Recent developments toward large-scale shell-model calculations

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Japanese “K computer” got rank 1 in the world. The construction will be completed at Nov. 2012. SPARC64 VIIIfx  548352 cores

What is the application program to run on it?
In view of truncation approaches to full LSSM space

Many efforts have been paid to develop truncation scheme consisting of form of basis and way of selection.

- \( t \)-particle \( t \)-hole truncation + Lanczos method
  spherical Slater determinant
- Generator coordinate method
  (J-projected) deformed Slater determinant or quasi-particle vacua
- **Monte Carlo Shell Model**
  J-projected deformed Slater determinants
- VAMPIR
  J-projected quasi-particle vacua
- Importance Truncated Shell Model
  spherical Slater determinant
- Projected CI
  J-projected deformed Slater determinants
- **Variational Monte Carlo method**, DMRG, and so on ...

They are variational approaches, which always provide us with upper limit of exact value. It is difficult to know how far it is from the exact one.

Energy variance extrapolation
Monte-Carlo Shell Model

A tool to go beyond the conventional diagonalization method

The shell-model wave function is described by a linear combination of parity, angular-momentum projected Slater determinants

\[
|\Psi\rangle = \sum_{i=k}^{N_{MCSM}} c_k P^\pi \sum_{K=-J}^{J} g_K P^J_{MK} |\phi(D^{(k)})\rangle
\]

MCSM basis, deformed Slater det.

Increase the MCSM basis, or number of defomed Slater det. till energy converges.

Angular-momentum projection ... 3-dimension integral (discretized)
Small disk I/O

Advantageous for parallel computation, bases and mesh points

\[
|\phi\rangle = \prod_{\alpha=1}^{N} \left( \sum_{i} c_i^\dagger D_{i\alpha} \right) |\rangle
\]

\[
|\phi(\sigma)\rangle = \prod e^{\Delta\beta \cdot h(\sigma)} \cdot |\phi^{(0)}\rangle
\]

\[\hat{h}(\sigma)\] one-body Hamiltonian
\[\sigma\]... auxiliary field
random numbers
generated stochastically
Developments of the Monte Carlo shell Model towards “K computer”

- Precise estimation of energy eigenvalue by variance extrapolation

Parallel efficiency

- OpenMP+MPI hybrid parallel
  - 1024 cores

Algorithm tuning for computation

- 8 times faster at maximum

OpenMP+MPI hybrid parallel

- 1024 cores

PC cluster

- 100CPU parallel

Improvement of the MCSM by Conjugate Gradient method

- 8 times faster at maximum


Parallel efficiency

- Full scalability

Algorithm tuning for computation

- MFLOPS

New algorithm for evaluating Hamiltonian matrix elements in the MCSM

hot spot: calculation of the matrix element of two-body int.

\[ \hat{V} = \sum_{i<j, k<l} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k \]

\[ \rho_{ij} = \frac{\langle \phi | c_j^\dagger c_i | \phi' \rangle}{\langle \phi | \phi' \rangle} \]

\[ \langle \phi | \hat{V} | \phi' \rangle = \sum_{i<j, k<l} v_{ijkl} (\rho_{ki} \rho_{lj} - \rho_{kj} \rho_{li}) \]

\[ \langle \phi | \hat{V} | \phi' \rangle = \frac{1}{2} \sum_{i,k} \rho_{ki} \left( \sum_{j,l} v_{ijkl} \rho_{lj} \right) = \frac{1}{2} \sum_{(kl)} \rho_{(ki)} \left( \sum_{jl} v_{(ki),(lj)} \rho_{(lj)} \right) \]

Product of a sparse matrix and a vector is replaced by the product of dense matrices

Matrix product is performed by DGEMM subroutine in BLAS library, which is highly tuned
Tuning by density matrix product

The performance reaches 80% of the theoretical peak at hot spot.

SPARC64 requires large $N_{\text{bunch}}$ in comparison to Xeon

Matrix product e.g. $(390 \times 390) \times (390 \times 2N_{\text{bunch}})$

Nshell = 5

N_{\text{bunch}}$ controllable tuning parameter chunk size

Courtesy of Y. Utsuno
How far from the exact eigenvalue?

$^{56}\text{Ni}$ in pf shell, $0^+_1$, $10^9$ m-scheme dimension

• Very small difference between the MCSM and exact solution
  – About 99% correlation energy (i.e., gain from HF) can be gained typically.
• It is not easy to see where the energy converges.
Extrapolation method: spherical basis vs. projected deformed basis

- Spherical basis with particle-hole truncation
- Angular-momentum projected deformed basis

Exponential convergence method

M. Horoi, B. A. Brown, V. Zelevinsky: PRC65, 027303

Extrapolation method using sorted submatrices

N. Yoshinaga and A. Arima: PRC81, 044316 (2010)

Needs extrapolation method which works independently of the basis representation

Exponential fit causes slow convergence and big uncertainty

Extrapolation method using energy variance

MCSM, PCI, VAMPiR, HMD, ITSM, ...
What is the energy-variance extrapolation?

Demonstrated by Mizusaki in the framework of conventional shell model

Energy variance is defined as

$$\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$$

If the wave function is an exact eigenstate of the Hamiltonian, energy variance is exactly zero

$$\langle \Delta H^2 \rangle = 0$$

A series of approximated wave functions:

$$\langle H \rangle = E_0 + a\langle \Delta H^2 \rangle + b\langle \Delta H^2 \rangle^2 + \ldots$$

With a sequence of approximate energies, extrapolate $$\langle \Delta H^2 \rangle \to 0$$ so that $$\langle H \rangle$$ becomes $$E_0$$, true energy.

Obstacle of the MCSM+extrapolation: computation time for energy variance, $\langle H^2 \rangle$

The expectation value of general four-body operator in deformed Slater determinants is obtained by Wick’s theorem:

2-body int. \[ \langle \phi | \hat{V} | \phi' \rangle = \sum_{i<j,k<l} v_{ijkl} (\rho_{ki} \rho_{lj} - \rho_{kj} \rho_{li}) \] 2-fold loops, 2 terms

4-body int. \[ \frac{\langle \phi | V^2 | \phi' \rangle}{\langle \phi | \phi' \rangle} = \frac{1}{16} \sum_{ijkl\alpha\beta\gamma\delta} \tilde{v}_{ijkl} \tilde{v}_{\alpha\beta\gamma\delta} \left( (1-\rho)_{k\alpha} (1-\rho)_{l\beta} \rho_{\gamma i} \rho_{\delta j} - (1-\rho)_{k\alpha} (1-\rho)_{l\beta} \rho_{\gamma j} \rho_{\delta i} \right) \\
- (1-\rho)_{l\alpha} (1-\rho)_{k\beta} \rho_{\gamma i} \rho_{\delta j} + (1-\rho)_{l\alpha} (1-\rho)_{k\beta} \rho_{\gamma j} \rho_{\delta i} \\
+ \rho_{\gamma \alpha} (1-\rho)_{l\beta} \rho_{k i} \rho_{\delta j} - \rho_{\gamma \alpha} (1-\rho)_{k\beta} \rho_{l i} \rho_{\delta j} \\
- \rho_{\delta \alpha} (1-\rho)_{l\beta} \rho_{k i} \rho_{\delta i} + \rho_{\delta \alpha} (1-\rho)_{k\beta} \rho_{l i} \rho_{\delta i} \\
- \rho_{\delta \alpha} (1-\rho)_{l\beta} \rho_{k i} \rho_{\delta j} + \rho_{\delta \alpha} (1-\rho)_{k\beta} \rho_{l i} \rho_{\delta j} \\
+ \rho_{\delta \alpha} (1-\rho)_{l\beta} \rho_{k i} \rho_{\delta i} - \rho_{\delta \alpha} (1-\rho)_{k\beta} \rho_{l i} \rho_{\delta i} \\
- \rho_{\beta \beta} (1-\rho)_{l\alpha} \rho_{k i} \rho_{\delta j} + \rho_{\beta \beta} (1-\rho)_{k\alpha} \rho_{l i} \rho_{\delta j} \\
+ \rho_{\beta \beta} (1-\rho)_{l\alpha} \rho_{k i} \rho_{\delta i} - \rho_{\beta \beta} (1-\rho)_{k\alpha} \rho_{l i} \rho_{\delta i} \\
- \rho_{\beta \beta} (1-\rho)_{l\alpha} \rho_{k i} \rho_{\delta j} + \rho_{\beta \beta} (1-\rho)_{k\alpha} \rho_{l i} \rho_{\delta j} \\
+ \rho_{\beta \beta} (1-\rho)_{l\alpha} \rho_{k i} \rho_{\delta i} - \rho_{\beta \beta} (1-\rho)_{k\alpha} \rho_{l i} \rho_{\delta i} \right) \]

8-fold loops, 24 terms

\[ \frac{\langle \phi | \hat{H}^2 | \psi \rangle}{\langle \phi | \psi \rangle} = \sum_{i<j, i'j'k<l} \sum_{k<l} v_{ijkl} \left( (1-\rho)_{k\alpha} (1-\rho)_{l\beta} \rho_{\gamma i} \rho_{\delta j} - (1-\rho)_{k\alpha} (1-\rho)_{l\beta} \rho_{\gamma j} \rho_{\delta i} \right) \left( \sum_{\gamma<\delta} v_{\alpha\beta\gamma\delta} (\rho_{\gamma i} \rho_{\delta j} - \rho_{\delta i} \rho_{\gamma j}) \right) \]

Separability of $H^2$

\[ \text{two independent inside loops} \]

6-fold loops, matrix-product form
Result of energy variance extrapolation in the MCSM: $^{56}$Ni in $pf$-shell

Red solid line: 2nd order extrapolation for the MCSM
Blue dashed line: 2nd order extrapolation of $t$-particle $t$-hole truncation in spherical basis

$\langle H \rangle_1, \langle H \rangle_2, \langle H \rangle_3, \ldots \ E_{\text{exact}}$

$\langle \Delta H^2 \rangle_1, \langle \Delta H^2 \rangle_2, \langle \Delta H^2 \rangle_3, \ldots \ 0$

$H_{ij} =$

Energy [MeV]

Energy Variance [MeV$^2$]

$J=0^+$
Extrapolation method in observables: $^{56}\text{Ni}$ in pf-shell

MCSM + 1st order extrapolation shows good predictive power in various physical quantities in addition to energy eigenvalues.
MCSM + energy-variance extrapolation $^{64}$Ge with $^{40}$Ca core

(24 valence particles in pf+g9/2 space, corresponding the diagonalization of $1.7 \times 10^{14}$ m-scheme dimension)


\[
H_{ij} = \langle \Delta H^2 \rangle_i \langle H \rangle_j
\]

exact: unknown
diagonalization with $t$-particle $t$-hole truncation
Monte Carlo Shell Model + extrapolation
extrapolated value
For more efficient computation

Monte-Carlo Shell Model method: Wave function of the nuclear shell model is described by a linear combination of angular-momentum (and parity) projected Slater determinants

\[ \left| \Psi \right\rangle = \sum_{i=k}^{N_{\text{MCSM}}} c_{k} P^\pi J P_{MK}^{J,\pi} \left| \phi(D^{(k)}) \right\rangle \]

\[ \left| \phi \right\rangle = \prod_{\alpha=1}^{N} \left( \sum_{i=1}^{N_{sp}} c_{i}^\dagger D_{i\alpha} \right) \left| - \right\rangle \]

MCSM basis, deformed Slater det.

By using the energy variance of the approximated wave functions, we estimate the exact eigenvalue precisely.

The computation of the energy variance needs a lot of computer resources, which is proportional to the number of bases squared.

Efficient computation with a small number of Slater det.
Energy minimization by Conjugate Gradient method

Evaluation of the energy variance is time consuming due to the four-body interaction.

\[
|\Psi(D)\rangle = \sum_{n=1}^{N_B} c_i \sum_{K=-J}^{J} g_K P^{J,\Pi}_{MK} |\phi(D^{(n)})\rangle \quad |\phi(D^{(n)})\rangle = \prod_{\alpha=1}^{N_p} \left( \sum_{i=1}^{N_{sp}} c_i^\dagger D^{(n)}_{\alpha i} \right) - \langle \right|
\]

\[
E(D) = \langle \Psi(D)|H|\Psi(D) \rangle
\]

Minimize \(E(D)\) as a function of \(D\) utilizing Conjugate Gradient method.

**Step 1**: Generate basis candidate by auxiliary field technique stochastically

\[
|\phi(\sigma)\rangle = \prod e^{\Delta \beta \cdot h(\sigma)} \cdot |\phi^{(0)}\rangle
\]

and select basis which lowers the energy

**Step 2**: Energy expectation value is taken as a function of \(D\), and optimize it using Conjugate Gradient method (VAP)

Iterate these steps every basis till the energy converges

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Few Determinant Approximation
M. Honma, B.A.Brown, T. Mizusaki, and T. Otsuka

Hybrid Multi-Determinant

VAMPIR
K.W. Schmid, F. Glummer, M. Kyotoku, and A. Faessler
Energy minimization by Conjugate Gradient method

Stochastic sampling before conjugate gradient to minimize the expectation value energy
reduce the number of basis function roughly 30%

$^{64}$Ge in pfg9-shell, $10^{14}$dim
Energy minimization by Conjugate Gradient method

Energy of $^{64}$Ge in pf+g9/2 model space

- $J=0^+$ MCSM + extrapol.
- $J=0^+$ MCSM+CG + extrapol.
- $J=2^+$ MCSM + extrapol.

$^{64}$Ge in pfg9-shell, $10^{14}$dim

- stochastic sampling before conjugate gradient
- minimize the expectation value energy
- reduce the number of basis function roughly 30%

number of basis functions

Energy [MeV]

Energy Variance [MeV$^2$]
The $0^{+}_1$ MCSM wave function up to 20 bases is trapped by the $0^{+}_2$ state.

This situation is rare, the structure of $0^{+}_2$ state is close to the projected Slater det. the ground state includes much many-body correlations.
Step 3: simultaneous optimization of many bases

$$\ket{\Psi(D)} = \sum_{n=1}^{N_B} c_n P^\Pi \sum_{K=-J}^{J} g_K P_{MK}^{J} \ket{\phi(D^{(n)})}$$

$$\ket{\phi(D^{(n)})} = \prod_{\alpha=1}^{N_p} \left( \sum_{i=1}^{N_{sp}} c_i^{\alpha} D_{i\alpha}^{(n)} \right)$$

$$E(D) = \langle \Psi(D) | H | \Psi(D) \rangle$$

minimization of all $D^{(n)}$, not sequential opt.

$^{72}$Ge, JUN45 int. 1.4x10^8 m-scheme dim.

sequential optimization of each base, 704 parameters resulting in 120 bases

optimization of 24 bases, 16896 parameters with simultaneous variation many-basis correlation is included from beginning
A possible problem: narrow region for fit

In some cases, the range of the variance is too small to make stable fit

$2^{\text{nd}}$ order polynomial fit causes large uncertainty of the extrapolation

N,Z=50~82, P+QQ int.
triaxial deformed Xe, Ba isotopes

$^{132}\text{Ba} 0^+ \text{ MCG}$
extrap. $E=-9.85 +/- 0.29$
Re-ordering of the basis functions

Ansatz: Energy-variance extrapolation method always works and the extrapolated value is independent of the ordering of basis functions...

A sequence of the approximated wave functions

\[ |\Psi_1\rangle = c_1^{(1)} |\phi_1\rangle \]
\[ |\Psi_2\rangle = c_1^{(2)} |\phi_1\rangle + c_2^{(2)} |\phi_2\rangle \]
\[ |\Psi_3\rangle = c_1^{(3)} |\phi_1\rangle + c_2^{(3)} |\phi_2\rangle + c_3^{(3)} |\phi_3\rangle \]
\[ \vdots \]
\[ |\Psi_N\rangle = \sum_{i=1}^{N} c_i^{(N)} |\phi_i\rangle \]

Re-ordering

\[ |\phi_1\rangle, |\phi_2\rangle, |\phi_2\rangle, \ldots, |\phi_N\rangle \]
to obtain another sequence and fit

A fit curve can be close to linear
A possible problem: narrow region for fit

In some cases, the range of the variance is too small to make stable fit

2nd order polynomial fit causes large uncertainty of the extrapolation

Reordering of the bases decreases the uncertainty of the extrapolated value

fit curve is close to linear

N,Z=50~82, P+QQ int. triaxial deformed Xe, Ba isotopes
Energy-variance extrapolation for ground state energy

$^{132}$Ba  50 bases

$^{134}$Ba  24 bases

$2 \times 10^{10}$ dim.

$8 \times 10^{8}$ dim.

exact N/A
non-yrast states

8 bases are optimized for $0^+_1$
additional 8 bases for $0^+_2$

$^{134}\text{Ba}$ 8 + 8 base

$^{72}\text{Ge}$, JUN45 16+16 bases

1$^{\text{st}}$ order extrapolation
2$^{\text{nd}}$ order extrapolation
Excitation energies of Xe isotopes

symbol: exp.
line: theory

Excitation energies Ba isotopes
The application of the MCSM+extrapolation method to no-core shell model calculations

T. Abe (Univ. of Tokyo), T. Otsuka (Univ. of Tokyo), N. Shimizu (Univ. of Tokyo), Y. Utsuno (JAEA), J. Vary (Iowa), P. Maris (Iowa)
JISP16 NN interaction

- JISP16: J-matrix Inverse Scattering Potential tuned B.E.s up to $^{16}\text{O}$ with phase-shift-equivalent unitary transformation

$$V = \sum_{\Gamma,\Gamma'} \sum_{n=0}^{N_{\Gamma}} \sum_{n'=0}^{N_{\Gamma'}} |n, \Gamma\rangle V_{n,n'}^{\Gamma,\Gamma'} \langle n', \Gamma'|$$

- Small matrix of the NN int. in the oscillator basis
- High quality description of NN potential thru. p-shell nuclei
  -> Reproduce the phase shift, deuteron properties, & B.E.s of some light nuclei
  -> In this sense, JISP16 is the “bare” interaction
- JISP16 NN int. seems to minimize 3N (many-body) int.

 feasibly for the large-scale computation of nuclear structure

References

Why we need to extrapolate the energies

- Definition: (Correlation Energy) \( \equiv \langle \Psi | H | \Psi \rangle_{\text{JHF}} - \langle \Psi | H | \Psi \rangle_{\text{Exact}} \)

NCSM wf w/ realistic NN int is more correlated (complicated) than SSM wf w/ effective int

Need energy-variance extrapolation for No-Core MCSM calc
Helium-4 & carbon-12 gs energies

$^{4}\text{He}(0^+;\text{gs})$

$^{12}\text{C}(0^+;\text{gs})$

Exact result is unknown

w/ optimum hw
w/o Coulomb force
w/o spurious CoM treatment
Energies of Light Nuclei

T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary

Energies of Light Nuclei

w/o the extrapolation method

MCSM

FCI

Performed only by MCSM

N\text{shell} = 2 (sp)
N\text{shell} = 3 (spsd)
N\text{shell} = 4 (spsdf)

E (MeV)

0

-10

-20

-30

-40

-50

-60

-70

-80

-90

-100

6He (0+)
7Li (1/2-)
8Be (0+)
10B (1+)
10B (3+)
12C (0+)
4He (0+)
6Li (1+)
7Li (3/2-)
10B (1+)

N\text{shell} = 4 (spsdf)
Energies of Light Nuclei

T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary

Performed only by MCSM

w/ the extrapolation method

E (MeV)

4He (0+)
6He (0+)
6Li (1+)
7Li (1/2-)
7Li (3/2-)
8Be (0+)
10B (1+)
10B (3+)
12C (0+)

MCSM
FCI

N\text{shell} = 2 (sp)
N\text{shell} = 3 (spsd)
N\text{shell} = 4 (spsdpf)
• Benchmark calculation of light nuclei with Nshell=5

- $^4\text{He}(0^+;\text{gs})$: $-29.893\text{ MeV (exact)}$ vs $-29.812\text{ MeV (extrap)}$
- $^6\text{Li}(1^+;\text{gs})$: $-26.079\text{ MeV (exact)}$ vs $-26.081\text{ MeV (extrap)}$
- $^6\text{He}(0^+;\text{gs})$: $-29.036\text{ MeV (exact)}$ vs $-29.036\text{ MeV (extrap)}$

- ~1 PFLOPS\text{*hour/state}
- ~3 PFLOPS\text{*hour/state}

- ~3x10^5 M-scheme dim
- ~1x10^8 M-scheme dim

• The extrapolated values are obtained within a few 10 keVs uncertainty.
M-scheme dimension

Moore’s law:

\#transistors doubles every two years. \(p = 2^{n/2}\)

\[x 5.7 \text{ after } 5 \text{ yrs}\]

\[x 32 \text{ after } 10 \text{ yrs}\]

aim at many-particle many-hole excited state
Summary

• Energy-variance extrapolation works well in the frameworks of the MCSM, conventional Lanczos method with truncation, and the Variational Monte Carlo. It demonstrates up to $10^{14}$ dimension system.
• Conjugate Gradient optimization method makes the MCSM calculation more efficiently.
• Many basis optimization enables us to avoid the trapping problem of higher excited state.
• No-core MCSM shows its feasibility in light nuclei.
• The MCSM code is under intensive developments for massive parallel computation and “K computer”.