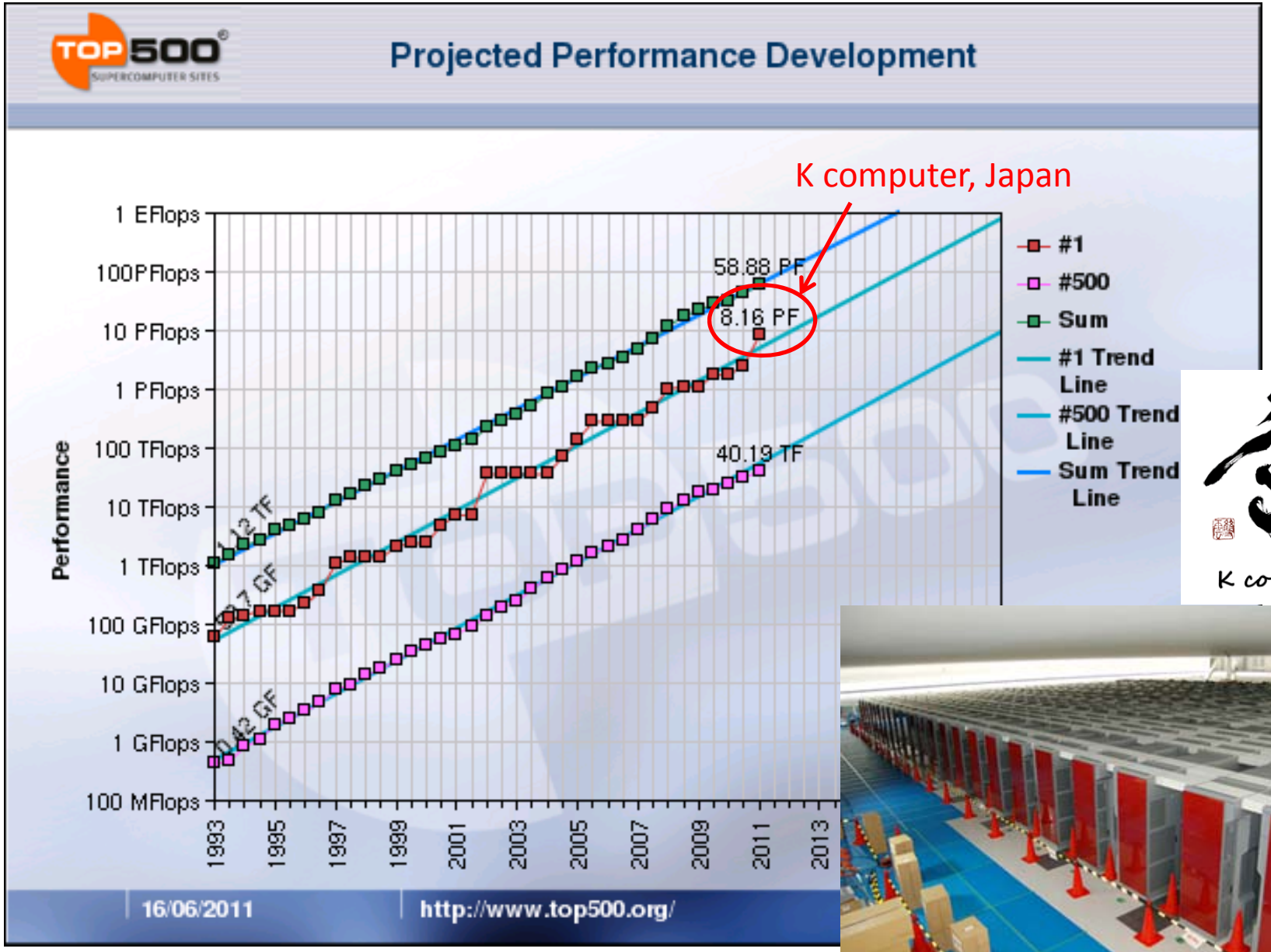
one-day workshop on
“ab initio study of nuclear structure and reaction”
RCNP 2012/12/11

New Generation of the Monte Carlo Shell Model for the K-Computer Era

Noritaka SHIMIZU (CNS, Univ. of Tokyo)

T. Abe (Tokyo), M. Honma (Aizu), P. Maris(Iowa),
T. Mizusaki (Senshu), T. Otsuka (Tokyo), Y. Tsunoda (Tokyo),
Y. Utsuno(JAEA), J. P. Vary(Iowa), T. Yoshida (CNS)



Japanese “K computer” got rank 1 in the world.

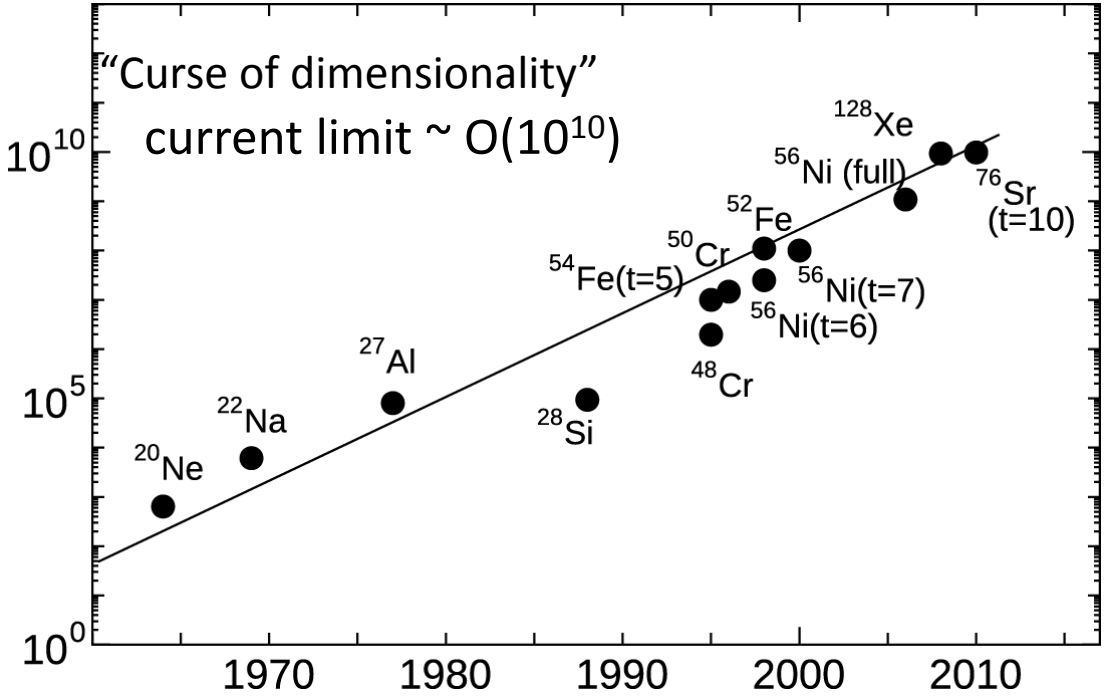
(Now rank 2)

SPARC64 VIIIfx (8 cores) 88128 nodes

What is the application program to run on it ?

Towards the limit of exact diagonalization method

m-scheme dimension:
dimension of Hamiltonian matrix
to be diagonalized
in conventional Lanczos method.



- *t*-particle *t*-hole, or exciation energy (*hw*) truncation
  + Lanczos method
- Generator coordinate method
- Monte Carlo Shell Model
- VAMPIR
- Importance Truncated Shell Model
- Projected CI
- Variational Monte Carlo method, DMRG, HMD, and so on ...

Computational challenges in large-scale shell-model calculations

- Lanczos method
  - (almost) exact eigenvalues and eigenstates
  - on-the-fly generation of the Hamiltonian matrix elements, store state vectors on memory
  - large I/O, large memory required (e.g. 10^{10} dim. = 40GB/w.f.)
    ... current limit *M*-scheme dim. ~O(10^{10})
  - rather large number of excited states
  - strength-function method

- Monte Carlo Shell Model (MCSM)
  - a tool to go beyond the Lanczos method
  - variational wave function + energy-variance extrapolation
  - obtain a few lowest eigenstates
  - small I/O, good parallel computation

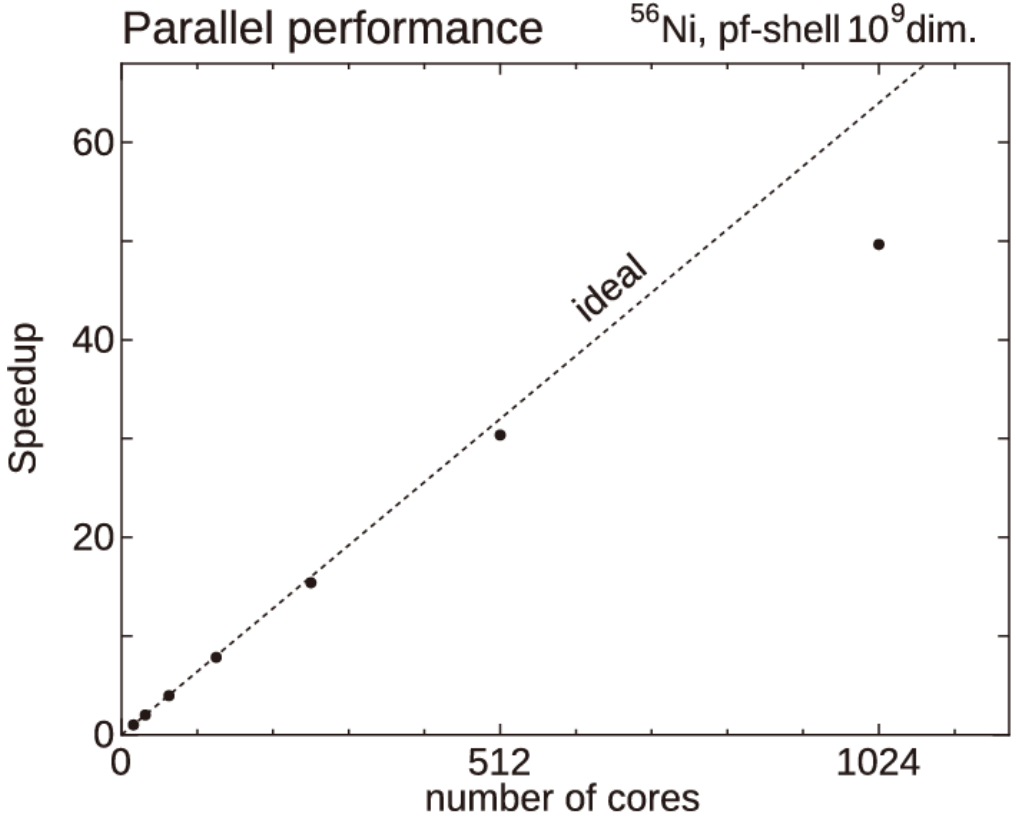
Lanczos method

applied to E1 excitation and GDR of Ca isotopes

Collaboration with Y. Utsuno(JAEA),
T. Mizusaki (Senshu), M. Honma (Aizu),
S. Ebata (CNS), T. Otsuka (Tokyo)

“Kshell” with OpenMP + MPI hybrid

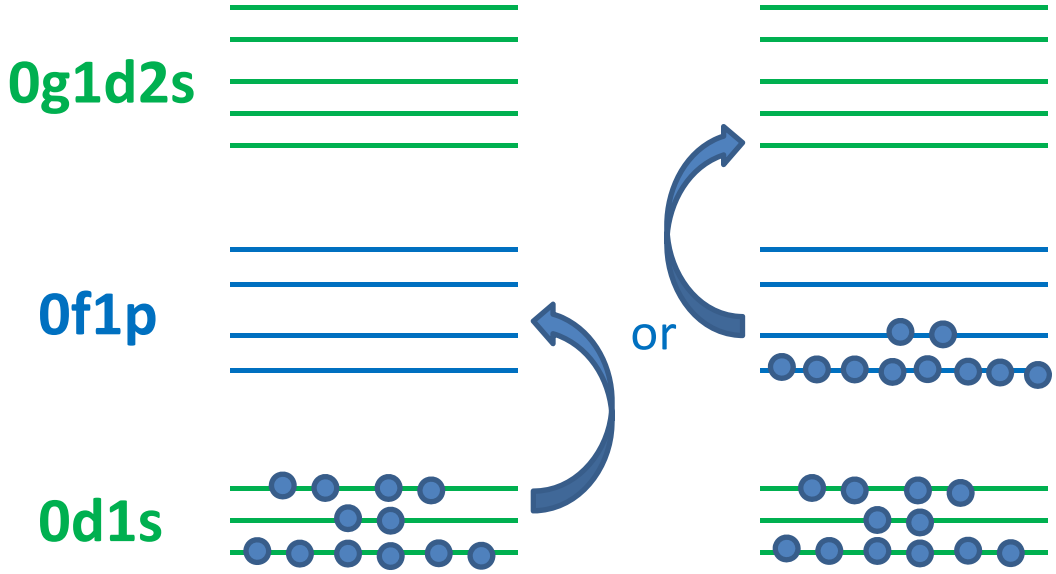
- *M*-scheme + “on the fly” computation of Hamiltonian matrix elements ... similar to *MSHELL64,* but code was redesigned for MPI parallel
- parallel in “partition”, or Slater determinant is categorized by occupation numbers of single-particle orbits
- program code is still under intensive developments for higher scalability



time/Lanczos iteration :: 25min.(16cores) ➡ 30sec.(1024cores)

Outline of the shell-model calculation

- Valance shell
  - full *sd-pf-sdg* shell
- 1hw truncation
  - full 0hw for the natural-parity states
  - full 1hw for the unnatural-parity states

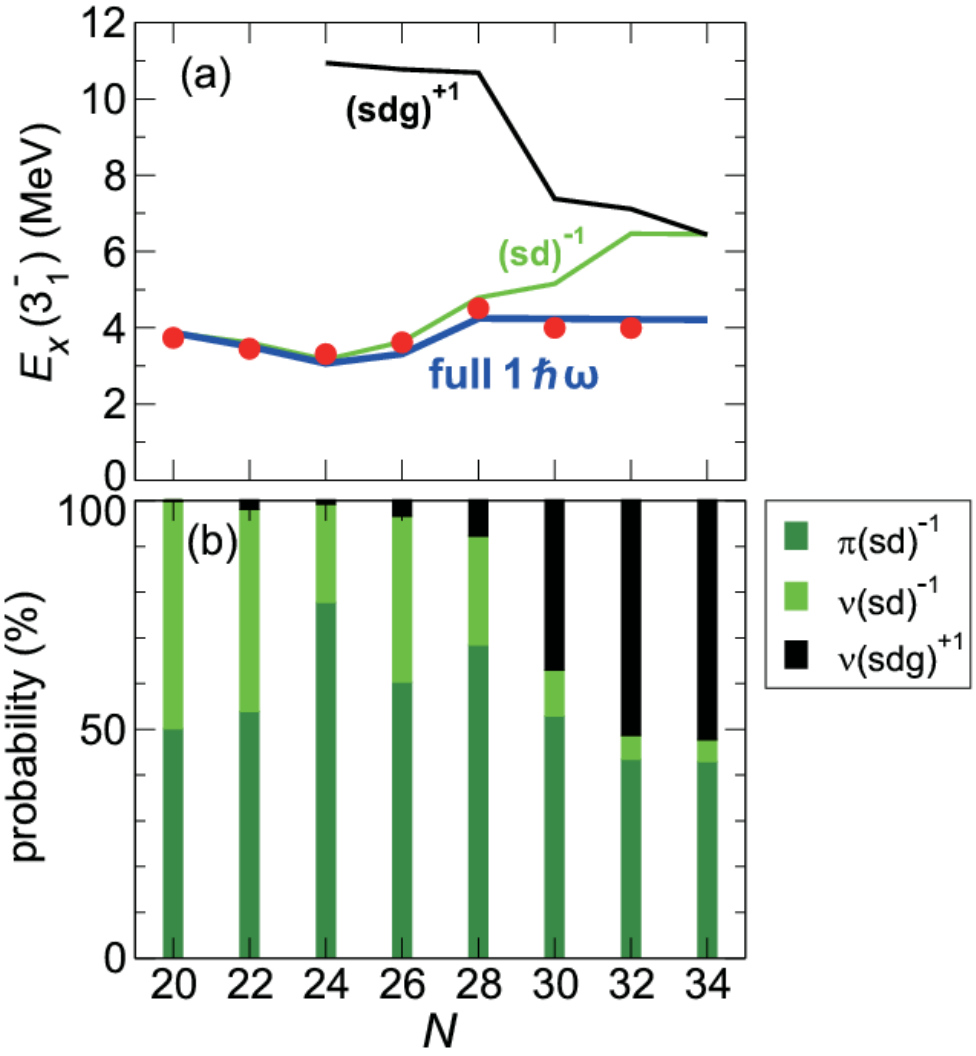


  - Either sd-to-pf or pf-to-sdg excitation is allowed.
  - Spurious components can be almost completely removed.
  - Somewhat similar to RPA but the 0hw correlation is fully included.
- 3hw truncation
  - full 2hw in *sd-pf-sdg* shell for the natural-parity states
  - full 3hw in *sd-pf-sdg* shell for the unnatural-parity states
- Effetive interatction USD+GXPF1B+VMU

Courtesy of Y. Utsuno

Systematics of the 3^-_1 state in even-A Ca

- Three calculations
  - excitations from sd to pf only
  - excitations from pf to sdg only
  - full 1$\hbar\omega$ configurations
- 3^-_1 levels
  - sd-pf calc.
    - good agreement for N≤28
    - large deviation for N>28 (no interaction dependence)
  - full 1hw calc.
    - Strong mixing with the sdg configuration accounts for the stable 3^- levels.



Lanczos strength-function method for E1 excitation

$|\varphi_0(1^-)\rangle = O(E1)|0^+(1)\rangle$

ground state

Lanczos iteration using $|\varphi_0(1^-)\rangle$ as an initial state.

Smoothing with Lorentz distribution

$$L(x, x_0, \Gamma) = \frac{1}{\pi} \frac{\gamma}{(x - x_0)^2 + \gamma^2}$$

$$\text{with } \gamma = \Gamma/2.$$

Good distribution obtained in a few hundred Lanczos iterations

$$\left\{H^n|\phi_0\rangle, H^{n-1}|\phi_0\rangle, \ldots, H^1|\phi_0\rangle, |\phi_0\rangle\right\}$$

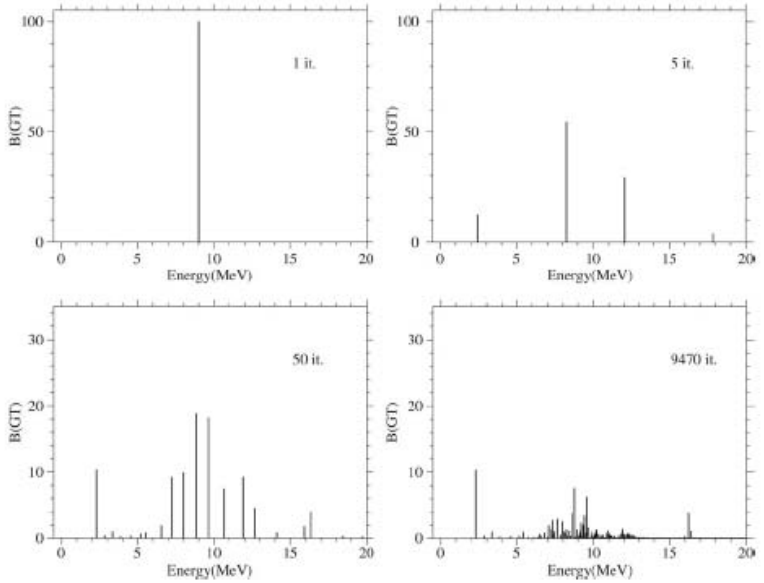


Fig. 6. Evolution of the *GT* strength function of ^{48}Ca with the number of Lanczos iterations.

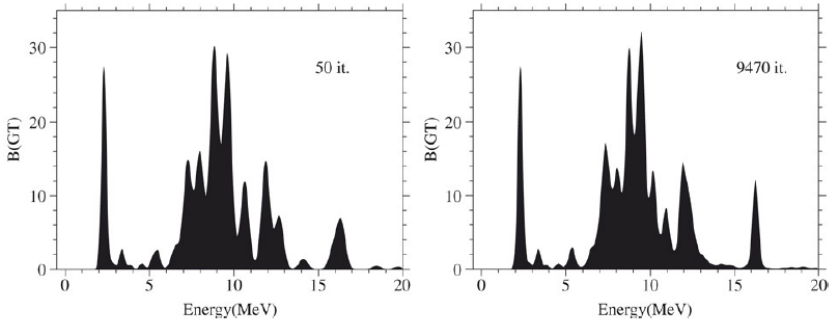


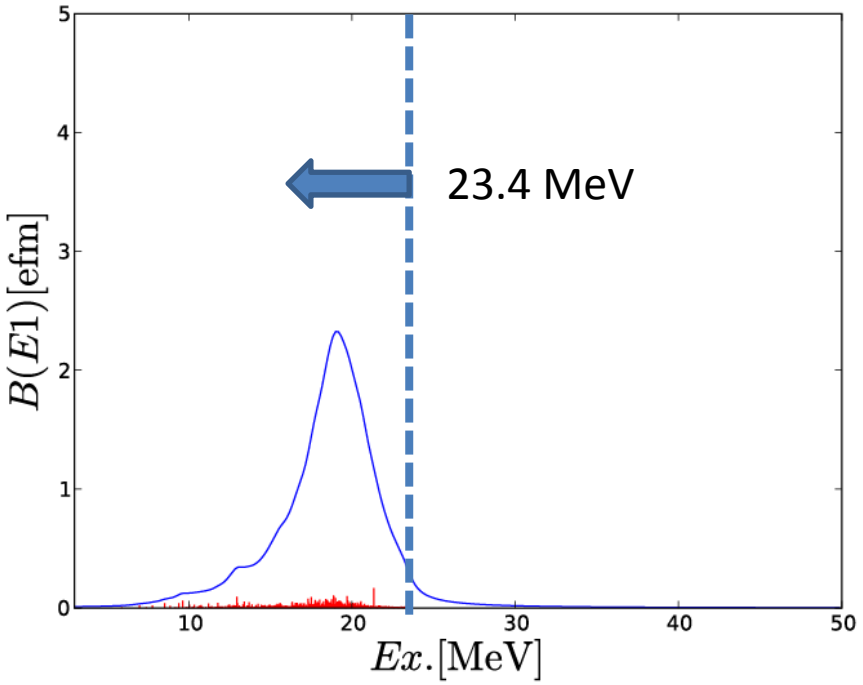
Fig. 7. Convolution of the *GT* strength function with Gaussians.

Ref. E. Caurier *et al.,* PPNP 59 226 (2007)

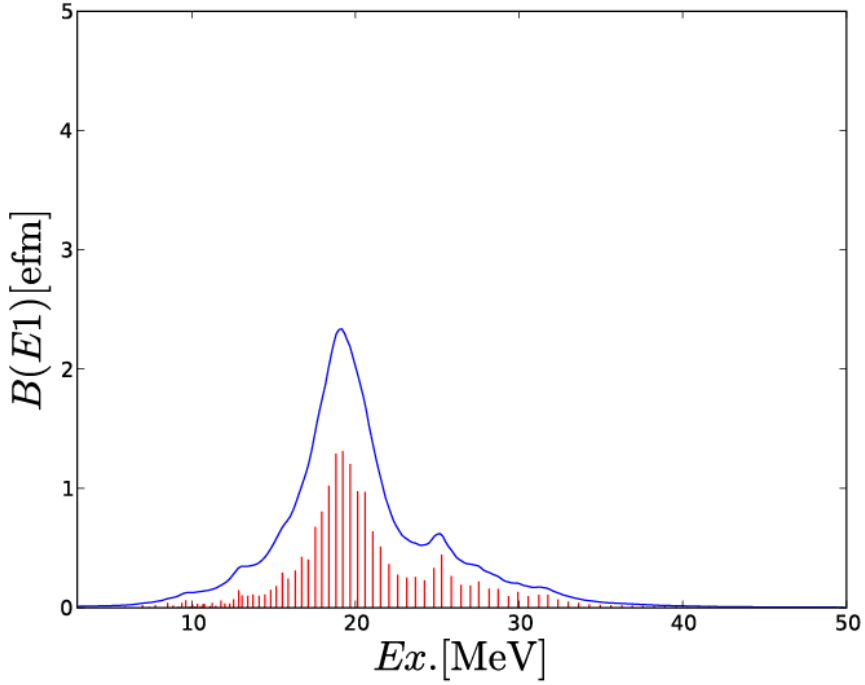
Exact diagonalization vs. strength function

48 Ca "1$\hbar\omega$ model space" 2.8 x 10^6 *M*-scheme dim.

Exact lowest 3,000 states



Lanczos strength function (300 iter.)

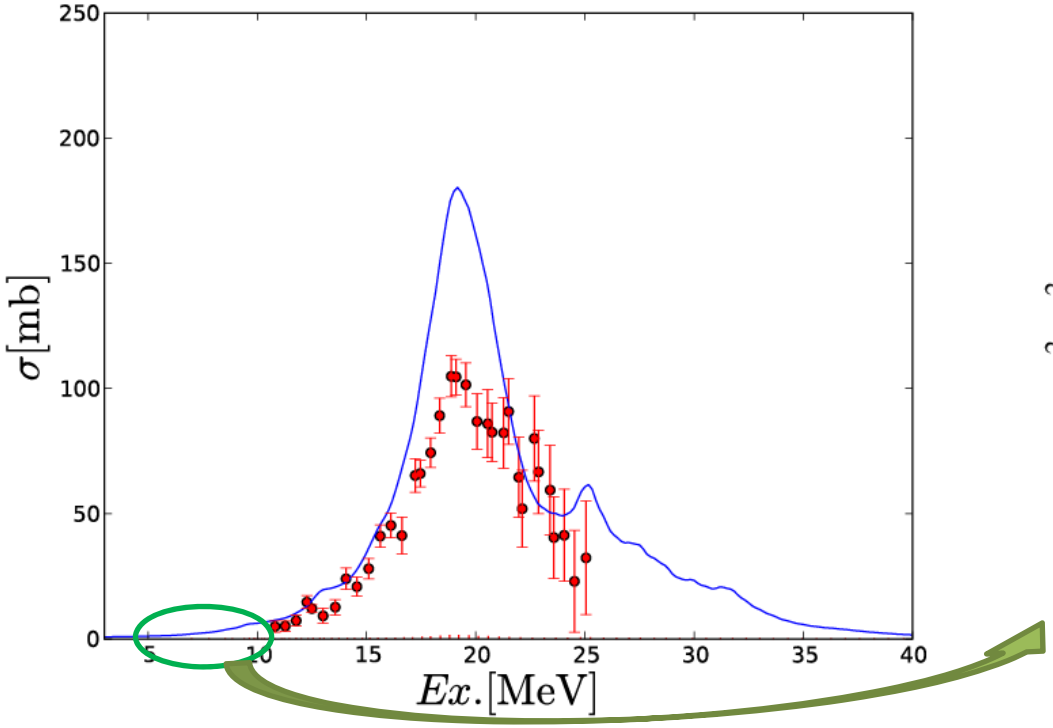


- Smearing width: Γ=1 MeV
- No visible difference between the two methods

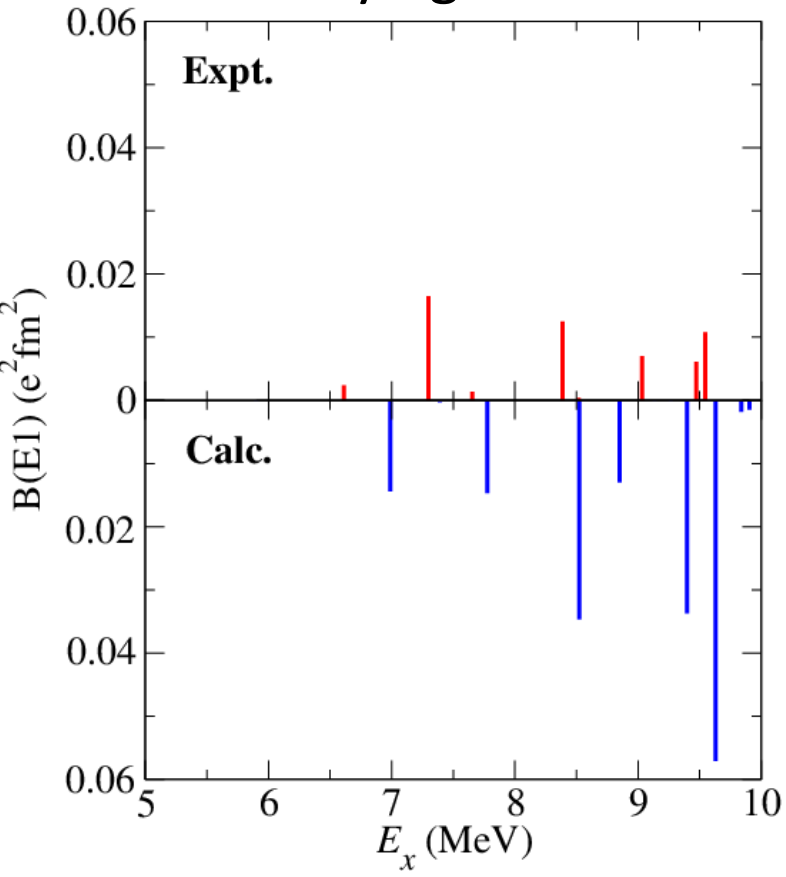
E1 excitation and Giant Dipole Resonance of ^{48}Ca

"$1\hbar\omega$ model space" 2.8 x 10^6 *M*-scheme dim.

GDR with Γ=1 MeV



Low-lying 1^- states



- GDR peak position: good
- GDR peak height: overestimated
- Low-lying states: shifted left or less fragmented

} need for $2\hbar\omega$ (g.s.) and $3\hbar\omega$ (1^-)?

Development of
the advanced Monte Carlo Shell Model

Monte-Carlo Shell Model

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

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

$$|\Psi\rangle = \sum_{i=1}^{N_{MCSM}} c_i \sum_{K=-J}^{J} g_K P^{J,\pi}_{MK} |\phi(D^{(i)})\rangle$$

MCSM basis, deformed Slater det.

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

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

$\hat{h}(\sigma)$ one-body Hamiltonian
σ... auxiliary field
random numbers
generated stochastically

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

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

Advantageous for parallel computation, bases and mesh points

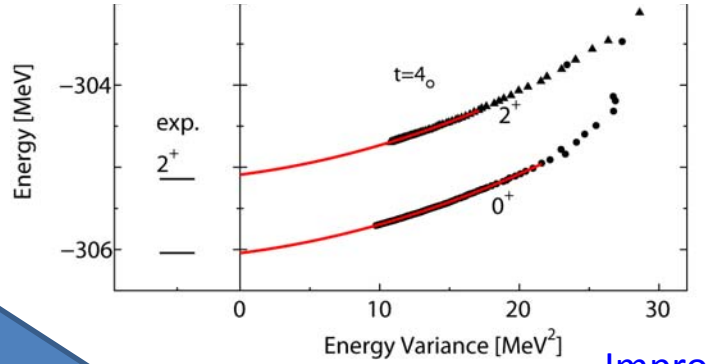
Developments of the Monte Carlo shell Model towards “K computer”

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

N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe, and M. Honma, Phys. Rev. C **82,** 061305(R) (2010).

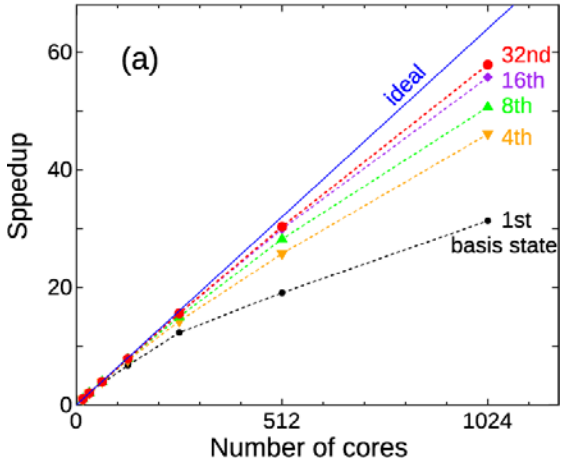
PC cluster
100CPU parallel

- Precise estimation of energy eigenvalue
  by variance extrapolation + reordering technique



N. Shimizu et al., Phys. Rev. C 85 054301(2012).

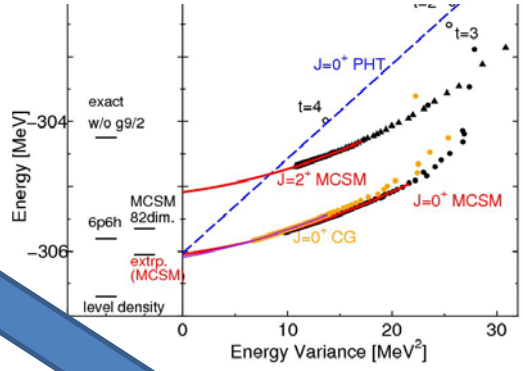
Parallel efficiency



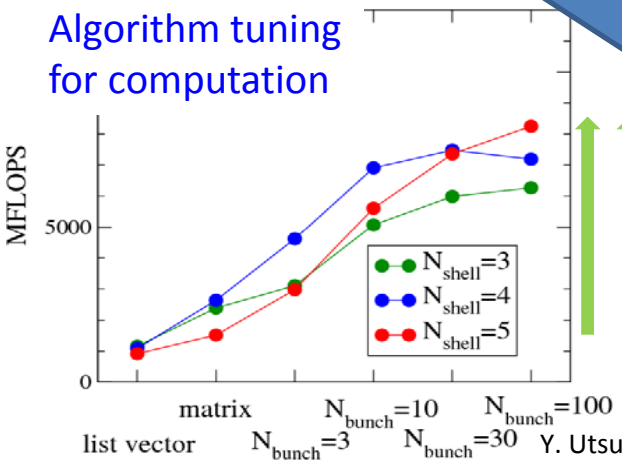
OpenMP+MPI hybrid parallel

N. Shimizu, *et al.* Prog. Theor. Exp. Phys. **2012** 01A205 (2012).

Improvement of the MCSM by Conjugate Gradient method



Algorithm tuning for computation



8 times faster at maximum

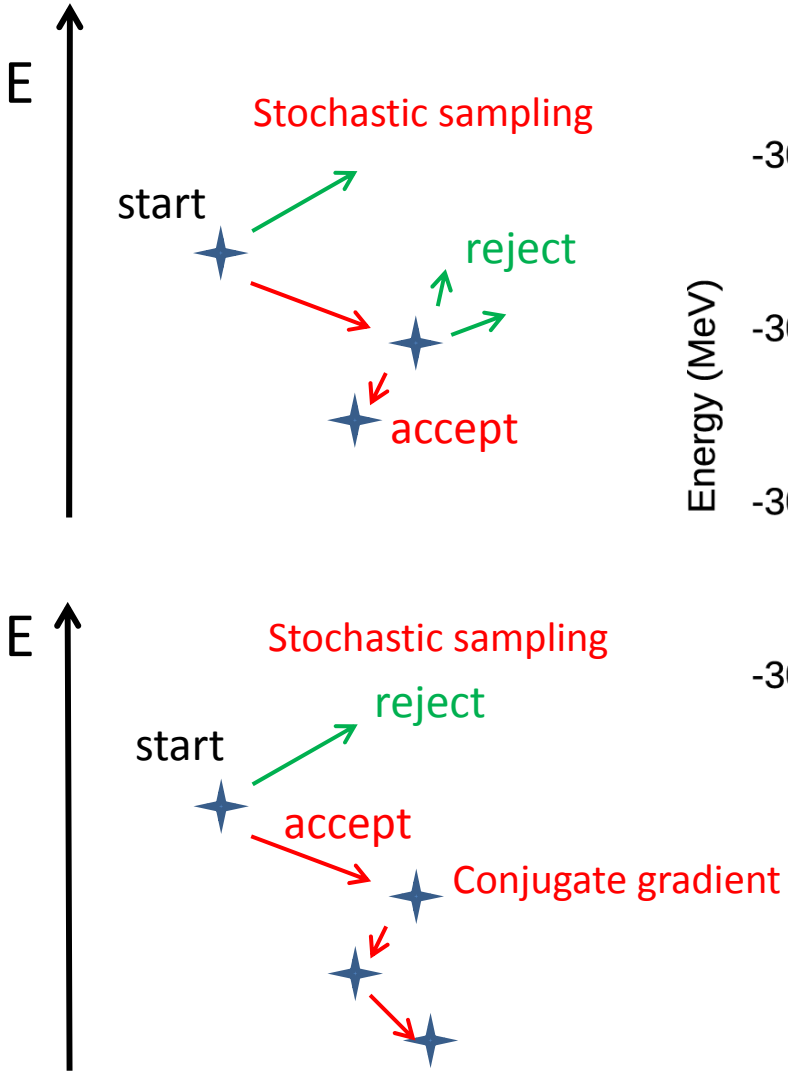
Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, Comp. Phys. Comm. 184 102 (2013).

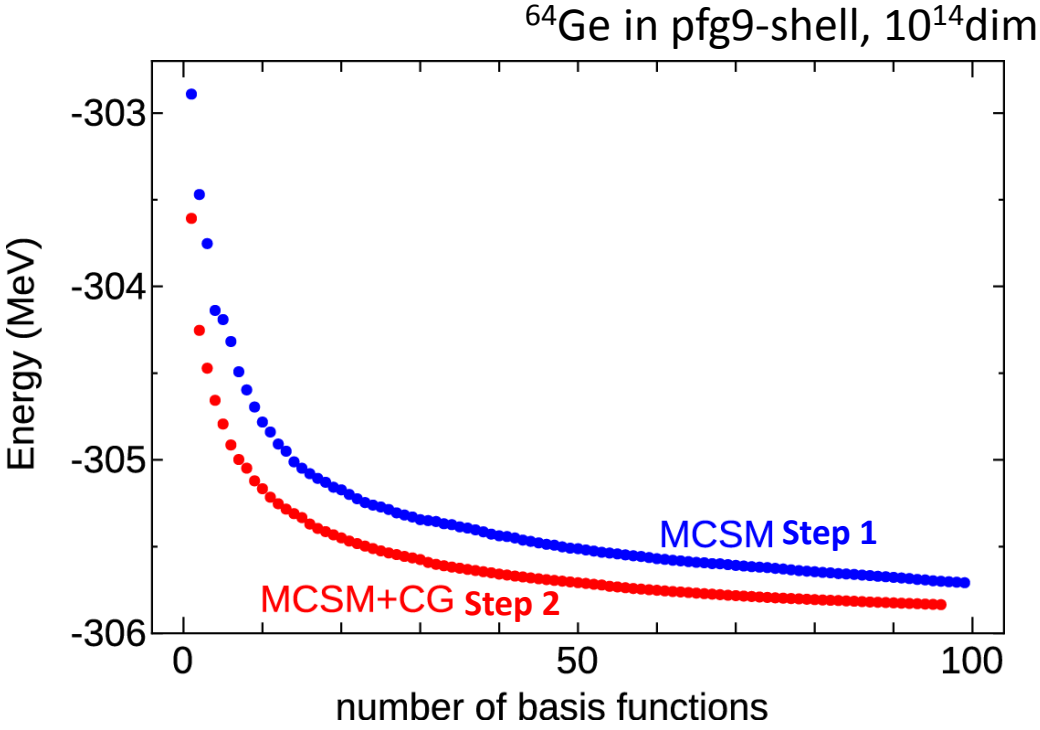
100 CPUs
→ Towards 10^5 cores

SPARC64 VIIIfx 705,024 cores

K computer

Energy minimization by Conjugate Gradient method

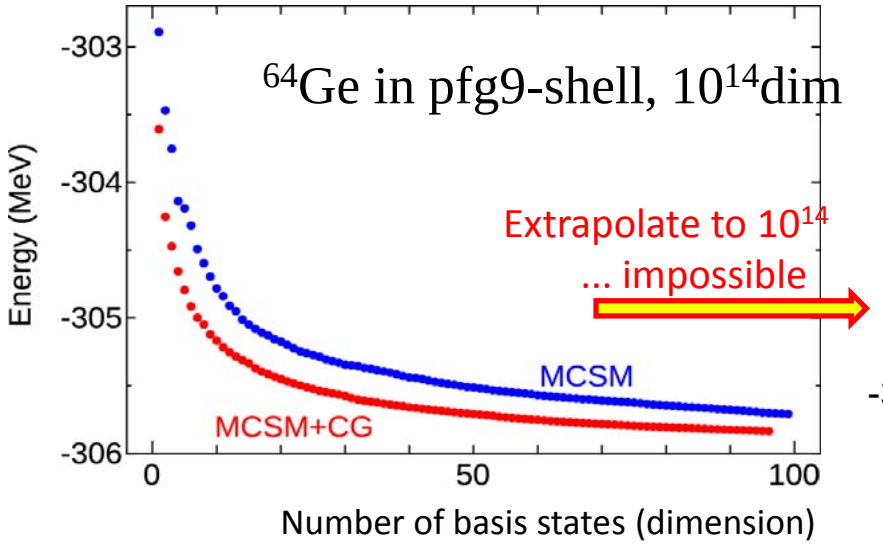




Stochastic sampling before conjugate gradient to minimize the expectation value energy

reduce the number of basis function roughly 30%

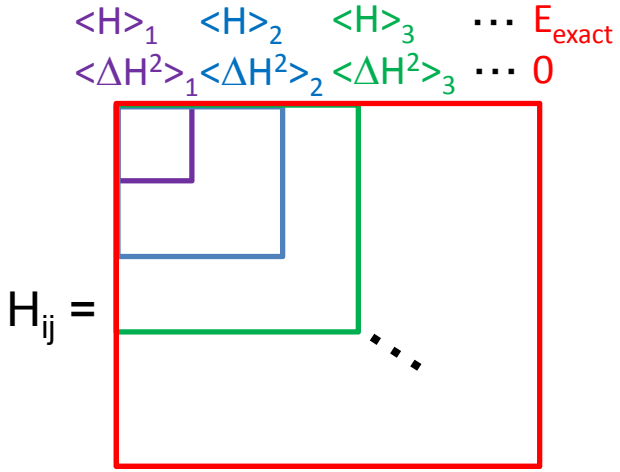
Energy variance extrapolation in the MCSM: ^{64}Ge in *pfg9*-shell

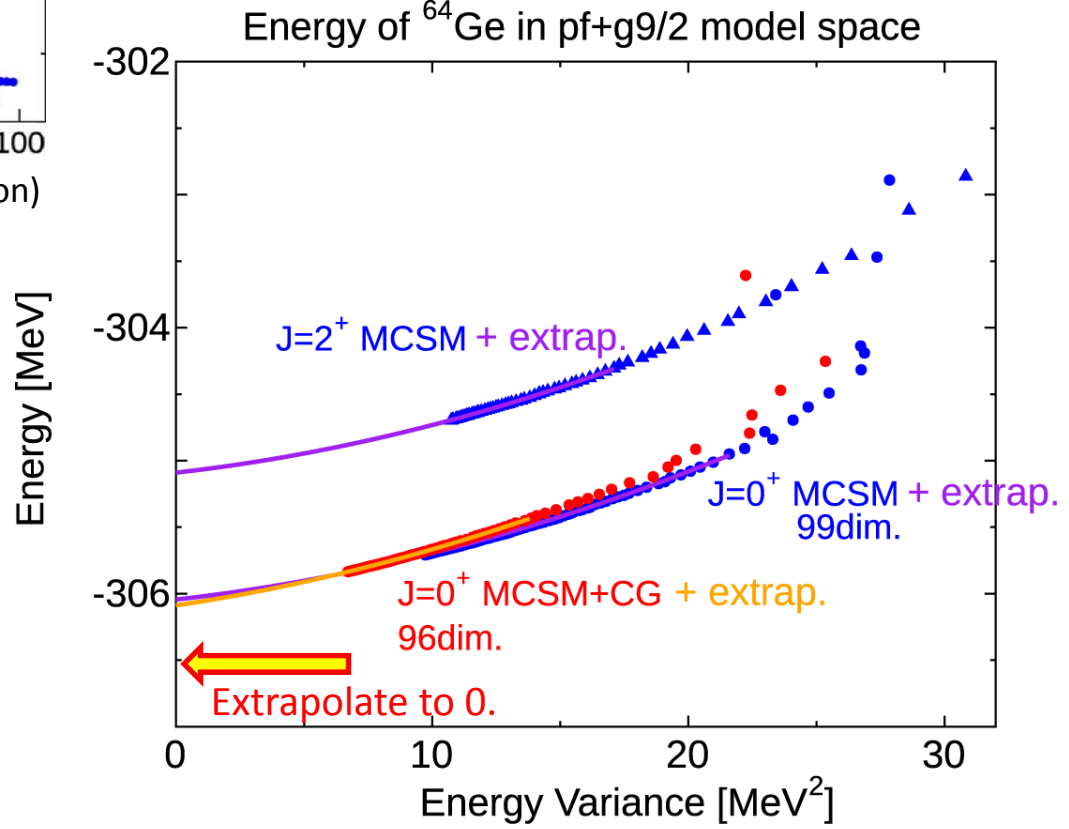


Energy variance : $\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$

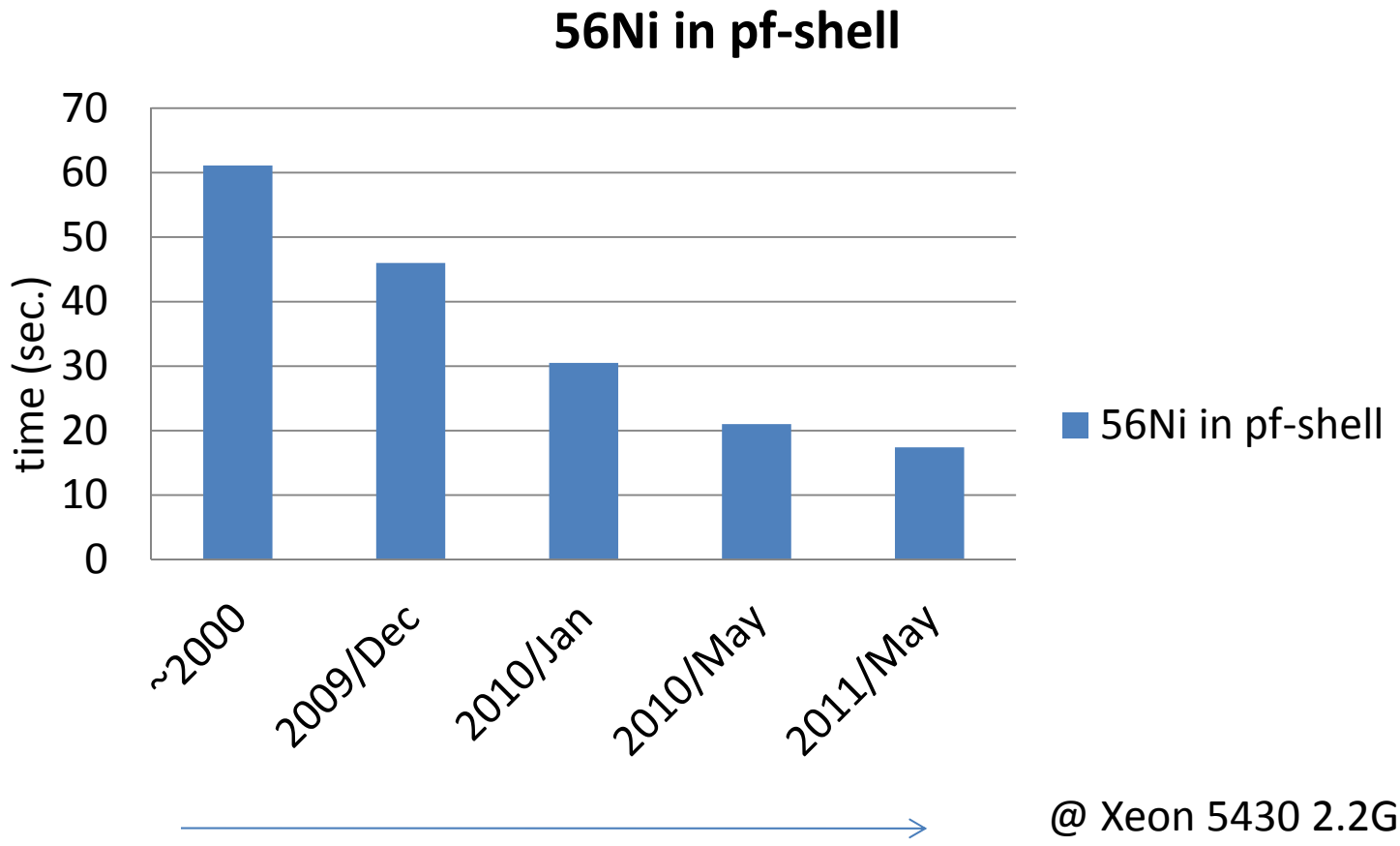
As the number of basis states increases,
the approximated w.f. approaches the exact one
and the energy variance approaches zero.

Extrapolate towards $\langle \Delta H^2 \rangle \to 0$





Performance improvement of the MCSM code in a single processor



@ Xeon 5430 2.2GHz

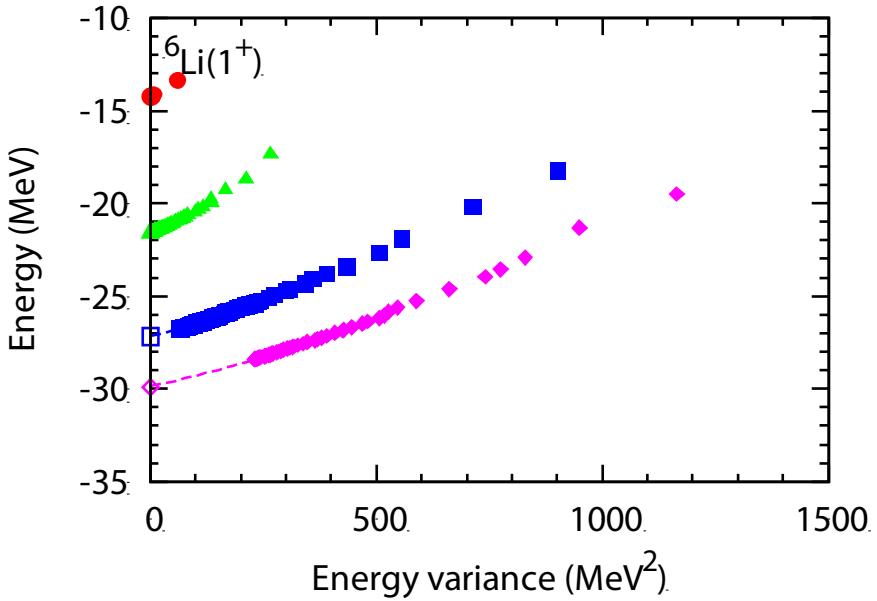
3.5 times speed up

10 times speed up for no-core shell model calc.

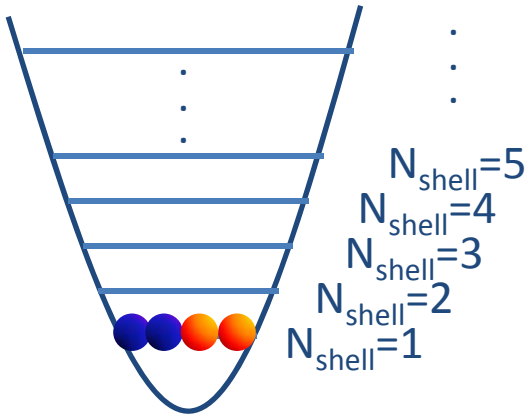
The performance improvement owes to the rewritten algorithm.

Application to
no-core shell model calculations

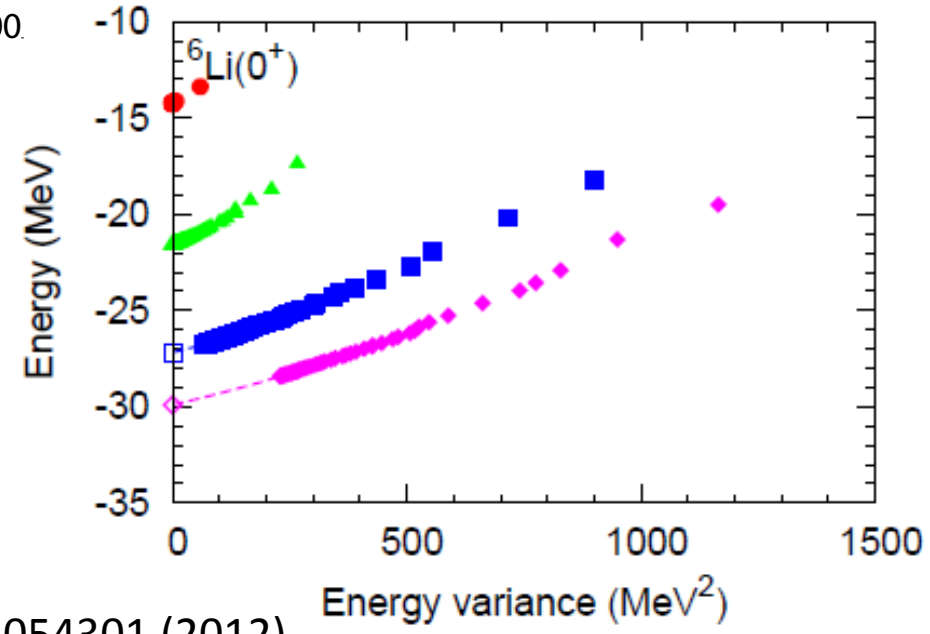
MCSM in light nuclei



Conergence vs. number of basis states



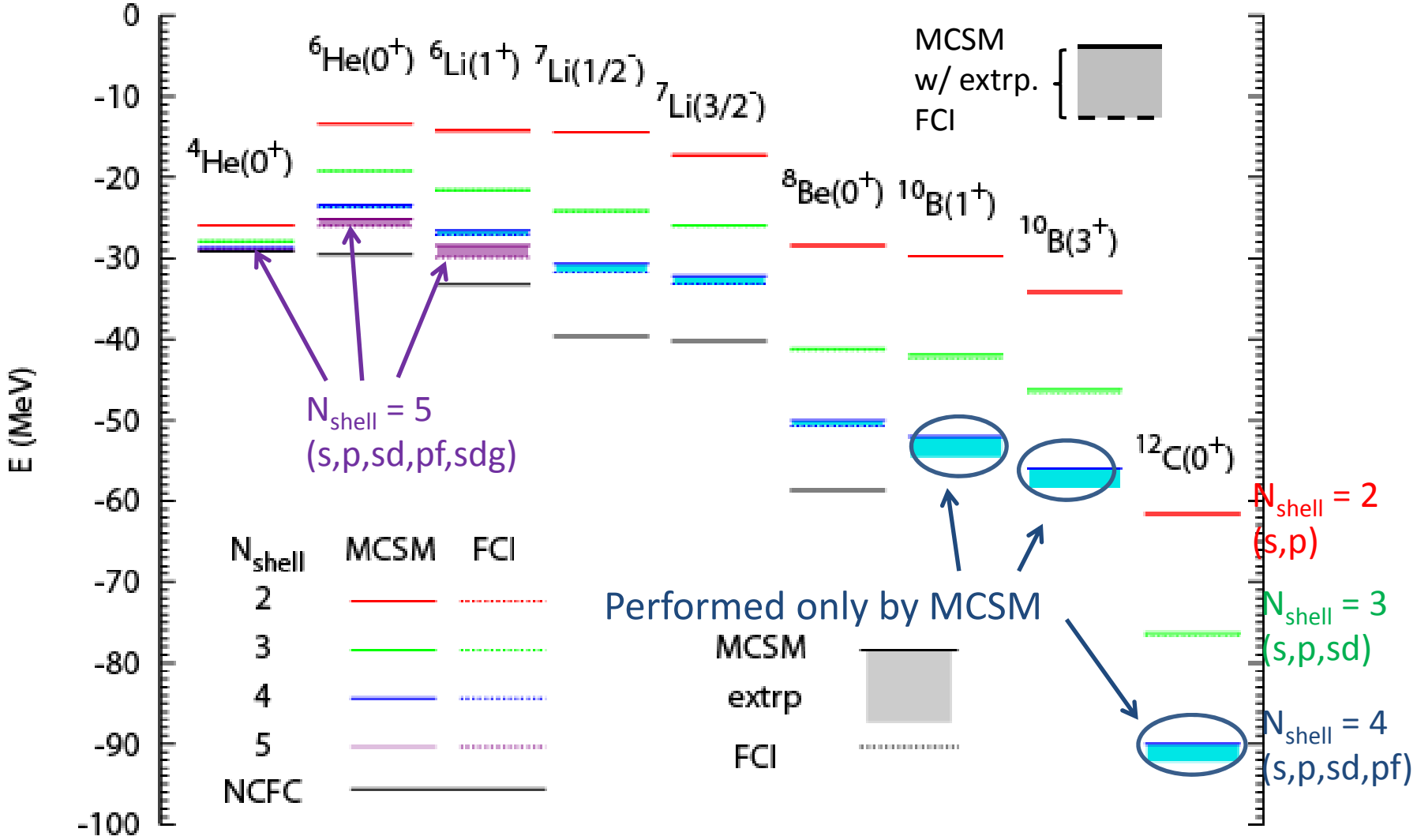
Energy variance extrapolation



Ref. T. Abe, P. Maris, T. Otsuka, N. Shimizu,
Y. Utsuno, and J. P. Vary, Phys. Rev. C 86 054301 (2012)

Ref. T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary,
Phys. Rev. C 86 054301 (2012)

Energies of the Light Nuclei



JISP16 interaction

Talk by T. Abe, QUCS 2012, Nara

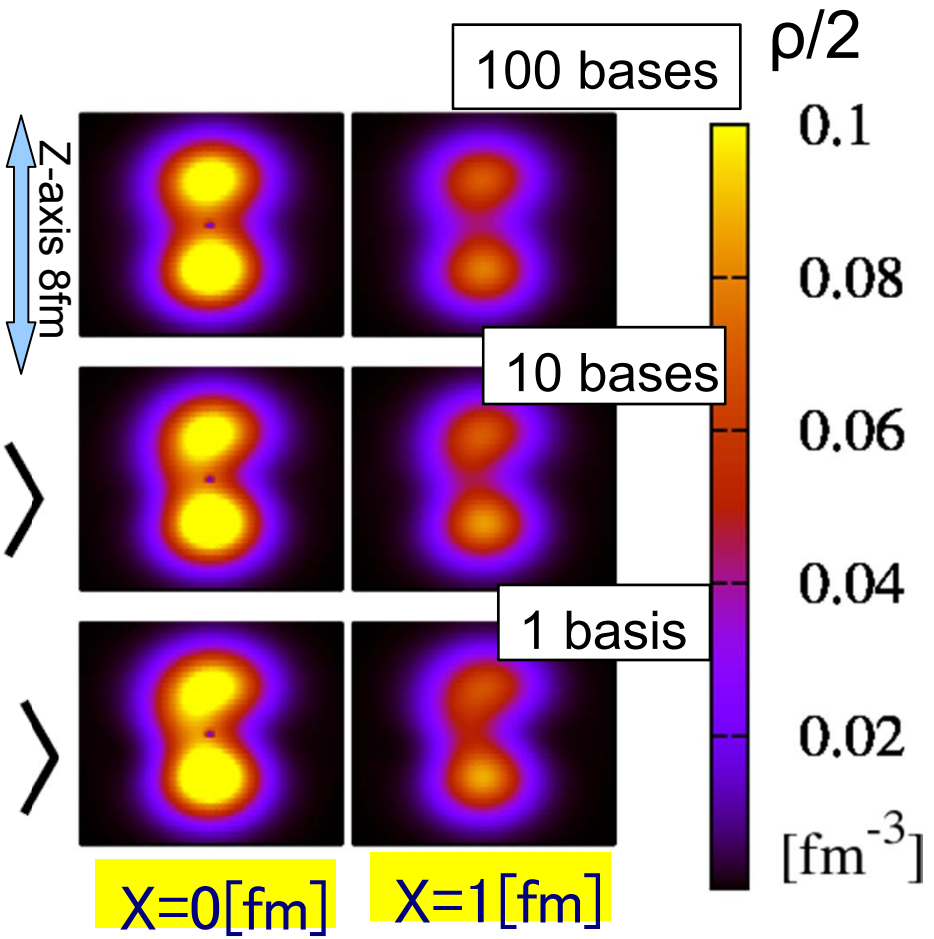
^{8}Be(0^{+}) intrinsic density profiles on YZ-plane

Nshell=4 100 basis states

$$|\Psi\rangle = P^{J,\pi}_{MK} \sum_{i=1}^{N_{MCSM}} c_i |\phi(D^{(i)})\rangle$$

$$= P^{J,\pi}_{MK} \Big| c_1 + c_2 + c_3 + \cdots + C_{98} + c_{99} + c_{100} \Big\rangle$$

$$= P^{J,\pi}_{MK} \Big| c_1 + c_2 + c_3 + \cdots + C_{98} + c_{99} + c_{100} \Big\rangle$$



2 alpha cluster structure emerges from scratch.

Basis number increases => alpha like structure manifested

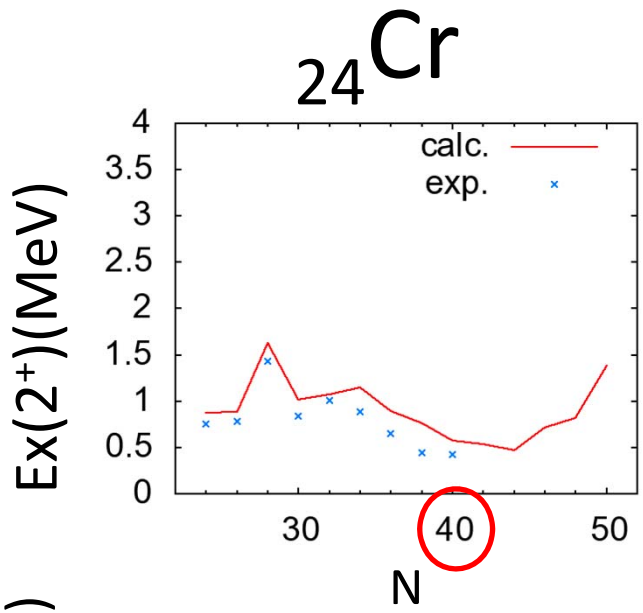
Ref. N. Shimizu, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma, and T. Otsuka, Prog. Theor. Exp. Phys. **2012** 01A205 (2012).

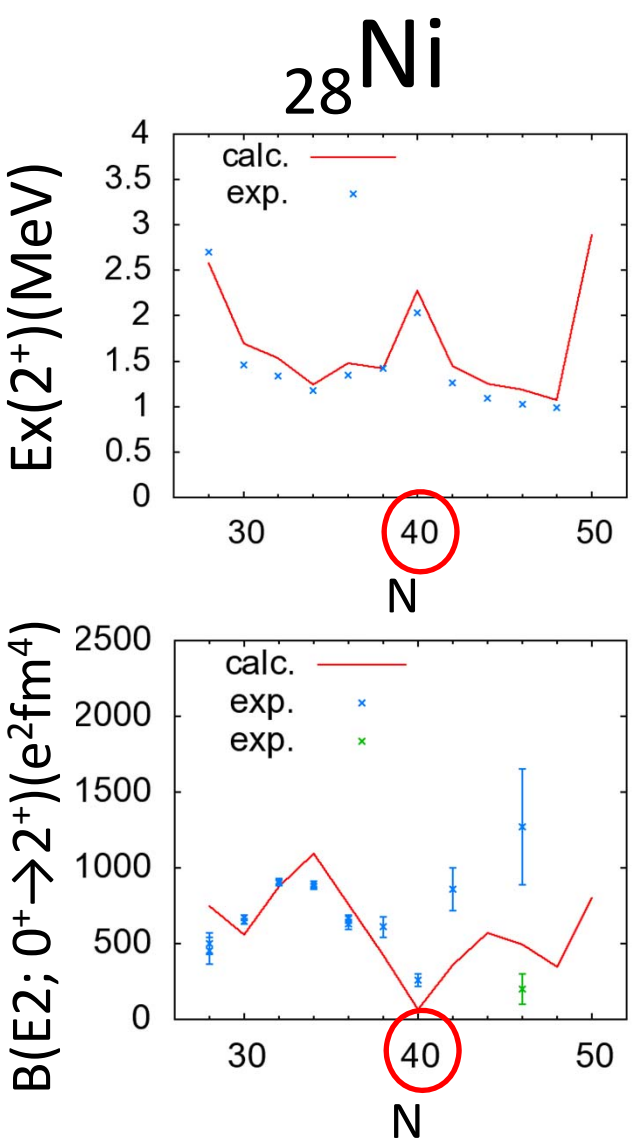
Application to shell model calculations in medium-heavy nuclei

Results of Cr and Ni

2^+ ex. energy

B(E2; $0^+ \rightarrow 2^+$): reduced transition probability

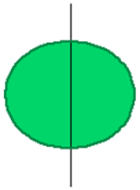




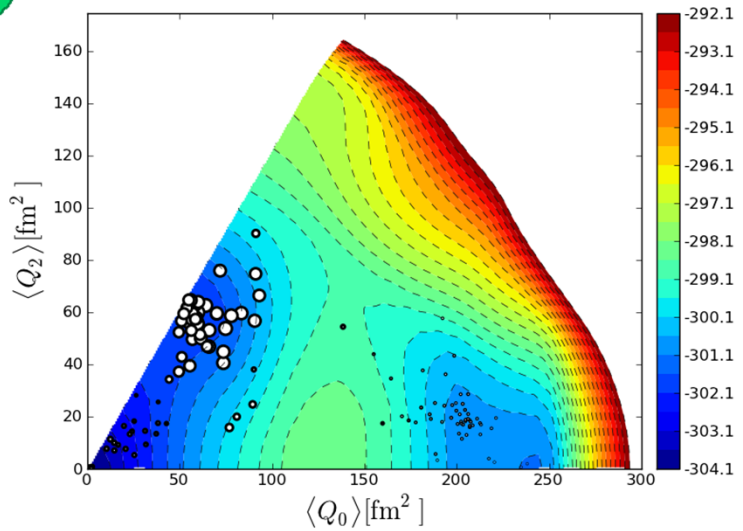
× B. Pritychenko, et al., arXiv:1102.3365v2 (2011)

× de Angelis, private communication

^{68}Ni 0^+ states ⇔ different shapes



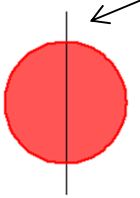
0^+_2 : oblate, β ~ -0.2



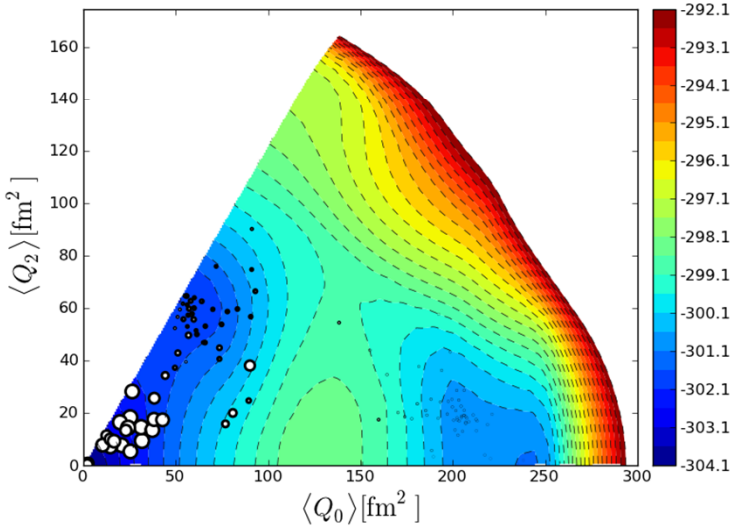
$$R(\theta) = R_0 \left[1 + \beta \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1) \right]$$

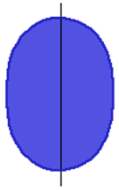
β: deformation parameter

symmetry axis

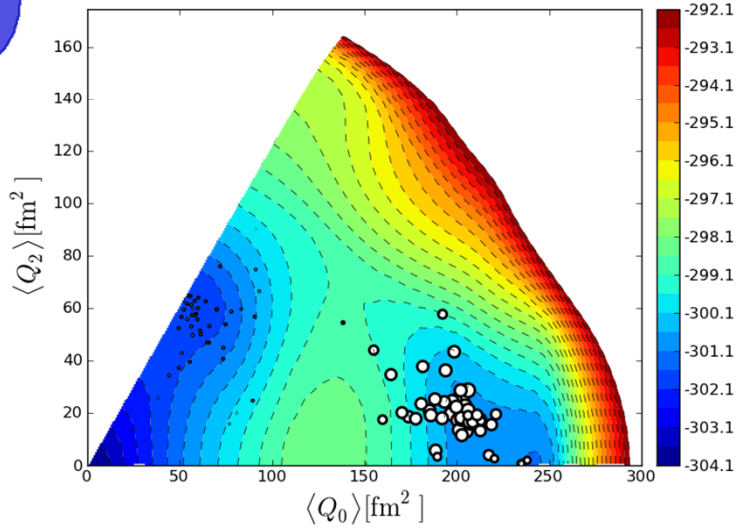


0^+_1 : spherical, β ~ 0

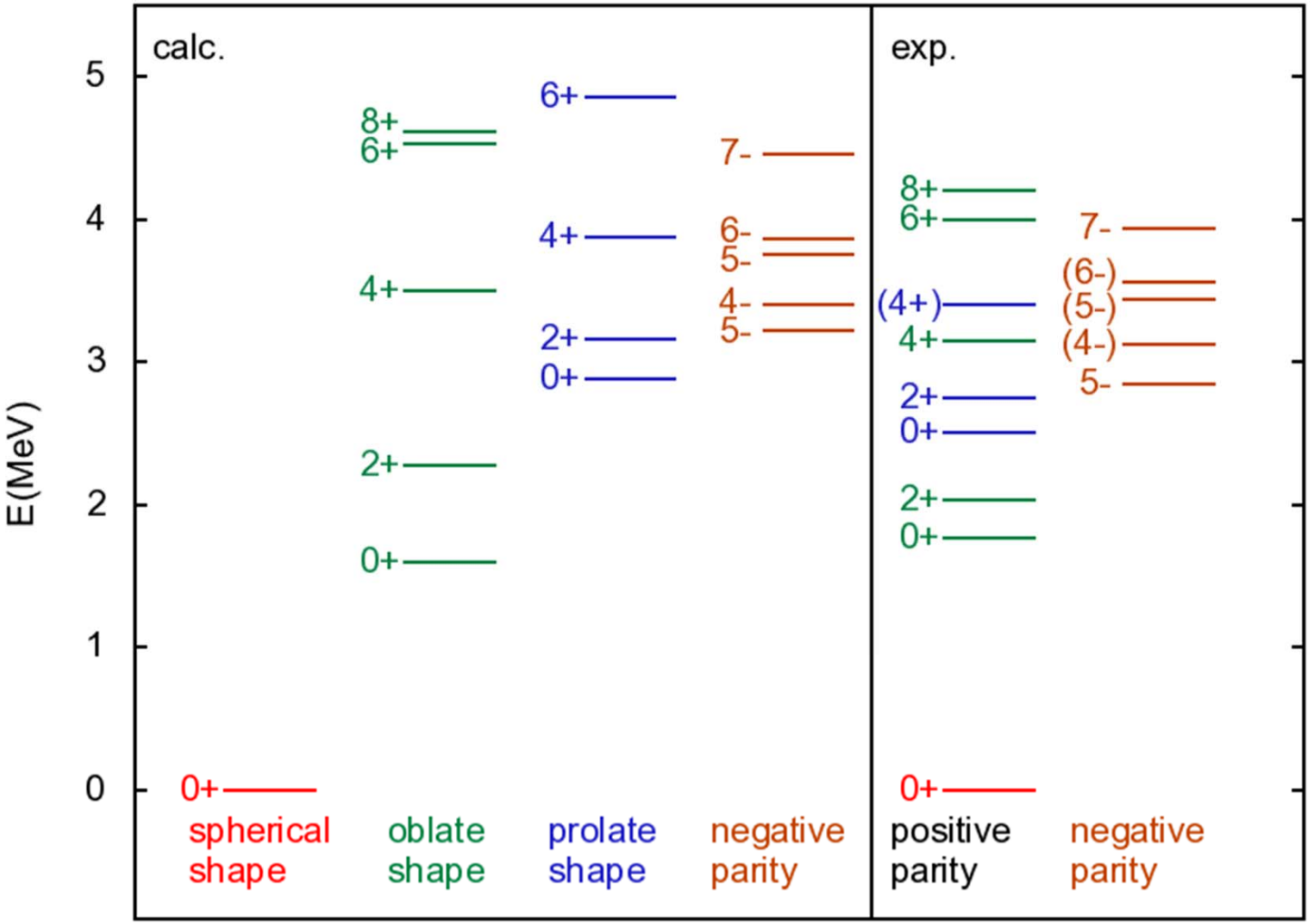


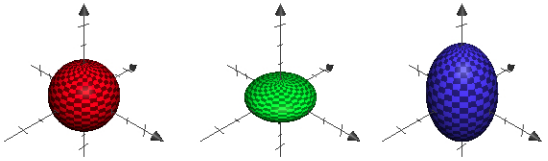


0^+_3 : prolate, β ~ +0.4



Level scheme of ^{68}Ni (a doubly magic nucleus)





$\beta \sim 0.0$ $\beta \sim -0.2$ $\beta \sim 0.4$ (superdeformed)

^{68}Ni in pf + g9 + d5 ... 5x10^{15} *M*-scheme dimension

Talk by Y. Tsunoda,
QUCS 2012, Nara

Summary

- New parallel code for Lanczos shell-model calculations with enables us to perform GDR in medium mass region. The $3\hbar\omega$ calculation successfully describe the GDR of ^{48}Ca.

- The MCSM was polished by algorithm tuning, conjugate gradient method, and energy-variance extrapolation.
- The MCSM program code was developed for massive parallel computer with 10^5 cores in “K computer”. Various applications are undergoing.