計算基礎科学連携拠点
研究報告会

サブ課題B 原子核

モンテカルロ殻模型による軽い核の第一原理計算

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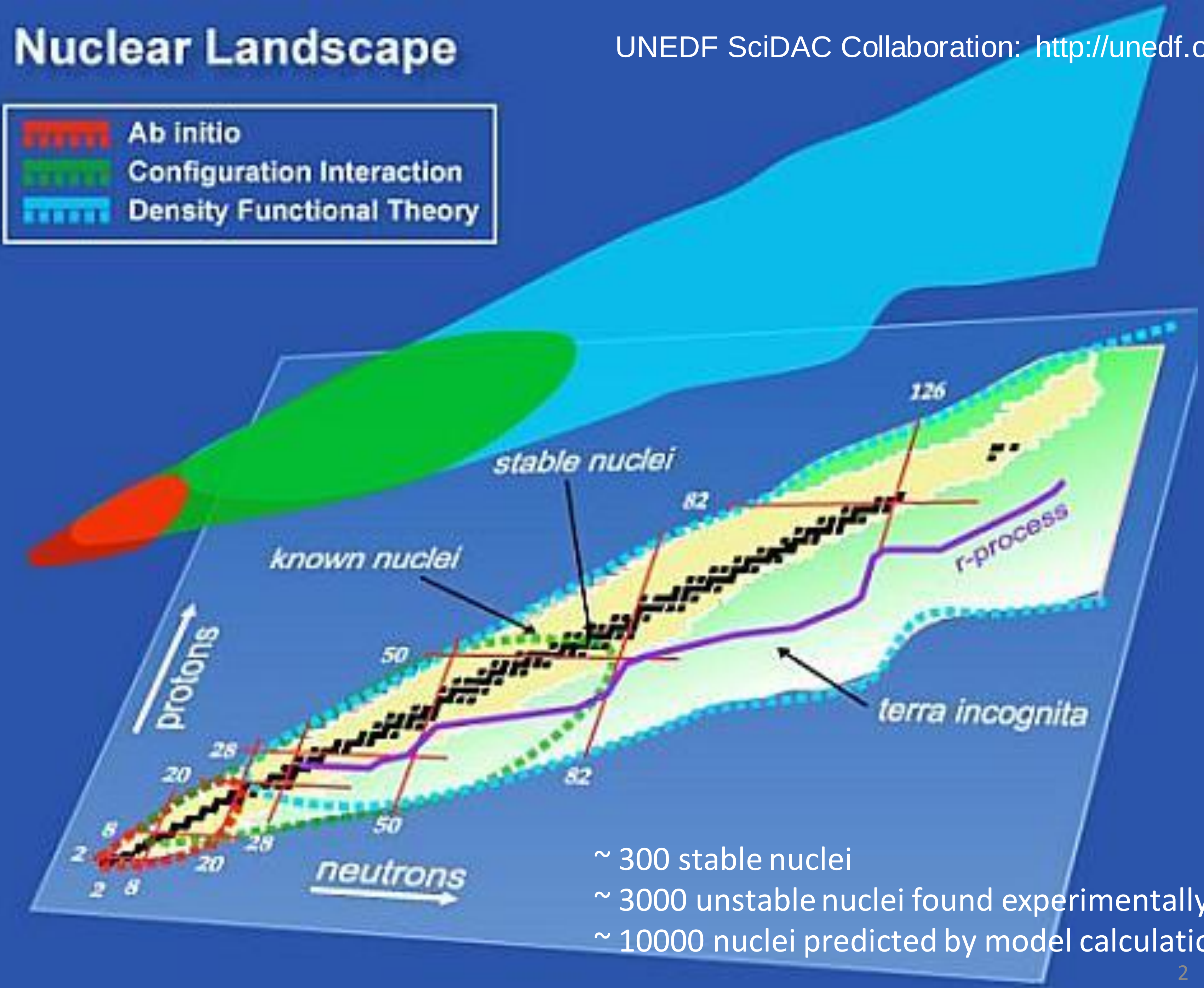
筑波大学計算科学研究センター
2016年10月14日

UNEDF SciDAC Collaboration: http://unedf.org/



~ 300 stable nuclei
~ 3000 unstable nuclei found experimentally
~ 10000 nuclei predicted by model calculations

Ab-inito approaches in low-energy nuclear physics

- Major challenge in nuclear physics

  \- Nuclear structure & reactions from *ab-initio* calculations w/ nuclear forces

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

  Green's Function Monte Carlo, No-Core Shell Model (A ~ 12),

  Coupled Cluster (sub-shell closure +/- 1,2),

  Self-consistent Green's Function theory, IM-SRG, Lattice EFT, …

  → computationally demanding

- Two main sources of uncertainties:
  - Many-body methods

    CI: Finite basis space (choice of basis function and truncation), (N_{shell}, $\hbar\omega$)

    we have to extrapolate to infinite basis dimensions

  ✓ need *ab-initio*(-like) approaches beyond standard NCSM

  → No-Core Monte Carlo Shell Model (MCSM)

  - Nuclear forces (interactions btw/among nucleons)

  → Chiral effective field theory (χEFT)

  ✓ In principle, they are hopefully obtained by (Lattice) QCD.

Shell model (Configuration Interaction, CI)

- Eigenvalue problem of large sparse Hamiltonian matirx

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

$$\underbrace{\begin{pmatrix} H_{11} & H_{12} & H_{13} & H_{14} & H_{15} & \cdots \\ H_{21} & H_{22} & H_{23} & H_{24} & & \\ H_{31} & H_{32} & H_{33} & & & \\ H_{41} & H_{33} & & \ddots & & \\ H_{51} & & & & & \\ \vdots & & & & & \end{pmatrix}}_{\text{Large sparse matrix (in M-scheme)}} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix} = \begin{pmatrix} E_1 & & & & 0 \\ & E_2 & & & \\ & & E_3 & & \\ & & & \ddots & \\ 0 & & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix}$$

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

non-zero MEs

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

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

Monte Carlo shell model (MCSM)

Standard shell model

$$\mathrm{H} = \underbrace{\begin{pmatrix} \star & \star & \star & \star & \star & \cdots \\ \star & \star & \star & \star & & \\ \star & \star & \star & & & \\ \star & \star & & \ddots & & \\ \star & & & & & \\ \vdots & & & & & \end{pmatrix}}_{\text{Large sparse matrix } \sim \mathcal{O}(10^{10})} \xrightarrow{\text{Diagonalization}} \begin{pmatrix} E_0 & & & 0 \\ & E_1 & & \\ & & E_2 & \\ 0 & & & \ddots \end{pmatrix}$$

\# non-zero MEs

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

- Importance truncation

T. Otsuka *et al*., Prog. Part. Nucl. Phys. 47, 319 (2001)

Monte Carlo shell model

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

Important bases stochastically selected

~ O(100)

$$|\Psi(J,M,\pi)\rangle = \sum_i^{N_{basis}} f_i |\Phi_i(J,M,\pi)\rangle$$

$$|\Phi(J,M,\pi)\rangle = \sum_K g_K P^J_{MK} P^\pi |\phi\rangle$$

diagonalization

$$|\phi\rangle = \prod_i^A a_i^\dagger |-\rangle$$

Deformed

$$a_i^\dagger = \sum_\alpha^{N_{sps}} c_\alpha^\dagger D_{\alpha i}$$

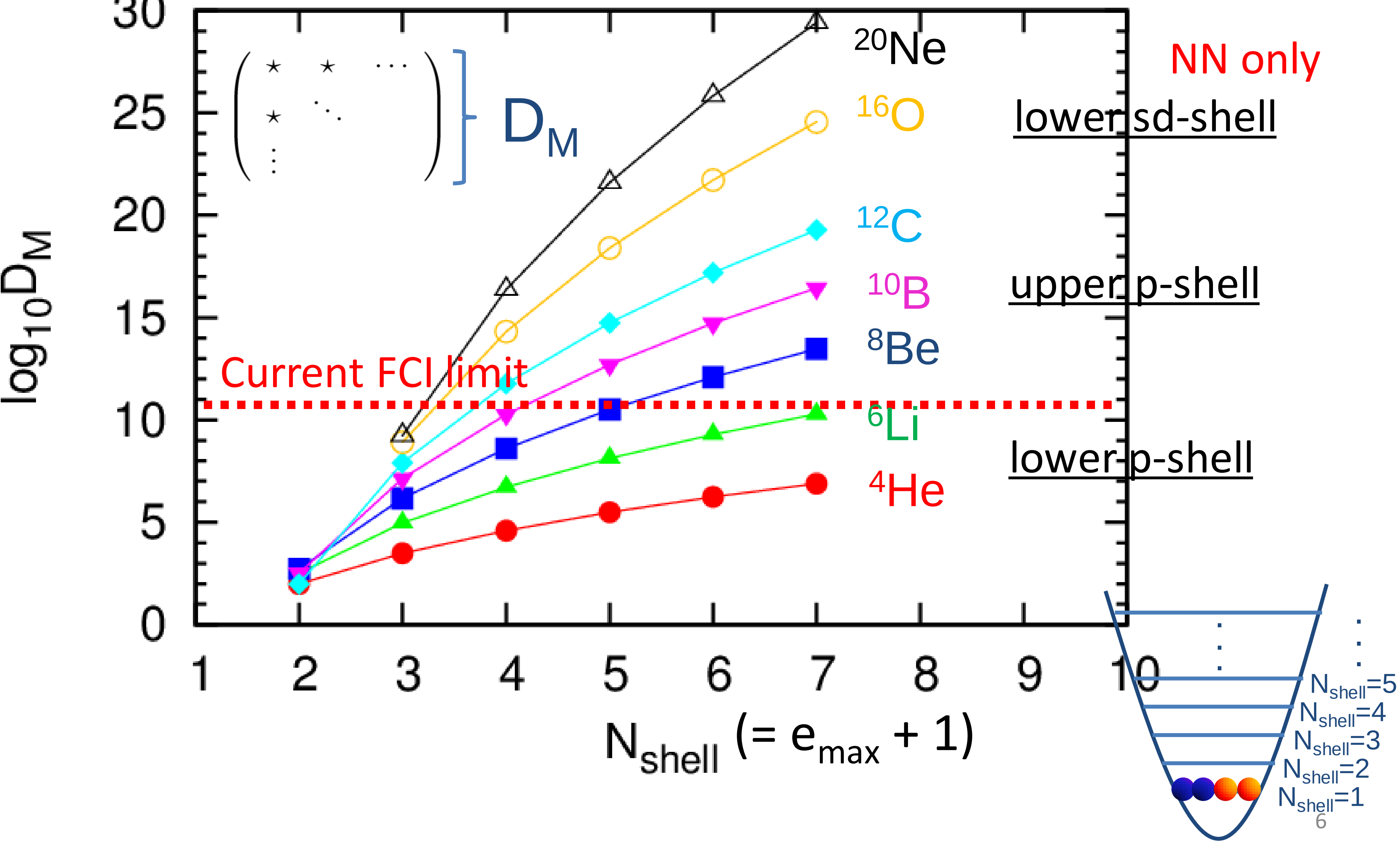
Spherical

stochastic sampling & CG

M-scheme dimension in N_{shell} truncation

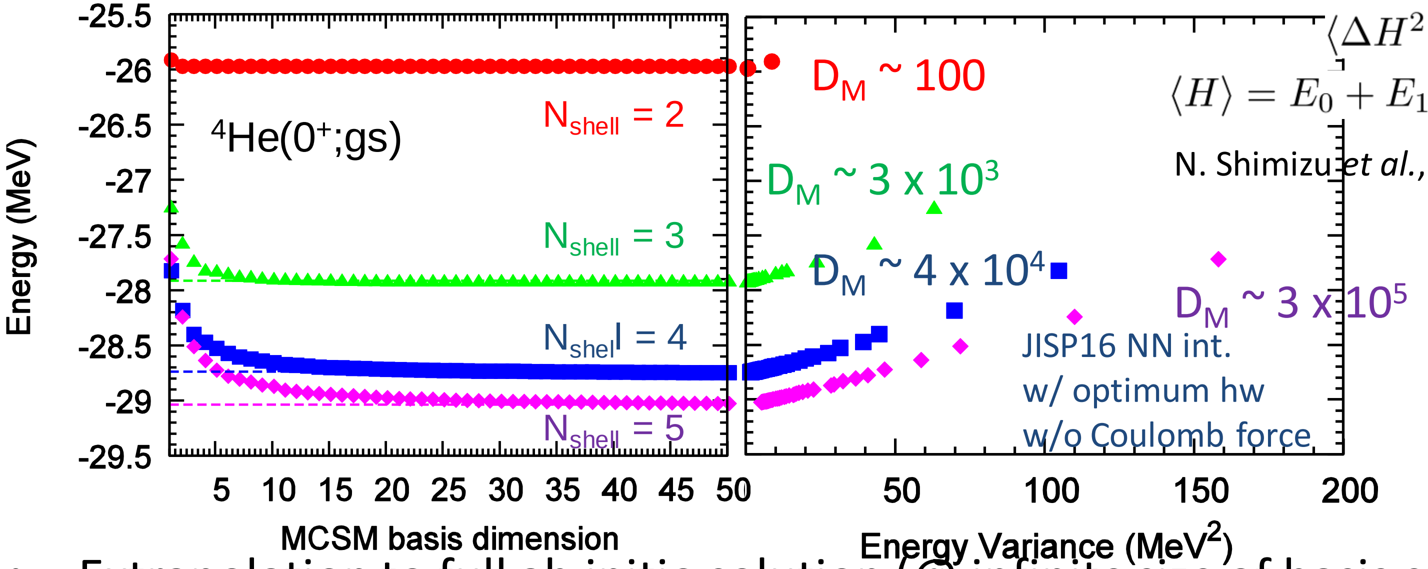
No-core calculations

NN only



Extrapolations

- Extrapolation to FCI results (@ fixed size of basis space) <- Energy variance

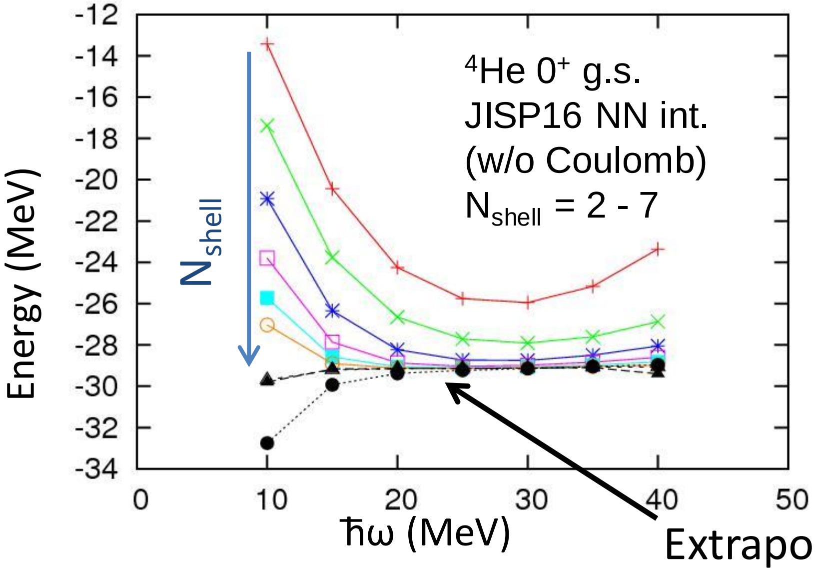


$$\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$$

$$\langle H \rangle = E_0 + E_1 \langle \Delta H^2 \rangle + E_2 \langle \Delta H^2 \rangle^2 + \cdots$$

N. Shimizu *et al.*, Phys. Rev. C82, 061305 (2010)

- Extrapolation to full ab initio solution (@ infinite size of basis space)

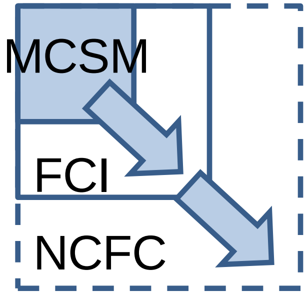


Extrapolations

(N_{shell}, ħω)

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

MCSM(traditional): -29.15(3) MeV
(N_{shell} = 3 - 7, ħw = 20 - 30 MeV)

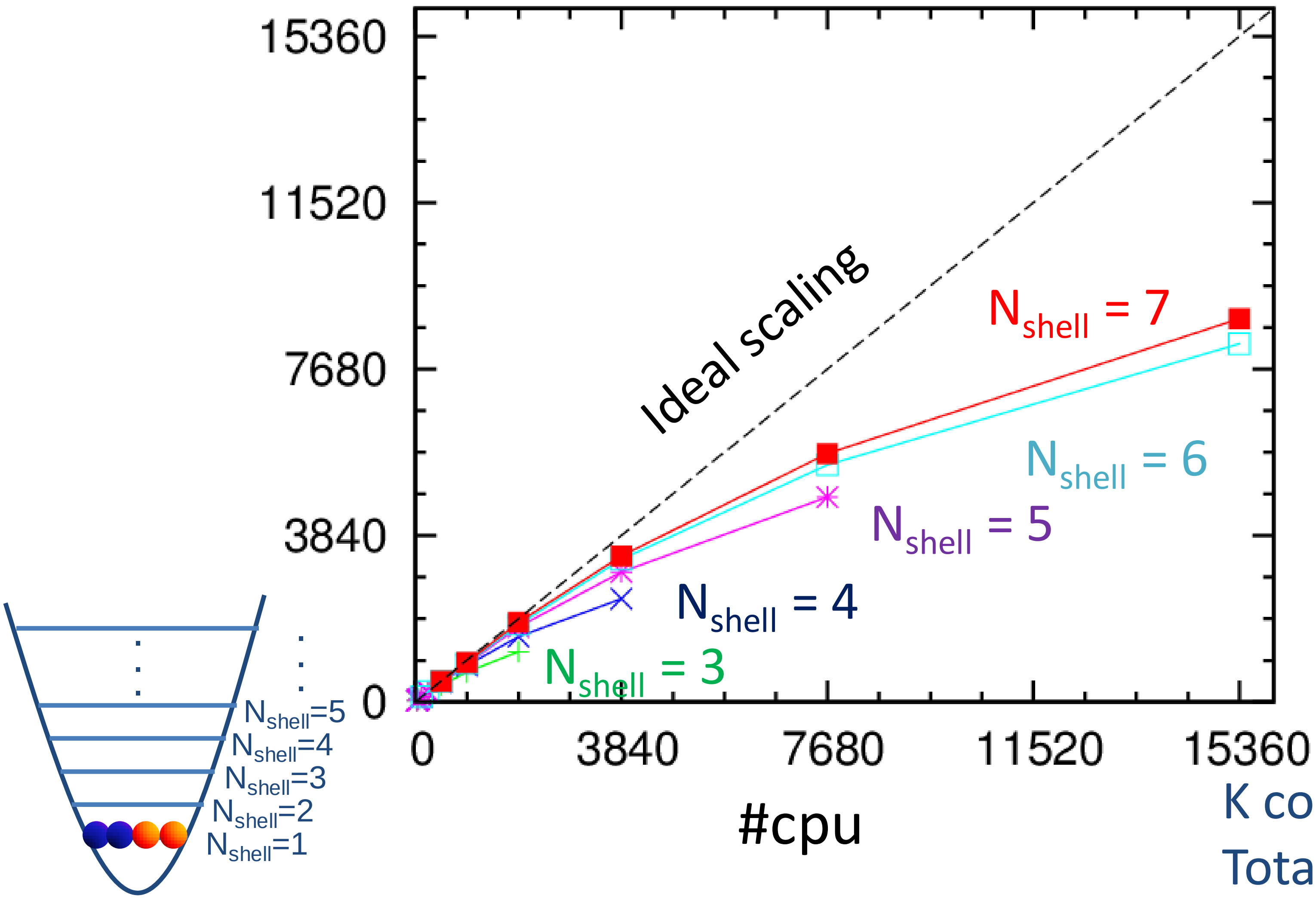


c.f.) NCFC: -29.164(2) MeV
Extrapolated results to infinite N_{max} space

Strong scaling (eigen functions & eigenvalues)

- Wave function (100 CG iterations @ 100th basis)

Scales up to ~ 60,000 cores @ $N_{shell} = 7$ (^{4}He) on K computer



8 cores/cpu

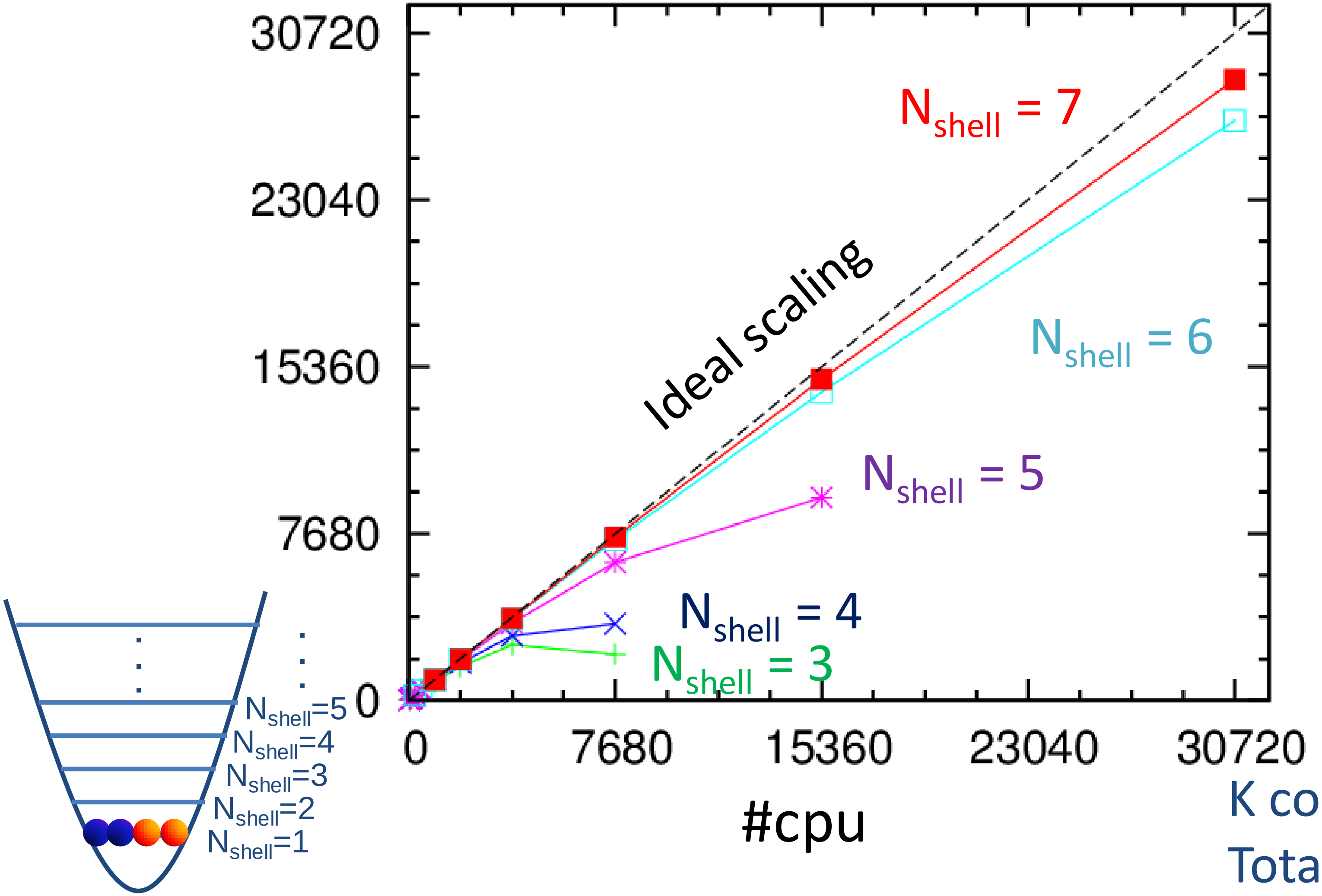
K computer

Total: 88,128 cpus

Strong scaling (energy variances)

- Energy variance (1^{st} – 100^{th} bases)

Scales over ~ 240,000 cores @ N_{shell} = 7 (^{4}He) on K computer

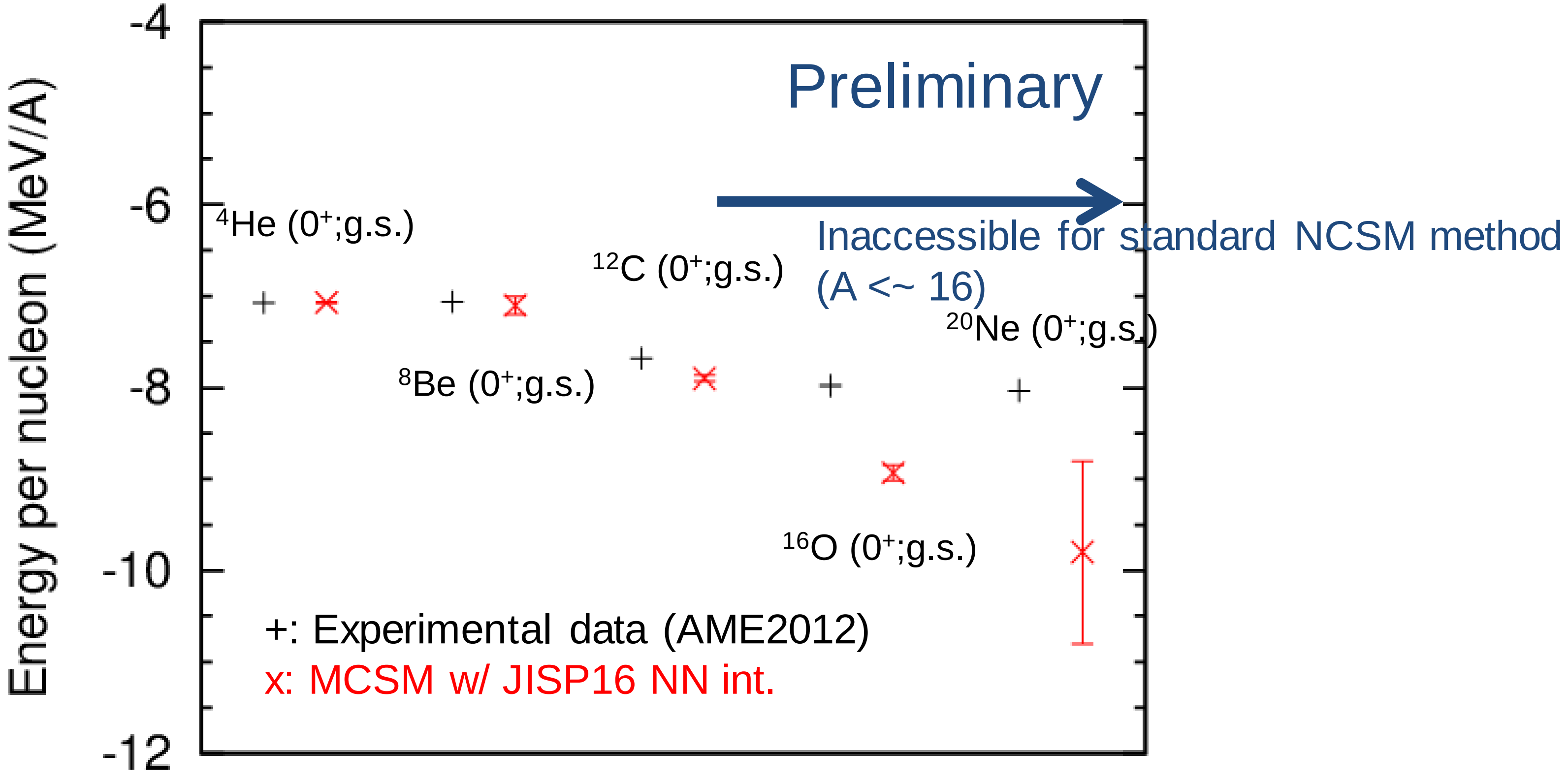


8 cores/cpu

K computer

Total: 88,128 cpus

Comparison of MCSM results w/ experiments



MCSM results are obtained using K computer by traditional extrapolation w/ optimum harmonic oscillator energies.
Coulomb interaction is included perturbatively.

MCSM results show good agreements w/ experimental data up to ^{12}C, slightly overbound for ^{16}O, and clearly overbound for ^{20}Ne.

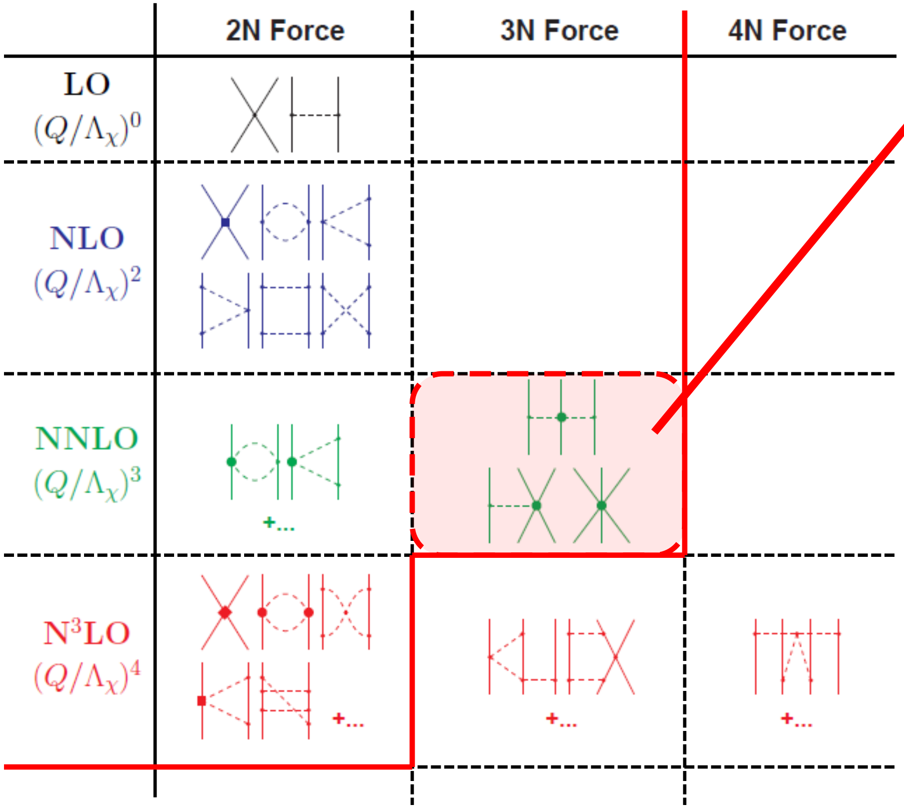
Nuclear force from χEFT

- Current standard input potential:

➢ Chiral effective field theory (χEFT) described by N & π DoF (Weinberg, van Kolck, …)

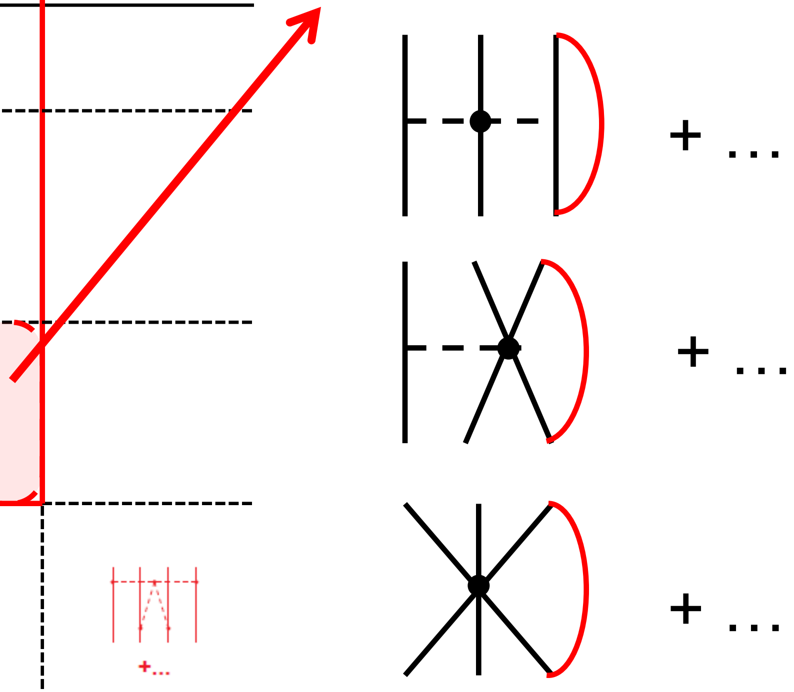
  - ✓ χEFT holds the effect of chiral symmetry breaking & the symmetries retained in low-energy QCD
  - ✓ χEFT N3LO NN + N2LO 3N
  - ✓ Renormalization technique: SRG, $V_{\text{low k}}$, UCOM, …
  - ✓ 3N interaction: Full, NO2B approx., …

E. Epelbaum, Prog. Part. Nucl. Phys. **57**, 654 (2006).
R. Machleidt and D. R. Entem, Phys. Rep. **503**, 1 (2011).



K. Hebeler, H. Krebs, E. Epelbaum, J. Golak, & R. Skibinski, arXiv:1502.02977

Effective NN forces from 3N forces



Effective 2N force from 3N force

Effective 2N potential from initial 3N potential in momentum space

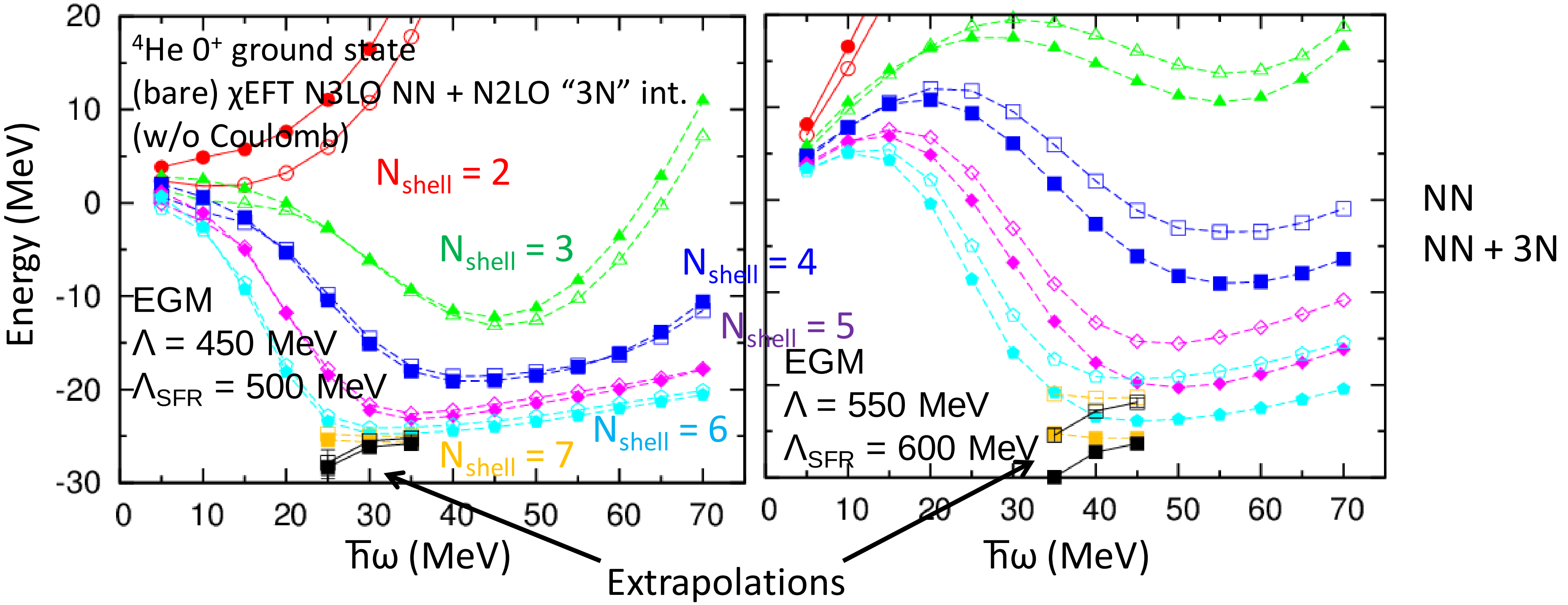
w/ M. Kohno (RCNP),
T. Miyagi (Tokyo),
S. Yoshida (Tokyo)

$$\frac{1}{2}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2}\langle \boldsymbol{k}_1\boldsymbol{k}_2|V_{12}|\boldsymbol{k}_1\boldsymbol{k}_2\rangle_A + \frac{1}{3!}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}\langle \boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3|V_{123}|\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\rangle_A$$

$$= \frac{1}{2}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2}\langle \boldsymbol{k}_1\boldsymbol{k}_2|V_{12}+\frac{1}{3}V_{12(3)}|\boldsymbol{k}_1\boldsymbol{k}_2\rangle_A.$$

$$\langle \boldsymbol{k}_1', \boldsymbol{k}_2'|V_{12(3)}|\boldsymbol{k}_1, \boldsymbol{k}_2\rangle_A \equiv \sum_{\boldsymbol{k}_3}\langle \boldsymbol{k}_1', \boldsymbol{k}_2', \boldsymbol{k}_3|V_{123}|\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{k}_3\rangle_A,$$

Preliminary

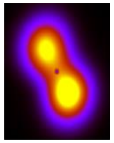
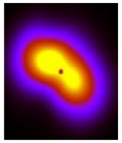
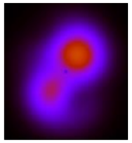
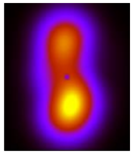


Extrapolations

Energies with 3NF in the different cutoff scales are consistent in a sufficiently large basis space

Density distribution in MCSM

T. Yoshida (CNS)

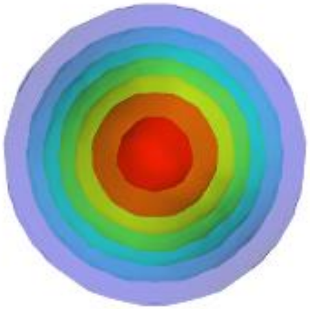
$|\Phi\rangle = \sum_{i=1}^{N_{basis}} c_i|\Phi_i\rangle =$ c_1  $+ c_2$  $+ c_3$  $+ c_4$  + …

Angular-momentum projection

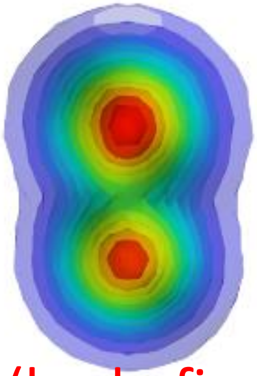
$$|\Psi\rangle = \sum_{i=1}^{N_{basis}} c_i P^J P^\pi |\Phi_i\rangle$$

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)

Density distribution of Be isotopes

T. Yoshida (CNS)

Preliminary

2-α structure is vanishing as A increases

^{8}Be $(0^+;\mathrm{gs})$

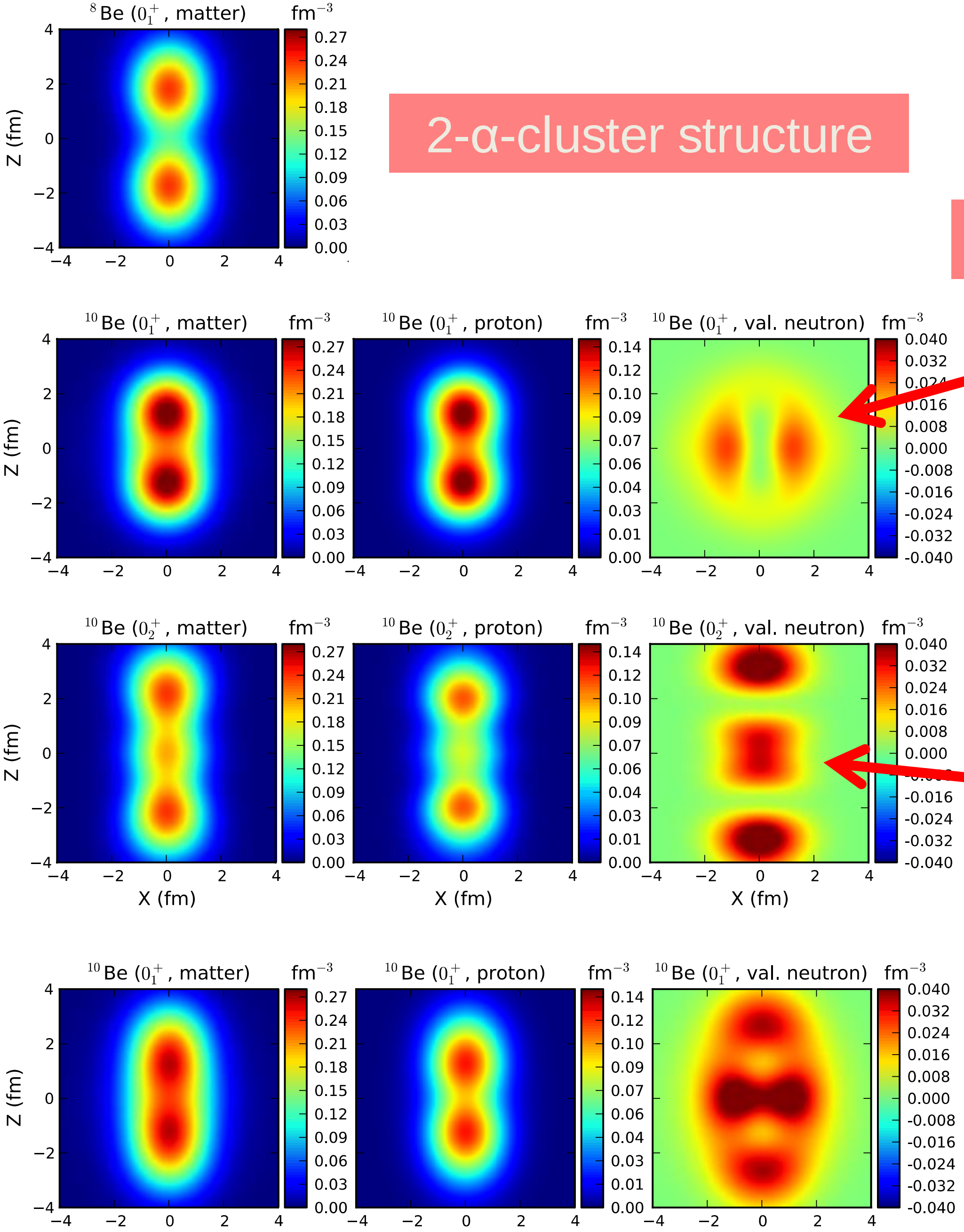
^{10}Be $(0^+;\mathrm{gs})$

0_2^+

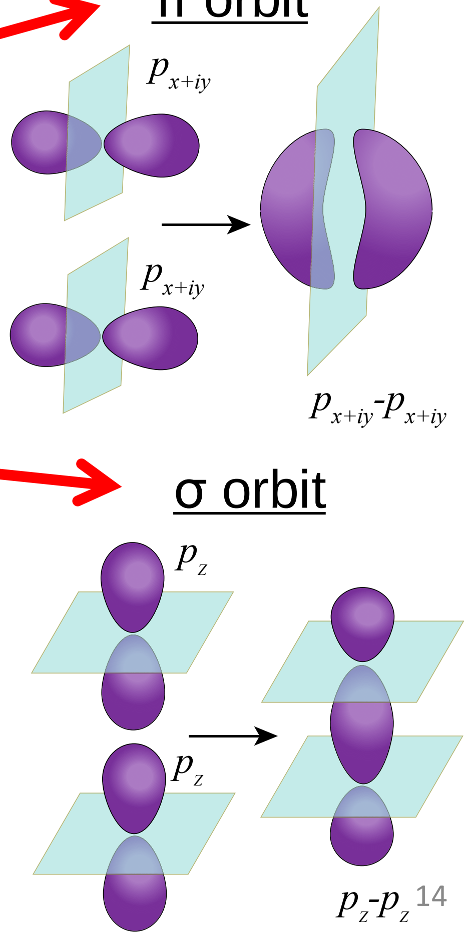
^{12}Be $(0^+;\mathrm{gs})$

2-α-cluster structure

Molecular-orbital states



π orbit



σ orbit

Summary

- MCSM results of g.s. energies for light nuclei (A<= 20) w/ a NN potential can be extrapolated to the infinite basis space.
  - JISP16 NN interaction gives good agreement w/ experimental data up to ^{12}C, slightly overbound for ^{16}O, and clearly overbound for ^{20}Ne.
- Effective 2NF from 3NF in the χEFT has been tested in the MCSM.
- Cluster structure of Be isotopes can be visualized using MCSM wave functions.

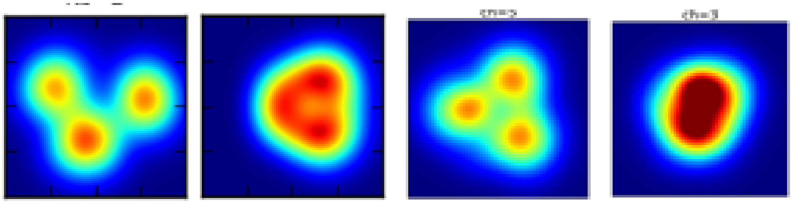
Future perspective

- MCSM w/ SRG evolved χEFT interactions
- Check of convergence w.r.t. the basis space & extrapolation
- Cluster structure of carbon isotopes (3α structure, Hoyle state, ...)

モンテカルロ殻模型による第一原理計算のまとめと今後の展望

素粒子・原子核・宇宙「京からポスト京に向けて」
シンポジウム@ワテラスコモンホール
（2016年3月30 – 31日）

- 京より前
  - A = 4 – 12 (^{4}He – ^{12}C) ← p殻核の全般
  - 模型空間：4 主殻まで
  - 二体力のみ
- 京で完了したこと
  - A = 20 (^{20}Ne)まで ← sd殻核の始め
  - 模型空間：7主殻（当初予定は6主殻）まで → 模型空間無限大への外挿が可能
  - ベリリウム同位体のクラスター構造の可視化（分子軌道状態も）
  - 有効二体化した三体力のテスト → 三体力の部分的な導入
- 引き続き京でやっていること
  - ^{12}CのHoyle状態
  - 三体力の本格的な導入



…

- ポスト京で
  - A ~ 40（sd殻核）、模型空間：8主殻
  - 炭素同位体（Hoyleを含む）のクラスター構造の解析
  - 三体力の本格的な導入 → χEFTや格子QCDによる核力

→ 軽・中重核の構造の核力に基づく第一原理計算による解明

Collaborators

- U of Tokyo
  - Takaharu Otsuka (Department of Physics)
  - Noritaka Shimizu (CNS)
  - Tooru Yoshida (CNS)
  - Takayuki Miyagi (Department of Physics)
  - Sota Yoshida (Department of Physics)
- JAEA
  - Yutaka Utsuno
- Iowa State U
  - James P. Vary
  - Pieter Maris
- Kyushu Institute of Technology
  - Ryoji Okamoto
- RCNP, Osaka U
  - Michio Kohno