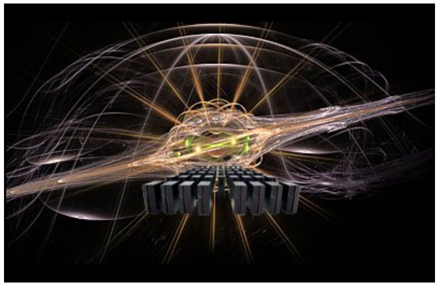


International Conference on
Nuclear Theory in the Supercomputing Era - 2013

Monte Carlo shell model towards ab initio calculations

Takashi Abe

THE UNIVERSITY OF TOKYO

Iowa State University, Ames, IA

May 16, 2013

Collaborators

- U of Tokyo
  - Takaharu Otsuka (Dept of Phys & CNS)
  - Noritaka Shimizu (CNS)
  - Tooru Yoshida (CNS)
- JAEA
  - Yutaka Utsuno
- Iowa State U
  - James P. Vary
  - Pieter Maris

Current status of ab inito approaches

- Major challenge of nuclear physics

  - Understand the nuclear structure from *ab-initio* calculations in non-relativistic quantum many-body system w/ realistic nuclear forces (potentials)

  - *ab-initio* approaches: GFMC, NCSM (A ~ 12-14), CC (closed subshell +/- 1,2), SCGF theory, IM-SRG, Lattice EFT, …

→ demand for extensive computational resources

✓ *ab-initio*(-like) SM approaches (which attempt to go) beyond standard methods

- IT-NCSM, IT-CI: R. Roth (TU Darmstadt), P. Navratil (TRIUMF), …
- SA-NCSM: T. Dytrych, K.D. Sviratcheva, J.P. Draayer, C. Bahri, J.P. Vary, … (Louisiana State U, Iowa State U)
- No-Core Monte Carlo Shell Model (MCSM)

“Ab initio” in low-energy nuclear structure physics

- Solve the non-relativistic Schroedinger eq.
  and obtain the eigenvalues and eigenvectors.

$$H|\Psi\rangle = E|\Psi\rangle$$

$$H = T + V_{\mathrm{NN}} + V_{\mathrm{3N}} + \cdots + V_{\mathrm{Coulomb}}$$

  – Ab initio: All nucleons are active, and Hamiltonian consists of realistic NN (+ 3N) potentials.
- Two main sources of errors:
  – Nuclear forces (interactions btw/among nucleons),
    in principle, they should be obtained (directly) by QCD.
  – Finite # of basis space (the choice of basis function and truncation),
    we have to extrapolate to infinite basis dimensions

Shell model (Configuration Interaction, CI)

- Eigenvalue problem of large sparse Hamiltonian matirx

$$H|\Psi\rangle = E|\Psi\rangle$$

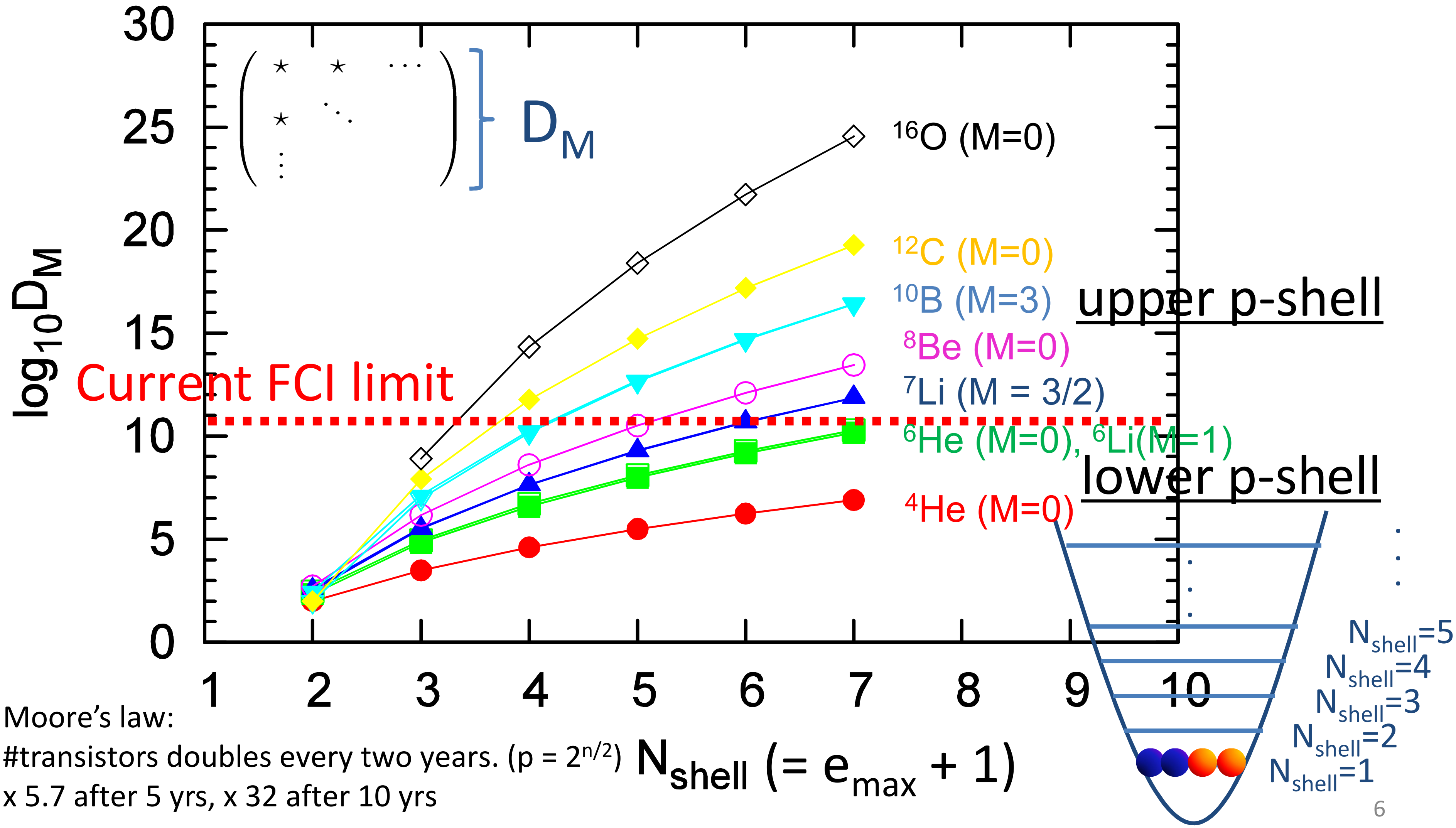
$$\begin{pmatrix} H_{11} & H_{12} & H_{13} & H_{14} & H_{15} & \cdots \\ H_{21} & H_{22} & H_{23} & H_{24} & & \\ H_{31} & H_{32} & H_{33} & & & \\ H_{41} & H_{33} & & \ddots & & \\ H_{51} & & & & & \\ \vdots & & & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix} = \begin{pmatrix} E_1 & & & & 0 \\ & E_2 & & & \\ & & E_3 & & \\ & & & \ddots & \\ 0 & & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix}$$

$$\sim \mathcal{O}(10^{10})$$

Large sparse matrix (in M-scheme)

$$\begin{cases} |\Psi_1\rangle = a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma \cdots |-\rangle \\ |\Psi_2\rangle = a^\dagger_{\alpha'} a^\dagger_{\beta'} a^\dagger_{\gamma'} \cdots |-\rangle \\ |\Psi_3\rangle = \cdots \\ \vdots \end{cases}$$

M-scheme dimension of the p-shell nuclei

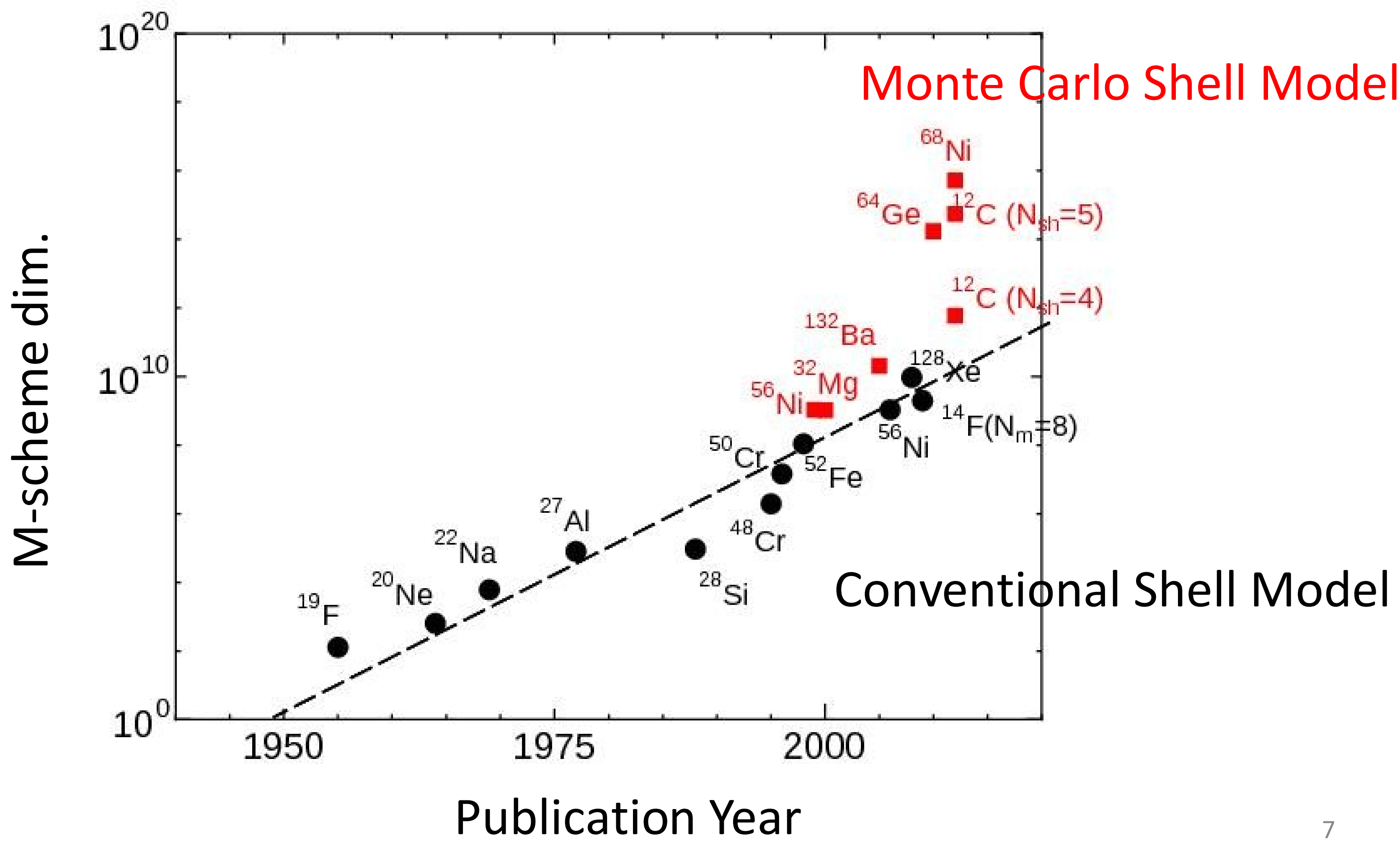


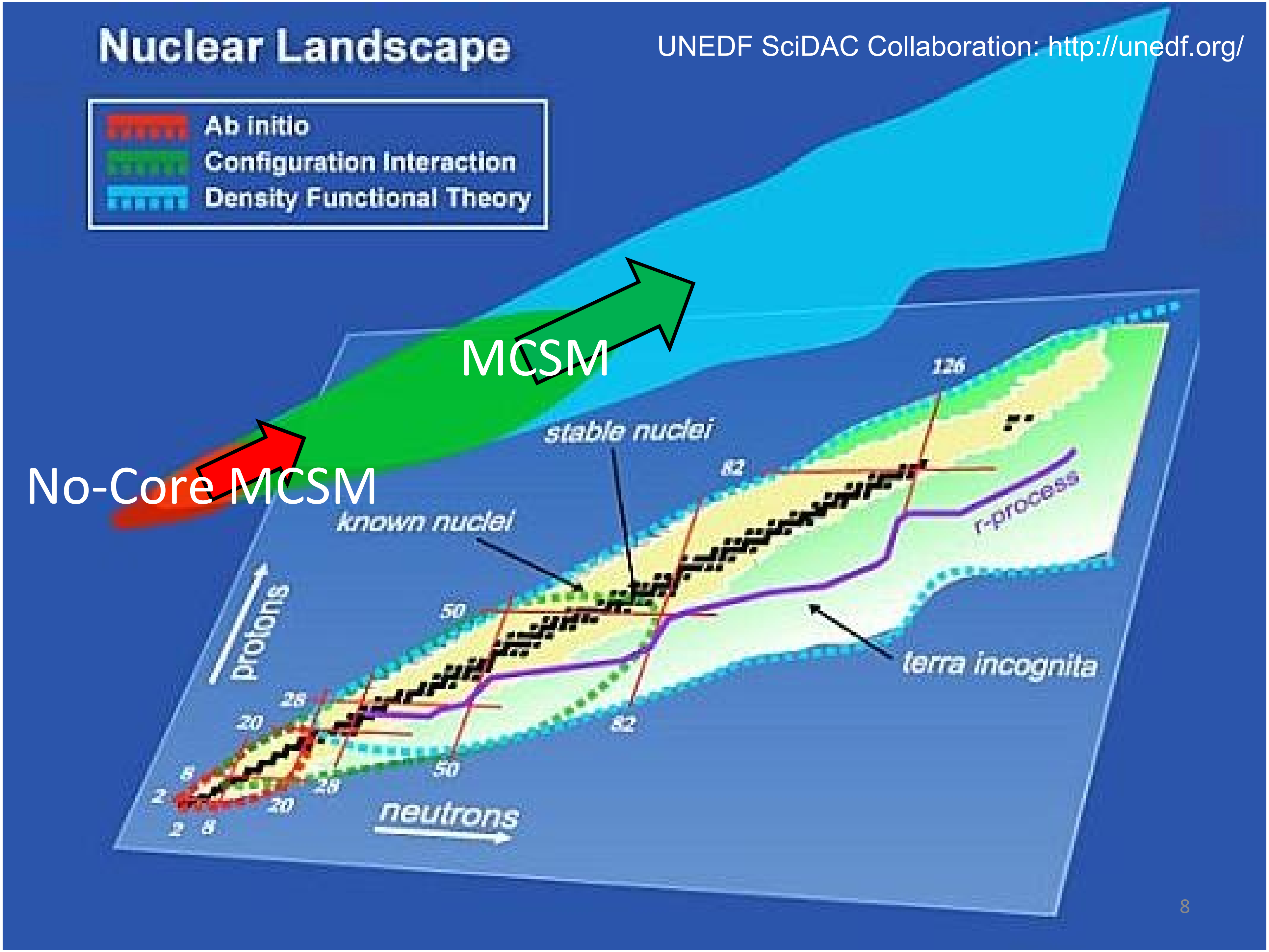
Moore's law:
#transistors doubles every two years. ($p = 2^{n/2}$)
x 5.7 after 5 yrs, x 32 after 10 yrs

Review: T. Otsuka , M. Honma, T. Mizusaki, N. Shimizu, Y. Utsuno, Prog. Part. Nucl. Phys. 47, 319 (2001)

Advantage of the MCSM

- MCSM w/ an assumed inert core is one of the powerful shell model algorithms.





Nuclear Landscape
UNEDF SciDAC Collaboration: http://unedf.org/
Ab initio
Configuration Interaction
Density Functional Theory
MCSM
No-Core MCSM
stable nuclei
known nuclei
terra incognita
r-process
protons
neutrons
126
82
50
28
20
8
2

Review: T. Otsuka , M. Honma, T. Mizusaki, N. Shimizu, Y. Utsuno, Prog. Part. Nucl. Phys. 47, 319 (2001)

Monte Carlo shell model (MCSM)

- Importance truncation

Standard shell model

$$H = \begin{pmatrix} \star & \star & \star & \star & \star & \cdots \\ \star & \star & \star & \star & & \\ \star & \star & \star & & & \\ \star & \star & & \ddots & & \\ \star & & & & & \\ \vdots & & & & & \end{pmatrix} \Rightarrow \begin{pmatrix} E_0 & & & & 0 \\ & E_1 & & & \\ & & E_2 & & \\ & & & \ddots & \\ 0 & & & & \end{pmatrix}$$

Diagonalization

All Slater determinants

d ~ $O(10^{10})$

Monte Carlo shell model

$$H \sim \begin{pmatrix} \star & \star & \cdots \\ \star & \ddots & \\ \vdots & & \end{pmatrix} \Rightarrow \begin{pmatrix} E'_0 & & 0 \\ & E'_1 & \\ 0 & & \ddots \end{pmatrix}$$

Diagonalization

Important bases stochastically selected

d_{MCSM} ~ O(100)

SM Hamiltonian & MCSM many-body w.f.

- 2nd-quantized non-rel. Hamiltonian (up to 2-body term, so far)

$$H = \sum_{\alpha\beta}^{N_{sps}} t_{\alpha\beta} c_\alpha^\dagger c_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta}^{N_{sps}} \bar{v}_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \quad \bar{v}_{ijkl} = v_{ijkl} - v_{ijlk}$$

- Eigenvalue problem

$$H|\Psi(J,M,\pi)\rangle = E|\Psi(J,M,\pi)\rangle$$

- MCSM many-body wave function & basis function

$$|\Psi(J,M,\pi)\rangle = \sum_{i=1}^{N_{basis}} f_i |\Phi_i(J,M,\pi)\rangle \qquad |\Phi(J,M,\pi)\rangle = \sum_{K=-J}^{J} g_K P_{MK}^J P^\pi |\phi\rangle$$

These coeff. are obtained by the diagonalization.

- Deformed SDs

This coeff. is obtained by a stochastic sampling.

$$|\phi\rangle = \prod_i^A a_i^\dagger |-\rangle \qquad a_i^\dagger = \sum_\alpha^{N_{sps}} c_\alpha^\dagger D_{\alpha i}$$

($c_\alpha^\dagger$ … spherical HO basis)

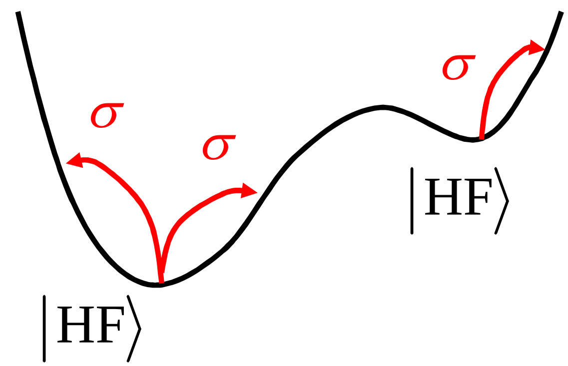
Sampling of basis functions

- Deformed Slater determinant basis

$$|\phi\rangle = \prod_i^A a_i^\dagger |-\rangle \qquad a_i^\dagger = \sum_\alpha^{N_{sps}} c_\alpha^\dagger D_{\alpha i}$$

($c_\alpha^\dagger$ … HO basis)

- Stochastic sampling of deformed SDs



$$|\phi(\sigma)\rangle = e^{-h(\sigma)}|\phi\rangle$$

$$h(\sigma) = h_{HF} + \sum_i^{N_{AF}} s_i V_i \sigma_i O_i$$

c.f.) Imaginary-time evolution & Hubbard-Stratonovich transf.

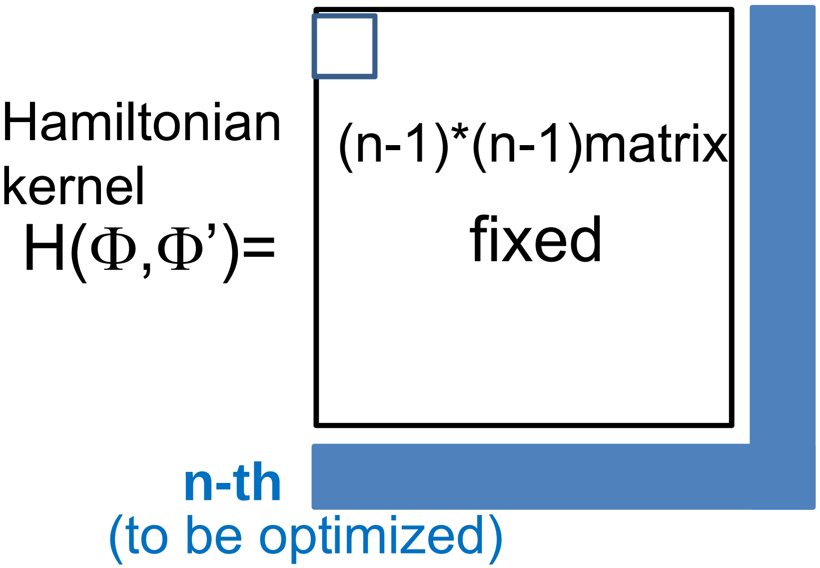
$$|\phi(\sigma)\rangle = \prod_{N_\tau} e^{-\Delta\beta h(\sigma)}|\phi\rangle \qquad e^{-\beta H} = \int_{-\infty}^{+\infty} \prod_i d\sigma_i \sqrt{\frac{\beta|V_i|}{2\pi}} e^{-\frac{\beta}{2}|V_i|\sigma_i^2} e^{-\beta h(\vec{\sigma})}$$

$$h(\sigma) = \sum_i^{N_{AF}} (\epsilon_i + s_i V_i \sigma_i) O_i \qquad H = \sum_i \epsilon_i O_i + \frac{1}{2}\sum_i V_i O_i^2$$

Rough image of the search steps

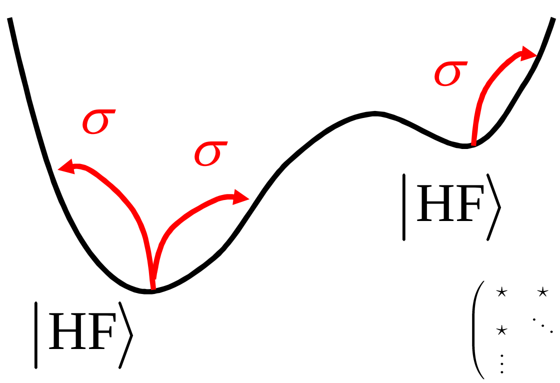
- Basis search
  - HF solution is taken as the 1st basis
  - Fix the n-1 basis states already taken
  - Requirement for the new basis: atopt the basis which makes the energy (of a many-body state) as low as possible by a stochastic sampling

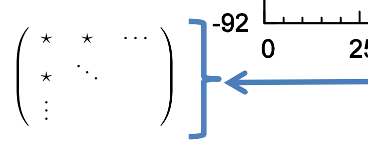
Hamiltonian kernel

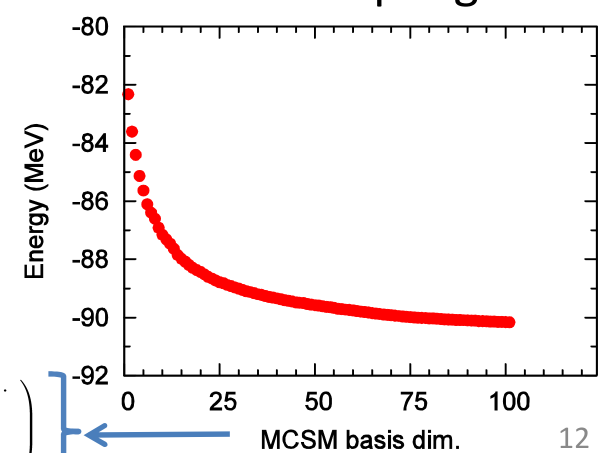


$$|\phi(\sigma)\rangle = \prod_n e^{-\Delta\beta h(\vec{\sigma}_n)} |\phi\rangle$$

$$h(\vec{\sigma}_n) = h_{HF} + \sum_\alpha \sigma_{\alpha n} O_\alpha$$







L. Liu, T. Otsuka, N. Shimizu, Y. Utsuno, R. Roth, Phys. Rev C86, 014302 (2012)

Feasibility study of MCSM for no-core calculations

PHYSICAL REVIEW C **86**, 014302 (2012)

No-core Monte Carlo shell-model calculation for ^{10}Be and ^{12}Be low-lying spectra

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Robert Roth
Institut für Kernphysik, Technische Universität Darmstadt, D-64289 Darmstadt, Germany
(Received 24 April 2011; revised manuscript received 1 June 2012; published 3 July 2012)

Recent developments in the MCSM

- Energy minimization by the CG method
  - N. Shimizu, Y. Utsuno, T. Mizusaki, M. Honma, Y. Tsunoda & T. Otsuka, Phys. Rev. C85, 054301 (2012)
- Efficient computation of TBMEs
  - Y. Utsuno, N. Shimizu, T. Otsuka & T. Abe, Compt. Phys. Comm. 184, 102 (2013)
- Energy variance extrapolation
  - N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe & M. Honma, Phys. Rev. C82, 061305 (2010)

- Summary of recent MCSM techniques
  - N. Shimizu, T. Abe, T. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma, T. Otsuka, Prog. Theor. Exp. Phys. 01A205 (2012)

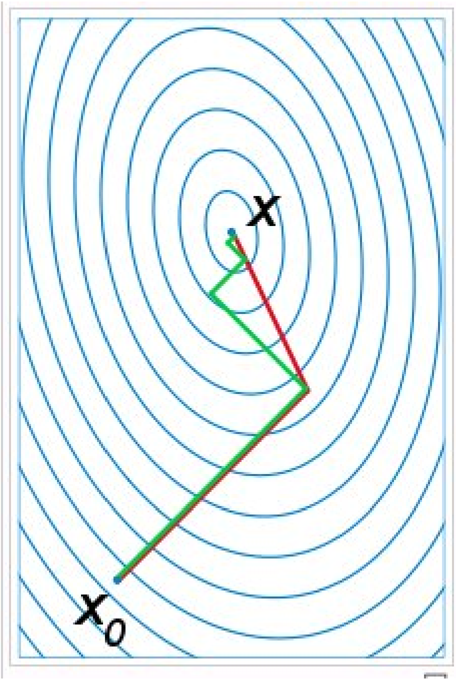
N. Shimizu, Y. Utsuno, T. Mizusaki, M. Honma, Y. Tsunoda, T. Otsuka, Phys. Rev. C85, 054301 (2012)

Energy minimization by Conjugate Gradient method

$$\left|\Psi(D)\right\rangle = \sum_{n=1}^{N_B} c_n \sum_{K=-J}^{J} g_K P_{MK}^{J,\Pi} \left|\phi(D^{(n)})\right\rangle$$

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

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



Conjugate gradient taken from wikipedia

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

Step1 : Generate basis candidate by auxiliary field technique stochastically

$$\left|\phi(\sigma)\right\rangle = \prod e^{\Delta\beta \cdot h(\sigma)} \cdot \left|\phi^{(0)}\right\rangle$$

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 until the energy converges

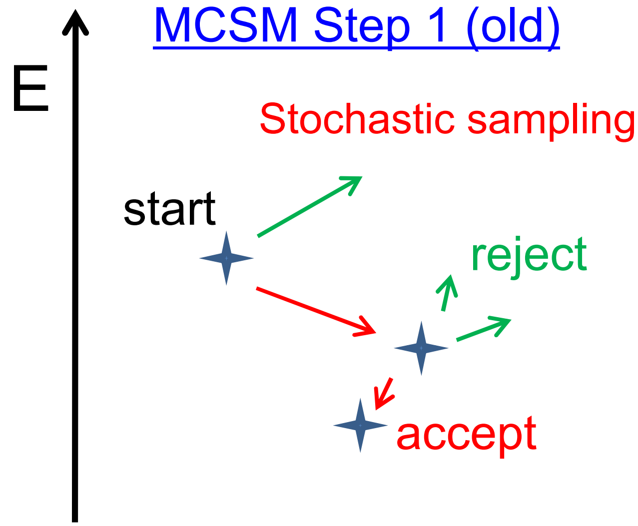
Few Determinant Approximation
M. Honma, B.A.Brown, T. Mizusaki, and T. Otsuka
Nucl. Phys. A 704, 134c (2002)

Hybrid Multi-Determinant
G. Puddu, Acta Phys. Polon. B42, 1287 (2011)

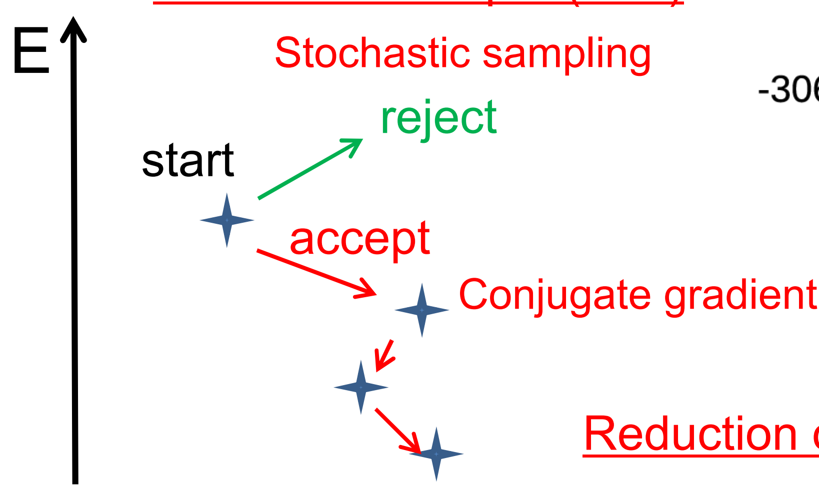
VAMPIR
K.W. Schmid, F. Glummer, M. Kyotoku, and A. Faessler
Nucl. Phys. A 452, 493 (1986)

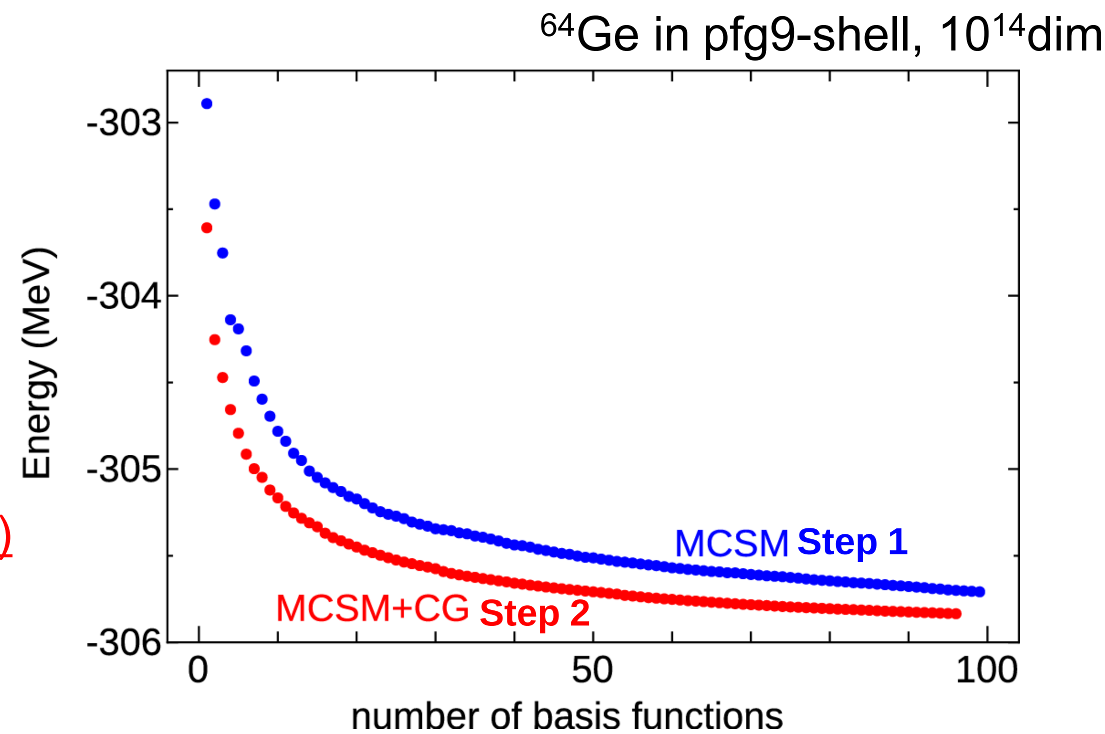
Energy minimization by Conjugate Gradient method

MCSM Step 1 (old)



MCSM+CG Step 2 (new)





Stochastic sampling before conjugate gradient to minimize the expectation value energy

Reduction of the number of basis function roughly 30%

Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, Compt. Phys. Comm. 184, 102 (2013)

Efficient computation of the TBMEs

- hot spot: Computation of the TBMEs

(w/o projections, for simplicity)

$$\frac{\langle\Phi'|V|\Phi\rangle}{\langle\Phi'|\Phi\rangle} = \frac{1}{2}\sum_{ijkl}\bar{v}_{ijkl}\rho_{ki}\rho_{lj}$$

c.f.) Indirect-index method (list-vector method)

- Utilization of the symmetry

$$j_z(i)+j_z(j) = j_z(k)+j_z(l) \rightarrow j_z(i)-j_z(k) = -(j_z(j)-j_z(l)) \equiv \Delta m$$

$$\sum_{ijkl}\bar{v}_{ijkl}\rho_{ki}\rho_{lj} = \sum_{\Delta m}\left[\sum_{a\in J_z(a)=-\Delta m}\tilde{\rho}_a\left(\sum_{b\in J_z(b)=\Delta m}\tilde{v}_{ab}\tilde{\rho}_b\right)\right]$$

$\bar{v}_{ijkl} \rightarrow \tilde{v}_{ab}$ $\rho_{ki} \rightarrow \tilde{\rho}_a$ $\rho_{lj} \rightarrow \tilde{\rho}_b$

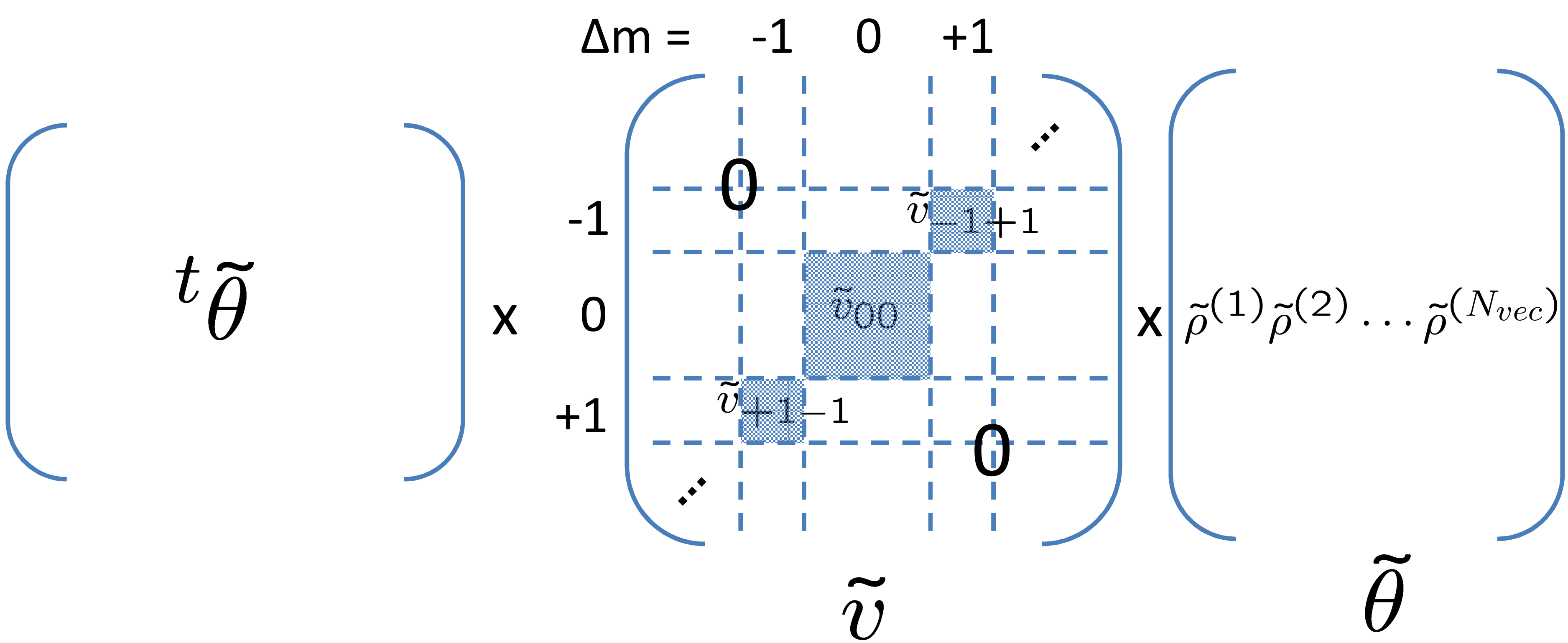
sparse dense

Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, Compt. Phys. Comm. 184, 102 (2013)

Schematic illustration of the computation of TBMEs

- Matrix-matrix method

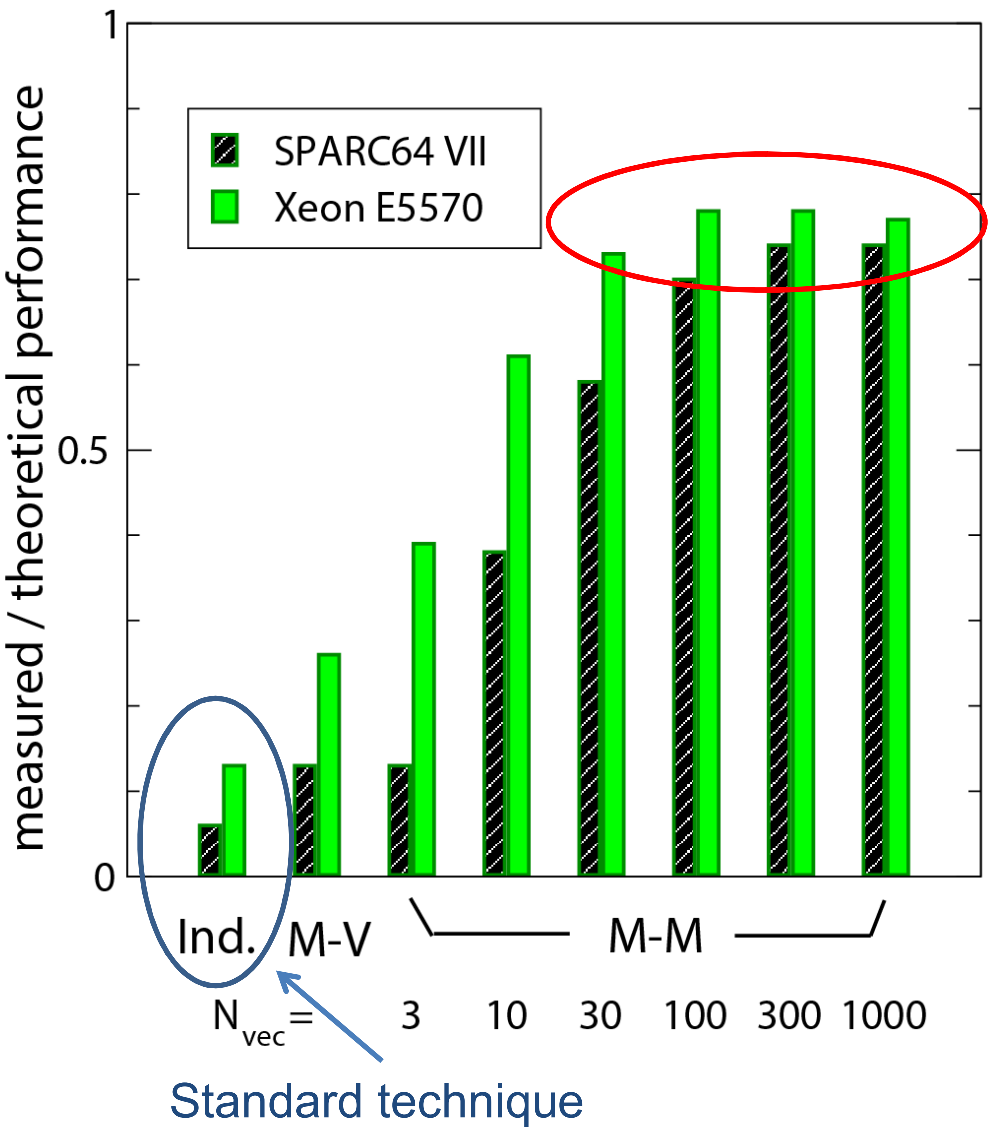
$$\sum_{ijkl} \bar{v}_{ijkl}\rho_{ki}\rho_{lj} = \sum_{\Delta m}\left[\sum_{a\in J_z(a)=-\Delta m}\tilde{\rho}_a\left(\sum_{b\in J_z(b)=\Delta m}\tilde{v}_{ab}\tilde{\rho}_b\right)\right]$$



→ BLAS Level 3

Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, Compt. Phys. Comm. 184, 102 (2013)

Tuning of the density matrix product



Nshell = 5

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

SPARC64 requires large N_{bunch} in comparison to Xeon

Matrix product e.g.
(390 x 390) x (390 x $2N_{bunch}$)

N_{bunch} controllable tuning parameter
chunk size

Extrapolations in the MCSM

- Two steps of the extrapolation

  1. Extrapolation of our MCSM (approx.) results to the FCI (exact) results in fixed model space

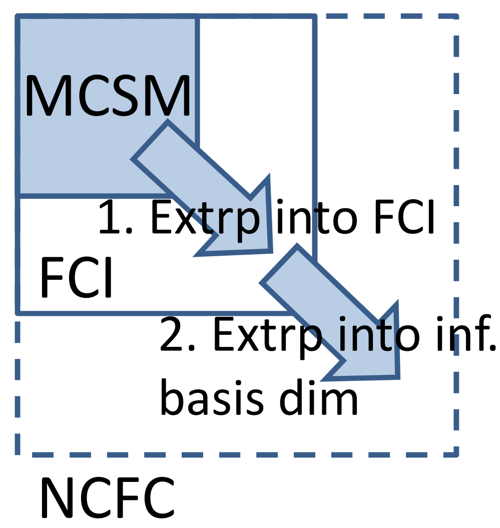
     Energy-variance extrapolation

  N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe, & M. Honma, Phys. Rev. C82, 061305(R) (2010)

  2. Extrapolation into the infinite model space

     Exponential fit w.r.t. Nmax in the NCFC

     Not applied in the MCSM, so far…



Energy-variance extrapolation

- Originally proposed in condensed matter physics

  Path Integral Renormalization Group method

  M. Imada and T. Kashima, J. Phys. Soc. Jpn 69, 2723 (2000)

- Imported to nuclear physics

  Lanczos diagonalization with particle-hole truncation

  T. Mizusaki and M. Imada Phys. Rev. C65 064319 (2002)

  T. Mizusaki and M. Imada Phys. Rev. C68 041301 (2003)

  single deformed Slater determinant

  T. Mizusaki, Phys. Rev. C70 044316 (2004)

→ Apply to the MCSM (multi deformed SDs)

N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe & M. Honma, Phys. Rev. C82, 061305 (2010)

Numerical effort

8-folded loop
~O(Nsps^8)

$$\frac{\langle\Phi'|\hat{V}^2|\Phi\rangle}{\langle\Phi'|\Phi\rangle} = \sum_{ijkl\alpha\beta\gamma\delta} \bar{v}_{ijkl}\bar{v}_{\alpha\beta\gamma\delta}\left[\frac{1}{4}(1-\rho)_{k\alpha}(1-\rho)_{l\beta}\rho_{\gamma i}\rho_{\delta j} + \rho_{\gamma\alpha}(1-\rho)_{l\beta}\rho_{ki}\rho_{\delta j} + \frac{1}{4}\rho_{ki}\rho_{lj}\rho_{\gamma\alpha}\rho_{\delta\beta}\right]$$

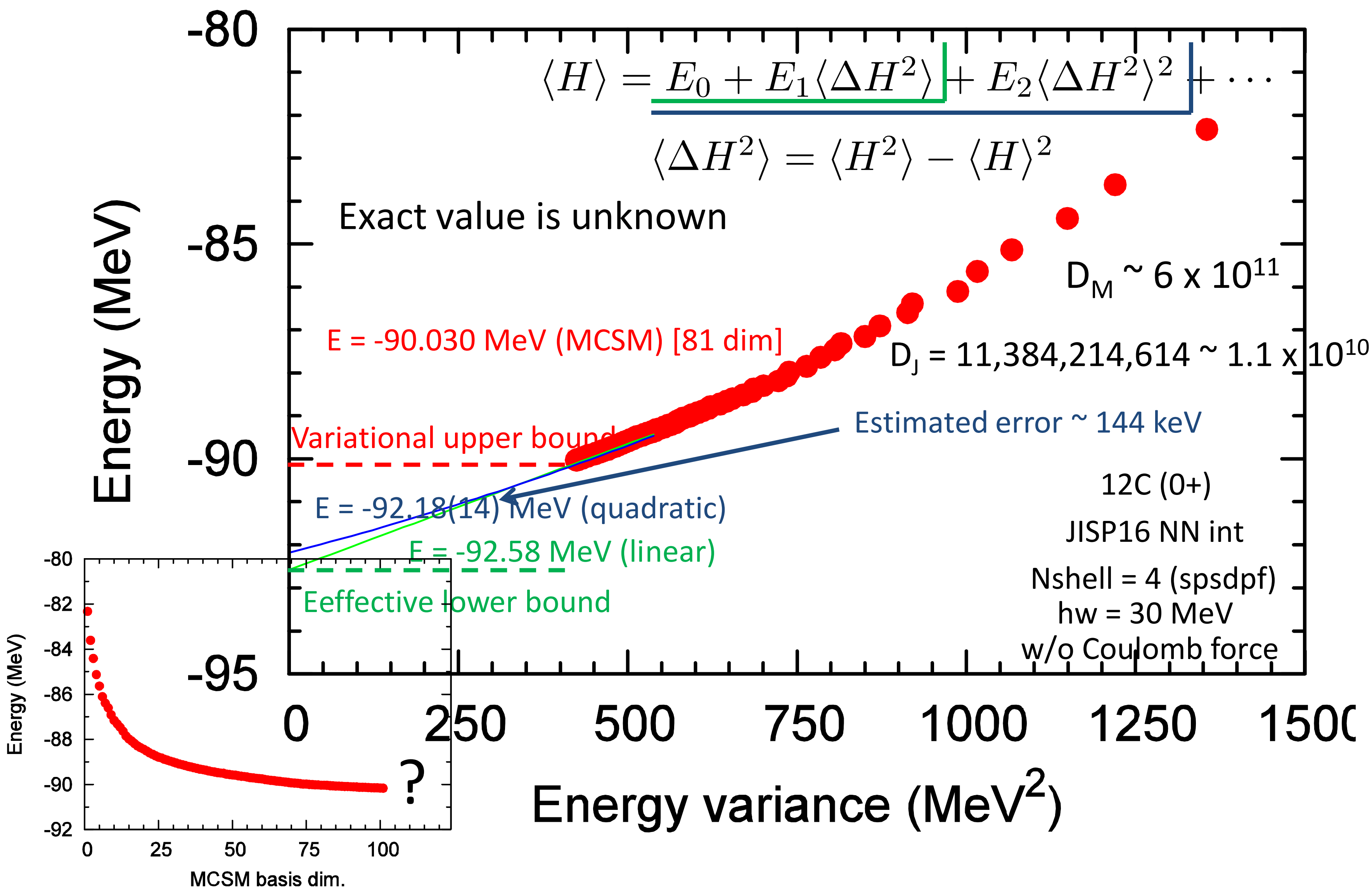
$$= \frac{1}{4}\sum_{ij\alpha\beta}\left(\sum_{kl}\bar{v}_{ijkl}(1-\rho)_{k\alpha}(1-\rho)_{l\beta}\right)\left(\sum_{\gamma\delta}\bar{v}_{\alpha\beta\gamma\delta}\rho_{\gamma i}\rho_{\delta j}\right) + \mathrm{Tr}(\Gamma(1-\rho)\Gamma\rho) + \frac{1}{4}[\mathrm{Tr}(\rho\Gamma)]^2$$

6-folded loop
~O(Nsps^6)

$$\rho_{\beta\alpha} = \frac{\langle\Phi'|c^\dagger_\alpha c_\beta|\Phi\rangle}{\langle\Phi'|\Phi\rangle} \quad \Gamma_{ik} = \sum_{jl}\bar{v}_{ijkl}\rho_{lj} \quad \frac{\langle\Phi'|V|\Phi\rangle}{\langle\Phi'|\Phi\rangle} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\bar{v}_{\alpha\beta\gamma\delta}\rho_{\gamma\alpha}\rho_{\delta\beta}$$

N. Shimizu, Y. Utsuno, T.Mizusaki, T. Otsuka, T. Abe, & M. Honma, Phys. Rev. C82, 061305(R) (2010)

Energy-variance Extrapolation of 12C 0+ g.s. Energy



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BERKELEY LAB Lawrence Berkeley National Laboratory

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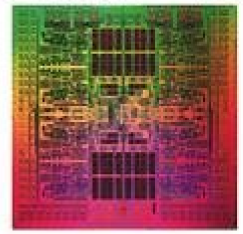
	NAME	SPECS	SITE	COUNTRY	CORES	RMAX PFLOP/S	POWER MW
1	TITAN	Cray XK7, Operon 6274 16C 2.2 GHz + Nvidia Kepler GPU, Custom interconnect	DOE/OS/ORNL	USA	560,640	17.6	8.3
2	SEQUOIA	IBM BlueGene/Q, Power BQC 16C 1.60 GHz, Custom interconnect	DOE/NNSA/LLNL	USA	1,572,864	16.3	7.9
3	K COMPUTER	Fujitsu SPARC64 VIIIfx 2.0GHz, Custom interconnect	RIKEN AICS	Japan	705,024	10.5	12.7
4	MIRA	IBM BlueGene/Q, Power BQC 16C 1.60 GHz, Custom interconnect	DOE/OS/ANL	USA	786,432	8.16	3.95
5	JUQUEEN	IBM BlueGene/Q, Power BQC 16C 1.60 GHz, Custom interconnect	Forschungszentrum Jülich	Germany	393,216	4.14	1.97

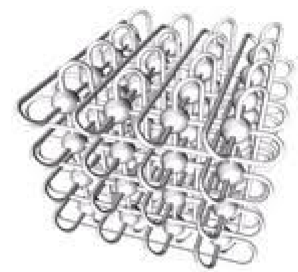
SPARC64 TM VIIIfx



128 GFLOPS/CPU
(8 cores/CPU)

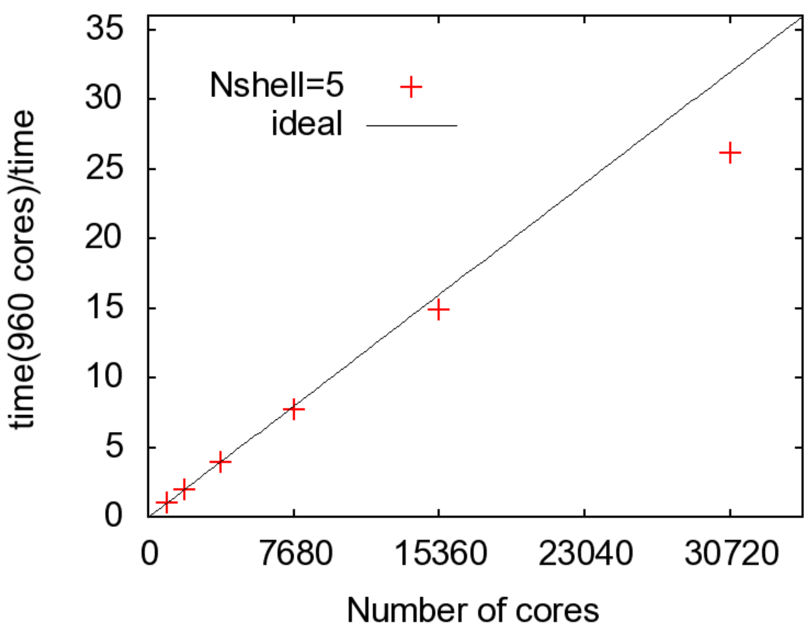
PERFORMANCE DEVELOPMENT

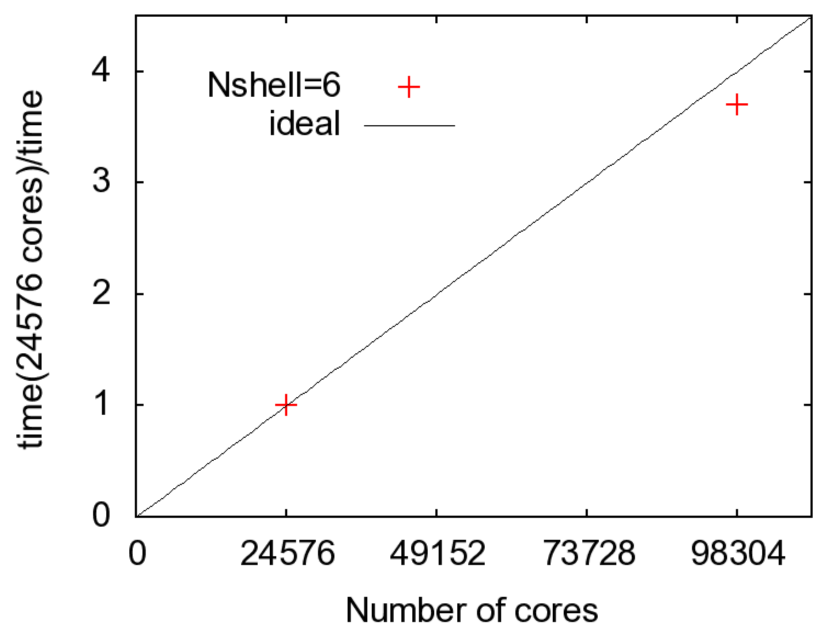
Tofu inter-connection
6D Mesh/Torus



Parallel efficiency @ K-computer

- Optimization of 15th basis dim. of the 4He (0+) w.f. in Nshell=5 w/ 100 CG iterations
- Optimization of 48th basis dim. of the 4He (0+) w.f. in Nshell=6 w/ 100 CG iterations

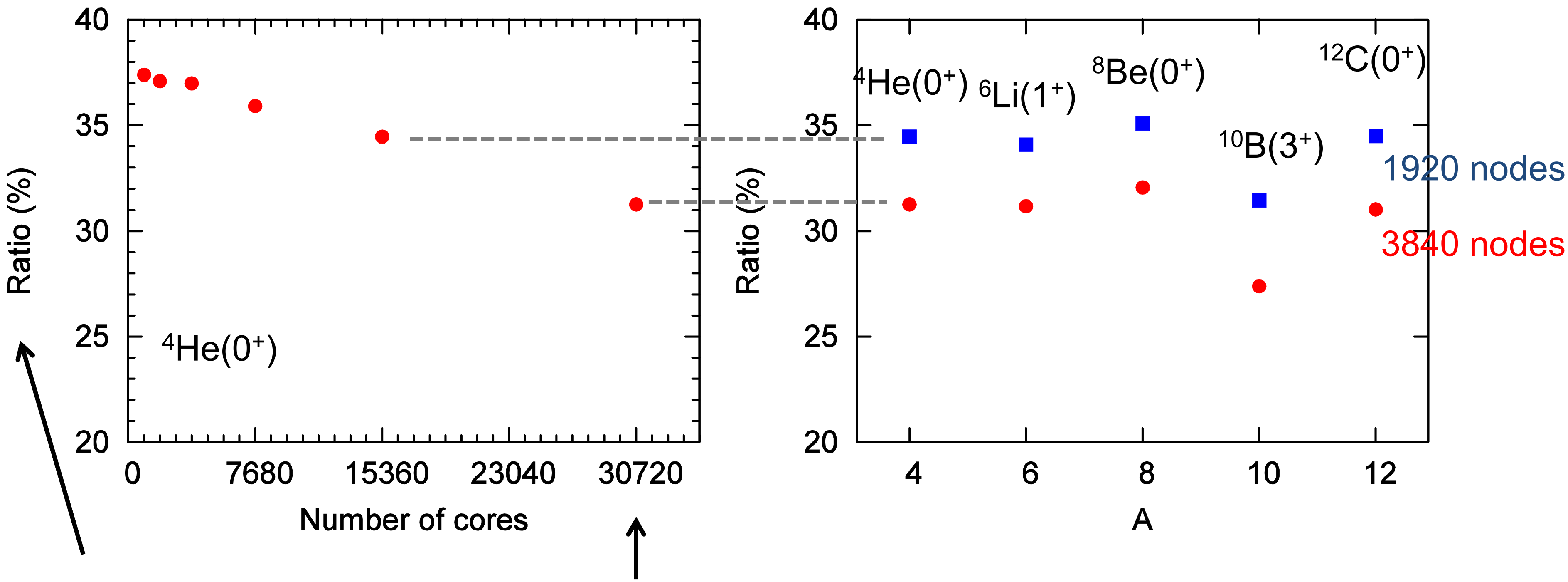




Note: it is a tentative result by early access to the K-computer at AICS, RIKEN.

Ratio to the peak performance @ K computer (phase IV-1)

- Test case: Optimization of 15th basis dim. of the w.f. in Nshell=5 w/ 100 CG iterations w/o preprocessing (MPI/OpenMP, 8 threads)



Ratio to the peak performance

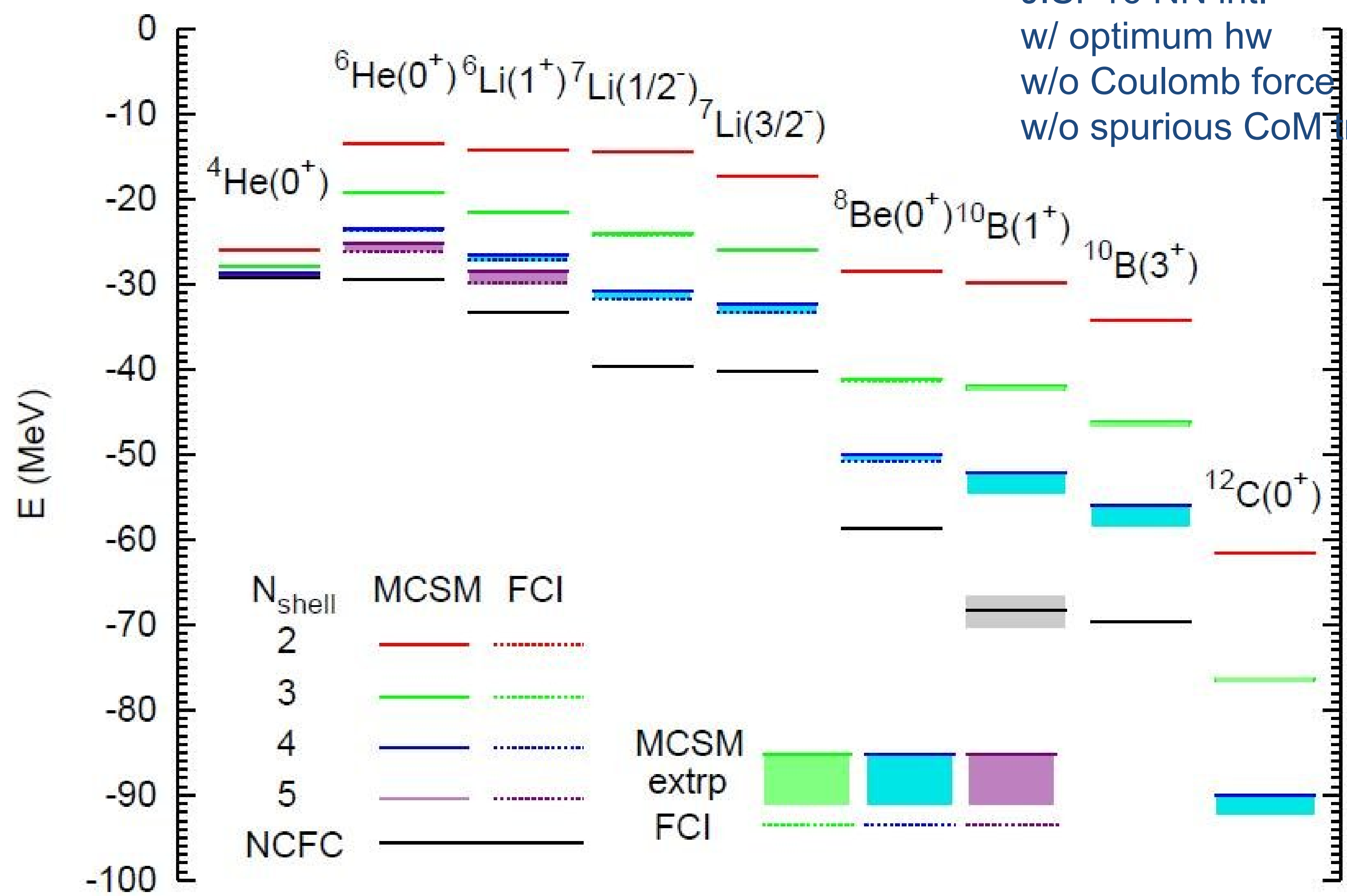
3840 nodes
(8 cores/node)

Note: it is a tentative result by early access to the K-computer at AICS, RIKEN.

T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary, Phys Rev C86, 054301 (2012)

Energies of the Light Nuclei

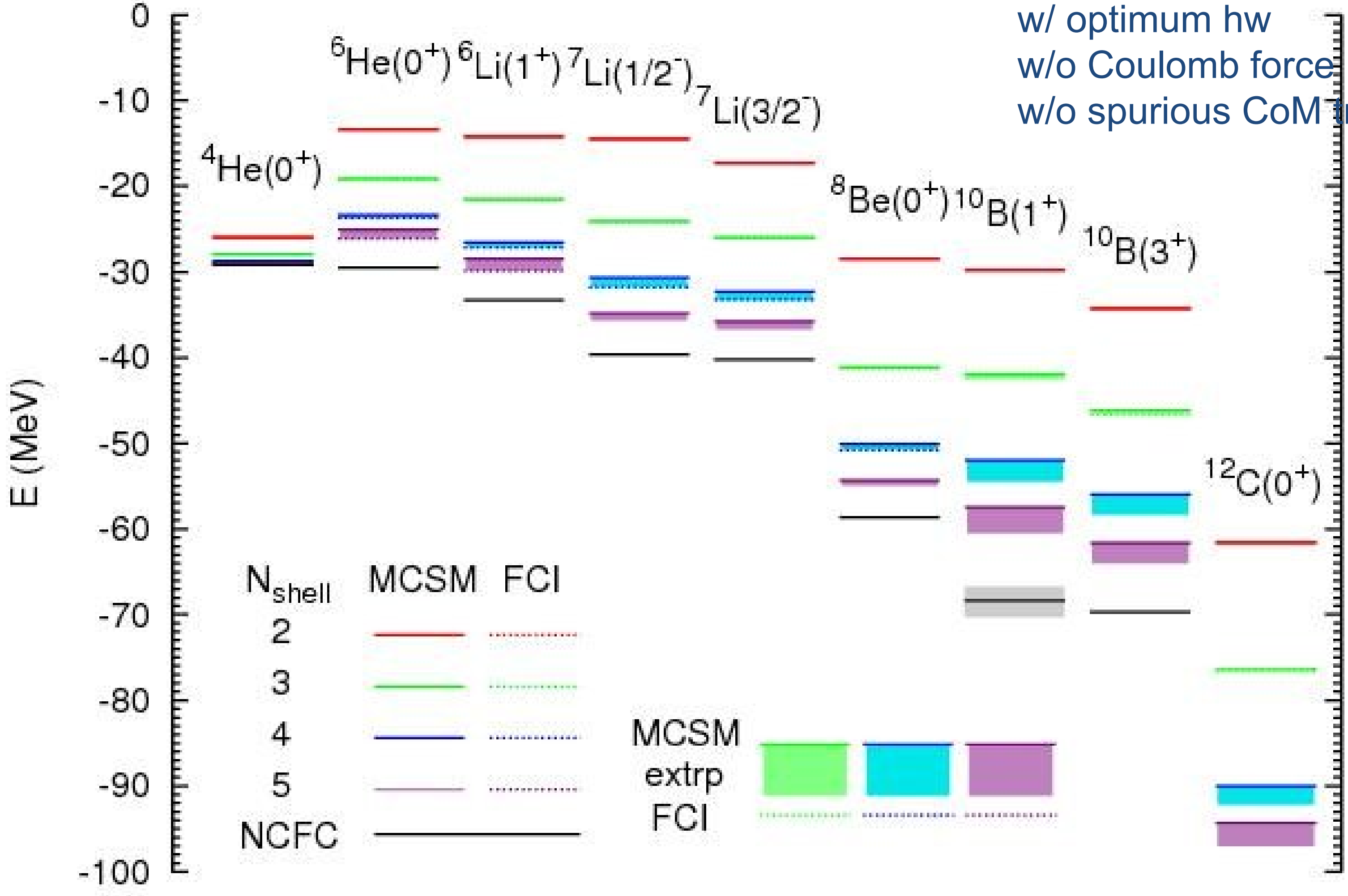
JISP16 NN int.
w/ optimum hw
w/o Coulomb force
w/o spurious CoM treatment



Preliminary

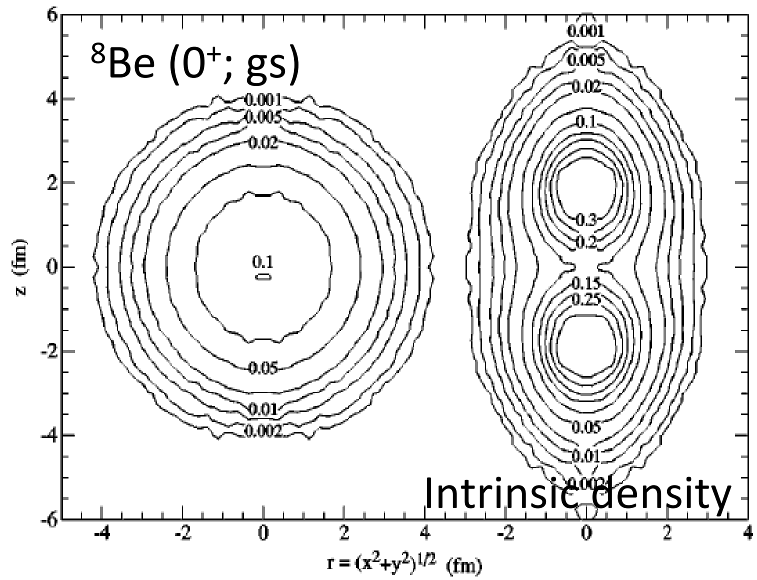
Energies of the Light Nuclei

JISP16 NN int.
w/ optimum hw
w/o Coulomb force
w/o spurious CoM treatment



Density Profile from ab initio calc.

VMC



- Green's function Monte Carlo (GFMC)
  - "Intrinsic" density is constructed by aligning the moment of inertia among samples

R. B. Wiringa, S. C. Pieper, J. Carlson & V. R. Pandharipande, Phys. Rev. C62, 014001 (2000)

- No-core full configuration (NCFC)
  - Translationally-invariant density is obtained by deconvoluting the intrinsic & CM w.f.

C. Cockrell J. P. Vary & P. Maris, Phys. Rev. C86, 034325 (2012)

^{8}Li (2$^+$; gs)

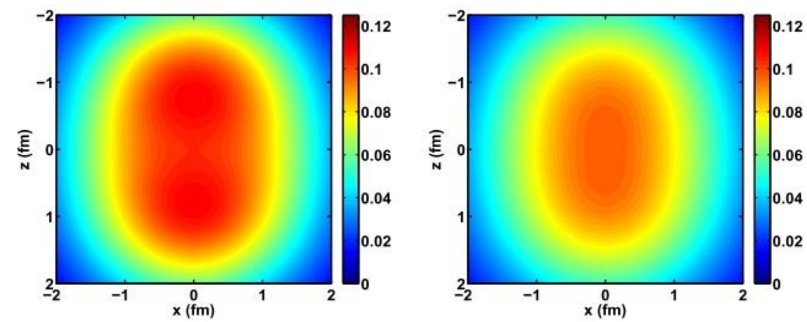


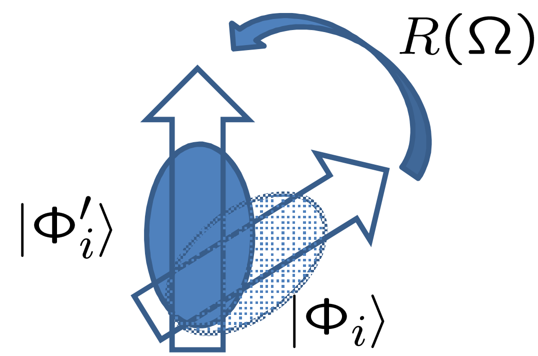
FIG. 12: (Color online) The $y = 0$ slice of the translationally-invariant neutron density (left) of the 2^+ gs of ^{8}Li. The space-fixed density for the same state is on the right. These densities were calculated at $N_{\max} = 12$ and $\hbar\Omega = 12.5$ MeV.

Translationally-invariant neutron density

Space-fixed neutron density

N. Shimizu, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma, T. Otsuka,
Progress in Theoretical and Experimental Physics, 01A205 (2012)

How to construct an “intrinsic” density from MCSM w.f.

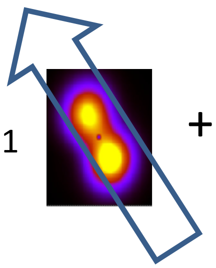
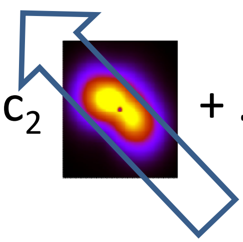
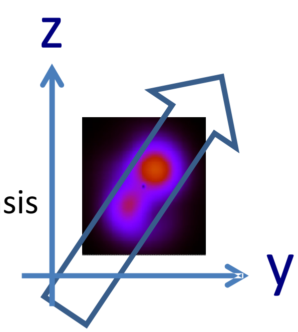


Rotation by diagonalizing Q-moment
(Qzz > Qyy > Qxx)

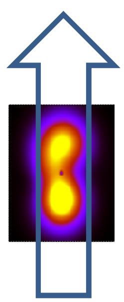
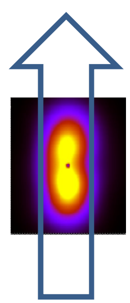
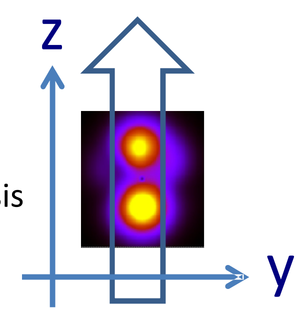
- MCSM wave function

$$|\Psi\rangle = \sum_{i=1}^{N_{basis}} c_i P^J P^\pi |\Phi_i\rangle$$

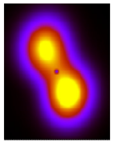
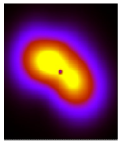
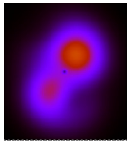
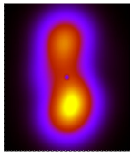
- Wave function w/o the projections

$$\sum_{i=1}^{N_{basis}} c_i |\Phi_i\rangle = c_1$$  $+ c_2$  $+ \ldots + c_{Nbasis}$ 

- Wave function w/o the projection w/ the alignment of Q-moment

$$\sum_{i=1}^{N_{basis}} c_i |\Phi'_i\rangle = c_1$$  $+ c_2$  $+ \ldots + c_{Nbasis}$ 

Density profiles in MCSM

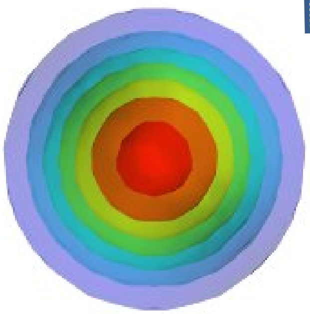
$|\Phi\rangle = \sum_{i=1}^{N_{basis}} c_i|\Phi_i\rangle =$ c_1  $+ c_2$  $+ c_3$  $+ c_4$  $+ \ldots$

Angular-momentum projection

$$|\Psi\rangle = \sum_{i=1}^{N_{basis}} c_i P^J P^\pi |\Phi_i\rangle$$

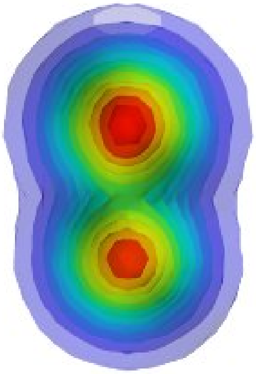
Rotation of each basis

$$|\Phi'\rangle = \sum_{i=1}^{N_{basis}} c_i R(\Omega_i)|\Phi_i\rangle$$



<u>Laboratory frame</u>

^{8}Be 0^+ g.s. state



<u>"Intrinsic" (body-fixed) frame</u>

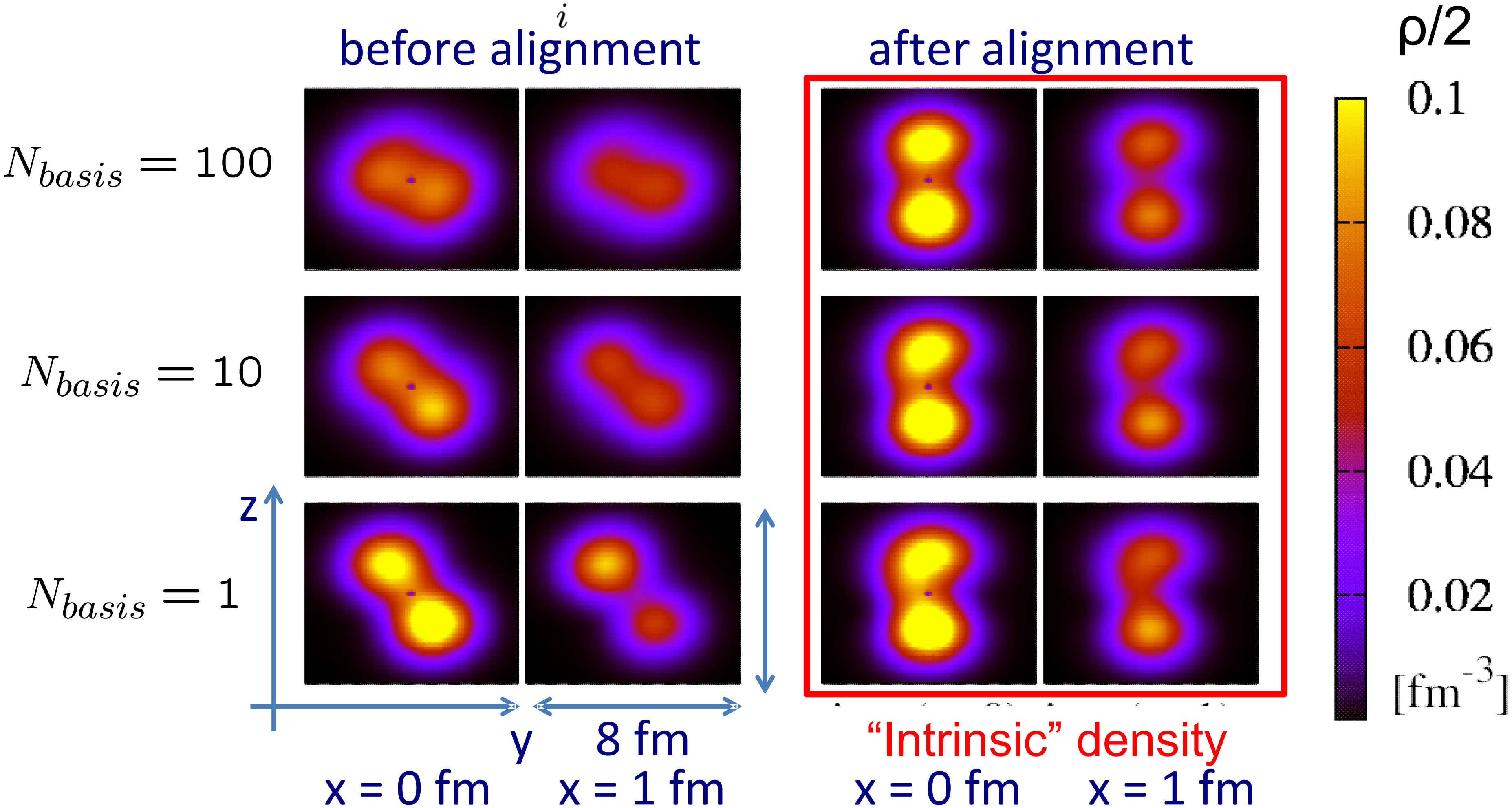
N. Shimizu, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma, T. Otsuka,
Progress in Theoretical and Experimental Physics, 01A205 (2012)

N. Shimizu, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma, T. Otsuka, Progress in Theoretical and Experimental Physics, 01A205 (2012)

Density profile of ^{8}Be 0^{+} g.s. state from MCSM w.f.

- Test calculation of the density by using the MCSM w.f. in Nshell = 4

$$\rho(\vec{r}) = \langle \Phi(\{\vec{r}_i{}'\}) | \sum_i \delta(\vec{r} - \vec{r}_i{}') | \Phi(\{\vec{r}_i{}'\}) \rangle$$



Summary

- MCSM can be applied to no-core calculations of the p-shell nuclei.

  - Benchmarks for the p-shell nuclei have been performed and gave good agreements w/ FCI results.

  - Density profiles from MCSM many-body w.f. are preliminarily investigated and the cluster-like distributions are reproduced.

Perspective

- MCSM algorithm/computation

  - Extension to larger model spaces (Nshell = 6, 7, …), extrapolation to infinite model space, & comparison with another truncations

  - Inclusion of the 3-body force (thru. effective 2-body force)

- Physics

  - Cluster(-like) states (He & Be isotopes, 12C Hoyle state, …)

  - sd-shell nuclei

Happy birthday, James!!