GFMC Benchmarks and Scattering

Steven C. Pieper

Work with
Ralph Butler (Middle Tennessee State U.)  Keneth M. Nollett (Argonne)
Joseph Carlson (Los Alamos)  Muslema Pervin (Argonne)
E. L. (Rusty) Lusk (Argonne)  Robert B. Wiringa (Argonne)

- 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

Argonne National Laboratory
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

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′

<table>
<thead>
<tr>
<th></th>
<th>$\langle r_p^2 \rangle^{1/2}$</th>
<th>Quadrupole Moment</th>
<th>Magnetic Moment*</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NCSM</td>
<td>GFMC</td>
<td>NCSM</td>
</tr>
<tr>
<td>$^4$He</td>
<td>1.51(1)</td>
<td>1.51(2)</td>
<td></td>
</tr>
<tr>
<td>$^6$Li</td>
<td>2.33(5)</td>
<td>2.55(4)</td>
<td>0.00(5)</td>
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<tr>
<td>$^6$He</td>
<td>1.88(5)</td>
<td>1.96(4)</td>
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<tr>
<td>$^7$Li</td>
<td>2.24(5)</td>
<td>2.42(4)</td>
<td>$\leq -2.85$</td>
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<tr>
<td>$^8$He</td>
<td>1.85(5)</td>
<td>1.83(5)</td>
<td></td>
</tr>
<tr>
<td>$^9$Be</td>
<td>2.32(5)</td>
<td>2.46(5)</td>
<td></td>
</tr>
</tbody>
</table>

*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

$^{12}\text{C}$ will have only ~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 $^7$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 $H$, $\Psi_T$, 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).

- $\Psi_T$ has BCS one-body part with pairs of $0S$, $0P$, $1S$, $0D$ neutrons
- $0S$, $0P$ shells basically full; $1S$, $0D$ occupations are variational parameters
- $\Psi_T$ 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 $\Psi_T$
- red contours for Jastrow+$f_6$
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.

\[\langle H \rangle' \text{ (MeV)}\]

\(n_u\) vs \(\langle H \rangle'\) for different models and constraints.
NEUTRON DROPS – SINGLE-NEUTRON DENSITY DISTRIBUTIONS

\[ \rho_n(r) \times r^2 \text{ (fm}^{-1} \text{)} \]

\[ \rho_n(r) \text{ (fm}^{-3} \text{)} \]

\[ r \text{ (fm)} \]

14\(^n\) - (-35.5, 3.0, 1.1) Well+AV8’+UIX – Jas & f\(_6\) Cor - \(\rho_n\) - 17 Jun 2008

14\(^n\) - (-35.5, 3.0, 1.1) Well+AV8’+UIX – Jas & f\(_6\) Cor - \(\rho_n\) - 20 Jun 2008
GFMC produces same final densities starting from very different $\Psi_T$ densities
**Neutron Drops – Dependence on External Well Depth**

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

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

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 $|p_i|; Q_{tot} = 0$
- Pairs with relative momentum $2–3$ fm$^{-1}$ show $10–20 \times np$ enhancement (preliminary).

- VMC calculations for $^3\text{He}$, $^4\text{He}$, and $^8\text{Be}$ show this effect
- Effect disappears when tensor correlations are turned off
- Shows importance of tensor correlations to $>3$ 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 \(q_{\text{rel}} = 300–500\ MeV/c\)
- Compares well with preliminary analysis of data
- Second JLAB experiment to demonstrate importance of tensor correlations at \(q \sim 2\ fm^{-1}\)

\[
\begin{align*}
\text{\(^3\text{He}\)} & \quad \text{\(^4\text{He}\)} \\
\begin{array}{c}
\text{\(q (fm^{-1})\)} \\
0 & 1 & 2 & 3 & 4 & 5 \\
0 & 0.5 & 1 & 1.5 & 2 \\
\end{array} \\
\begin{array}{c}
\text{\(R_{pp/pn}\)} \\
0.0 & 0.1 & 0.2 & 0.3 & 0.4 & 0.5 & 0.6 \\
0 & 0.5 & 1 & 1.5 & 2 \\
\end{array}
\end{align*}
\]

Magnetic Moments

No effective charges or effective nucleon magnetic moments!
$M1, E2, F, GT$ transitions

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

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

\[ F = \sum_k \tau_{k\pm} ; \quad GT = \sum_k \sigma_k \tau_{k\pm} \]

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, $\gamma$)$^6$Li, $^7$Be(p, $\gamma$)$^8$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 $\nu'$?) would be useful
GFMC for Scattering States – Method

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

![Graph showing $E(\tau)$ vs $\tau$ with data points and fitted lines. The graph includes markers for "bound state" and log-deriv = -0.168 fm$^{-1}$.]
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

NEW ILLINOIS POTENTIALS – PROGRESS REPORT

  - 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 $A_\sigma$ in $V^{3\pi}_{ijk}$
  - Formula was published correctly, but incorrectly programmed
  - Increased attraction for all nuclei

- New fit made with corrected $A_\sigma$: 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 $V^R_{ijk}$
  - 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 $^{12}\text{C}$ 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 $^{12}\text{C} \Psi_T$
- First $^{12}\text{C}$ calculations using ADLB version of GFMC (Benchmark $NN$ potentials?)

Next year

- Continuing ADLB work and start multithreading of GFMC
- Many $^{12}\text{C}$ 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?