基研研究会
「核力に基づいた原子核の構造と反応」

モンテカルロ殻模型による第一原理計算の進展

阿部　喬（理研）

Collaborators:

P. Maris (Iowa State U), T. Otsuka (RIKEN/U Tokyo),

N. Shimizu (U Tokyo), Y. Tsunoda (U Tokyo), Y. Utsuno (JAEA),

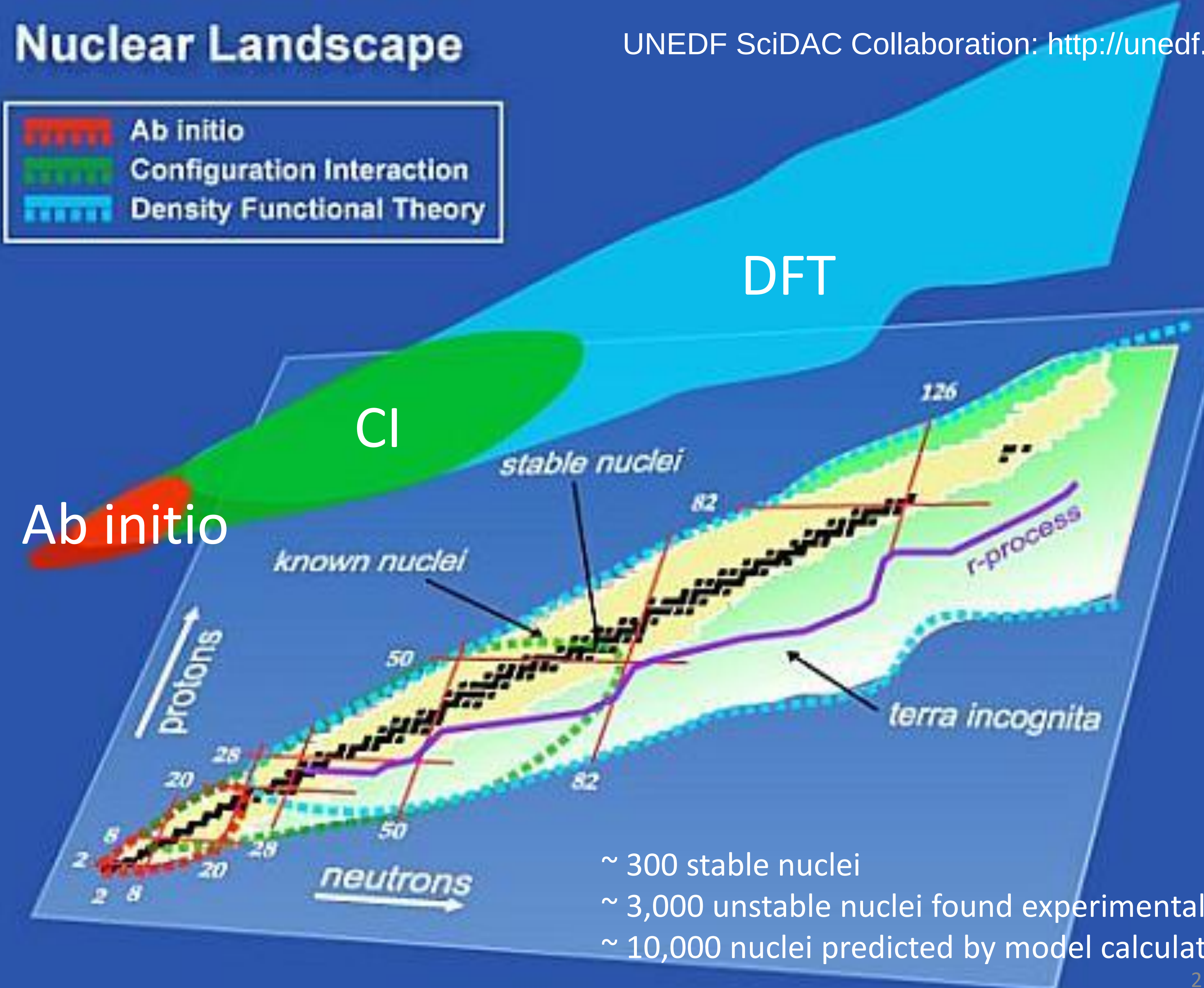
J. P. Vary (Iowa State U), T. Yoshida (RIST)

Reference: Phys. Rev. C 104, 054315 (2021)

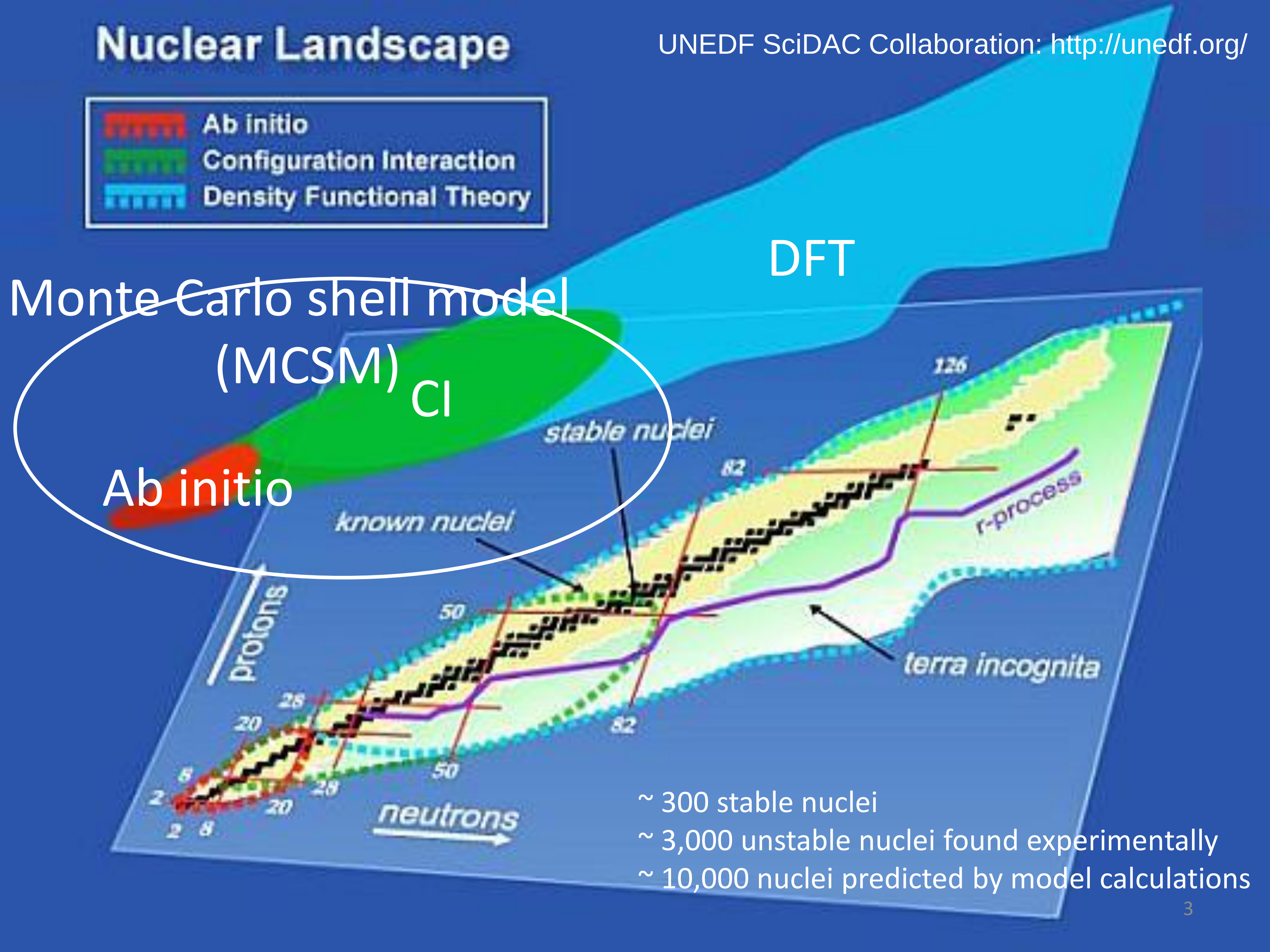
Hybrid (YITP, Kyoto U)

December 7-10, 2021

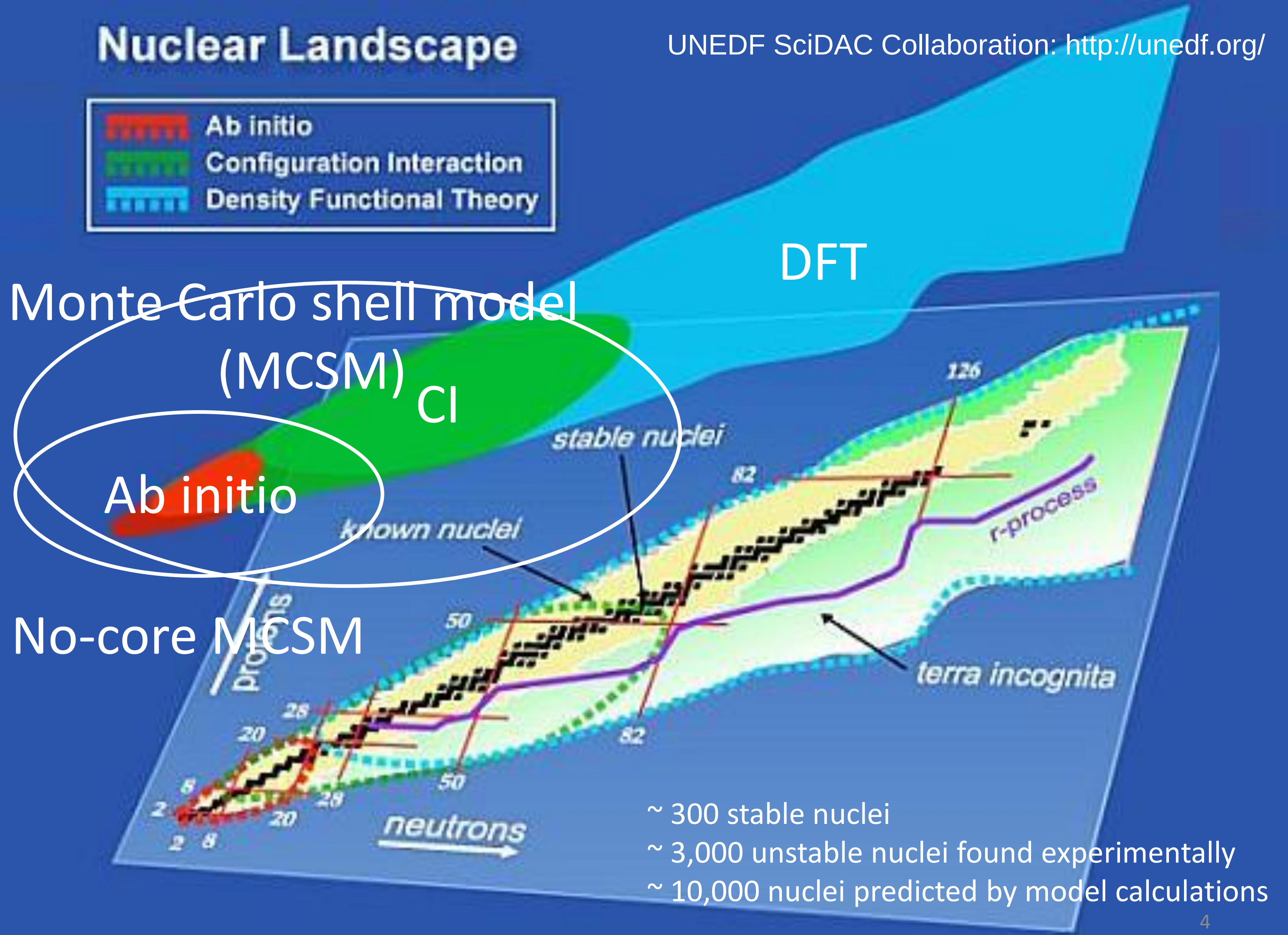
UNEDF SciDAC Collaboration: http://unedf.org/



~ 300 stable nuclei
~ 3,000 unstable nuclei found experimentally
~ 10,000 nuclei predicted by model calculations



Nuclear Landscape
UNEDF SciDAC Collaboration: http://unedf.org/
Ab initio
Configuration Interaction
Density Functional Theory
DFT
Monte Carlo shell model
(MCSM)
CI
Ab initio
stable nuclei
known nuclei
126
82
50
28
20
8
2
protons
neutrons
r-process
terra incognita
~ 300 stable nuclei
~ 3,000 unstable nuclei found experimentally
~ 10,000 nuclei predicted by model calculations



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~ 3,000 unstable nuclei found experimentally
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"Ab initio" in low-energy nuclear structure physics

- Major challenge in nuclear physics
  - Nuclear structure & reactions directly from *ab-initio* calc. w/ nuclear forces
  - *ab-initio* approaches in nuclear structure calculations (A > 4):
    Light mass: Green's Function Monte Carlo, No-Core Shell Model (A ~ 12),
    Medium/heavy mass: Coupled Cluster, IM-SRG,
    Self-consistent Green's Function theory, Lattice EFT, UMOA, …
  * SM + eff. Int. from ab initio approaches (CC, IM-SRG, NCSM, MBPT, …)

S. Yoshida
T. Fukui
T. Otsuka

- Solve the non-relativistic many-body 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.

→ Computationally demanding → Monte Carlo shell model (MCSM)

Configuration Interaction (CI)

- Eigenvalue problem of large and 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 and sparse real symmetric

$$\sim \mathcal{O}(10^{11})$$

\# non-zero MEs

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

Lanczos method for diagonalization

Slater determinants

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

Monte Carlo shell model (MCSM)

Standard shell-model calculation

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

Diagonalization

Spanned by Slater determinants

$$d \lesssim \mathcal{O}(10^{11})$$

Monte Carlo shell model

Importance truncation

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

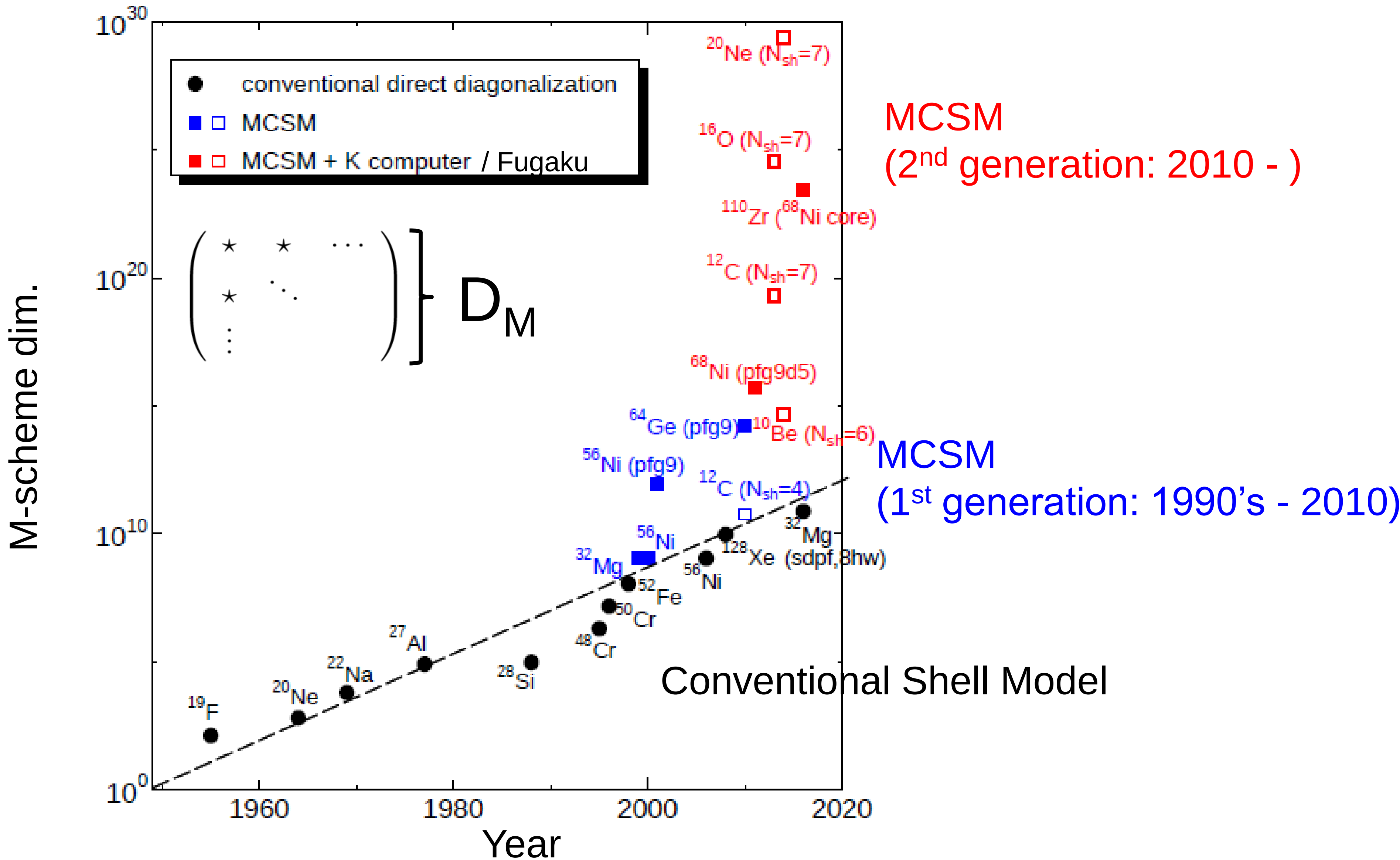
Diagonalization

Spanned by “important” bases
selected stochastically and variationally

$$d_{\mathrm{MCSM}} \sim \mathcal{O}(10^2)$$

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

Dimensionality of shell-model calculations



N. Shimizu et al., Phys. Scr. 92, 063001 (2017).

MCSM wave function

- Superposition of quantum-number projected SDs

\# of MCSM basis states ~ 100

$$|\Psi^{J M \pi}(N_b)\rangle = \sum_{d=1}^{N_b} f^{(d)} \sum_{K=-J}^{J} g_K^{(d)} \hat{P}^{\pi} \hat{P}^{J}_{MK} |\Phi(D^{(d)})\rangle$$

Superposition — Projection on to good spin & parity — Deformed SD

$$|\Phi(D^{(d)})\rangle = \prod_i \hat{a}_i^\dagger(D^{(d)})|\text{core}\rangle \qquad \hat{a}_i^\dagger(D^{(d)}) = \sum_\ell D_{\ell i}^{(d)} \hat{c}_\ell^\dagger$$

$$|\text{vacuum}\rangle$$

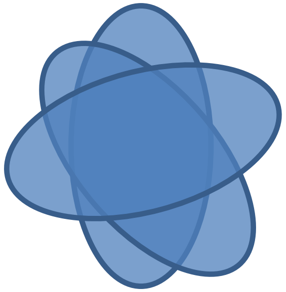
\- Angular momentum projection

Restoration of symmetries

$$\hat{P}^I_{MK} = \frac{2I+1}{8\pi^2} \int D^{I*}_{MK}(\Omega) \hat{R}(\Omega) d\Omega$$

$$\to \sum_\Omega W(\Omega) \cdots$$

O(~10^4)



Favorable for massively parallel computation

How to obtain ab-initio results from no-core MCSM

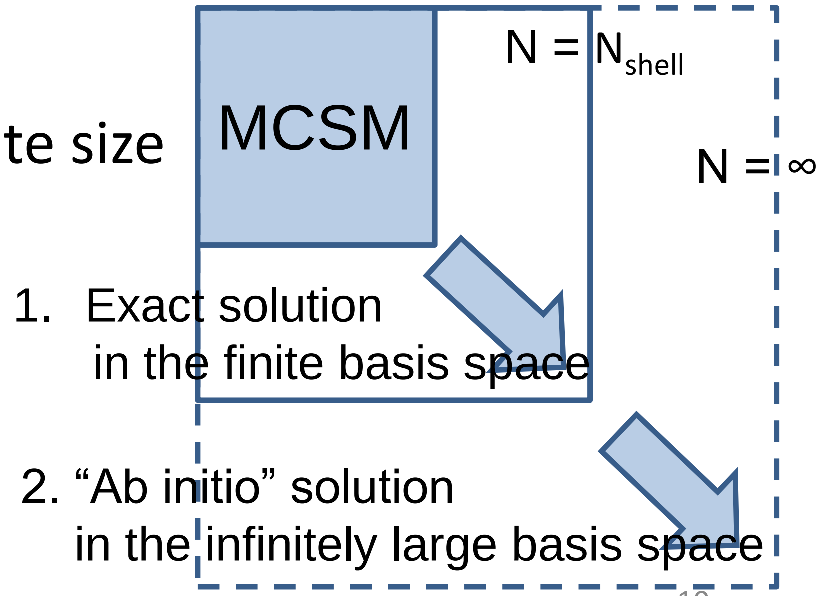
- Two steps of the extrapolation

Same as in the MCSM w/ an inert core

1. Extrapolation of our MCSM (approx.) results
   to exact results in the finite size of 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 of the results in the finite size
   to the infinitely large basis space
   - Empirical extrapolation w.r.t. N_{shell}
   - IR- & UV-cutoff extrapolations

→ Ab initio solution

Inter-nucleon potentials

- JISP16:

  J-matrix Inversion Scattering Potential tuned up to O-16

  - Derived from nucleon-nucleon scattering phase shifts
  by J-matrix inversion scattering method.
  Then, adjusted via a phase-shift equivalent transformations
  (PETs) to better describe light nuclei with A < 16

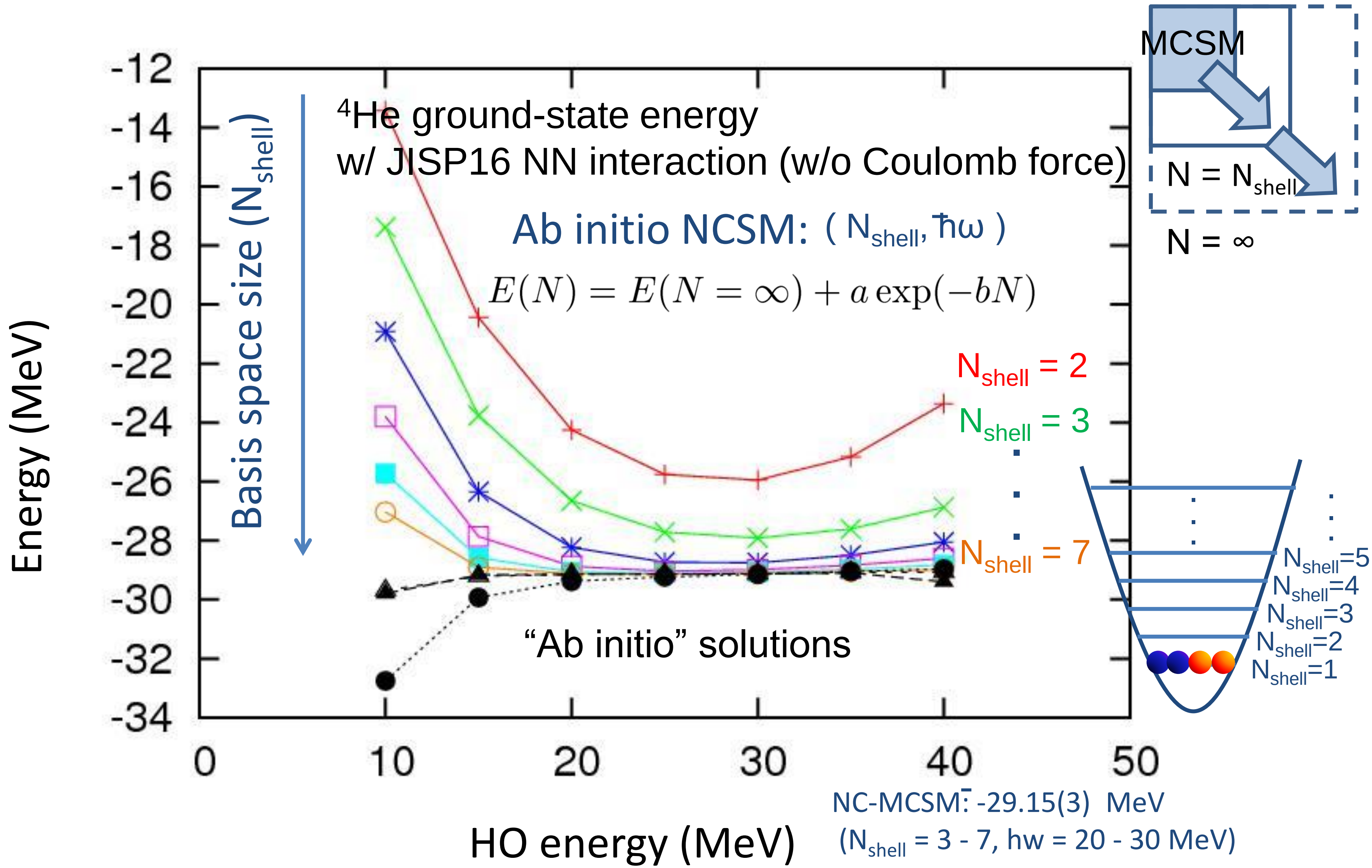
  A. M. Shirokov, J. P. Vary, A. I. Mazur and T. A. Weber, PLB644, 33 (2007).

- Daejeon16:

  - Starting from χEFT N3LO NN interaction (EM) + PETs

A. M. Shirokov, I. J. Shin, Y. Kim, M. Sosonkina, P. Maris and J. P. Vary, PLB761, 87 (2016).

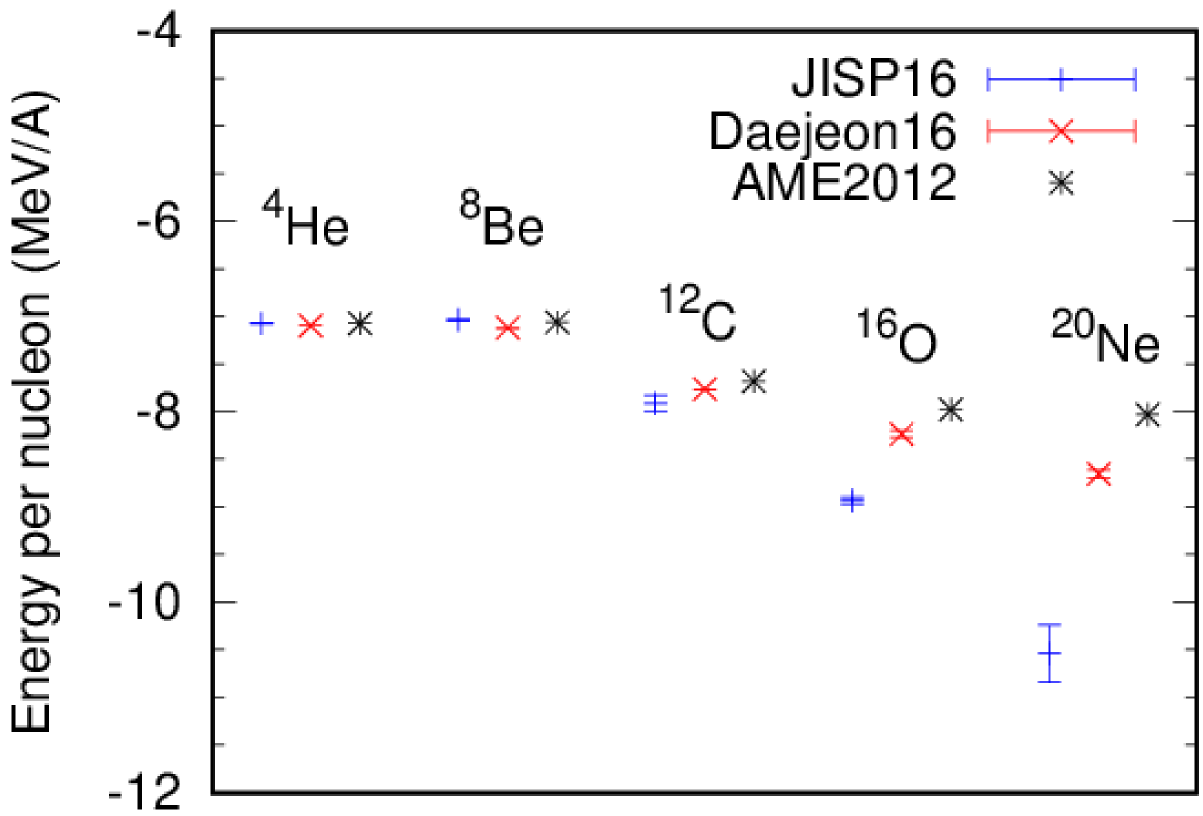
Extrapolation to the infinitely large basis space



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

c.f.) NCFC: -29.164(2) MeV

Ground-state energies of light nuclei



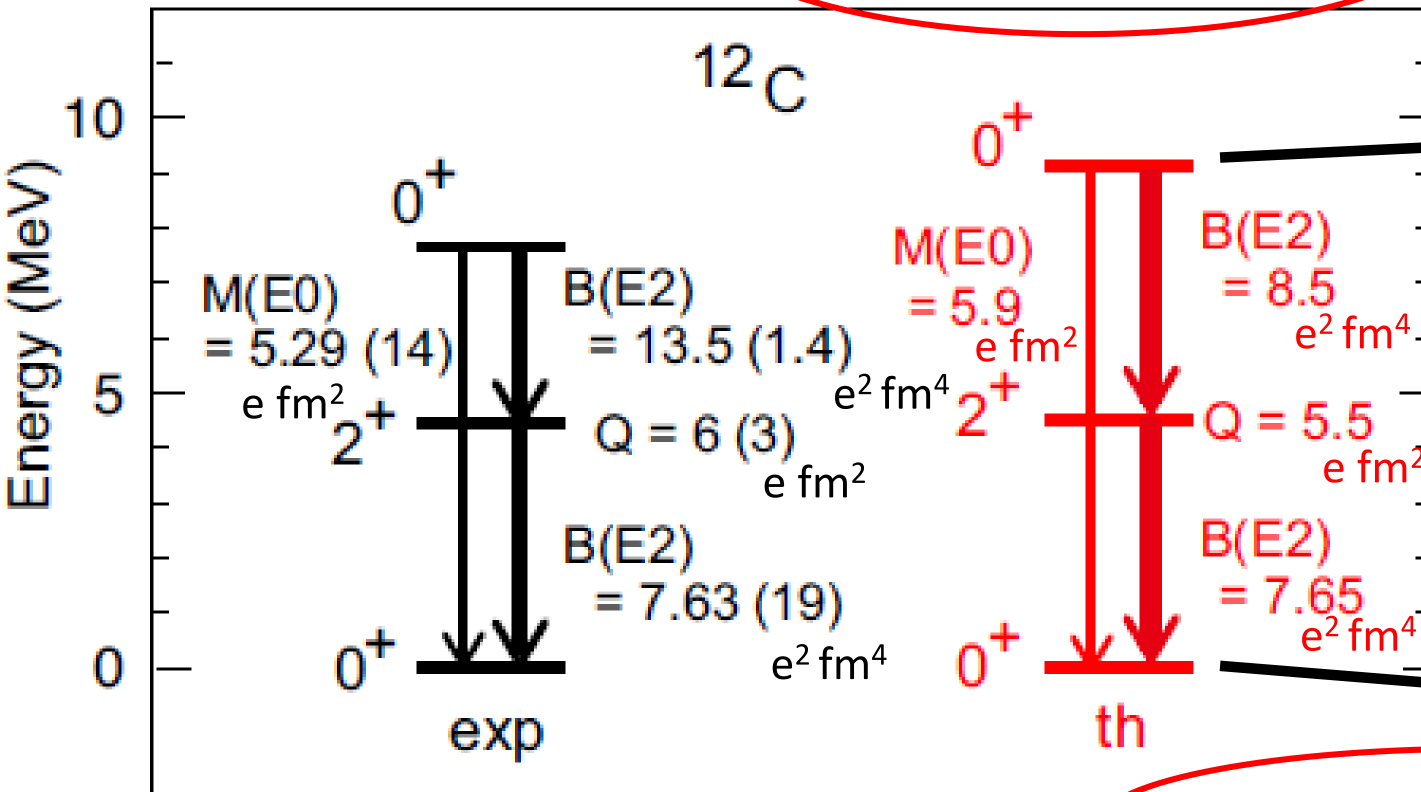
MCSM results are obtained using K computer by traditional extrapolation w/ optimum harmonic oscillator energies.

JISP16 results show good agreements w/ experimental data up to ^{12}C, slightly overbound for ^{16}O, and clearly overbound for ^{20}Ne.

Daejeon16 results show good agreements w/ experimental data up to ^{20}Ne.

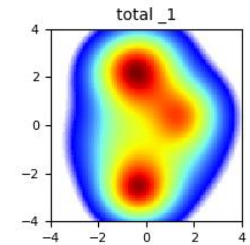
^{12}C excitation spectra and transitions

Single particle (liquid) like ~ 1/3
Alpha cluster like ~ 2/3



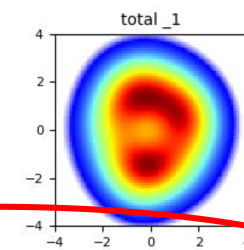
Intrinsic density

1st excited 0^+ state
(Hoyle state?)



r_{pp} = 2.60 fm

Ground state



Single particle (liquid) like ~ 94 %

Daejeon16 NN, N_{shell} = 7, hw = 20 MeV

K computer / Supercomputer Fugaku

r_{pp} = 2.28 fm

r_{pp} = 2.32(2) fm (exp)

Summary

- Ab initio calculations in NC-MCSM can be performed up to A ~ 20 on state-of-the-art supercomputers.
- NC-MCSM results can be extrapolated to the infinitely large basis space to obtain an ab initio solution.
  - Daejoen16 NN interaction provides good agreement w/ experimental data for light nuclei.
- Low-lying level structure of 12C can be examined by NC-MCSM, including alpha-cluster structure of the Hoyle state.

← T. Otsuka

Future perspective

- Di-neutron structure of the He isotopes
- Second 0+ state of 16O
- Beta decay
- Something long-standing challenges in low-energy nuclear physics (Please let me know!)