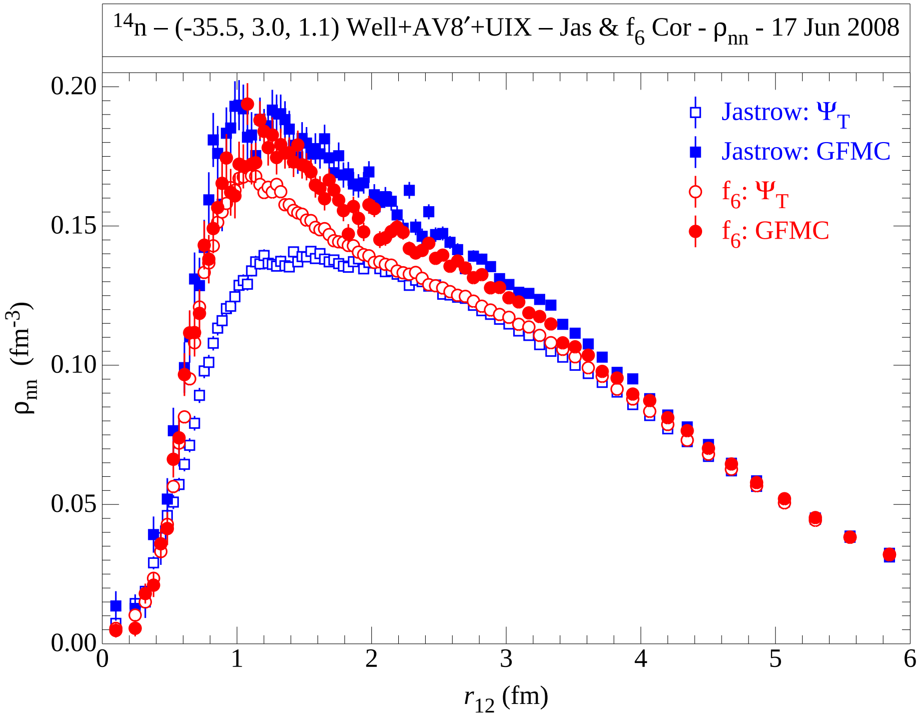


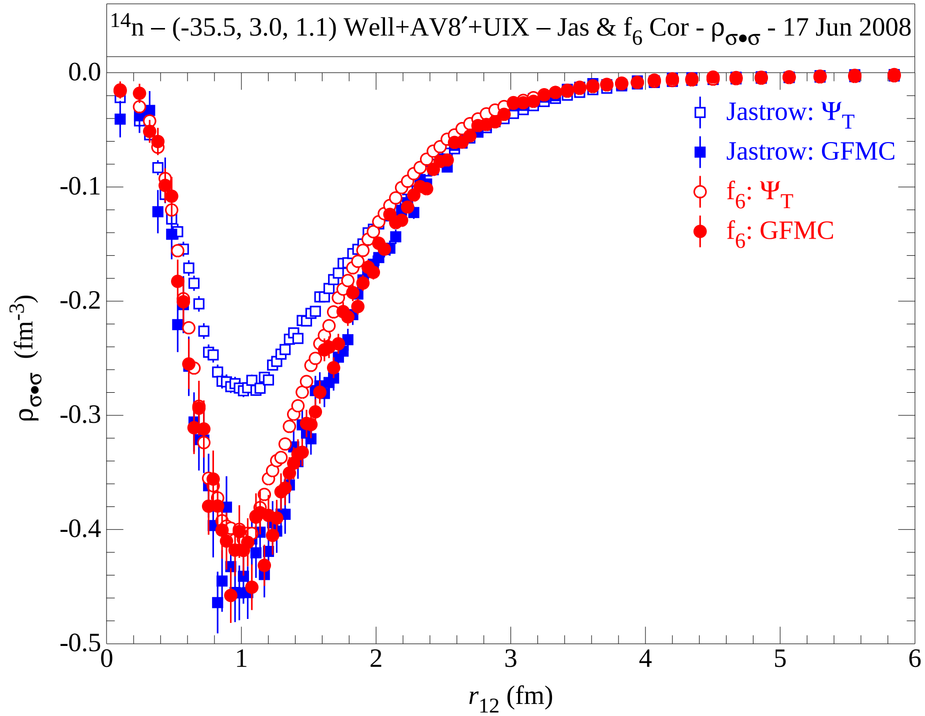
NEUTRON DROPS - GFMC CONSTRAINED-PATH CONVERGENCE

- 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.



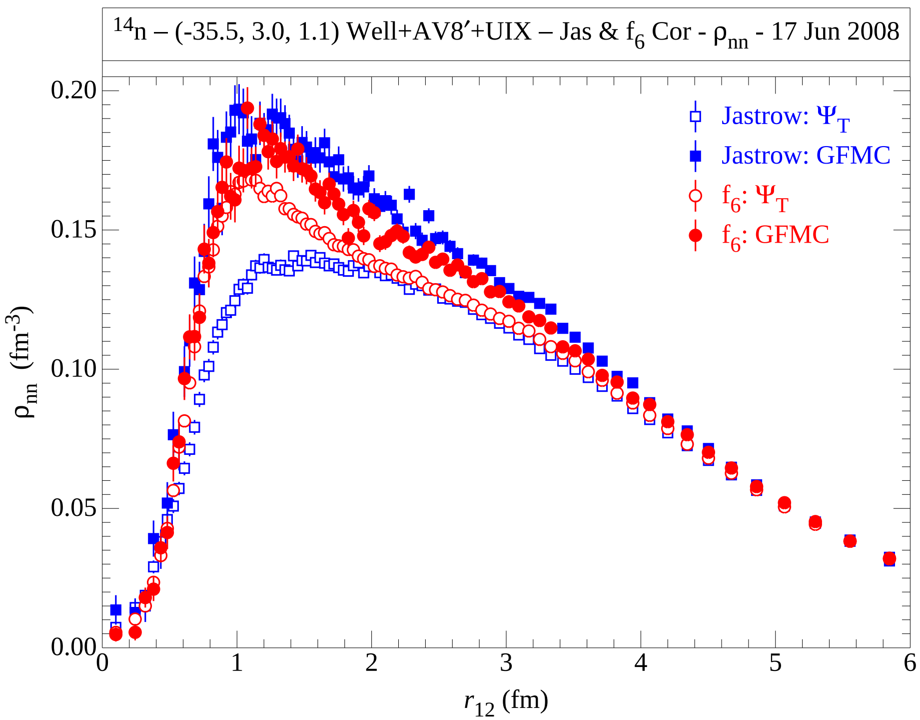
TWO-NEUTRON PAIR AND $\sigma \cdot \sigma$ DENSITY DISTRIBUTIONS

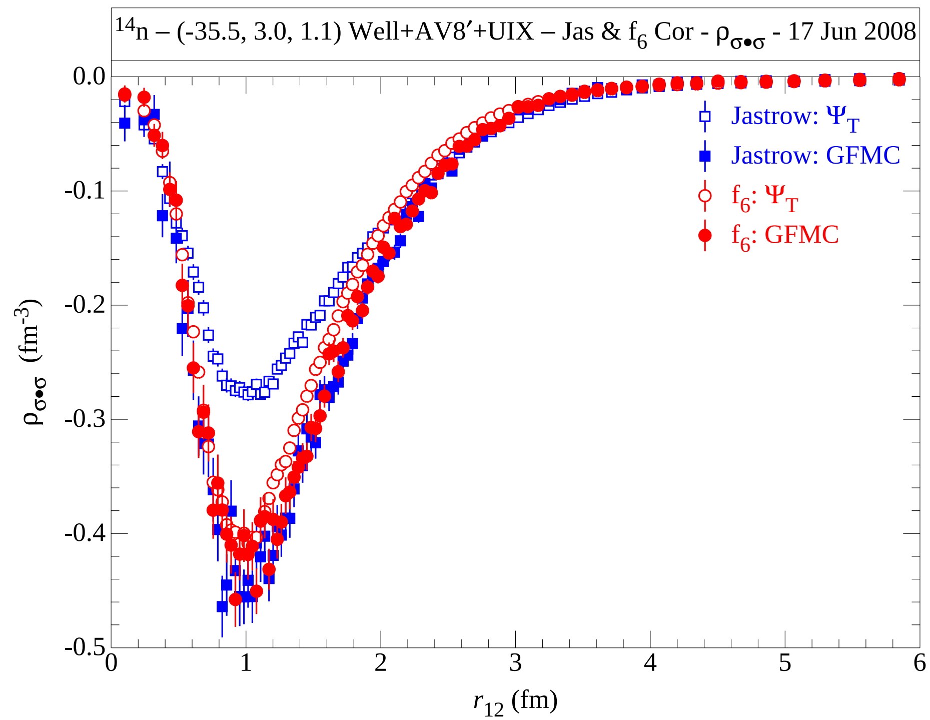




GFMC produces same final densities starting from very different Ψ_T densities

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





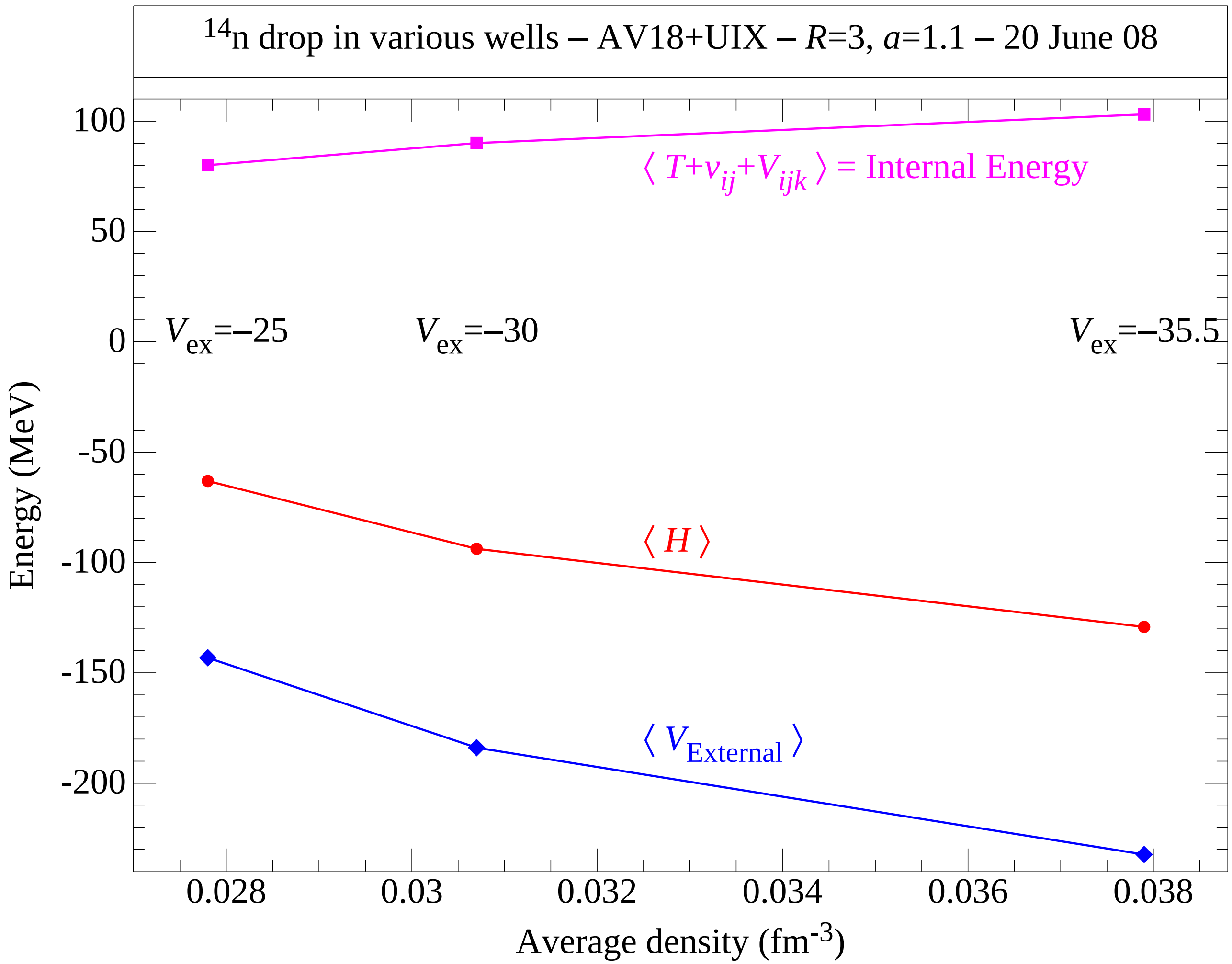
GFMC produces same final densities starting from very different Ψ_T densities

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



NN Benchmark Potentials

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

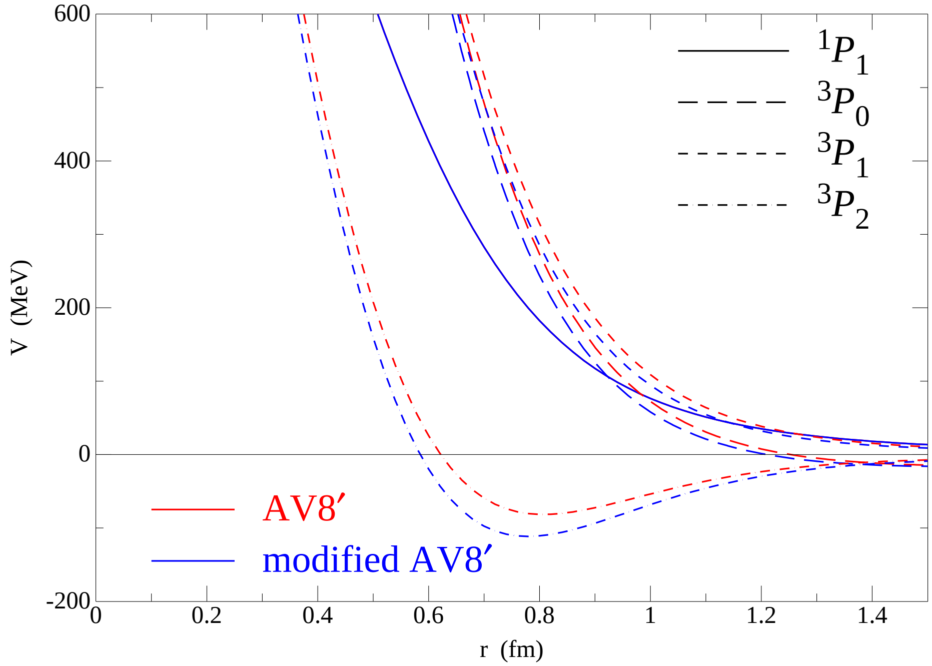
Ultimately we want a ^{12}C benchmark using AV8′ and AV8′ with some V_{ijk} (UIX or TM′).

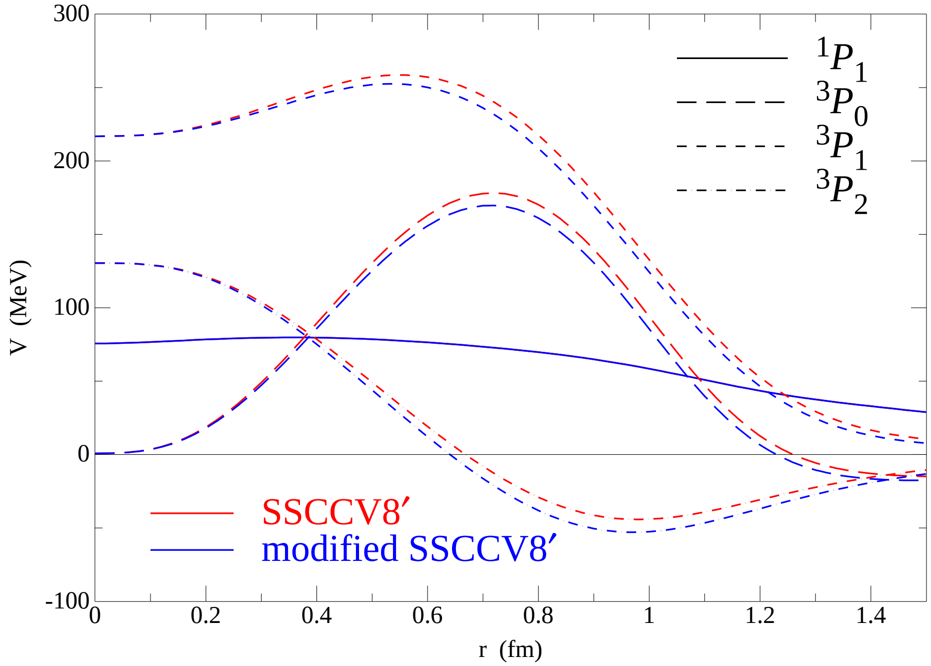
However it was felt that

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:

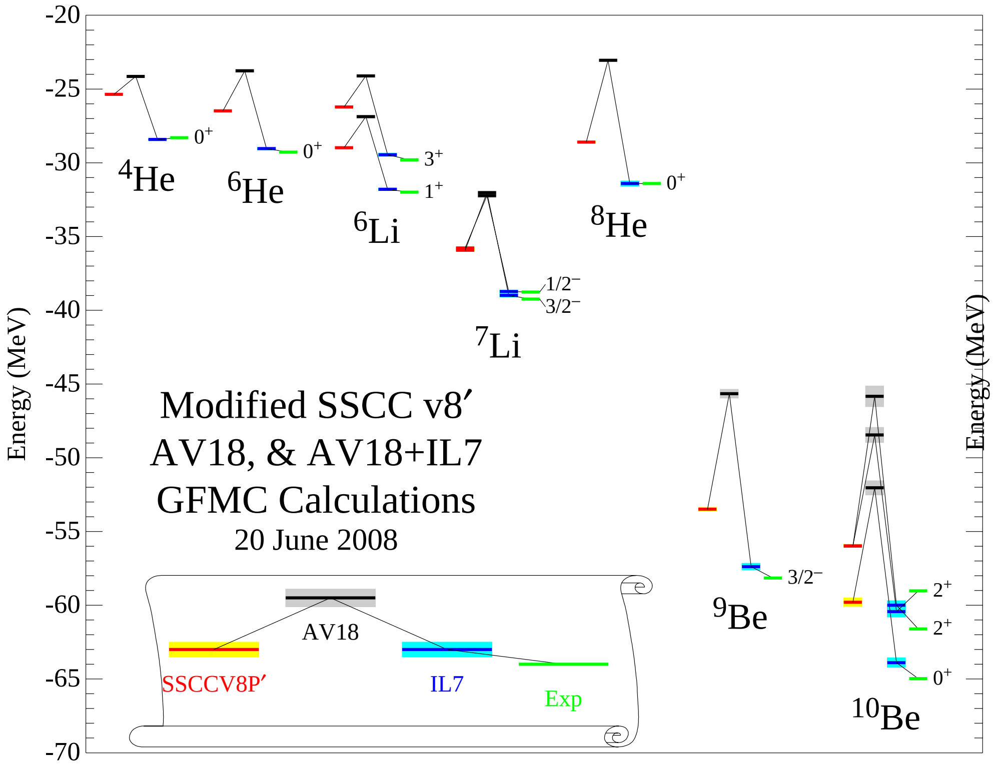


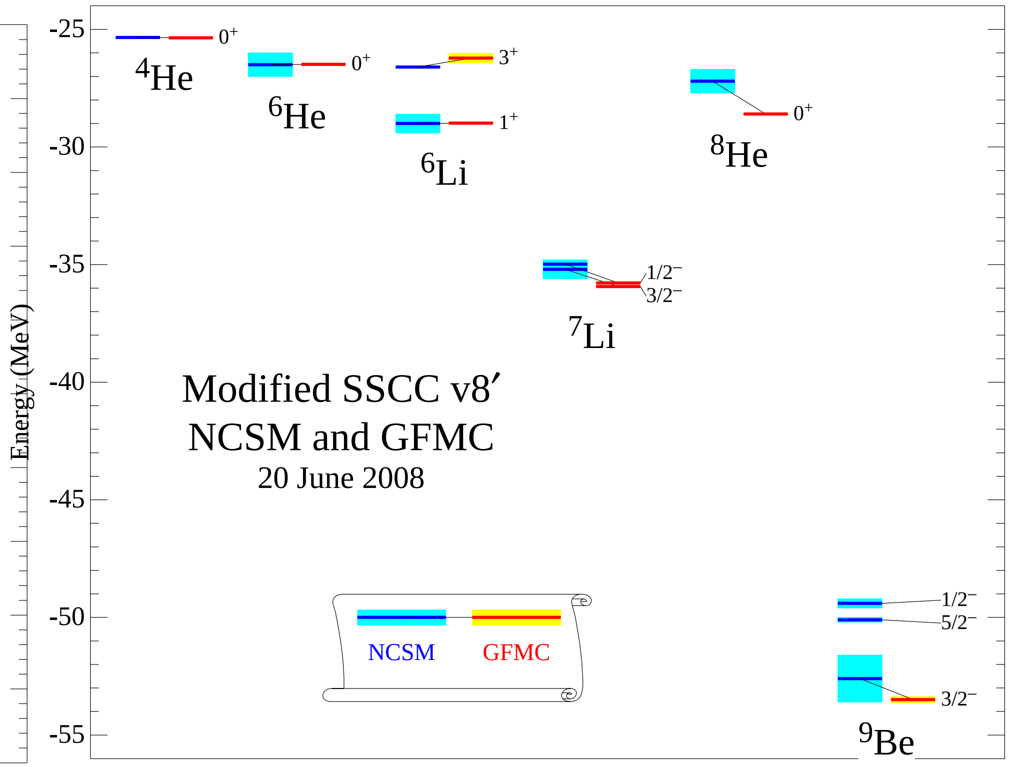


No changes in all even and singlet-odd partial waves

*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