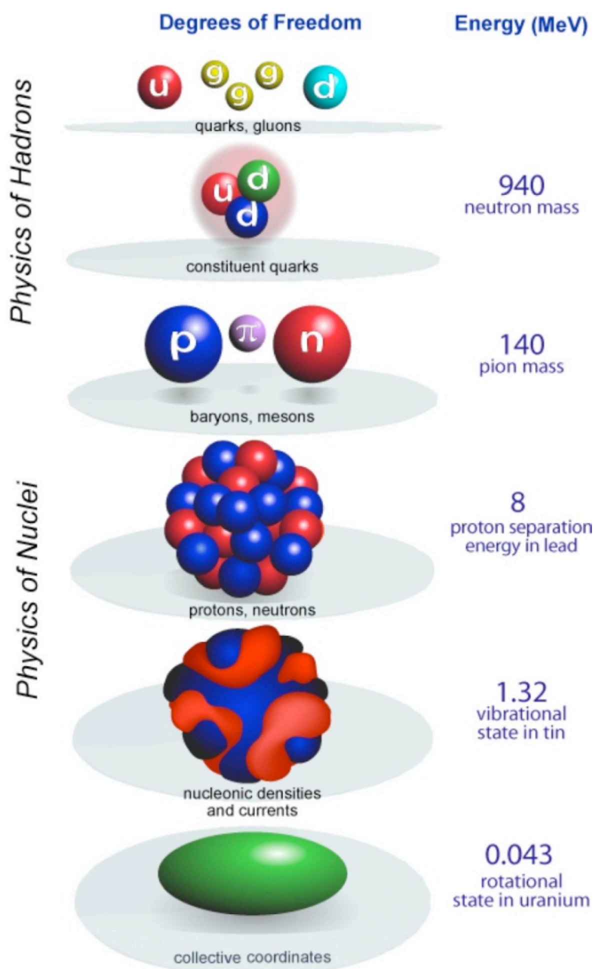
ab initio Nuclear Structure/Reactions: Progress and Outlook

James P. Vary
Iowa State University

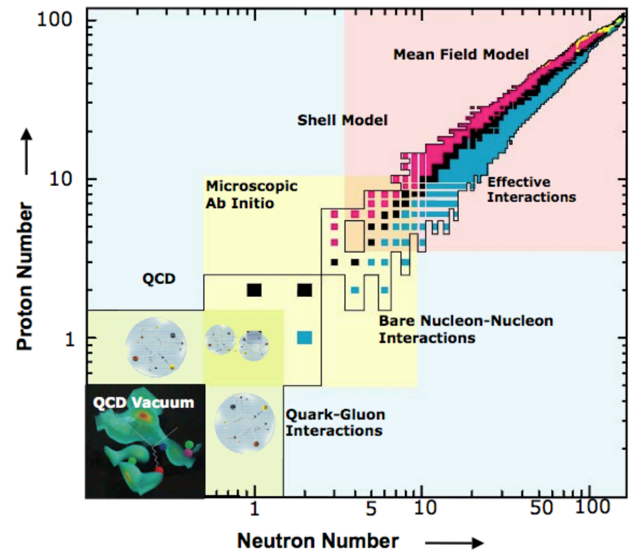
Nuclear Energy Fuel Cycle R&D
Nuclear Physics Working Group Meeting
November 5-6, 2009
Brookhaven National Laboratory

In collaboration with
P. Maris, A. Negoita, A. Shirokov, A. Mazur

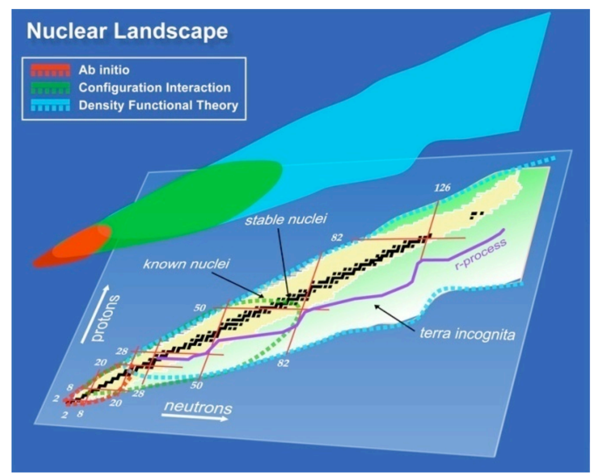
Exa-scale computing will unify nuclear physics



QCD



Nuclear
Structure



Applications in astrophysics,
defense, energy, and medicine

- D. Dean, JUSTIPEN Meeting, February 2009

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

QCD
Theory of strong interactions

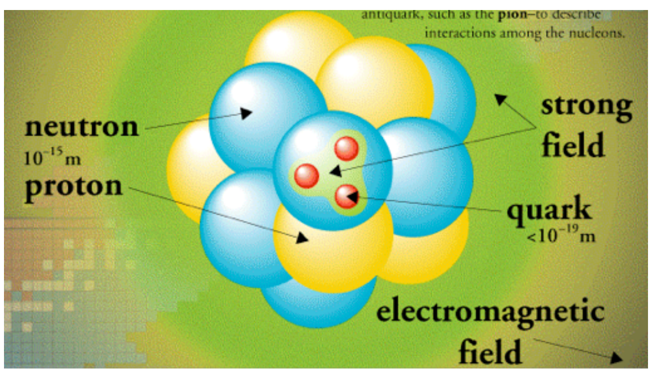
χEFT
Chiral Effective Field Theory

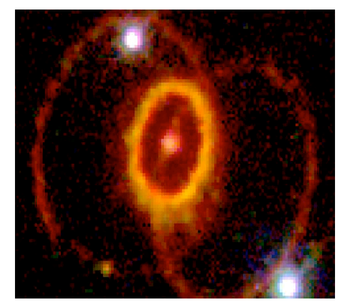
Inter-Nucleon
NN, NNN Interactions
AV18, EFT, $V_{\text{low-k}}$

Theory of Light Nuclei
Spectroscopy and selected reactions
Verification: NCSM=GFMC=CC
Validation: nuclei with A<16

Big Bang
Nucleosynthesis
& Stellar Reactions

Density Functional Theory
improved functionals
remove computationally-imposed constraints
properties for all nuclei with A>16





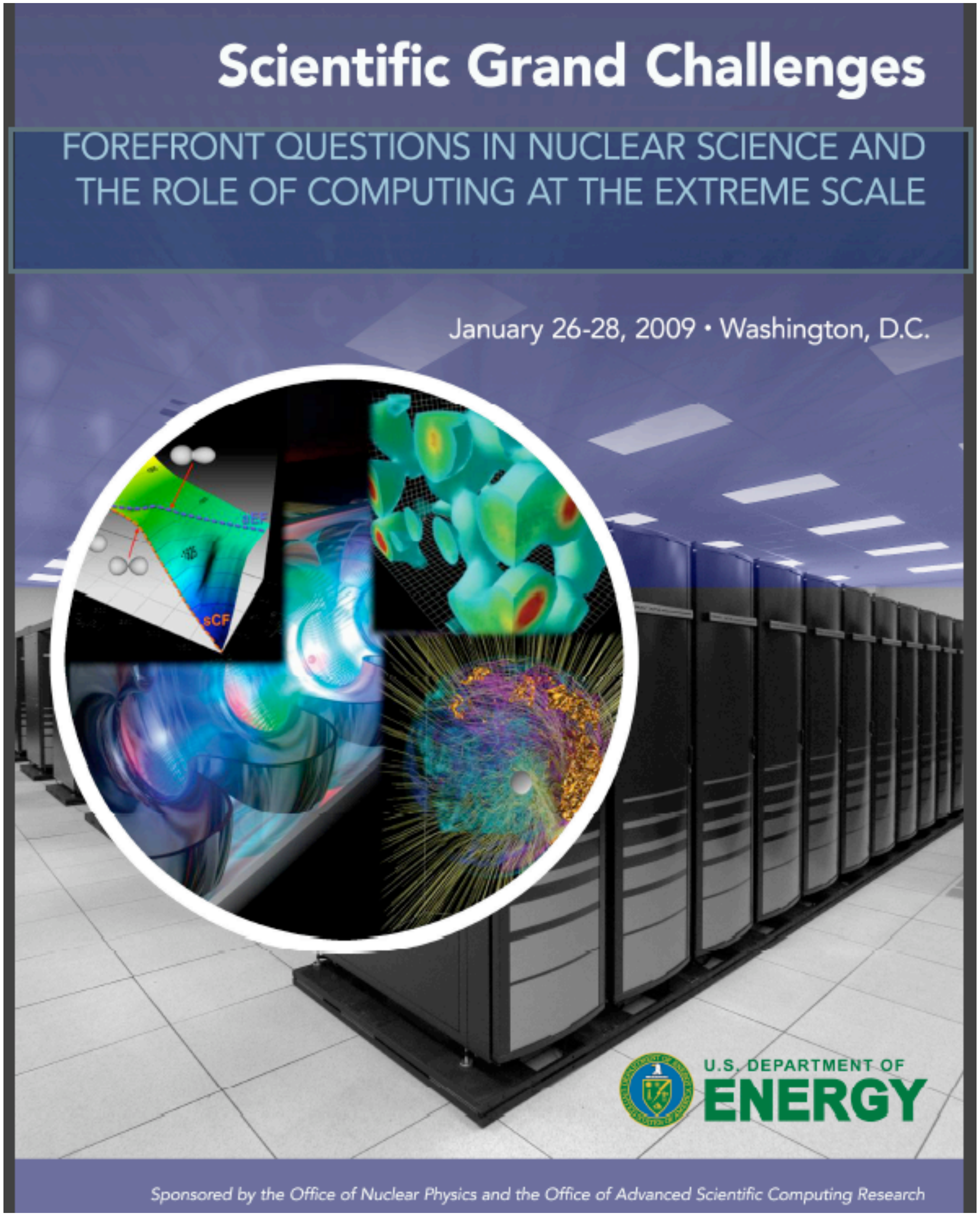
Dynamic Extensions of DFT
LACM by GCM,TDDFT,QRPA
Level densites

Low-energy Reactions
Hauser-Feshbach
Feshbach-Kerman-Koonin
Fission
mass and energy distributions

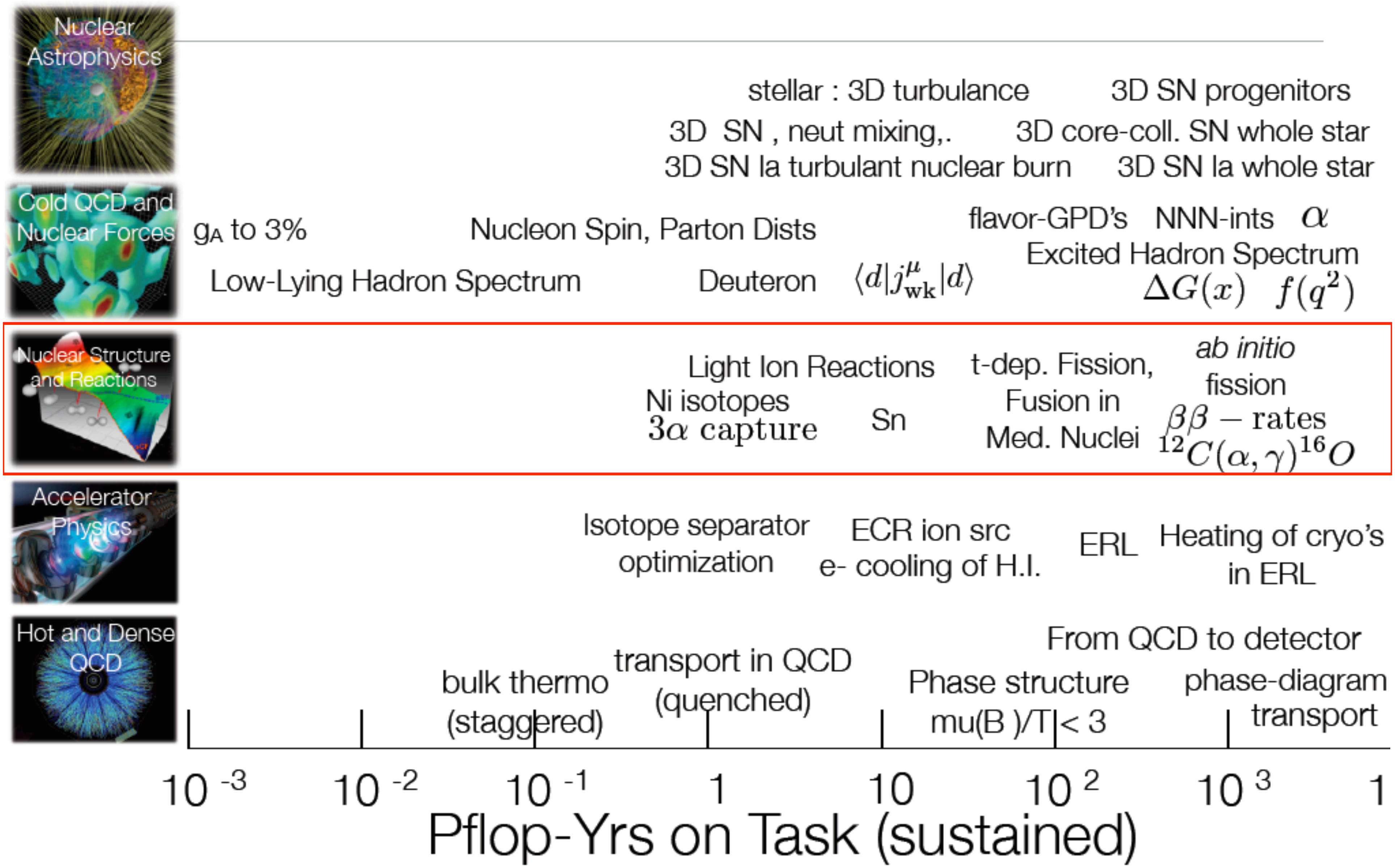
r,s processes
& Supernovae

www.unedf.org

http://extremecomputing.labworks.org/nuclearphysics/report.stm



Nuclear Physics Requires Exa-scale Computation

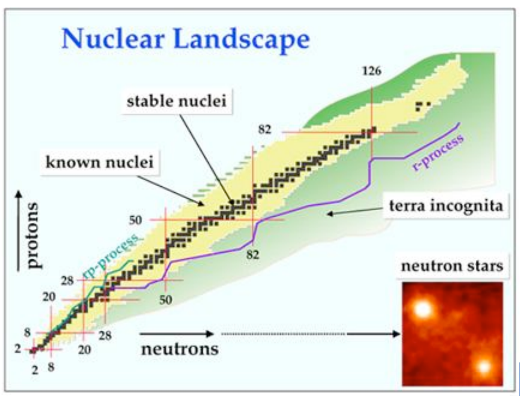


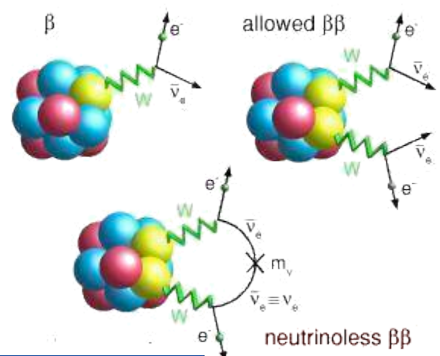
- M. Savage, Summary Talk

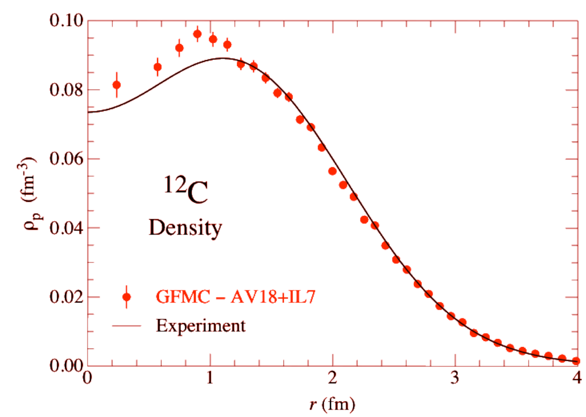
DOE Workshop on Forefront Questions in Nuclear Science
and the Role of High Performance Computing,
Gaithersburg, MD, January 26-28, 2009
Nuclear Structure and Nuclear Reactions

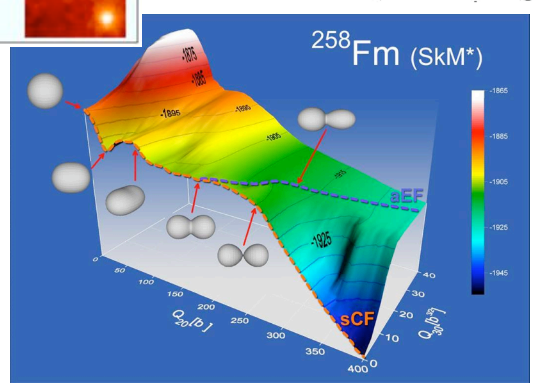
List of Priority Research Directions

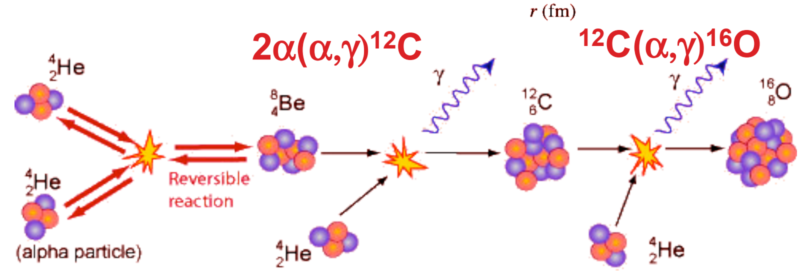
- **Physics of extreme neutron-rich nuclei and matter**
- **Microscopic description of nuclear fission**
- **Nuclei as neutrino physics laboratories**
- **Reactions that made us - triple α process and $^{12}C(\alpha,\gamma)^{16}O$**

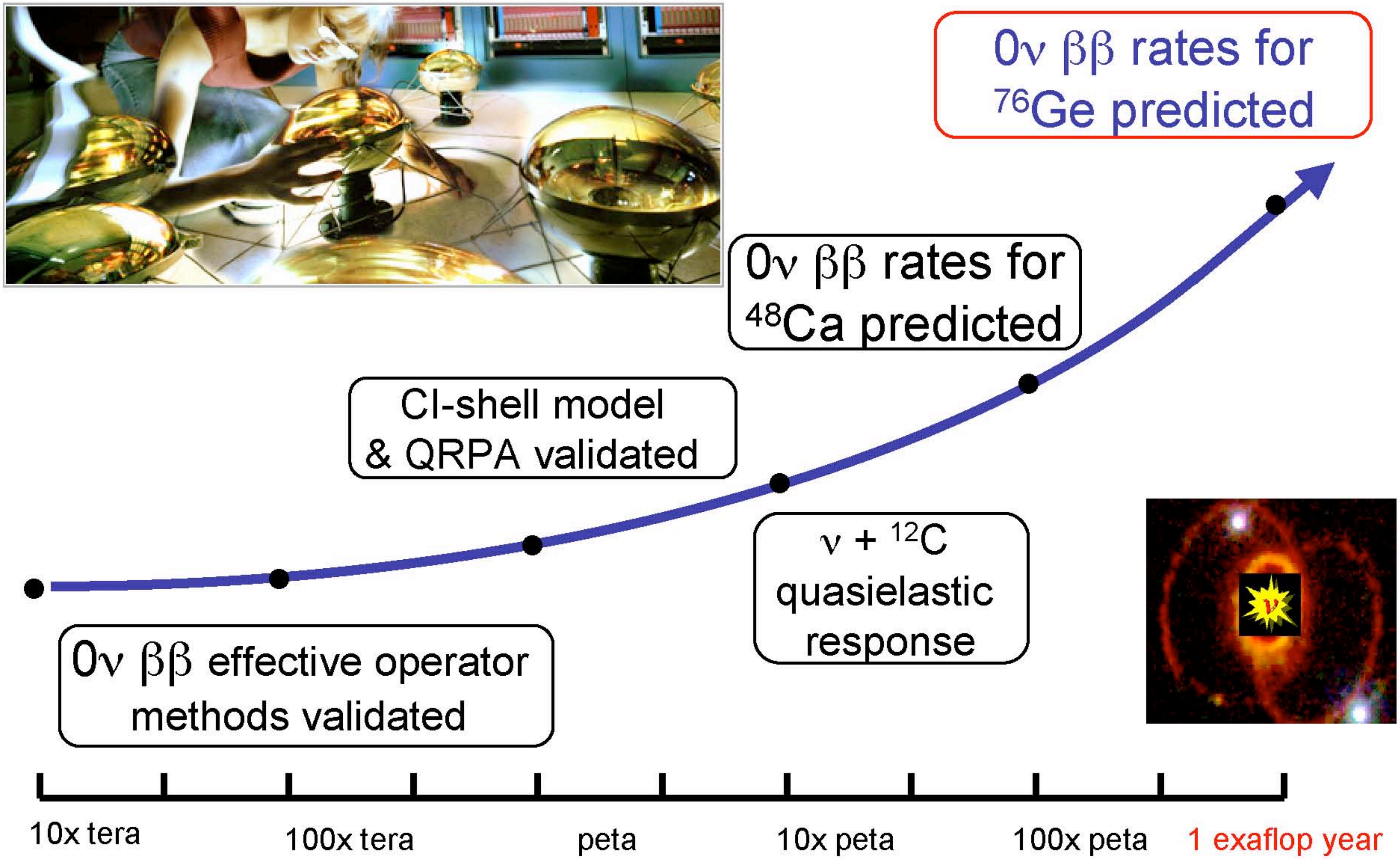




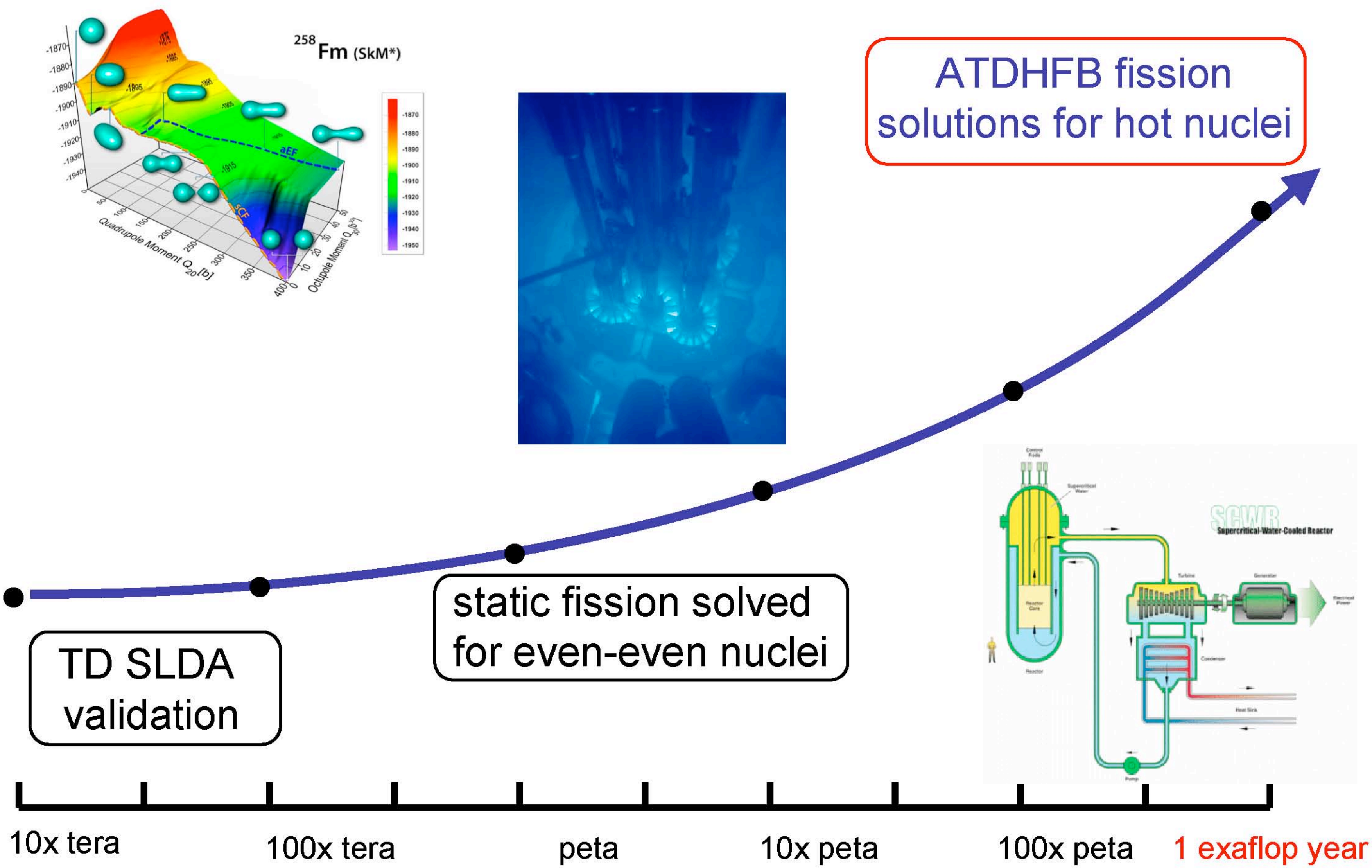








http://extremecomputing.labworks.org/nuclearphysics/report.stm



http://extremecomputing.labworks.org/nuclearphysics/report.stm

The 3-fold physics challenge = computationally hard

Multiple scales - keV to GeV (collective modes, fission, fusion, EOS, SRC's)
Strong interaction - SRC's, renormalization, NN+NNN potentials
Self-bound quantum N-body systems - preserve all underlying symmetries

DOE major facilities with related experimental programs

Facility for Rare Isotope Beams (FRIB)
Thomas Jefferson Lab (TJ Lab)
Neutrino detector facilities (several)
National Ignition Facility (NIF)

Nuclear physics interfaces with other disciplines - input/benefits

Math/Comp Sci
Particle physics
Astrophysics/Cosmology
Many-body physics
Nuclear physics applications

Realistic NN & NNN interactions
High quality fits to 2- & 3- body data

Need
Consistent
EW operators

Meson-exchange

NN: AV18, CD-Bonn, Nijmegen, . . .
NNN: Tucson-Melbourne, UIX, IL7, . . .

Need
Improved NNN

Chiral EFT (Idaho)

NN: N3LO
NNN: N2LO
4N: predicted & needed for consistent N3LO

Need
Fully derived/coded
N3LO

Inverse Scattering

NN: JISP16

Need
JISP40
Consistent NNN

The Nuclear Many-Body Problem

The many-body Schroedinger equation for bound states consists of $2\binom{A}{Z}$ coupled second-order differential equations in 3A coordinates using strong (NN & NNN) and electromagnetic interactions.

Ab initio approaches projected for exascale machines

Stochastic approach in coordinate space
Greens Function Monte Carlo (**GFMC**)

Hamiltonian matrix in basis function space
No Core Shell Model (**NCSM**)

Cluster hierarchy in basis function space
Coupled Cluster (**CC**)

Comments

All work to preserve and exploit symmetries
Extensions of each to scattering/reactions are well-underway
They have different advantages and limitations

Computational challenge:
large sparse matrix eigenvalue problem

$$H = T_{rel} + V_{NN} + V_{3N} + \bullet\bullet\bullet$$

$$H\left|\Psi_i\right\rangle = E_i\left|\Psi_i\right\rangle$$

$$\left|\Psi_i\right\rangle = \sum_{n=0}^{\infty} A_n^i \left|\Phi_n\right\rangle$$

$$\text{Diagonalize } \left\{\left\langle\Phi_m\right|H\left|\Phi_n\right\rangle\right\}$$

- Adopt realistic NN (and NNN) interaction(s) & renormalize as needed - retain induced many-body interactions: Chiral EFT interactions and JISP16
- Adopt the 3-D Harmonic Oscillator (HO) for the single-nucleon basis states, α, β,…
- Evaluate the nuclear Hamiltonian, H, in basis space of HO (Slater) determinants (manages the bookkeeping of anti-symmetrization)
- Diagonalize this sparse many-body H in its “m-scheme” basis where [α =(n,l,j,$m_{j,}$ τ_z)]

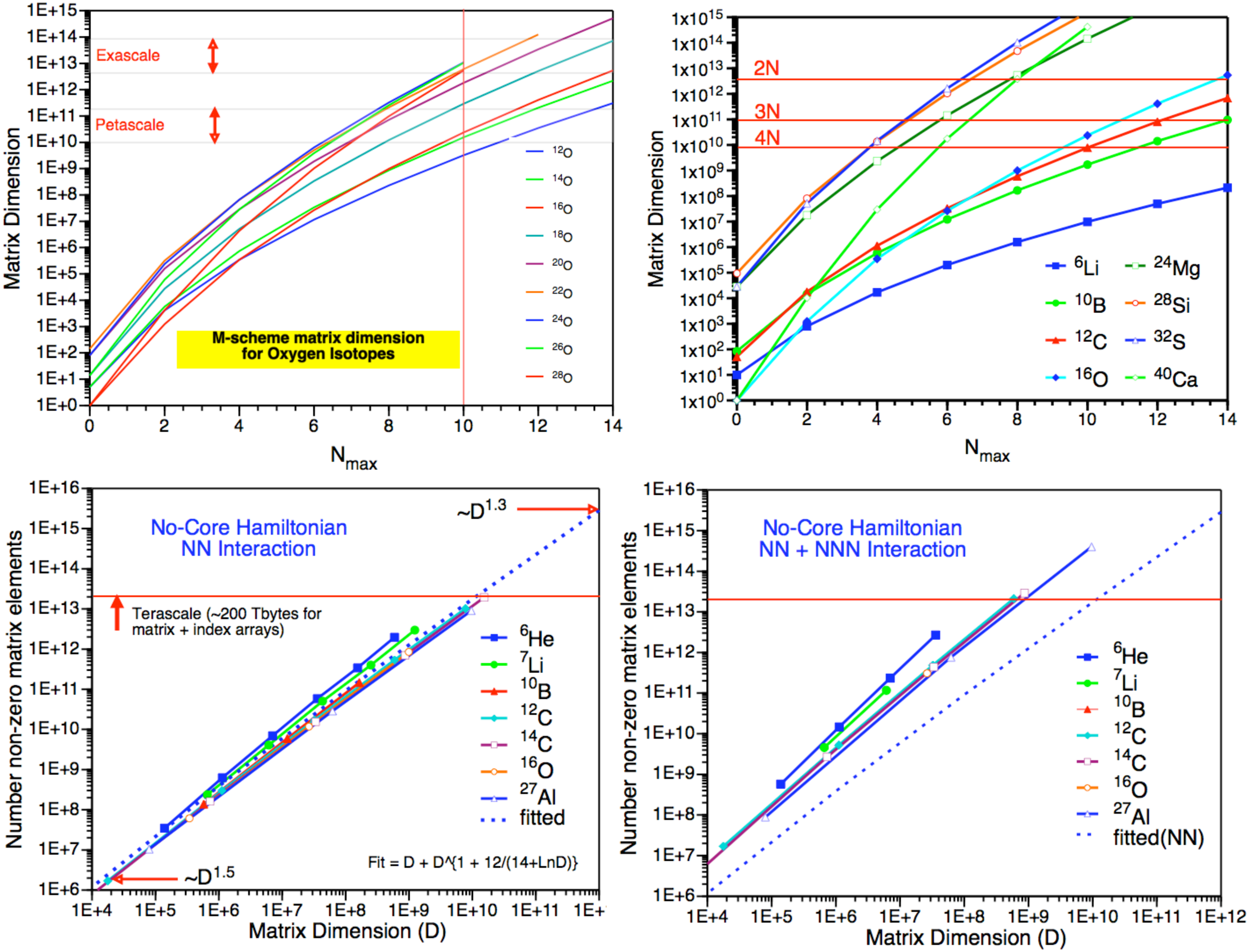
$$\left|\Phi_n\right\rangle = [a_\alpha^+ \bullet\bullet\bullet a_\varsigma^+]_n \left|0\right\rangle$$

$$n = 1,2,\ldots,10^{10} \text{ or more!}$$

- Evaluate observables and compare with experiment

Comments

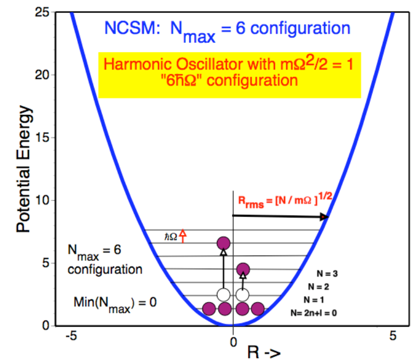
- Straightforward but computationally demanding => new algorithms/computers
- Requires convergence assessments and extrapolation tools
- Achievable for nuclei up to A=16 (40) today with largest computers available

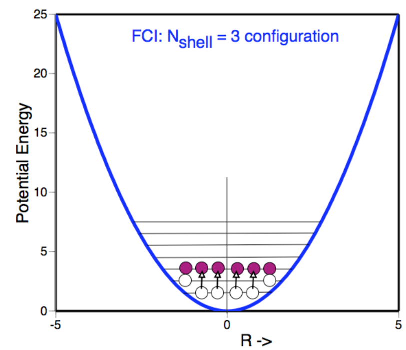


Matrix Dimension
Exascale
Petascale
M-scheme matrix dimension for Oxygen Isotopes
12O
14O
16O
18O
20O
22O
24O
26O
28O
N max
Matrix Dimension
2N
3N
4N
6Li
10B
12C
16O
24Mg
28Si
32S
40Ca
N max
No-Core Hamiltonian
NN Interaction
~D1.3
Terascale (~200 Tbytes for matrix + index arrays)
6He
7Li
10B
12C
14C
16O
27Al
fitted
Fit = D + D^{1 + 12/(14+LnD)}
~D1.5
Number non-zero matrix elements
Matrix Dimension (D)
No-Core Hamiltonian
NN + NNN Interaction
6He
7Li
10B
12C
14C
16O
27Al
fitted(NN)
Number non-zero matrix elements
Matrix Dimension (D)

Work in progress: Different truncation schemes

- No-Core Shell Model, No-Core Full Configuration
  - truncation on total number of H.O. quanta, N_{max}, in many-body basis space
- Full Configuration Interaction
  - truncation on single-particle basis space, retaining all many-body states allowed by the symmetries





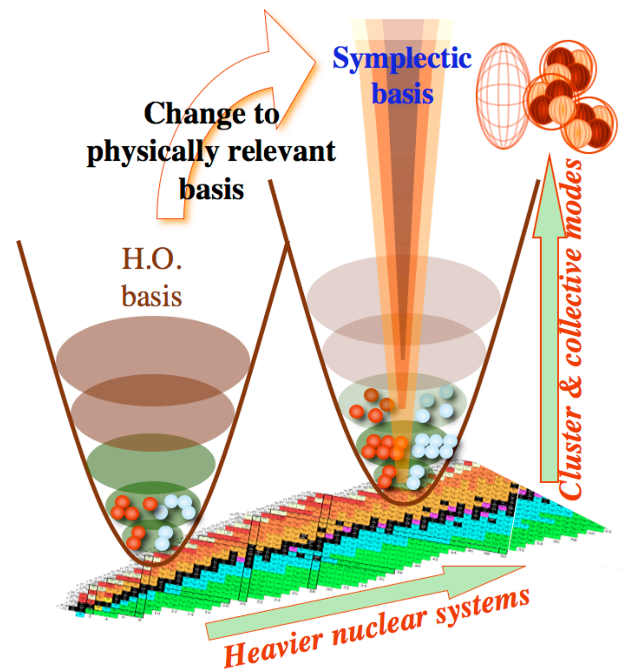
- Monte-Carlo Shell Model
  Abe, Otsuka, Shimizu, Utsuno
  - sampling of the many-body basis in a FCI truncation
- Importance Sampling
  Navratil, Roth
  - sampling of the many-body basis in a N_{max} truncation
- Symplectic No-Core Shell Model   Draayer *et.al.*, PetaApps grant

Taming the scale explosion in nuclear calculations
NSF PetaApps - Louisiana State, Iowa State, Ohio State collaboration

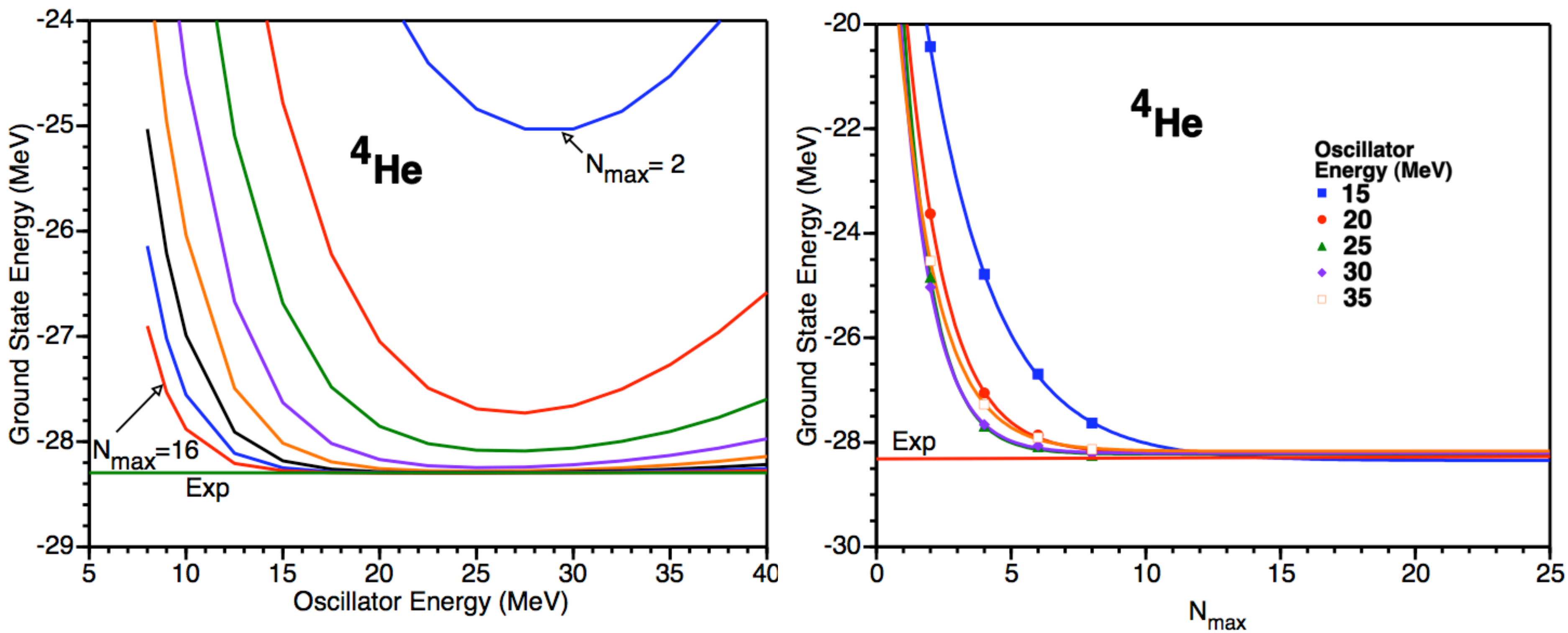
- **Goals**
  - Ab initio calculations of nuclei with unprecedented accuracy using basis-space expansions
  - Current calculations limited to nuclei with A ≤ 16 (up to 20 billion basis states with 2-body forces)

- **Progress**
  - Scalable CI code for nuclei
  - Sp(3,R)/SU(3)-symmetry vital
- **Challenges/Promises**
  - Constructing hybrid Sp-CI code
  - Publicly available peta-scale software for nuclear science

- **Novel approach**
  - Sp-CI: exploiting symmetries of nuclear dynamics
  - Innovative workload balancing techniques & representations of multiple levels of parallelism for ultra-large realistic problems
- **Impact**
  - Applications for nuclear science and astrophysics

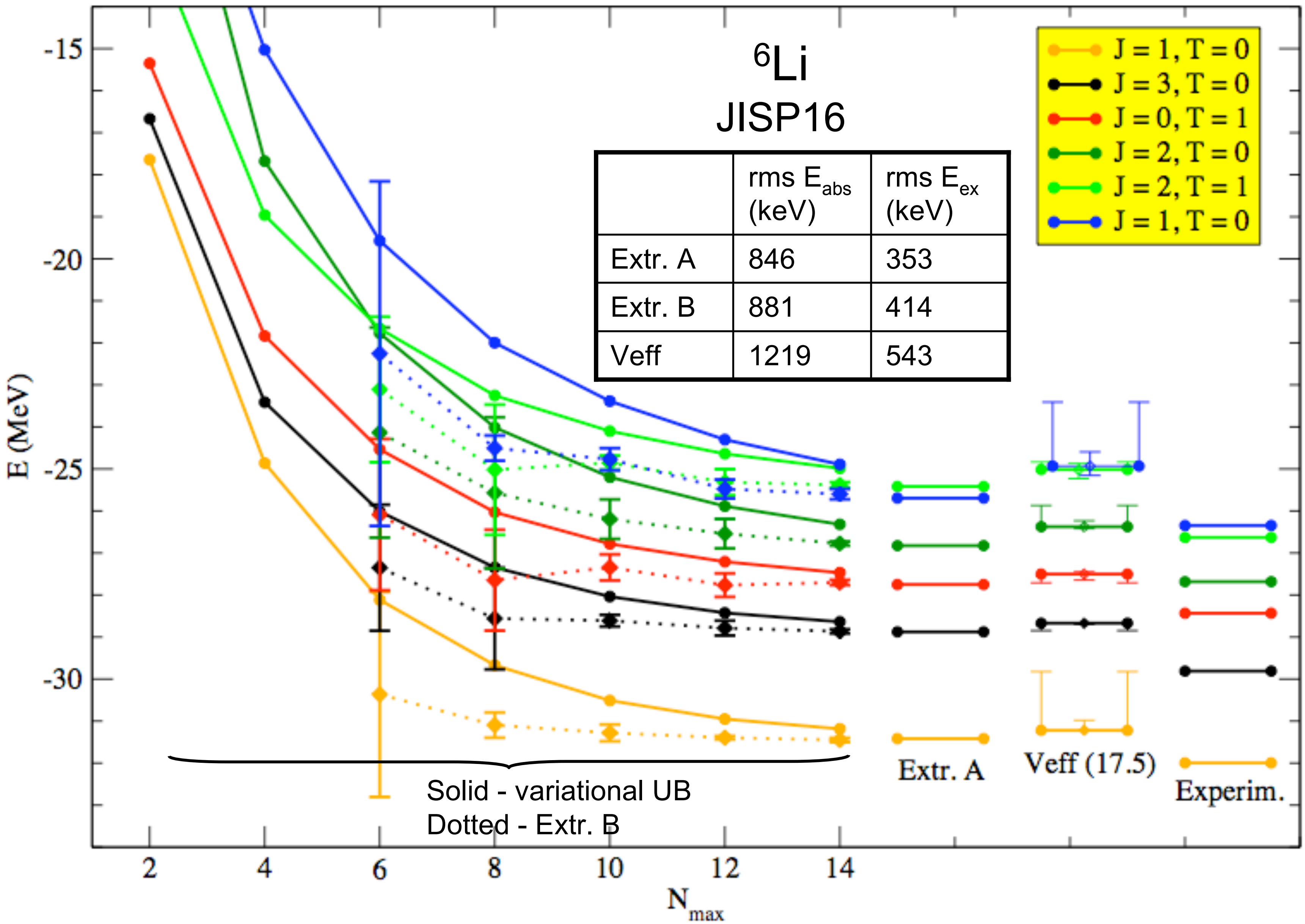


Convergence Pattern for “Bare” NCSM
JISP16 NN interaction



P. Maris, J.P. Vary and A. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420

Exponential extrapolation applied to excited states

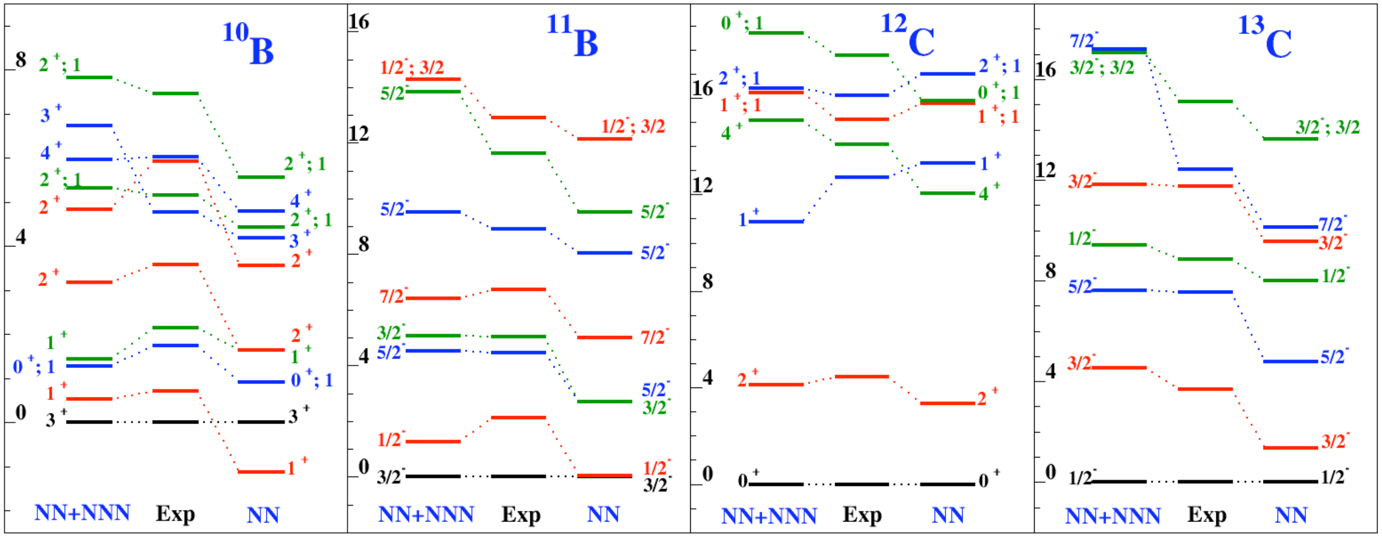


	rms E_{abs} (keV)	rms E_{ex} (keV)
Extr. A	846	353
Extr. B	881	414
Veff	1219	543

P. Maris, A. M. Shirokov and J.P. Vary, ArXiv 0911.2281

ab initio NCSM with χ_{EFT} Interactions

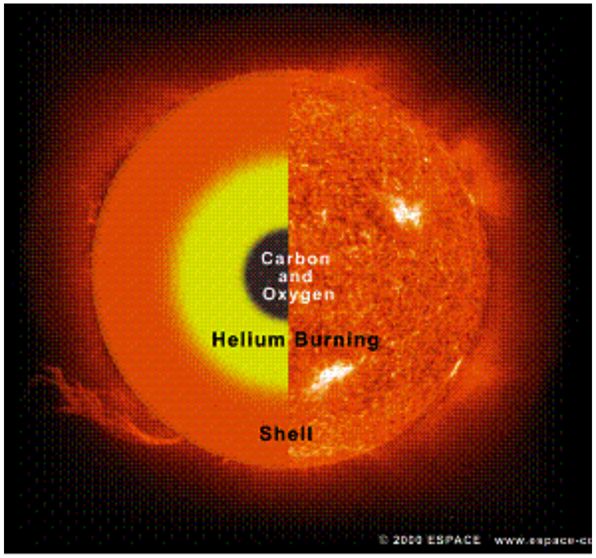
- *Only method capable to apply the χ_{EFT} NN+NNN interactions to all p-shell nuclei*
- *Importance of NNN interactions for describing nuclear structure and transition rates*



P. Navratil, V.G. Gueorguiev, J. P. Vary, W. E. Ormand and A. Nogga, PRL 99, 042501(2007); ArXiV: nucl-th 0701038.

Extensions and work in progress

- *Better determination of the NNN force itself, feedback to χ_{EFT}* (LLNL, OSU, MSU, TRIUMF)
- *Implement Vlowk & SRG renormalizations (Bogner, Furnstahl, Maris, Perry, Schwenk & Vary, NPA 801, 21(2008); ArXiv 0708.3754)*
- *Response to external fields - bridges to DFT/DME/EDF (SciDAC/UNEDF)*
  - *- Axially symmetric quadratic external fields - in progress*
  - *- Triaxial and spin-dependent external fields - planning process*
- *Cold trapped atoms (Stetcu, Barrett, van Kolck & Vary, PRA 76, 063613(2007); ArXiv 0706.4123) and applications to other fields of physics (e.g. quantum field theory)*
- *Effective interactions with a core (Lisetsky, Barrett, Navratil, Stetcu, Vary)*
- *Nuclear reactions & scattering (Forssen, Navratil, Quaglioni, Shirokov, Mazur, Vary)*



^{12}C - At the heart of matter

The first excited 0+ state of ^{12}C, the "Hoyle state", is the key state of ^{12}C formation in the triple-alpha fusion process that occurs in stars.

Due to its role in astrophysics and the fact that carbon is central to life, some refer to this as one of the "holy grails" of nuclear theory.

Many important unsolved problems of the Hoyle state:

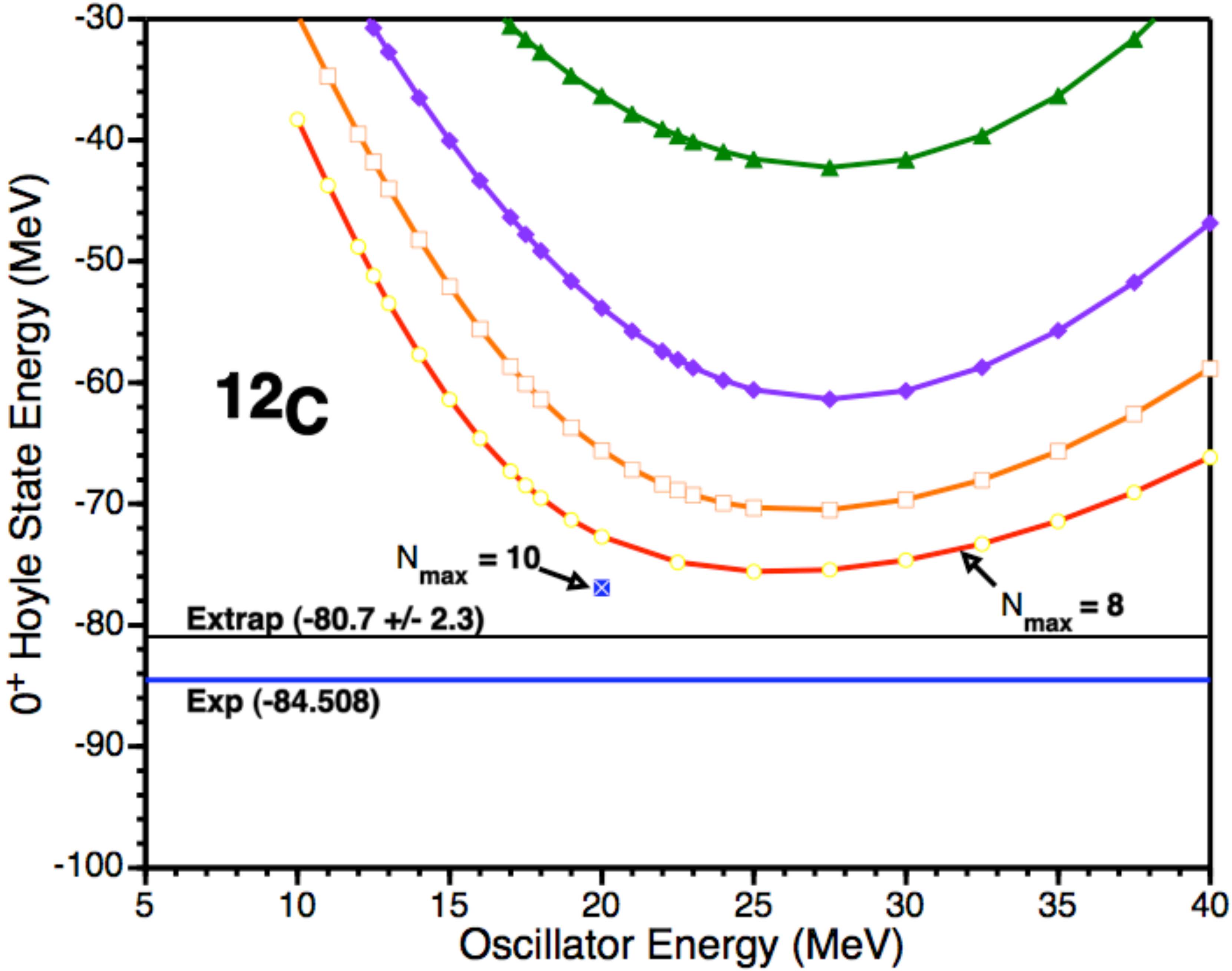
Microscopic origins of the triple-alpha structure are unsolved

Breathing mode puzzle - experiments disagree on sum rule fraction

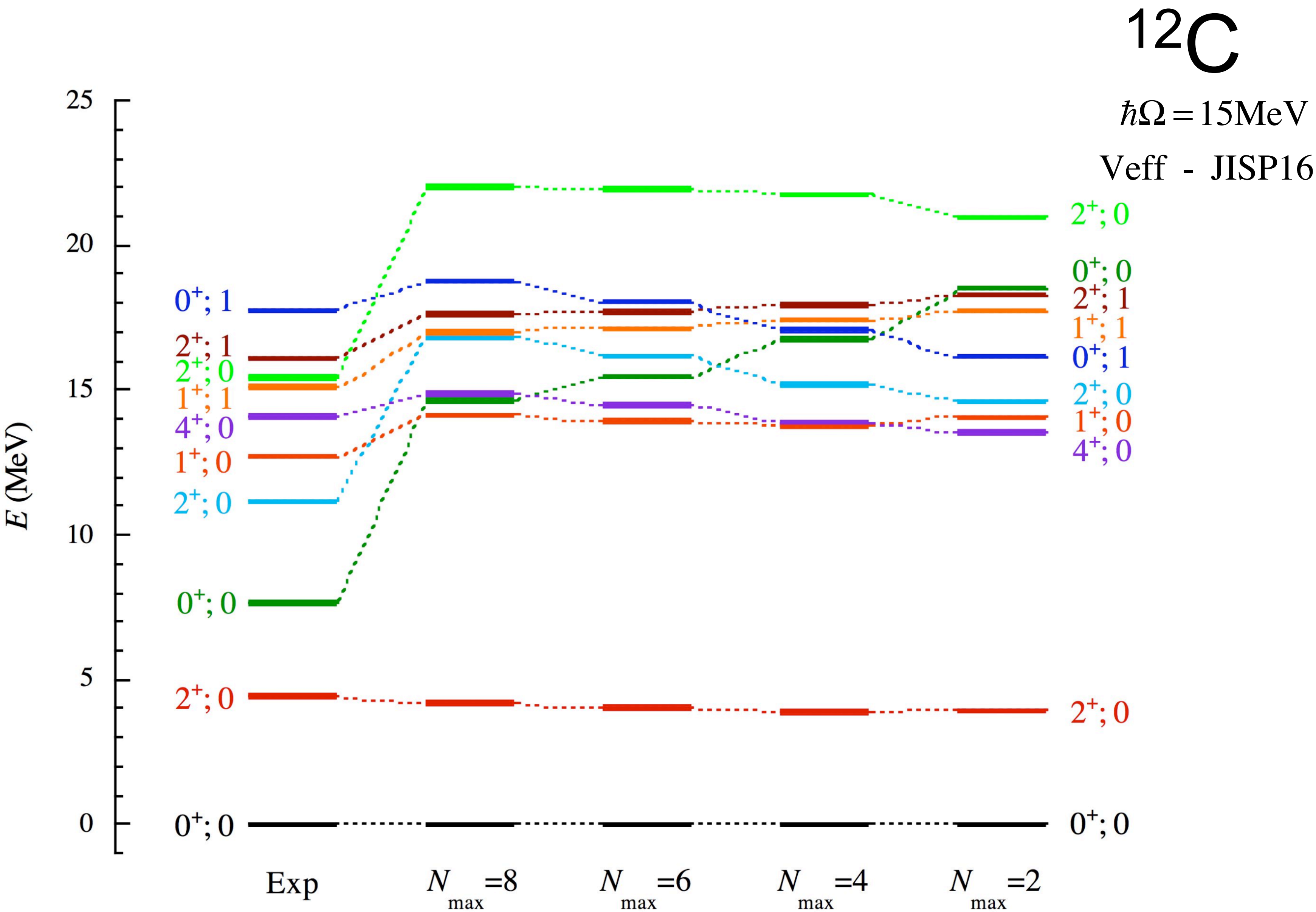
Laboratory experiments to measure the formation rate are very difficult - resulting uncertainties are too large for predicting the ^{12}C formation rate through this state that dictates the size of the iron core in pre-supernova stars

Conclusion: Need *ab initio* solutions of the Hoyle state with no-core method that accurately predicts the ground state binding energy

==> parameter free predictions for the Hoyle state achievable with petascale within 1-2 years



P. Maris, J.P. Vary and A. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420; and to be published



12C
ħΩ = 15MeV
Veff - JISP16
E (MeV)
25
20
15
10
5
0
0+; 1
2+; 1
2+; 0
1+; 1
4+; 0
1+; 0
2+; 0
0+; 0
2+; 0
0+; 0
2+; 0
0+; 0
2+; 1
1+; 1
0+; 1
2+; 0
1+; 0
4+; 0
2+; 0
0+; 0
Exp
N max =8
N max =6
N max =4
N max =2

Jaguar PF award of 30,000,000 cpu hours

Petascale Early Science – Ab-initio structure of Carbon-14

Puzzling to scientists …

What is the nuclear structure of ^{14}C that leads to its anomalously long half-life?

$\tau_{1/2}$ = 5730 years

^{10}Be and ^{14}C have extremely long half-lives compared to other light nuclei (1.6×10^6 years / 5,730 years) . Their long half-lives make both isotopes useful for radioactive dating.

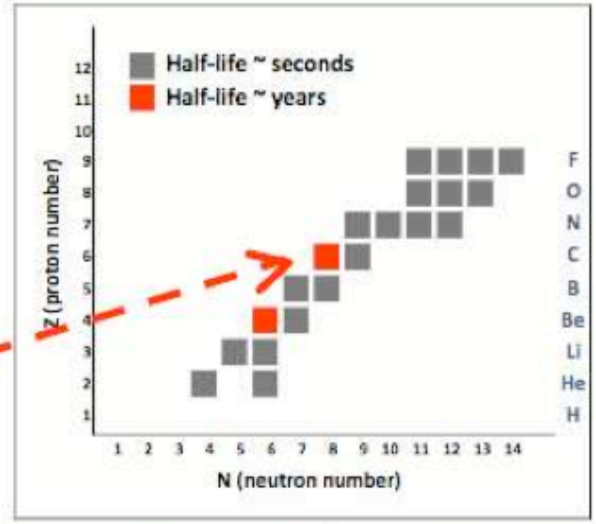
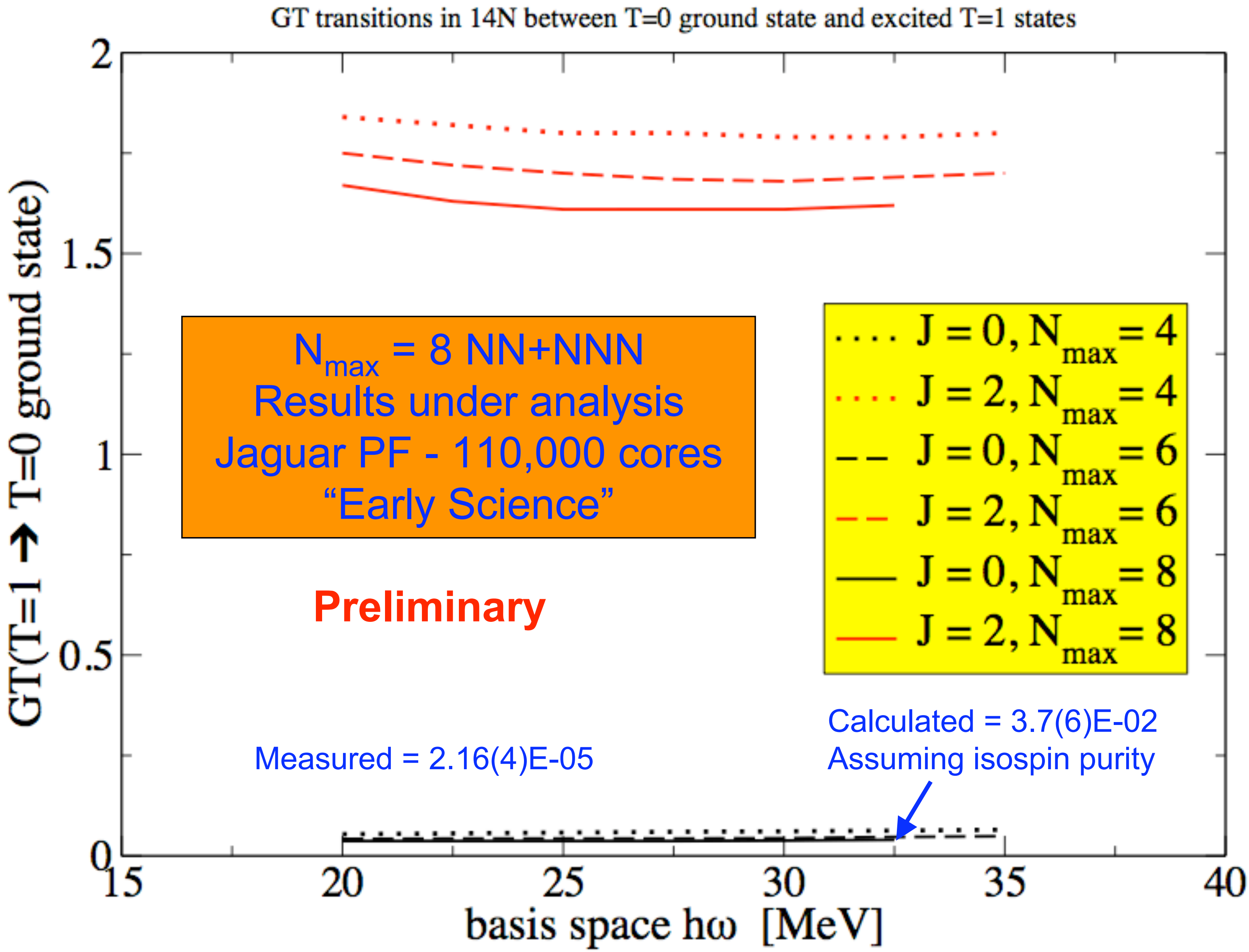


Chart of light nuclei that decay via beta emissions

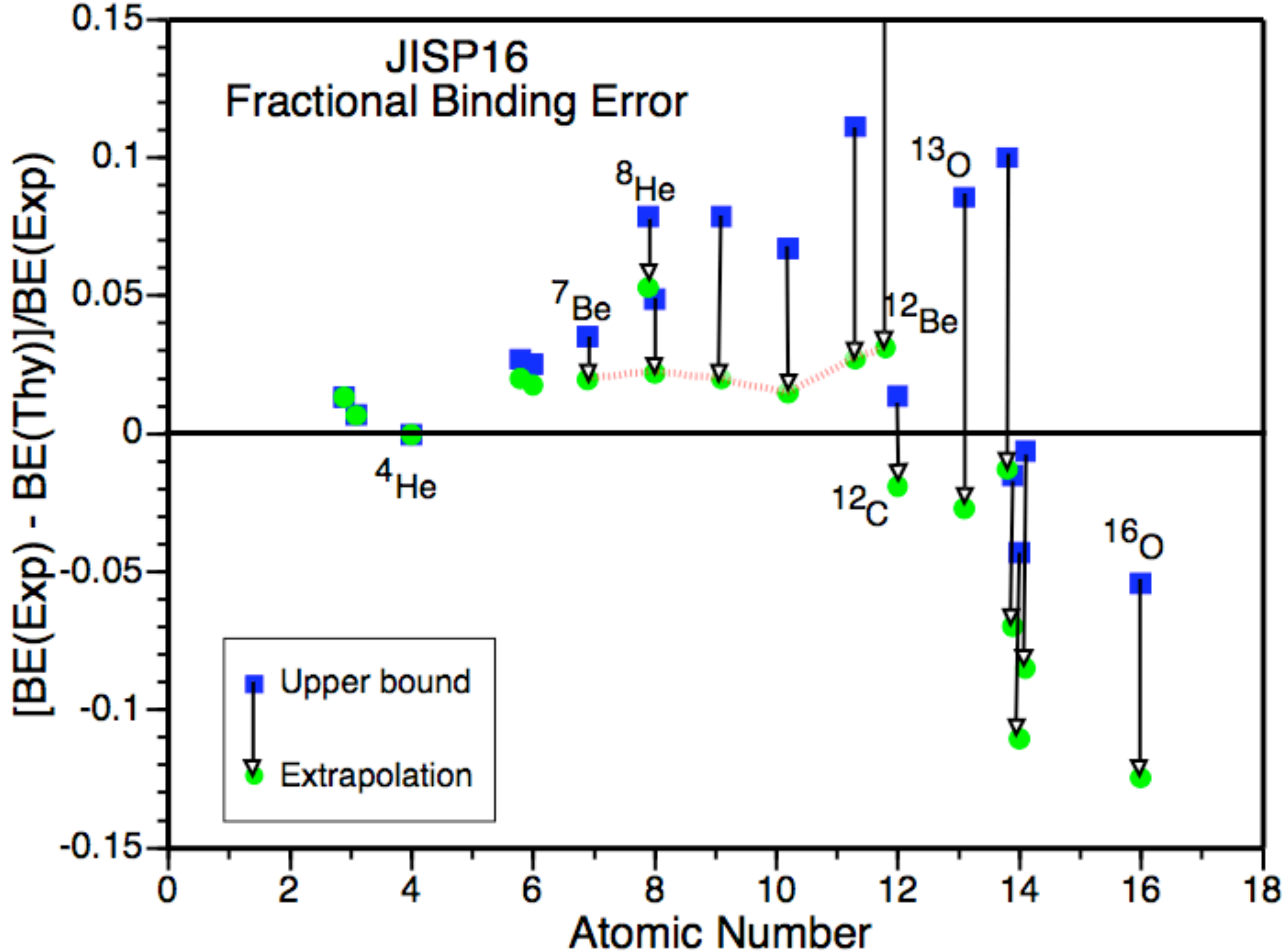
$n \rightarrow p + e^- + n_e$

Transition	Experimental	Calculated
$B(GT): {}^{10}Be \rightarrow {}^{10}B$	0.08	0.06 (3 - body : 0.066)
$B(GT): {}^{14}N \rightarrow {}^{14}C(\Sigma 2^+)$	0.92(33)	2.61 (CD - Bonn)
		1.62 (JISP16)

Collaborators: David Dean, Pieter Maris, Hai Ah Nam, Petr Navratil, Erich Ormand



Iowa State - ORNL - LLNL collaboration

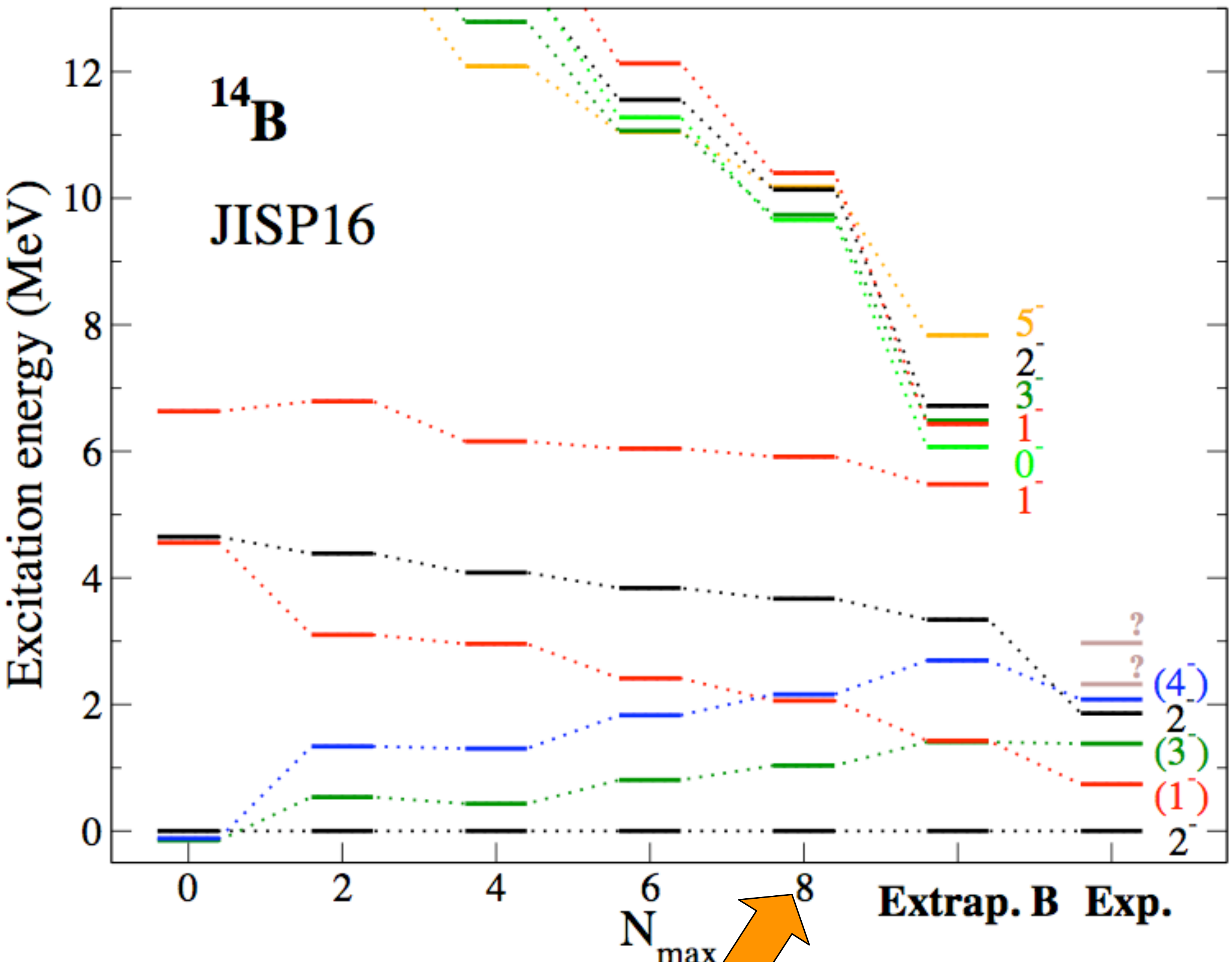


P. Maris, J.P. Vary and A. M. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420

Descriptive Science

$\Big\downarrow$

Predictive Science



2.5 hours on 30,628 cores
INCITE/Jaguar

P. Maris, A. M. Shirokov and J.P. Vary, ArXiv 0911.2281

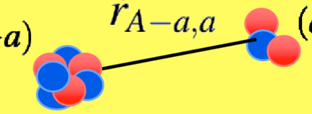
Ab initio Nuclear Structure

Ab initio Nuclear Reactions

Ab initio no-core shell model / resonating-group method (NCSM/RGM) in a snapshot

- Ansatz: $\Psi^{(A)} = \sum_\nu \int d\vec{r}\, \varphi_\nu(\vec{r})\, \hat{\mathcal{A}}\, \Phi^{(A-a,a)}_{\nu\vec{r}}$

$(A-a)$ $\vec{r}_{A-a,a}$ (a)



$$\psi^{(A-a)}_{1\nu}\, \psi^{(a)}_{2\nu}\, \delta(\vec{r} - \vec{r}_{A-a,a})$$

eigenstates of $H_{(A-a)}$ and $H_{(a)}$ in the *ab initio* NCSM basis

- Many-body Schrödinger equation:

$$H\Psi^{(A)} = E\Psi^{(A)}$$

$$T_{\rm rel}(r) + \mathcal{V}_{\rm rel} + \bar{V}_{\rm Coul}(r) + H_{(A-a)} + H_{(a)}$$

either bare interaction or NCSM effective interaction

$$\sum_\nu \int d\vec{r} \left[\mathcal{H}^{(A-a,a)}_{\mu\nu}(\vec{r}\,',\vec{r}) - E\mathcal{N}^{(A-a,a)}_{\mu\nu}(\vec{r}\,',\vec{r})\right] \varphi_\nu(\vec{r}) = 0$$

$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}} H \hat{\mathcal{A}} | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$$

Hamiltonian kernel

$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}}^2 | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$$

Norm kernel

Navratil

Introduced in PRL101, 092501 (2008)

Details:**PRC79, 044606 (2009); arXiv0901.0950**

- Non-local integro-differential coupled-channel equations:

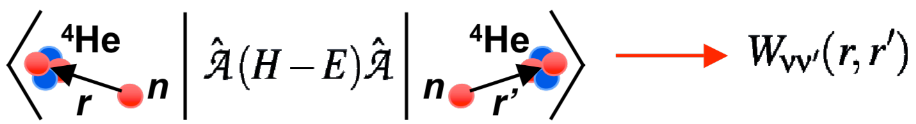
$$[\hat{T}_{\rm rel}(r) + \bar{V}_{\rm C}(r) - (E - E_\nu)]\, u_\nu(r) + \sum_\nu \int dr'\, r'\, W_{\nu\nu'}(r,r')\, u_\nu(r') = 0$$

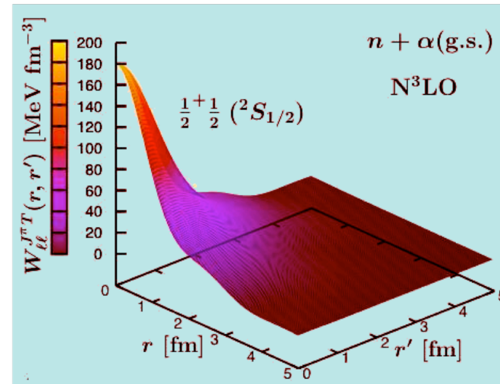
Fully implemented and tested for single-nucleon projectile (nucleon-nucleus) basis

Ab initio NCSM/RGM: nucleon-^{4}He scattering

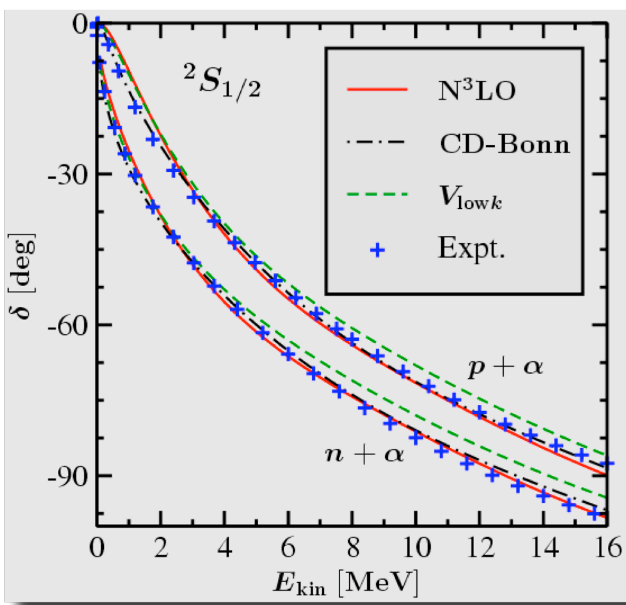
Navratil

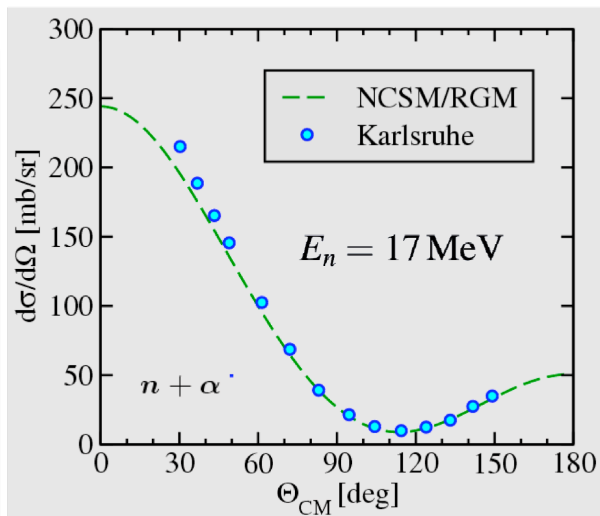
- The N-^{4}He potential is calculated microscopically from the many-body realistic Hamiltonian and the NCSM eigenstates of the ^{4}He

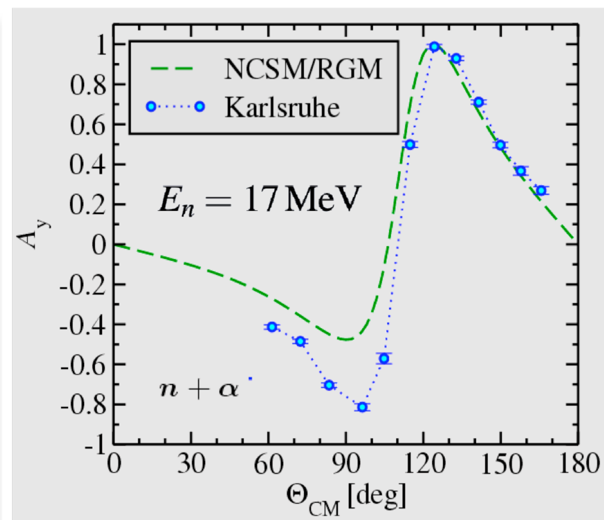




- Solving the non-local integro-differential coupled-channel equations for the N-^{4}He relative motion: phase shifts, cross sections, polarization observables



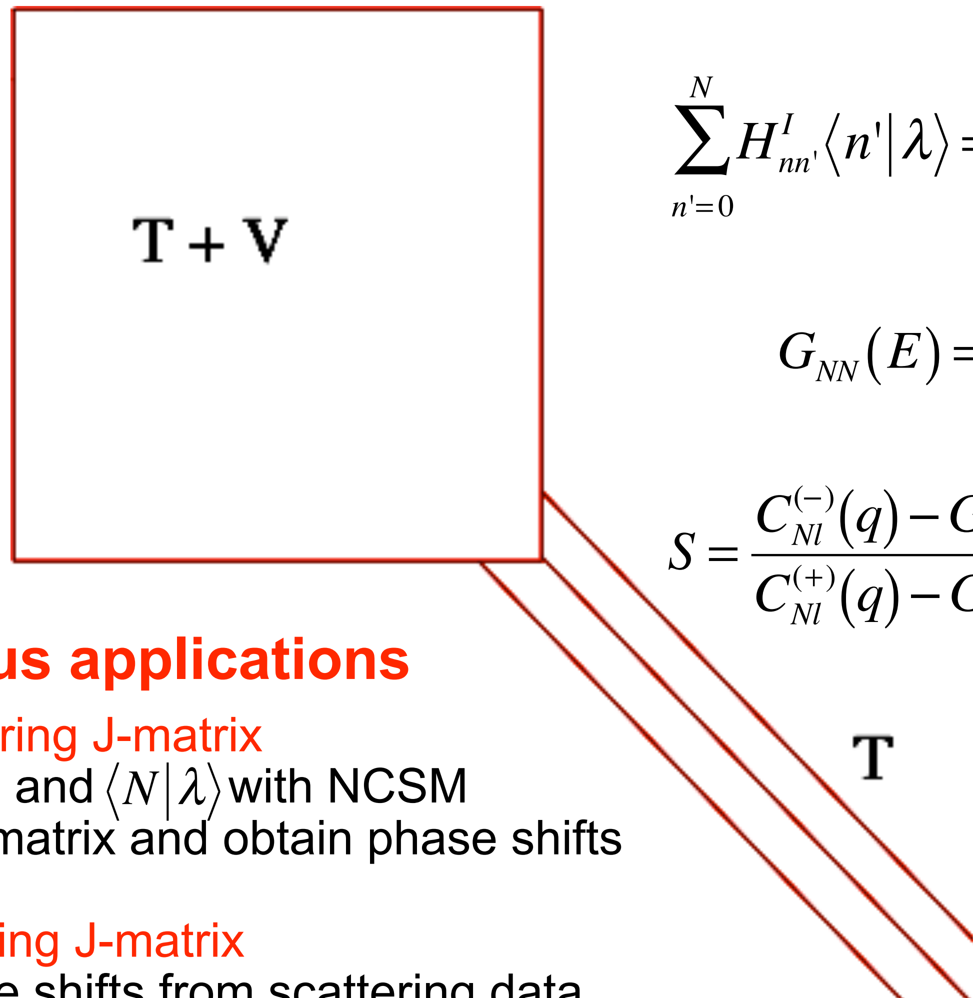




Phase shifts in PRL101, 092501 (2008)
and PRC79, 044606 (2009); arXiv0901.0950;
Cross sections and polarizations to be published

J-matrix formalism:

scattering in the oscillator basis



$$\sum_{n'=0}^{N} H^{I}_{nn'} \langle n' | \lambda \rangle = E_{\lambda} \langle n | \lambda \rangle, \qquad n \le N$$

$$G_{NN}(E) = -\sum_{\lambda=0}^{N} \frac{\langle N | \lambda \rangle^{2}}{E_{\lambda} - E}$$

$$S = \frac{C^{(-)}_{Nl}(q) - G_{NN}(E) T^{I}_{N,N+1} C^{(-)}_{N+1,l}(q)}{C^{(+)}_{Nl}(q) - G_{NN}(E) T^{I}_{N,N+1} C^{(+)}_{N+1,l}(q)}$$

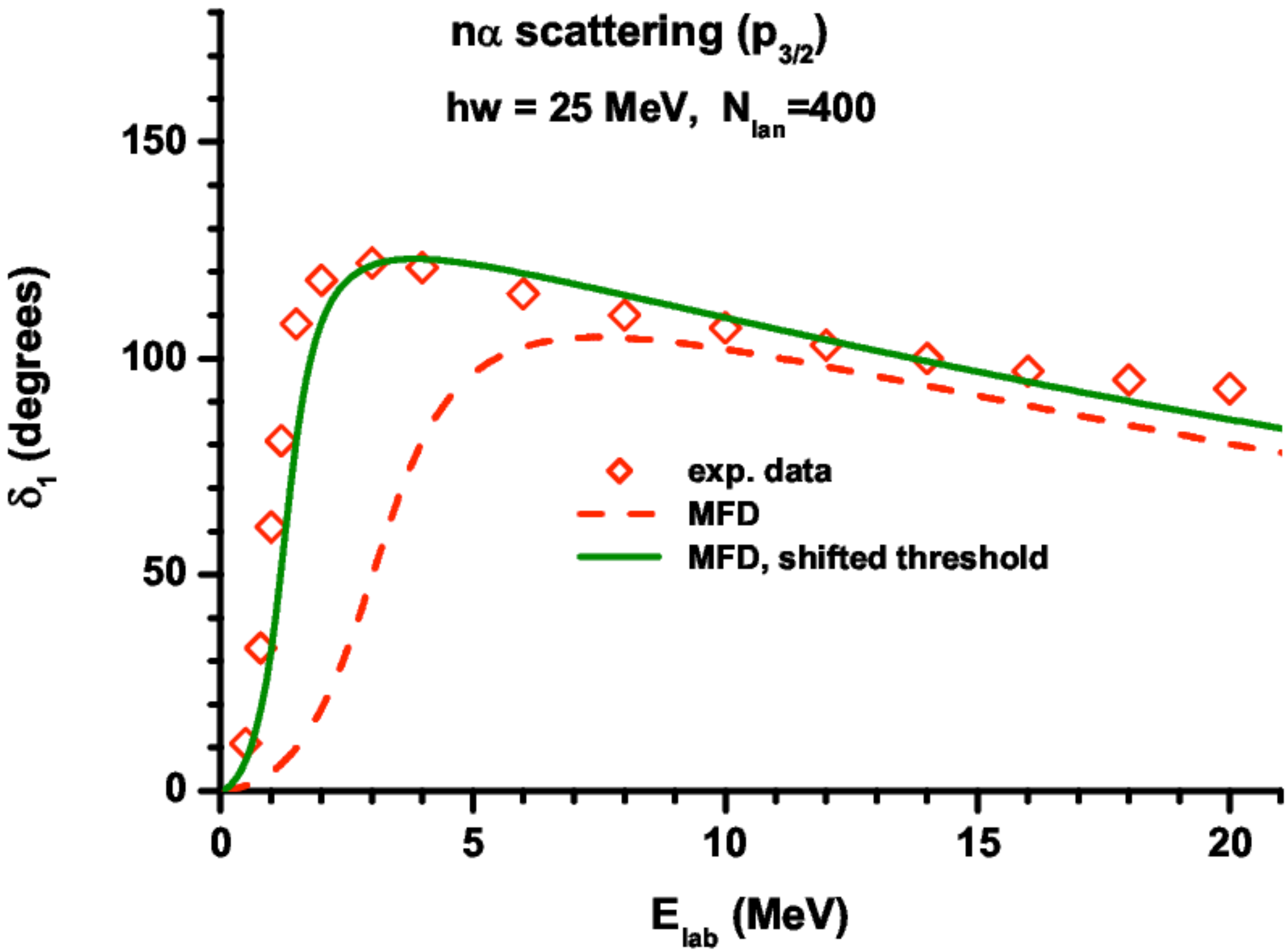
n(p)+nucleus applications

Forward scattering J-matrix
1. Calculate E_{λ} and $\langle N | \lambda \rangle$ with NCSM
2. Solve for S-matrix and obtain phase shifts

Inverse scattering J-matrix
1. Obtain phase shifts from scattering data
2. Solve for n(p)+nucleus potential, resonance params

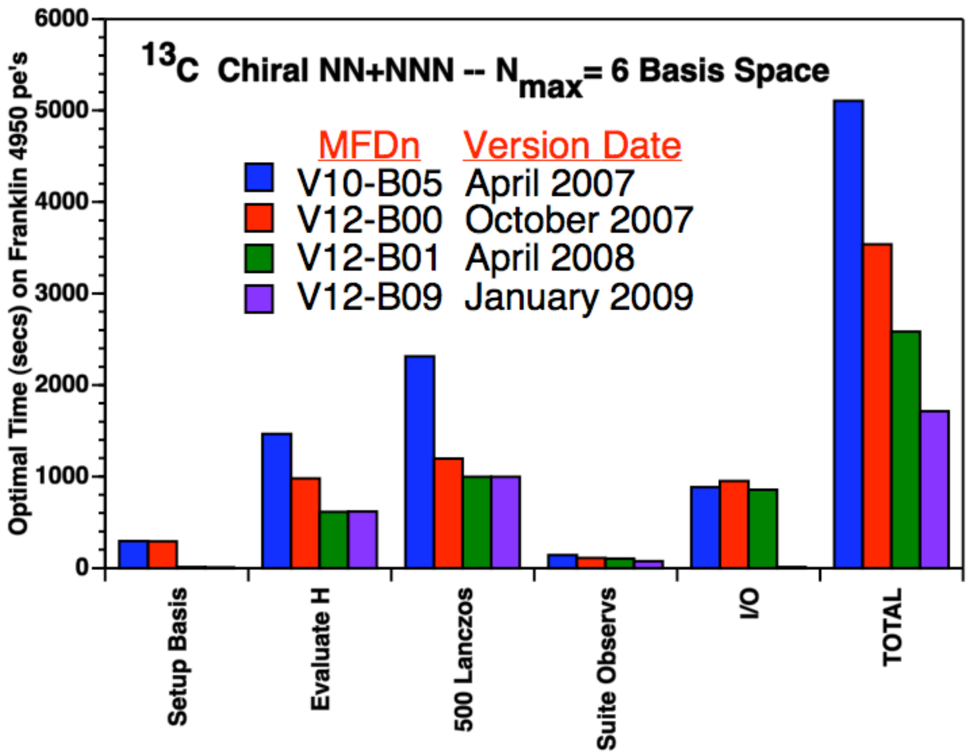
A.M. Shirokov, A.I. Mazur, J.P. Vary, and E.A. Mazur, Phys. Rev. C. 79, 014610 (2009), arXiv:0806.4018; and references therein

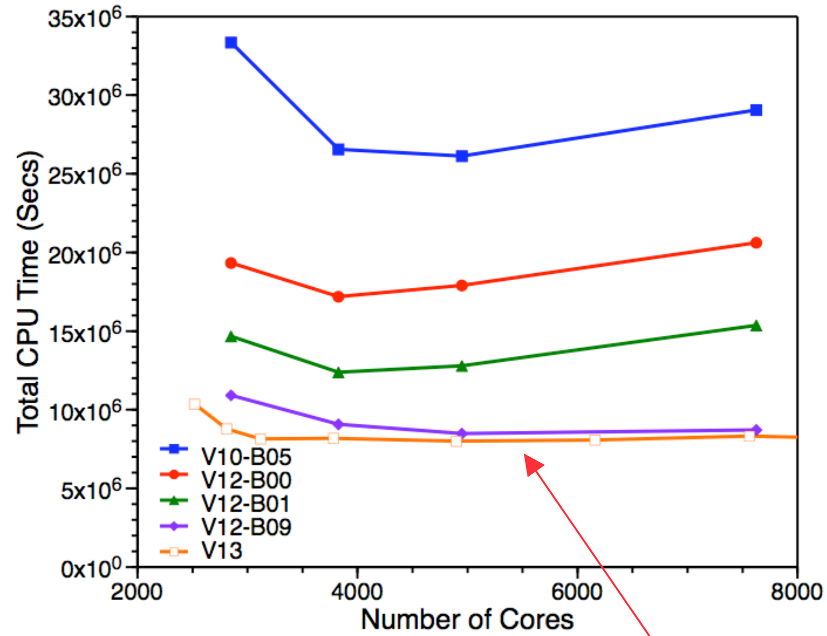
$n\alpha$ scattering



A. M. Shirokov, A. I. Mazur, J. P. Vary and E. A. Mazur, Phys. Rev. C. 79, 014610 (2009), arXiv 0806.4018

Improvements to MFDn under SciDAC





Note large range with near-perfect scaling

Dimension	38×10^6
# nonzero matrix elements	56×10^{10}
Input 3b matrix elements	3 Gbytes

J.P. Vary, P. Maris, E. Ng, C. Yang and M. Sosonkina, Journal of Physics: Conference Series **180**, 12083 (2009); arXiv nucl-th 0907.0209

Observation

Ab initio nuclear physics maximizes predictive power
and represents a computational physics challenge

Key issue

How to optimize use of computational resources
to achieve the physics potential of *ab initio* theory

Conclusions

We are entering an era of first principles, high precision,
nuclear theory

It is valuable to engage in dialog on the needs
that can best be served by the
rapidly evolving *ab initio* approach to structure/reactions

Suggested discussion topics

Near term (2-4 yr) development of ab initio approach
LCCI code development initiative
NPWG access to codes under development
Development of Nuclear Physics “Calculators”

Nuclear Physics Calculator: *ab initio* NCSM demonstration project

nuclear.physics.iastate.edu

- Select the NCSM application
- Enter your email address
- Select the number of neutrons and protons
- Select the N_{max}
- Select the oscillator energy, $\hbar\Omega$

Results file with the JISP16 interaction will be emailed to you in a few minutes

Note that this is a demonstration project and will evolve as funding permits