International Workshop
"Nuclear Theory in the Supercomputing Era"

No-core Monte Carlo shell model in light nuclei

Takashi Abe (U of Tokyo)

Pacific National University,
Khabarovsk, Russia
June 23 – 28, 2014

Collaborators

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

Ab inito approaches

- Major challenge of nuclear physics

  - Understand the nuclear structure & reactions from *ab-initio* calculations w/ realistic nuclear forces (potentials)

  - *ab-initio* approaches in nuclear structure physics (A > 4):

    GFMC, NCSM (A ~ 12-14), CC (sub-shell closure +/- 1,2),

    Green's Function 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, J.P. Draayer (Louisiana 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 uncertainties:
  – Nuclear forces (interactions btw/among nucleons)

    In principle, they should be obtained (directly) by QCD.
  – Many-body methods

    CI: Finite basis space (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 matrix

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

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

Large sparse matrix (in M-scheme)

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

non-zero MEs

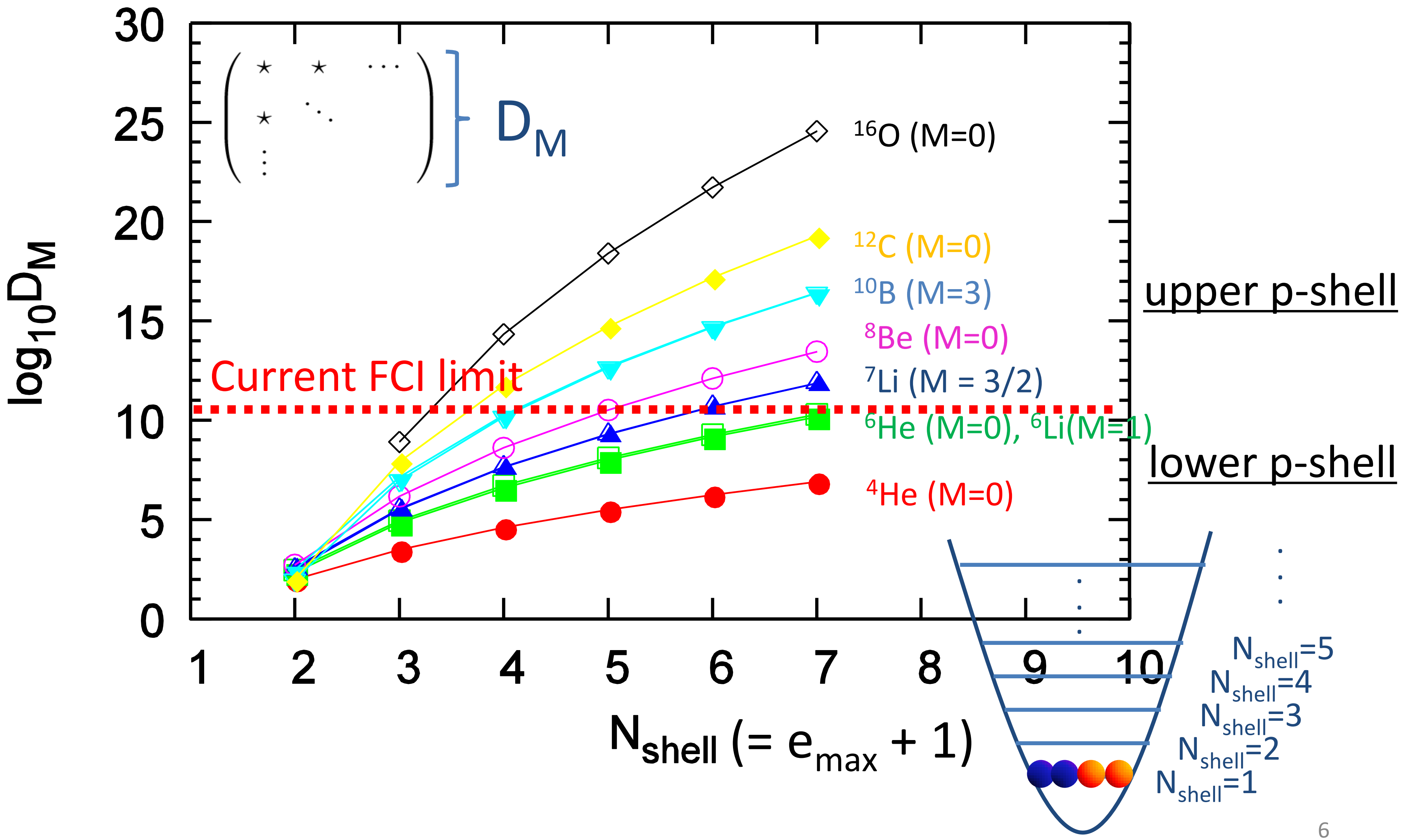
$$\sim \mathcal{O}(10^{13-14})$$

Slater determinants

$$\left\{ \begin{array}{lcl} |\Psi_1\rangle & = & a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma \cdots |-\rangle \\ |\Psi_2\rangle & = & a^\dagger_{\alpha'} a^\dagger_{\beta'} a^\dagger_{\gamma'} \cdots |-\rangle \\ |\Psi_3\rangle & = & \cdots \\ & \vdots & \end{array} \right.$$

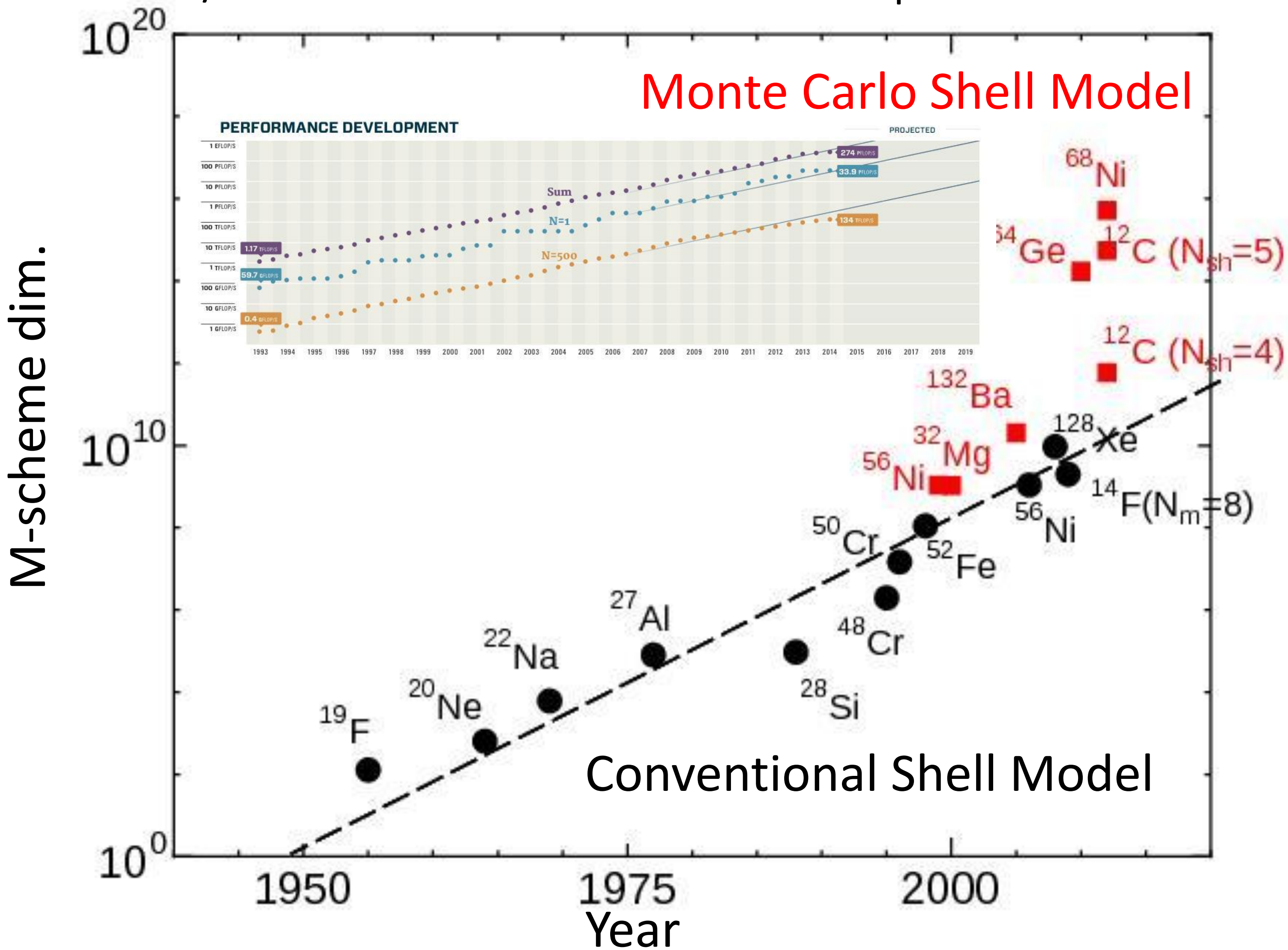
M-scheme dimension in N_{shell} truncation

No-core calculations

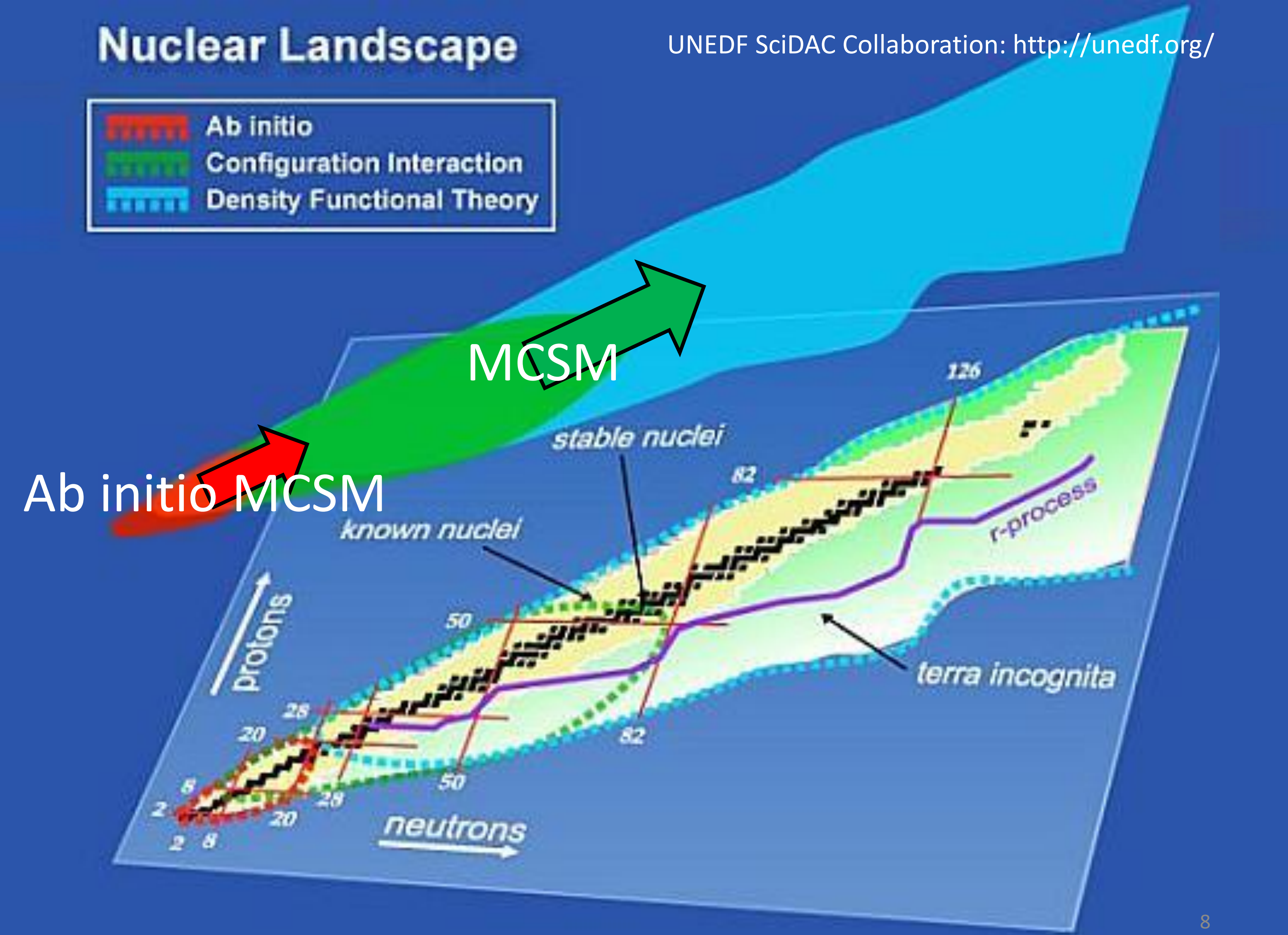


Historical evolution/development of the MCSM

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



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



Nuclear Landscape
UNEDF SciDAC Collaboration: http://unedf.org/
Ab initio
Configuration Interaction
Density Functional Theory
MCSM
Ab initio MCSM
stable nuclei
known nuclei
terra incognita
r-process
protons
neutrons
126
82
50
28
20
8
2
82
50
28
20
8
2

Monte Carlo shell model (MCSM)

- Importance truncation

Standard shell model

$$H = \begin{pmatrix} \star & \star & \star & \star & \star & \cdots \\ \star & \star & \star & \star & & \\ \star & \star & \star & & & \\ \star & \star & & \ddots & & \\ \star & & & & & \\ \vdots & & & & & \end{pmatrix} \quad \xrightarrow{\text{Diagonalization}} \quad \begin{pmatrix} E_0 & & & & 0 \\ & E_1 & & & \\ & & E_2 & & \\ & & & \ddots & \\ 0 & & & & \end{pmatrix}$$

All Slater determinants

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

Monte Carlo shell model

$$H \sim \begin{pmatrix} \star & \star & \cdots \\ \star & \ddots & \\ \vdots & & \end{pmatrix} \quad \xrightarrow{\text{Diagonalization}} \quad \begin{pmatrix} E'_0 & & 0 \\ & E'_1 & \\ 0 & & \ddots \end{pmatrix}$$

Important bases stochastically selected

$d_{MCSM} < O(100)$

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

SM Hamiltonian & MCSM many-body w.f.

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

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

- Eigenvalue problem

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

- MCSM many-body wave function & basis function

$$|\Psi(J,M,\pi)\rangle = \sum_i^{N_{basis}} f_i |\Phi_i(J,M,\pi)\rangle \qquad |\Phi(J,M,\pi)\rangle = \sum_K g_K P_{MK}^J P^\pi |\phi\rangle$$

These coeff. are obtained by the diagonalization.

- Deformed SDs

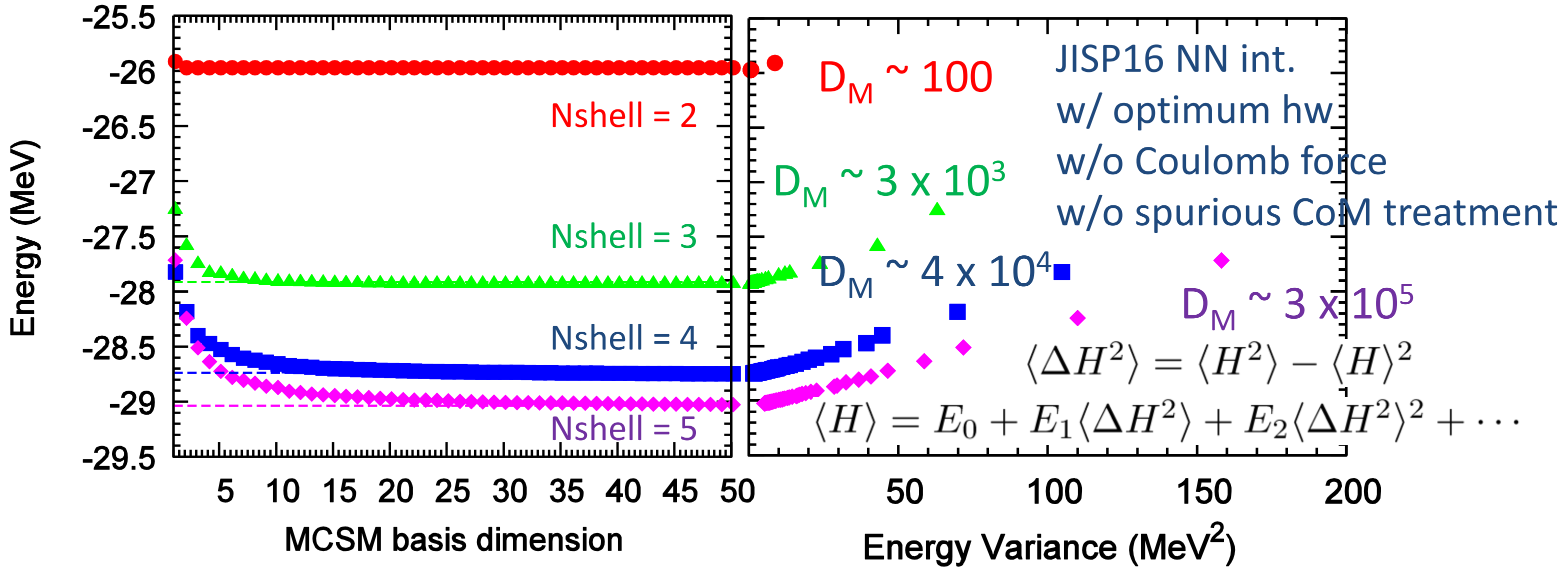
This coeff. is obtained by a stochastic sampling & CG.

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

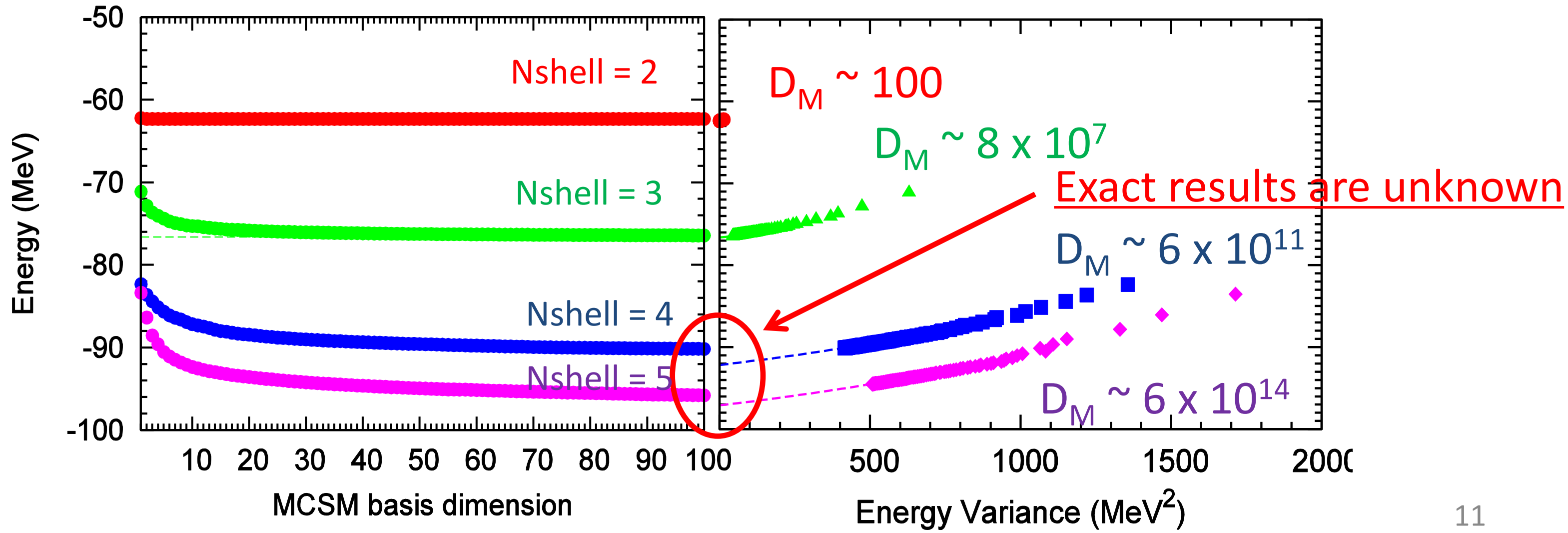
($c_\alpha^\dagger$ … spherical HO basis)

Energies w.r.t. # of basis & energy variance

^{4}He(0^+;gs)



^{12}C(0^+;gs)



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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(Received 24 April 2011; revised manuscript received 1 June 2012; published 3 July 2012)

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

~ 30% reduction of # basis

- Efficient computation of TBMEs
  - Y. Utsuno, N. Shimizu, T. Otsuka & T. Abe, Compt. Phys. Comm. 184, 102 (2013)

~ 80% of the peack performance

(~ 10-20% in the old MCSM)

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

Evaluation of exact eignvalue w/ error estimate

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

TOP500 JUNE 2014

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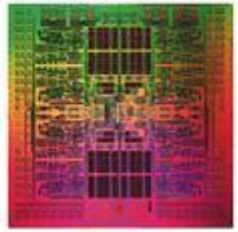
	NAME	SPECS	SITE	COUNTRY	CORES	RMAX PFLOP/S	POWER MW
1	Tianhe-2 (Milkyway-2)	NUDT, Intel Ivy Bridge (12C, 2.2 GHz) & Xeon Phi (57C, 1.1 GHz), Custom interconnect	NSCC Guangzhou	China	3,120,000	33.9	17.8
2	Titan	Cray XK7, Operon 6274 (16C 2.2 GHz) + Nvidia Kepler GPU, Custom interconnect	DOE/SC/ORNL	USA	560,640	17.6	8.2
3	Sequoia	IBM BlueGene/Q, Power BQC (16C 1.60 GHz), Custom interconnect	DOE/NNSA/LLNL	USA	1,572,864	17.2	7.9
4	K computer	Fujitsu SPARC64 VIIIfx (8C, 2.0GHz), Custom interconnect	RIKEN AICS	Japan	705,024	10.5	12.7
5	Mira	IBM BlueGene/Q, Power BQC (16C, 1.60 GHz), Custom interconnect	DOE/SC/ANL	USA	786,432	8.59	3.95

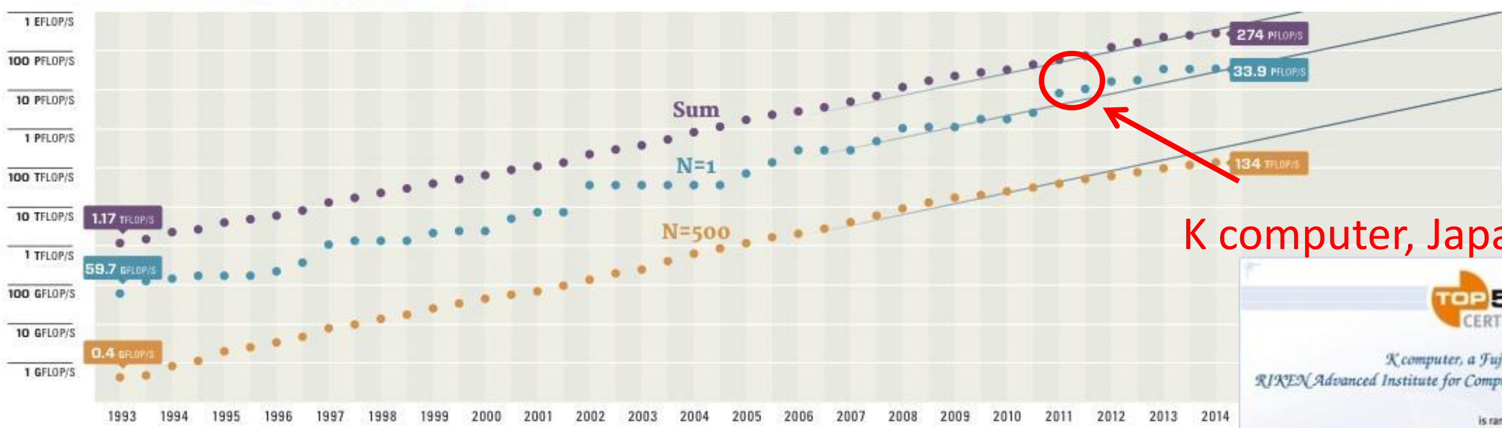
SPARC64 ™ VIIIfx



128 GFLOPS/CPU
(8 cores/CPU)

Tofu inter-connection
6D Mesh/Torus

PERFORMANCE DEVELOPMENT



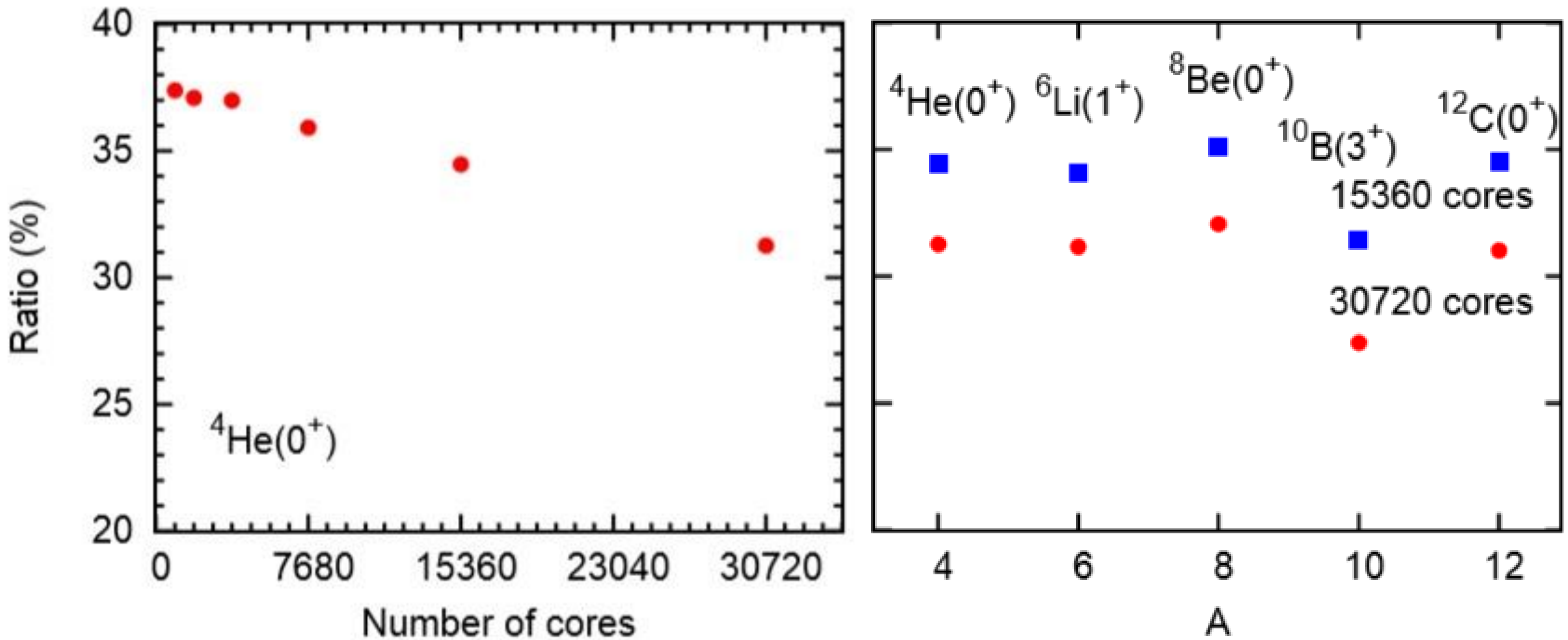
K computer, Japan

HPCI Strategic Program Field 5
"The origin of matter and the universe"

Peak performance on the K computer

Peak performance

- Optimization of 15th basis dim. of the w.f. in N_{shell} = 5 w/ 100 CG iterations (MPI/OpenMP, 8 threads)

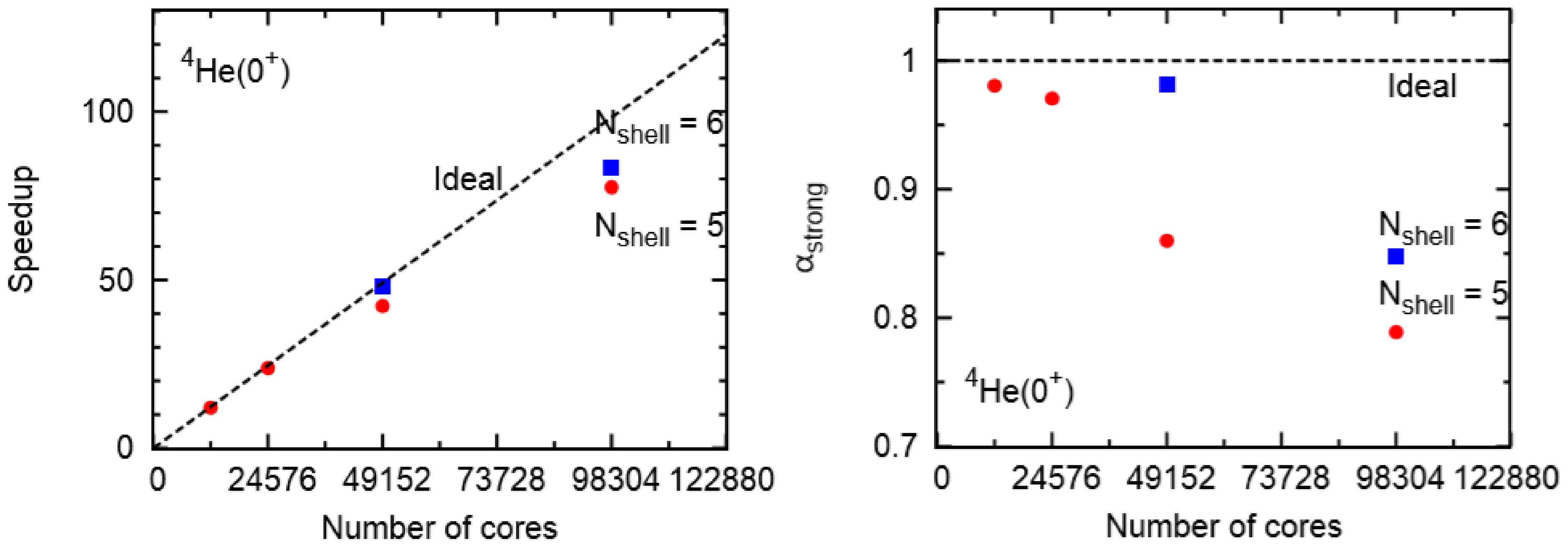


~30 % thru p-shell nuclei

Speed-up & strong scaling on the K computer

Speed-up (strong scaling)

- Optimization of 48th basis dim. of the $^4He\ (0^+)$ w.f. in $N_{shell} = 6$ w/ 100 CG iterations



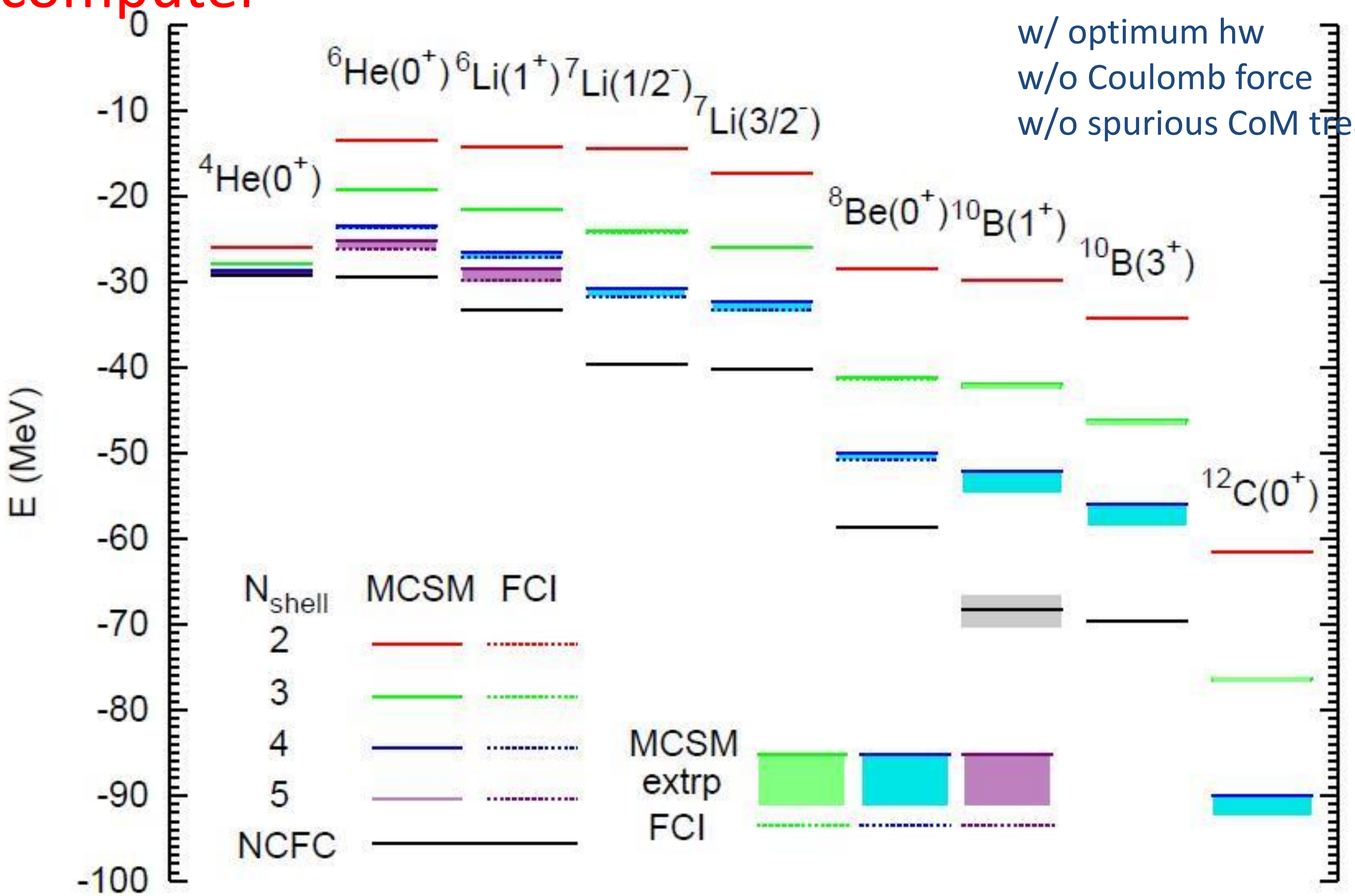
Scaling up to ~ 100,000 cores

Energies of the Light Nuclei

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

Pre K computer

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

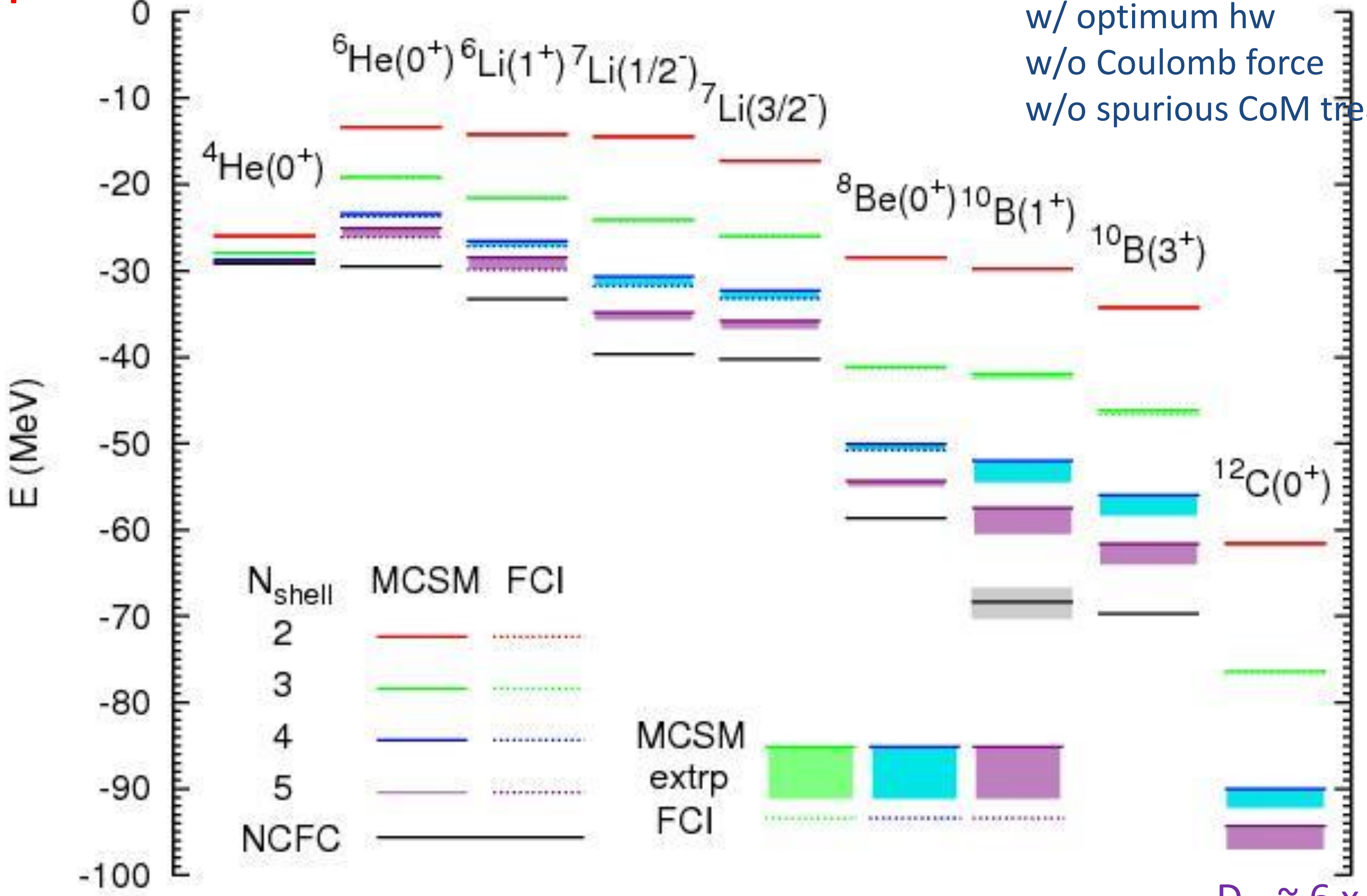


MCSM results w/ E-var extrp are consistent w/ FCI results

Energies of the Light Nuclei

K computer

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



$D_M \sim 6 \times 10^{14}$

Some MCSM results are not reachable in the current FCI

CPU time

core * hours

	N_{shell} = 2	N_{shell} = 3	N_{shell} = 4	N_{shell} = 5	N_{shell} = 6	N_{shell} = 7
$^{4}He\ (0^{+})$	1,300	2,000	2,400	10,000	70,000	400,000
$^{8}Be\ (0^{+})$	1,500	5,000	10,000	40,000	200,000	1,000,000
$^{12}C\ (0^{+})$	1,400	6,000	17,000	50,000	250,000	1,300,000
$^{16}O\ (0^{+})$	-------	6,000	15,000	70,000	280,000	1,400,000

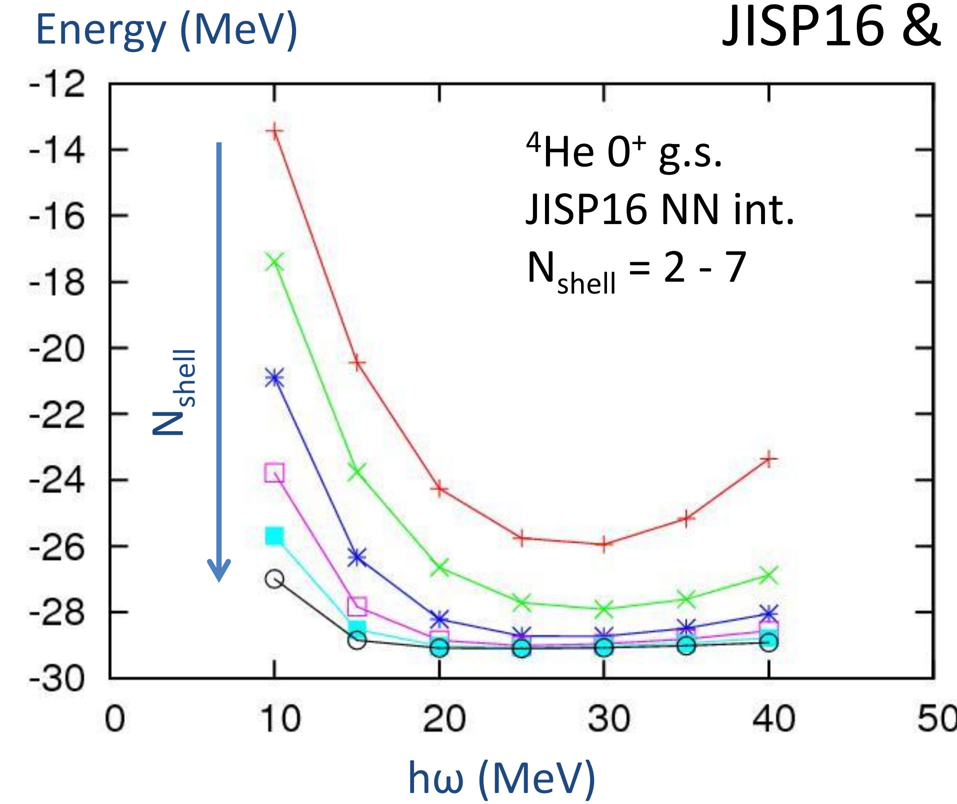
FX10 @ U of Tokyo

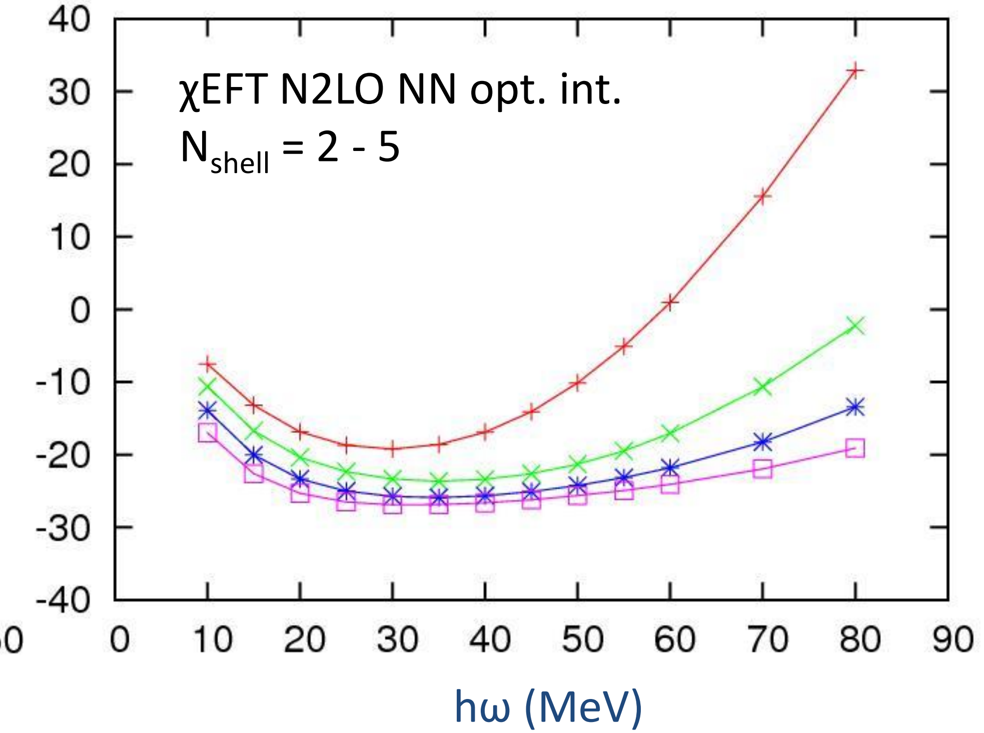
K computer

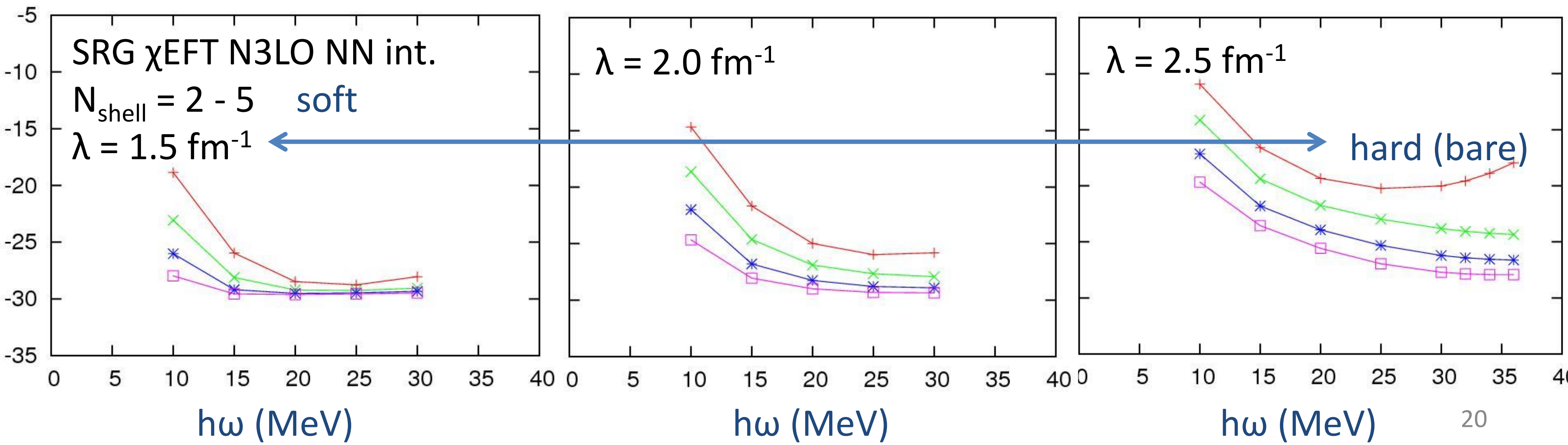
For 100 bases

JISP16 & χEFT NN int.

Preliminary







“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 uncertainties:
  – Nuclear forces (interactions btw/among nucleons)

    In principle, they should be obtained (directly) by QCD.
  – Many-body methods

    CI: Finite basis space (choice of basis function and truncation),

    we have to extrapolate to infinite basis dimensions

Extrapolations in the MCSM

- Two steps of the extrapolation

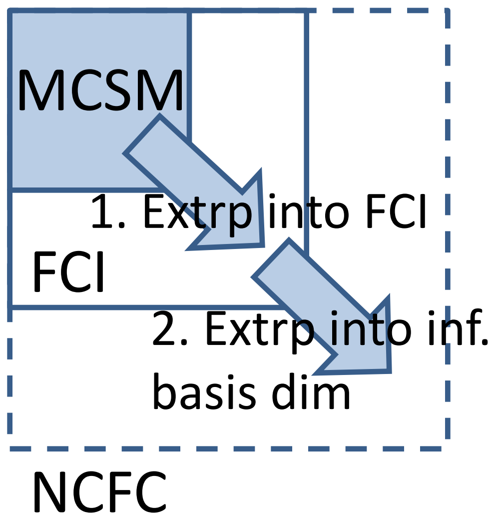
1. Extrapolation of our MCSM (approx.) results to the FCI (exact) results in fixed model space

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. N_{max} in the NCFC
   - IR- & UV-cutoff extrapolations

Not applied on the MCSM, so far…



Extrapolation to the infinite basis space

- Two ways of the extrapolation to the infinite basis space

1. Empirical exponential form (w/ fixed hw)

$$E(N) = E(N = \infty) + a\exp(-bN)$$

P. Maris, A. M. Shirokov, & J. P. Vary, Phys. Rev. C79, 014308 (2009)

2. Cutoff extrapolations

- IR-cutoff extrapolation (w/ UV-saturated data)

$$E(\lambda) = E(\lambda = 0) + a\exp(-b/\lambda)$$

- IR- & UV-cutoff extrapolations (w/ any data, ideally)

$$E(\lambda, \Lambda) = E(\lambda = 0, \Lambda = \infty) + a\exp(-b/\lambda) + c\exp(-\Lambda^2/d^2)$$

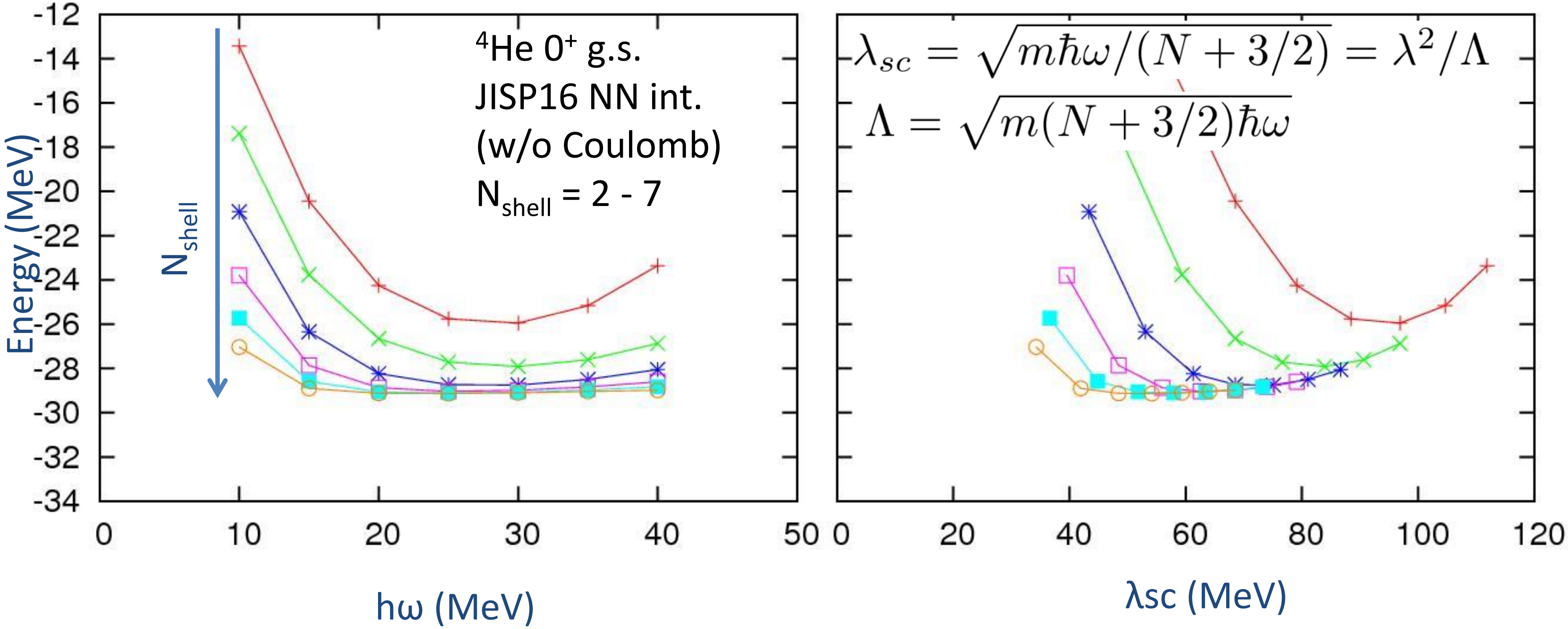
S. A. Coon, M. I. Avetian, M. K. G. Kruse, U. van Kolck, P. Maris, J. P. Vary, Phys. Rev. C86, 054002 (2012)
S. A. Coon, arXiv:1303.6358

R. J. Furnstahl, G, Hagen, T. Papenbrock, Phys. Rev. C86, 031301(R) (2012)
S. N. More, A. Ekstrom, R. J. Furnstahl, G. Hagen, T. Papenbrock, Phys. Rev. C87, 044326 (2013)
R. J. Furnstahl, S. N. More, T. Papenbrock, arXiv:1312.6876

E. D. Jurgenson, P. Maris, R. J. Furnstahl, W. E. Ormand & J. P. Vary, Phys. Rev. C87, 054312 (2013)

Preliminary

Empirical & IR-cutoff extrapolations



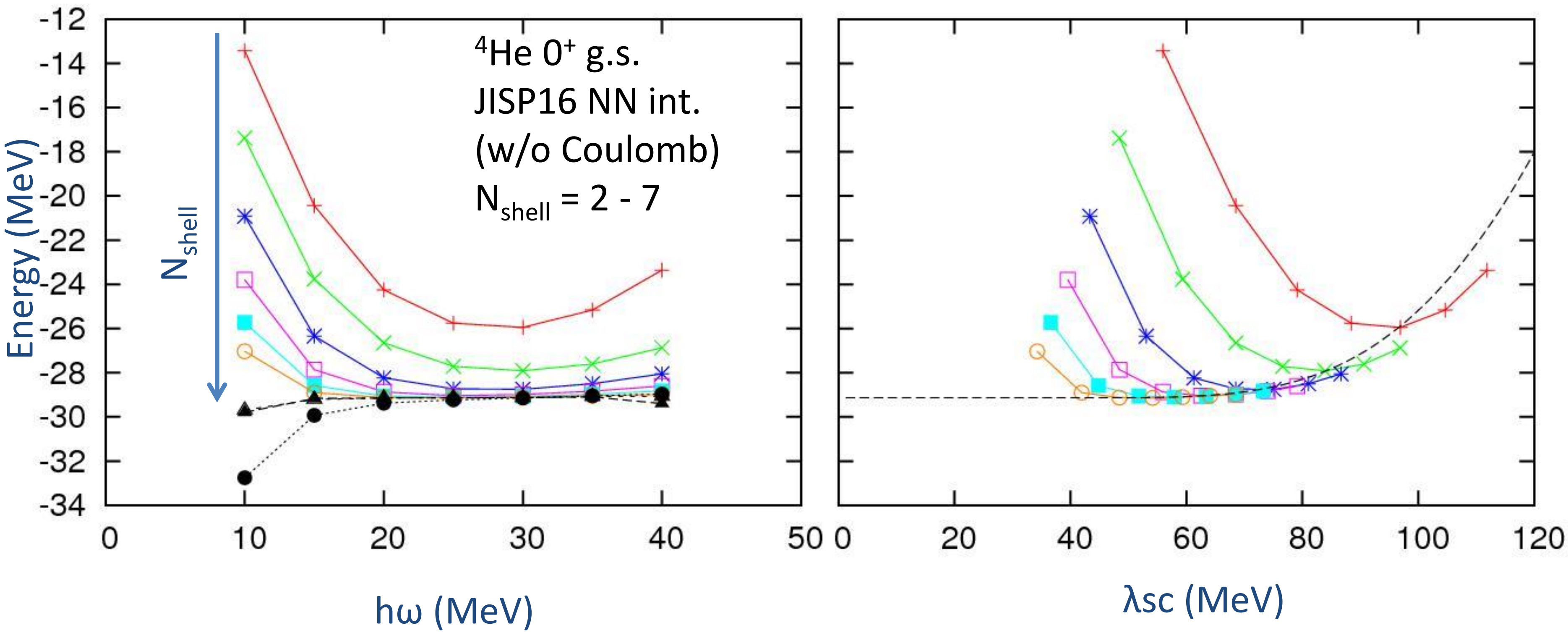
(N_{shell}, hω) ⟷ (Λ, λsc)

Λ: UV cutoff λsc: IR cutoff

IR cutoff scaling w/ UV saturated data

Preliminary

Empirical & IR-cutoff extrapolations



MCSM(empirical): -29.389 ~ -29.077 MeV
(Nshell = 3 - 7, hw = 15 - 35 MeV)

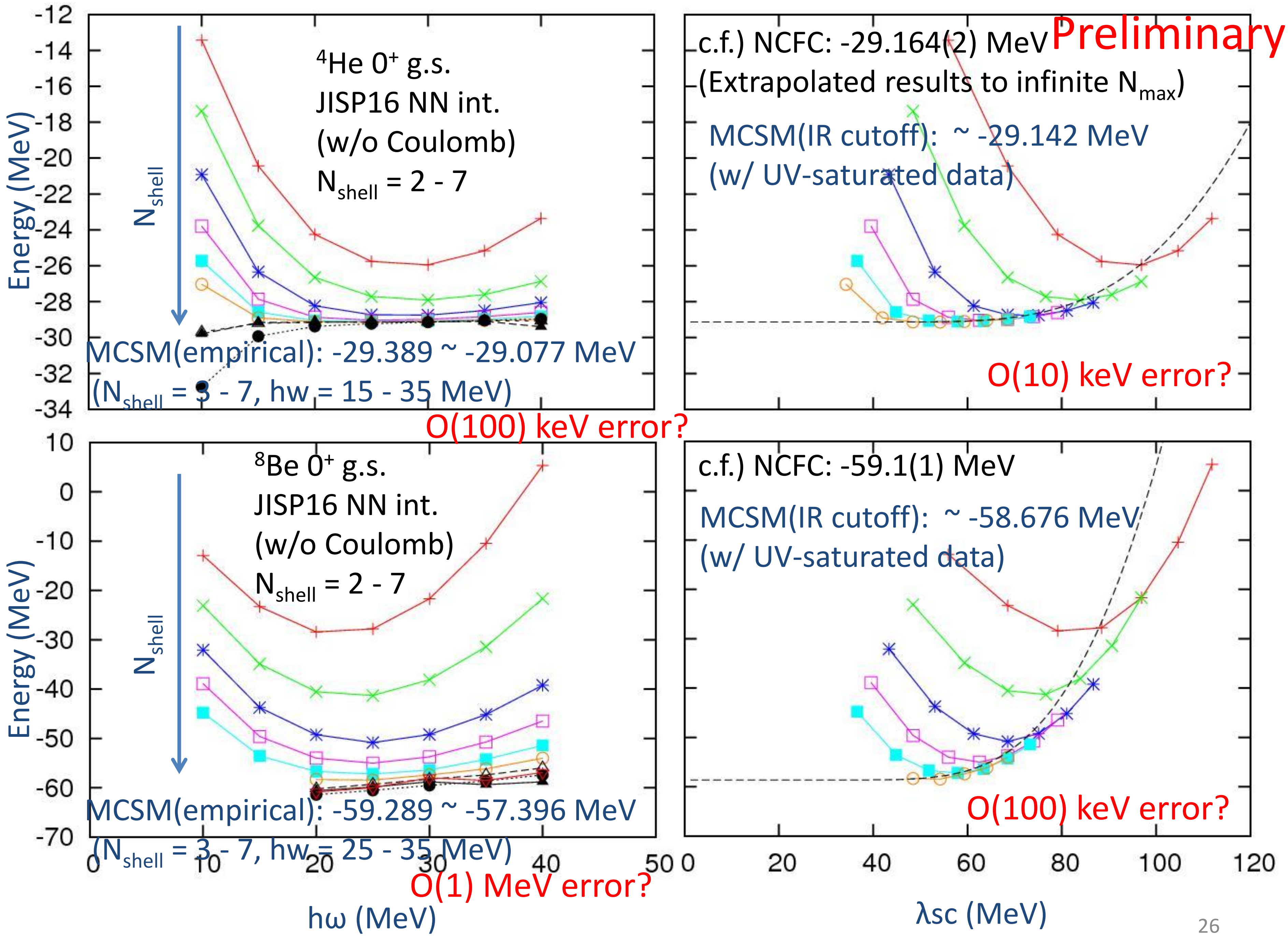
O(100) keV error?

MCSM(IR cutoff): ~ -29.142 MeV
(w/ UV-saturated data)

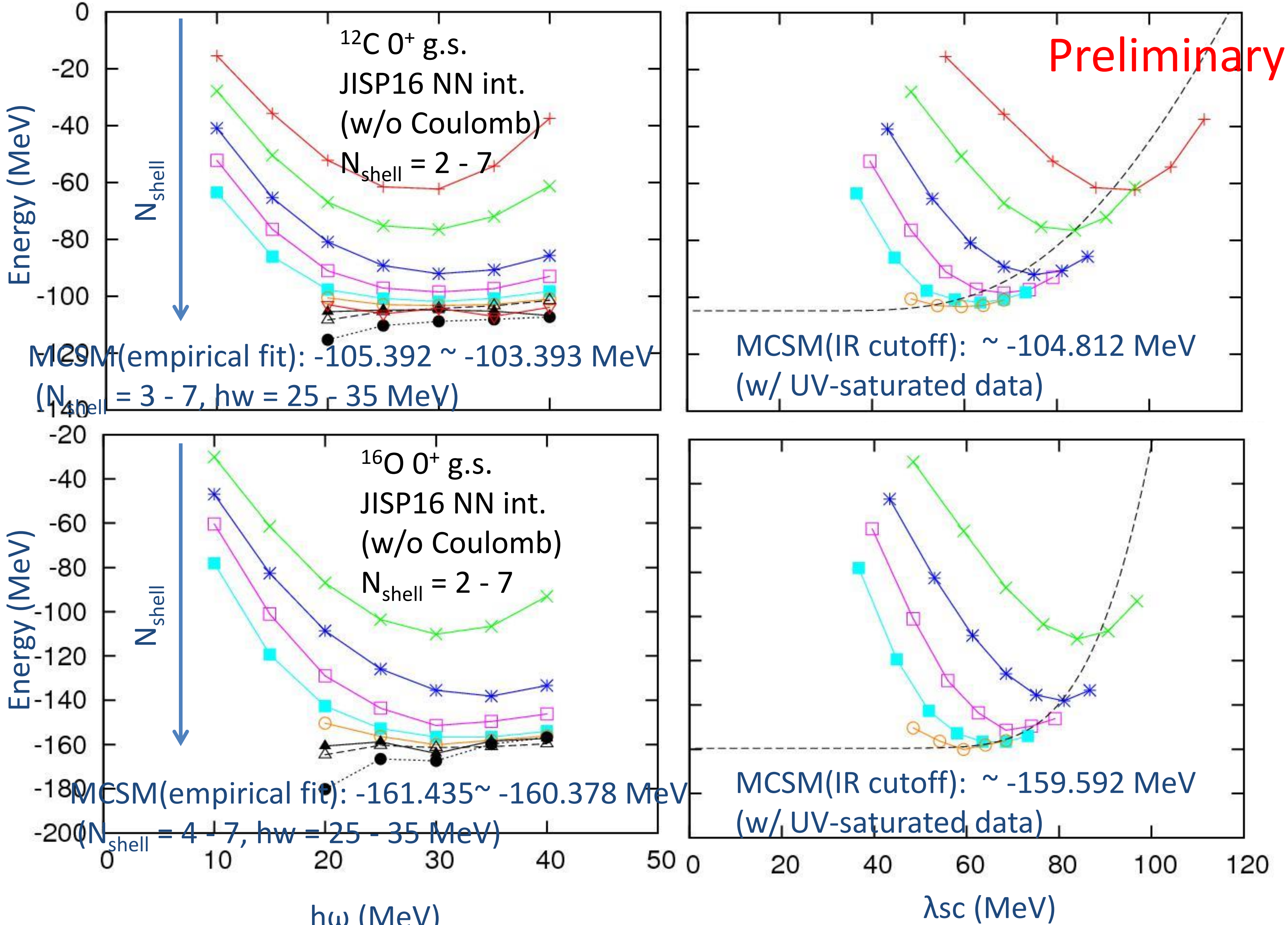
O(10) keV error?

c.f.) NCFC: -29.164(2) MeV
Extrapolated results to infinite N_{max}

Error estimates are needed.



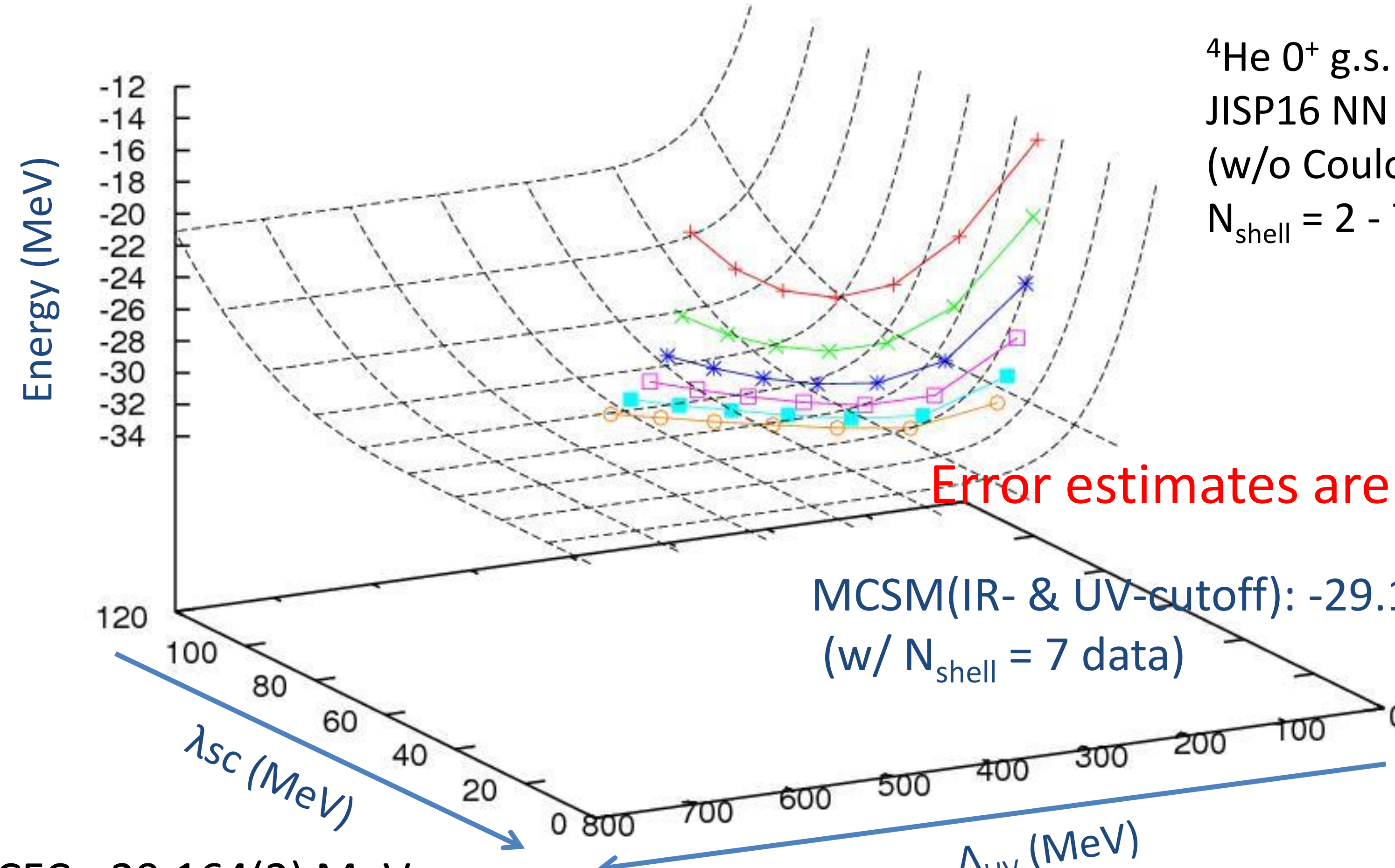
Preliminary
^{4}He 0^+ g.s.
JISP16 NN int.
(w/o Coulomb)
N_{shell} = 2 - 7
N_{shell}
MCSM(empirical): -29.389 ~ -29.077 MeV
(N_{shell} = 3 - 7, hw = 15 - 35 MeV)
O(100) keV error?
c.f.) NCFC: -29.164(2) MeV
(Extrapolated results to infinite N_{max})
MCSM(IR cutoff): ~ -29.142 MeV
(w/ UV-saturated data)
O(10) keV error?
^{8}Be 0^+ g.s.
JISP16 NN int.
(w/o Coulomb)
N_{shell} = 2 - 7
MCSM(empirical): -59.289 ~ -57.396 MeV
(N_{shell} = 3 - 7, hw = 25 - 35 MeV)
O(1) MeV error?
c.f.) NCFC: -59.1(1) MeV
MCSM(IR cutoff): ~ -58.676 MeV
(w/ UV-saturated data)
O(100) keV error?
Energy (MeV)
hω (MeV)
λsc (MeV)


Preliminary
^{12}C 0$^+$ g.s.
JISP16 NN int.
(w/o Coulomb)
N_{shell} = 2 - 7
N_{shell}
MCSM(empirical fit): -105.392 ~ -103.393 MeV
(N_{shell} = 3 - 7, hw = 25 - 35 MeV)
MCSM(IR cutoff): ~ -104.812 MeV
(w/ UV-saturated data)
^{16}O 0$^+$ g.s.
JISP16 NN int.
(w/o Coulomb)
N_{shell} = 2 - 7
N_{shell}
MCSM(empirical fit): -161.435~ -160.378 MeV
(N_{shell} = 4 - 7, hw = 25 - 35 MeV)
MCSM(IR cutoff): ~ -159.592 MeV
(w/ UV-saturated data)
Energy (MeV)
hω (MeV)
λsc (MeV)

Preliminary

IR- & UV-cutoff extrapolation

$$E(\lambda, \Lambda) = E(\lambda = 0, \Lambda = \infty) + a\exp(-b/\lambda) + c\exp(-\Lambda^2/d^2)$$



^{4}He 0$^+$ g.s.
JISP16 NN int.
(w/o Coulomb)
N_{shell} = 2 - 7

Error estimates are needed.

MCSM(IR- & UV-cutoff): -29.139 MeV
(w/ N_{shell} = 7 data)

c.f.) NCFC: -29.164(2) MeV
Extrapolated results to infinite N_{max}

on going: ^{8}Be, ^{12}C, ^{16}O, …

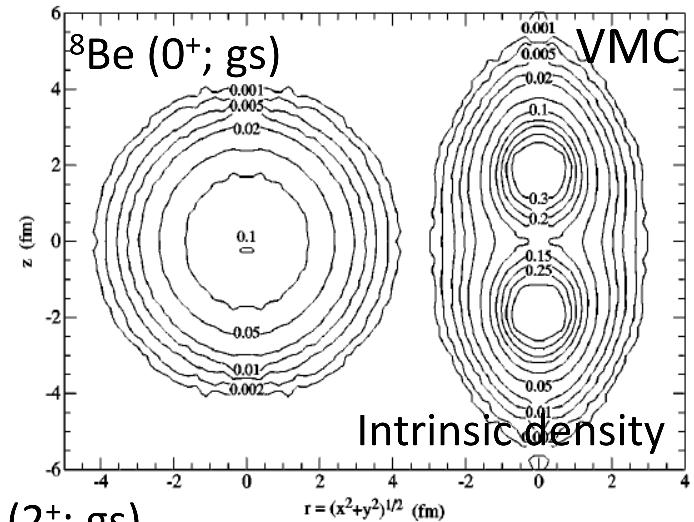
Density Plots from ab initio calc.

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

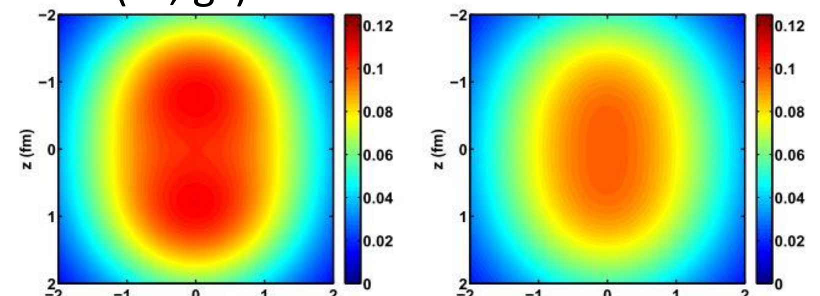
    R. B. Wiringa, S. C. Pieper, J. Carlson, & V. R. Pandharipande, Phys. Rev. C62, 014001 (2000)
- No-core full configuration (NCFC)
  - Translationally-invariant density is obtained by deconvoluting the intrinsic & CM w.f.

    C. Cockrell J. P. Vary & P. Maris, Phys. Rev. C86, 034325 (2012)
- Lattice EFT
  - Triangle structure in carbon-12

    E. Epelbaum, H. Krebs, T. A. Lahde, D. Lee, & U.-G. Meissner, Phys. Rev. Lett. 109, 252501 (2012)

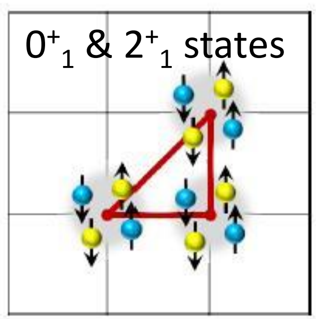


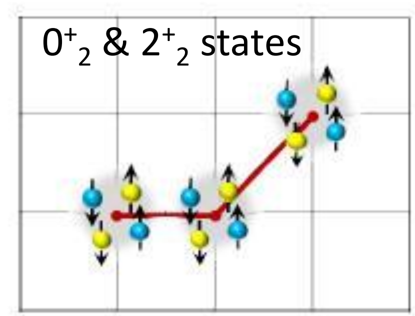
^{8}Li (2$^+$; gs)



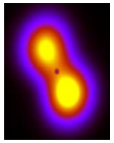
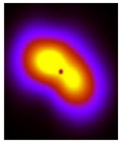
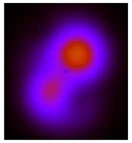
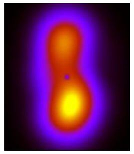
Translationally-invariant neutron density

Space-fixed neutron density





Density plots in MCSM

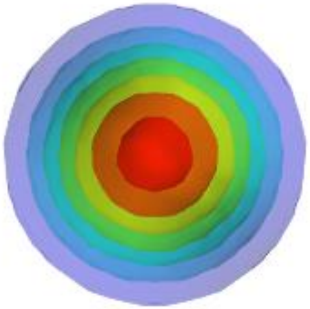
$$|\Phi\rangle = \sum_{i=1}^{N_{basis}} c_i |\Phi_i\rangle =$$ c_1  $+ c_2$  $+ c_3$  $+ c_4$  + ...

Angular-momentum projection

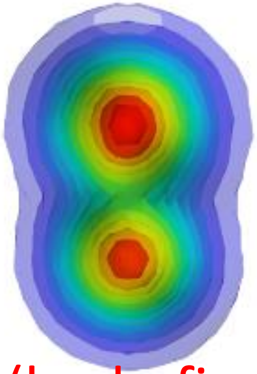
$$|\Psi\rangle = \sum_{i=1}^{N_{basis}} c_i P^J P^\pi |\Phi_i\rangle$$

Rotation of each basis by diagonalizing Q-moment

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



^{8}Be 0^+ ground state



Laboratory frame

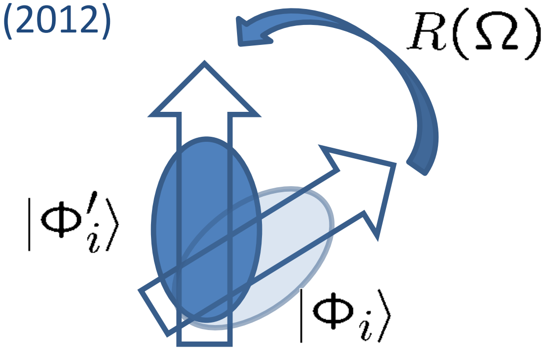
"Intrinsic" (body-fixed) frame

Densities in lab. & body-fixed frames can be constructed by MCSM

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.

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

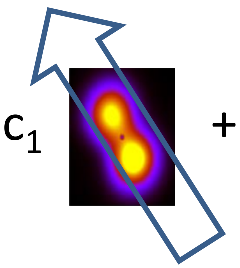
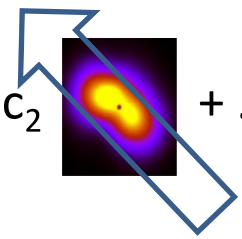
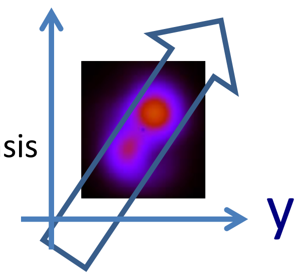


Rotation by diagonalizing Q-moment ($Q_{zz} > Q_{yy} > Q_{xx}$)

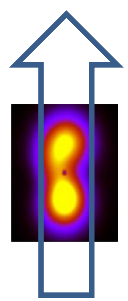
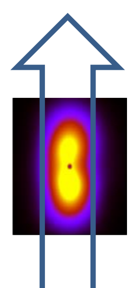
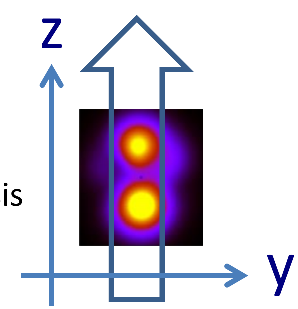
- MCSM wave function

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

- Wave function w/o the projections

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

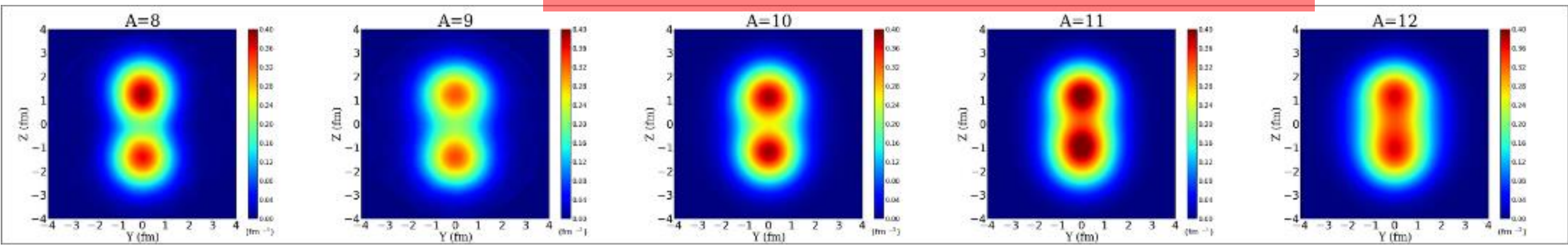
Preliminary Density plots of Be isotopes (0_1^+)

(N_{shell} = 4, hw = 25 MeV, β = 0, JISP16 NN w/o Coulomb)

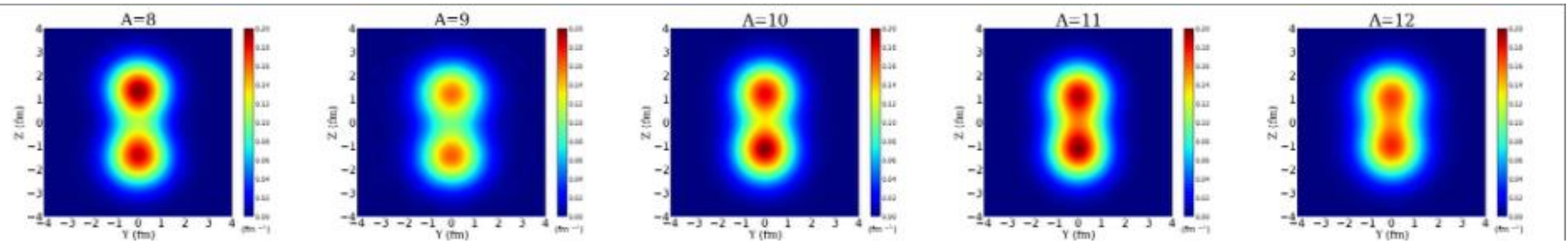
A = 8 A = 9 A = 10 A = 11 A = 12

2-α structure is vanishing as A increases

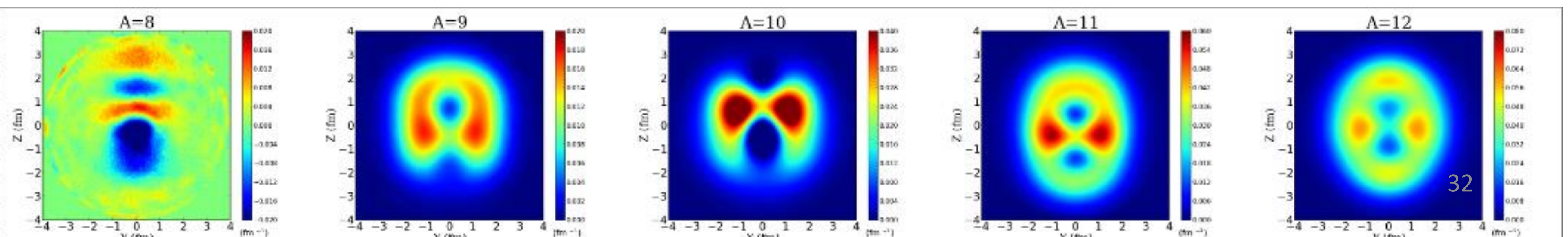
Matter density



Proton density



Neutron density – Proton density



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. Some results are obtained only by MCSM.

  - Extension to larger model spaces (N_{shell} = 6, 7, …), extrapolation to infinite basis space, & comparison with the another truncation (N_{max})

Perspective

- MCSM algorithm/computation

  - Error estimates of the extrapolations

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

  - GPGPU

- Physics

  - Cluster states, non-yrast states, unnatural parity states, …

  - sd-shell nuclei

END