Success Story from SciDAC2:
Solution of Long-Standing Mystery - Anomalous Lifetime of Carbon-14

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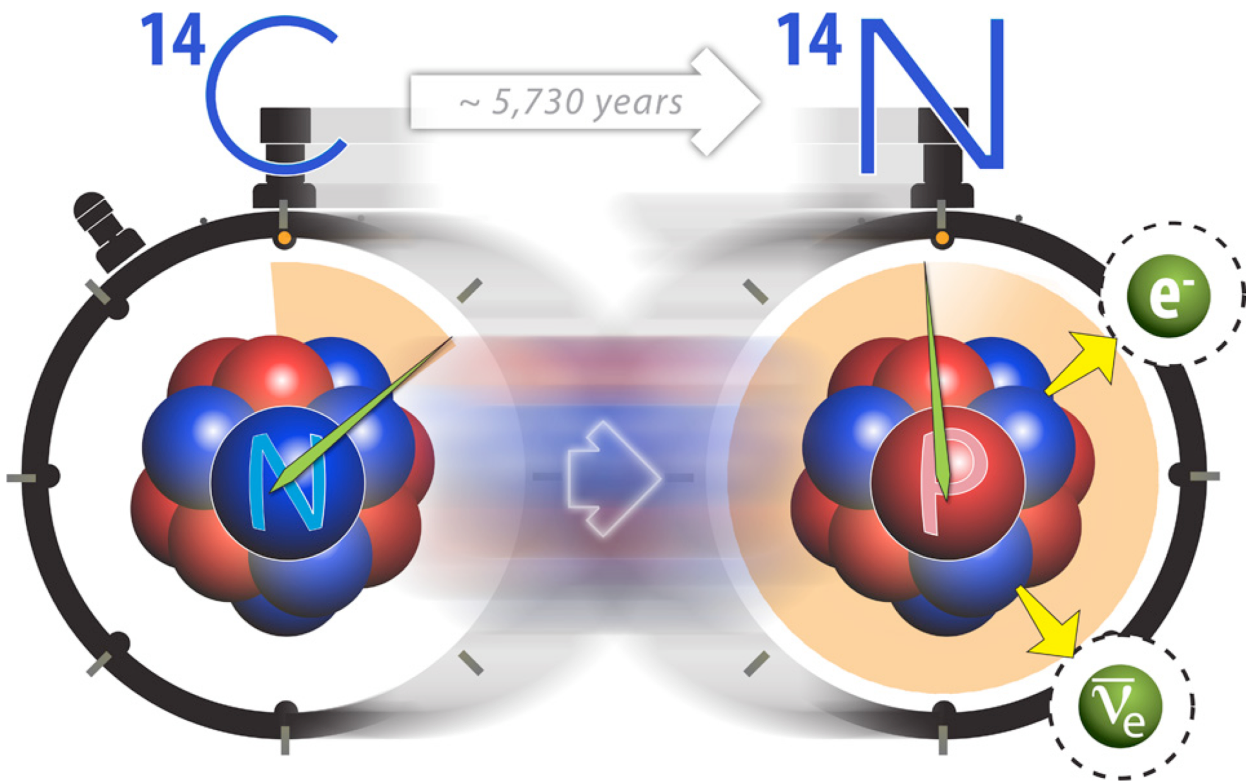
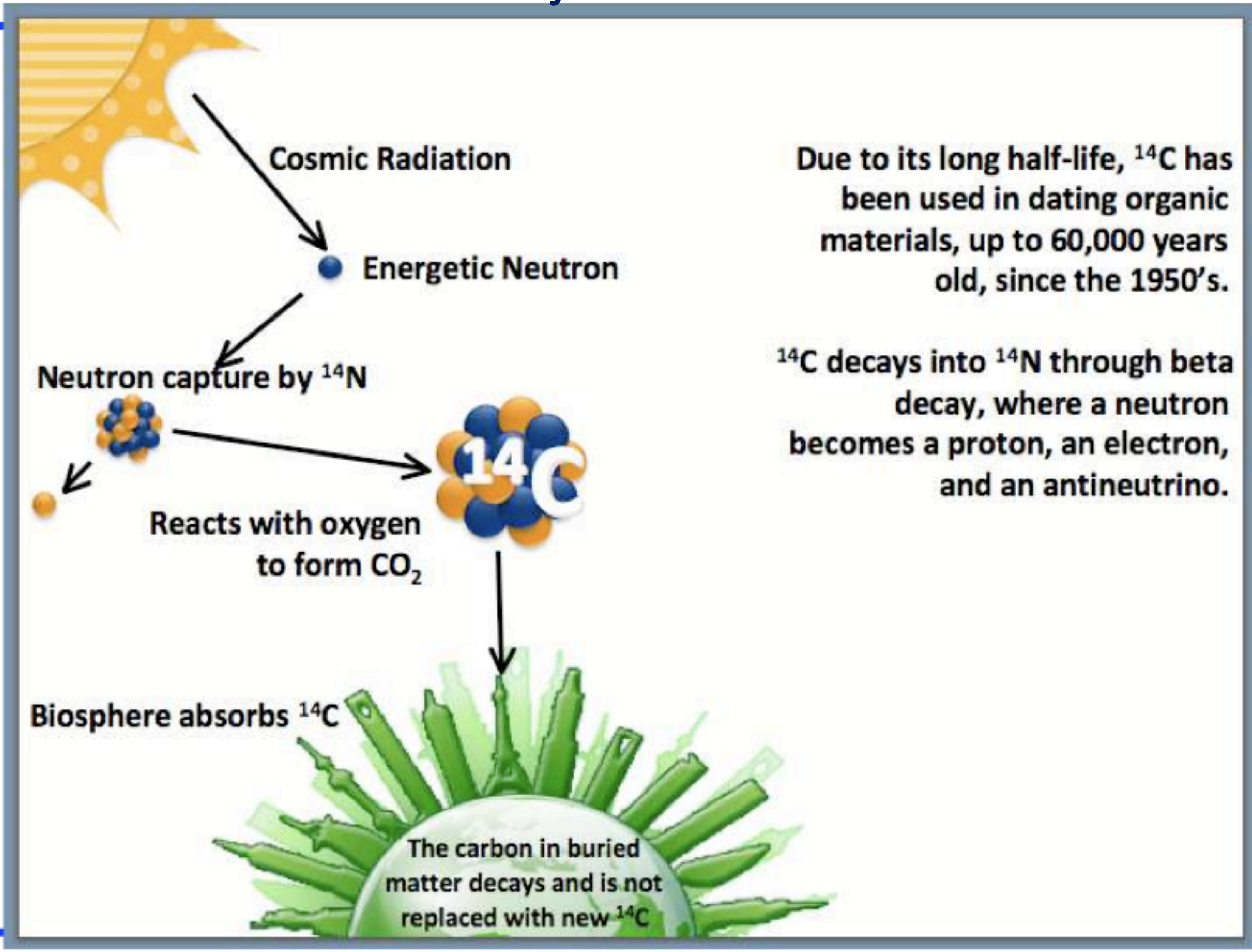
Iowa State University



P. Maris, J. P. Vary, P. Navratil, W.E. Ormand, H. Nam, D. J. Dean,
"Origin of the anomalous long lifetime of 14C," Phys. Rev. Lett. 106, 202502(2011)

How is ^{14}C made and why is it useful as a chronometer?



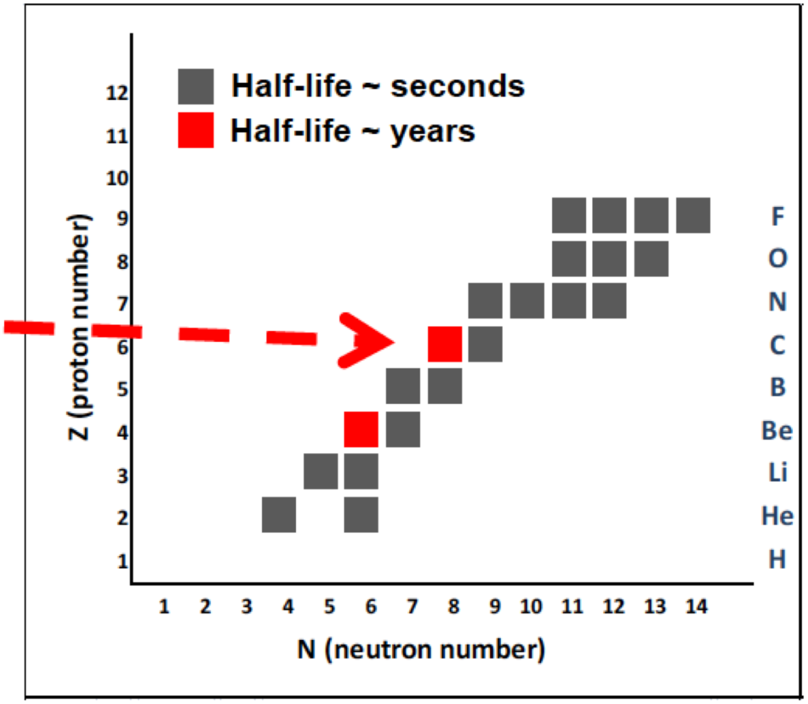
Puzzling to Scientists...

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

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

Chart of light nuclei that decay via beta emissions

$$n \rightarrow p + e^- + \bar{\nu}_e$$



Previous nuclear theory calculations yielded a very short half-life for ^{14}C, like its short-lived neighbors in the chart of isotopes.

Some studies has suggested the possibility that an exotic force, a three-nucleon force, could play a role in resolving this mystery but those studies lacked predictive power => Need an ab initio approach!

ab initio Nuclear Theory

Standard Model (QCD + Electroweak)

↓

Chiral EFT interactions & effective EW operators

↓

quantum many-body theory

↓

describe/predict experimental data => New Physics?

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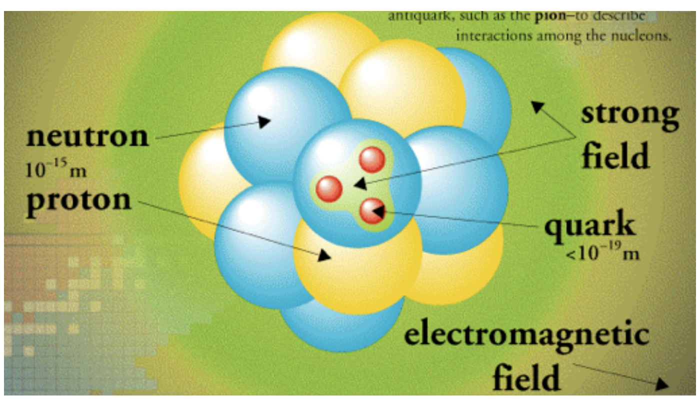
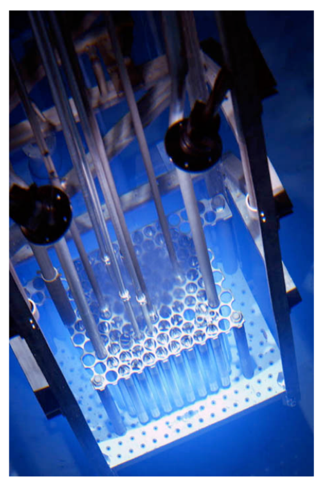
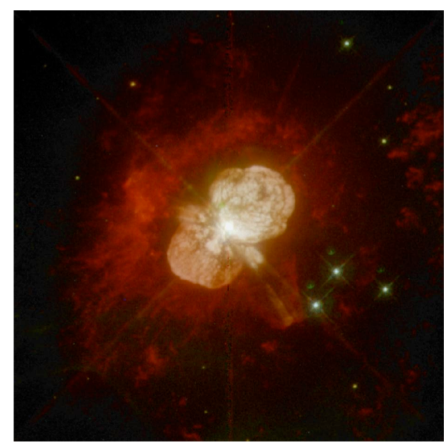






No Core Shell Model (NCSM)
A large sparse matrix eigenvalue problem

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

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

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

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

- Adopt realistic NN (and NNN) interaction(s) & renormalize as needed - retain induced many-body interactions: Chiral Effective Field Theory (EFT) interactions
- 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 bookkeepping of anti-symmetrization)
- Diagonalize this sparse many-body H in its “m-scheme” basis where [α =(n,l,j,$m_{j,}$$\tau_z$)]

HO basis space (configurations)

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

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

- Evaluate observables and compare with experiment

Comments

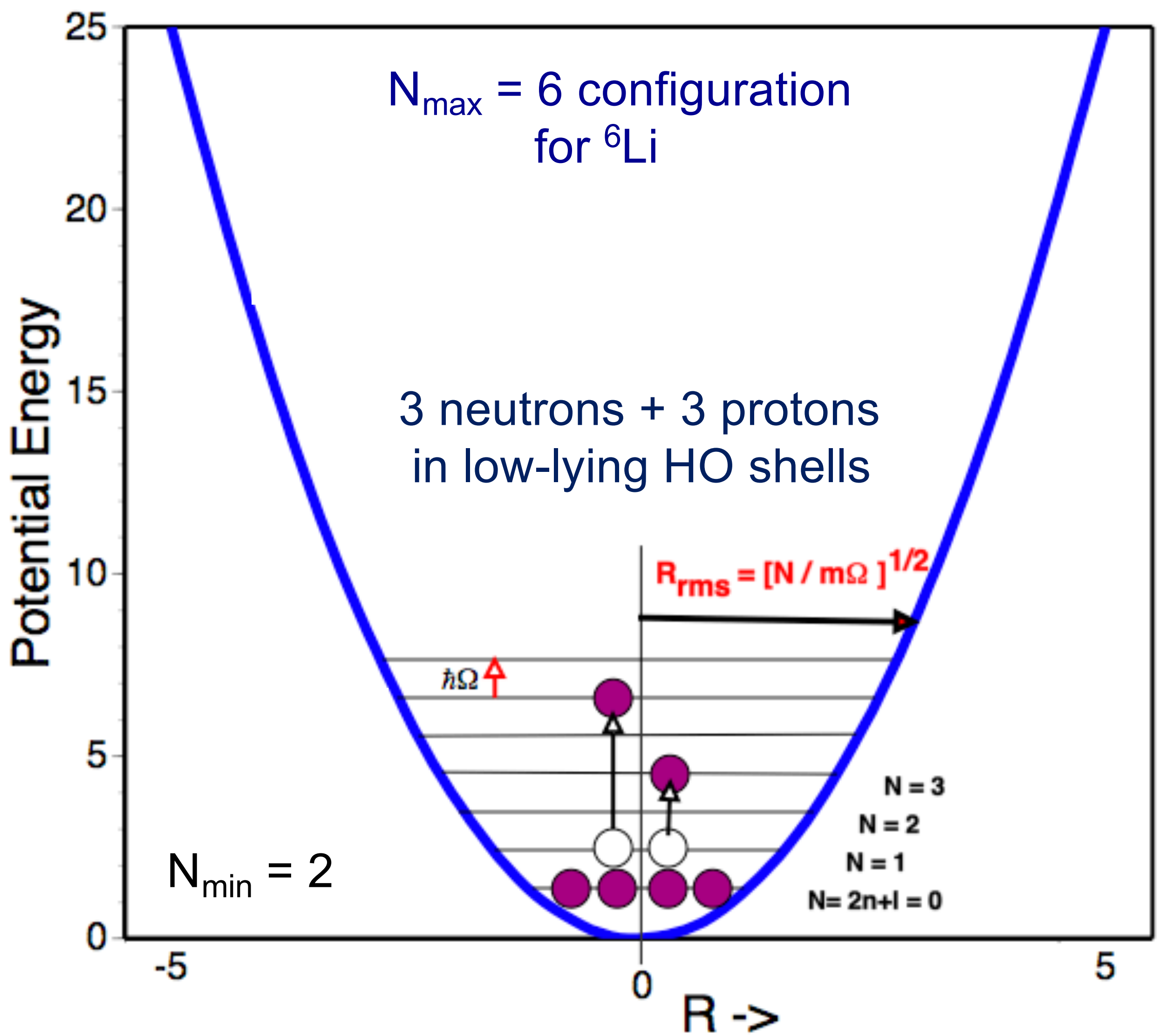
- Computationally demanding => needs new algorithms & high-performance computers
- Requires convergence assessments and extrapolation tools to retain predictive power
- Achievable for nuclei up to atomic number of about 20 with largest computers available (See poster by Pieter Maris)

$N_{\min} \equiv$ HO quanta of lowest configuration

$N_{\max} \equiv$ maximum HO quanta above the lowest configuration

Retain configurations with $N_{\min} \leq \sum_{i=1}^{A}(2n_i + l_i) \leq N_{\min} + N_{\max}$

consistent with symmetry constraints (parity, M_J,...)

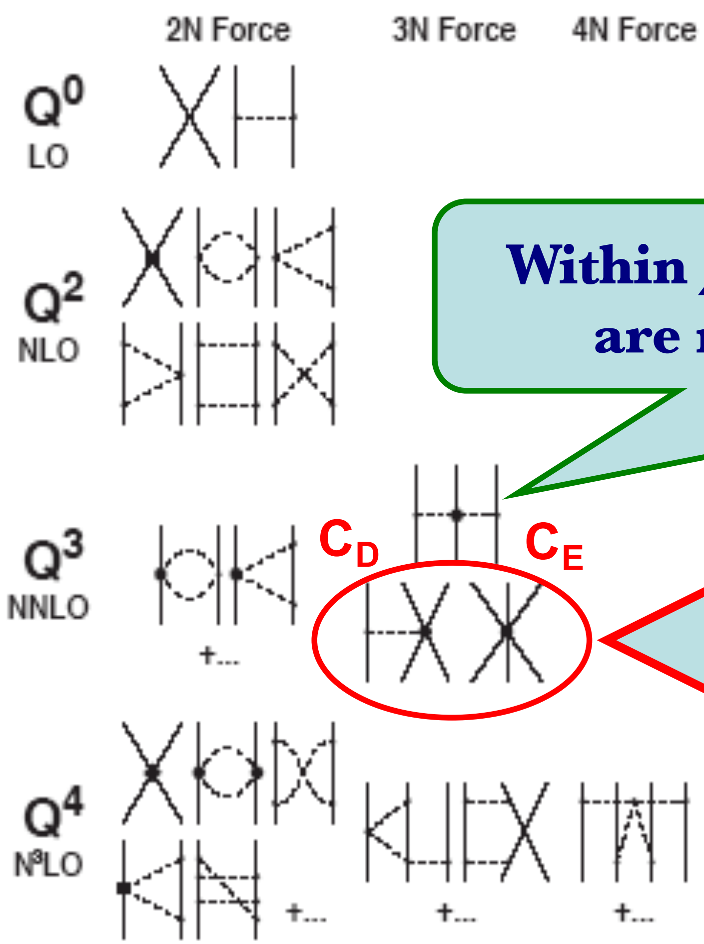


QCD => Chiral Effective Field Theory For Strong Inter-Nucleon Interactions

Chiral perturbation theory (χPT) allows for controlled power series expansion

Expansion parameter : $\left(\frac{Q}{\Lambda_\chi}\right)^{\upsilon}$, Q – momentum transfer,

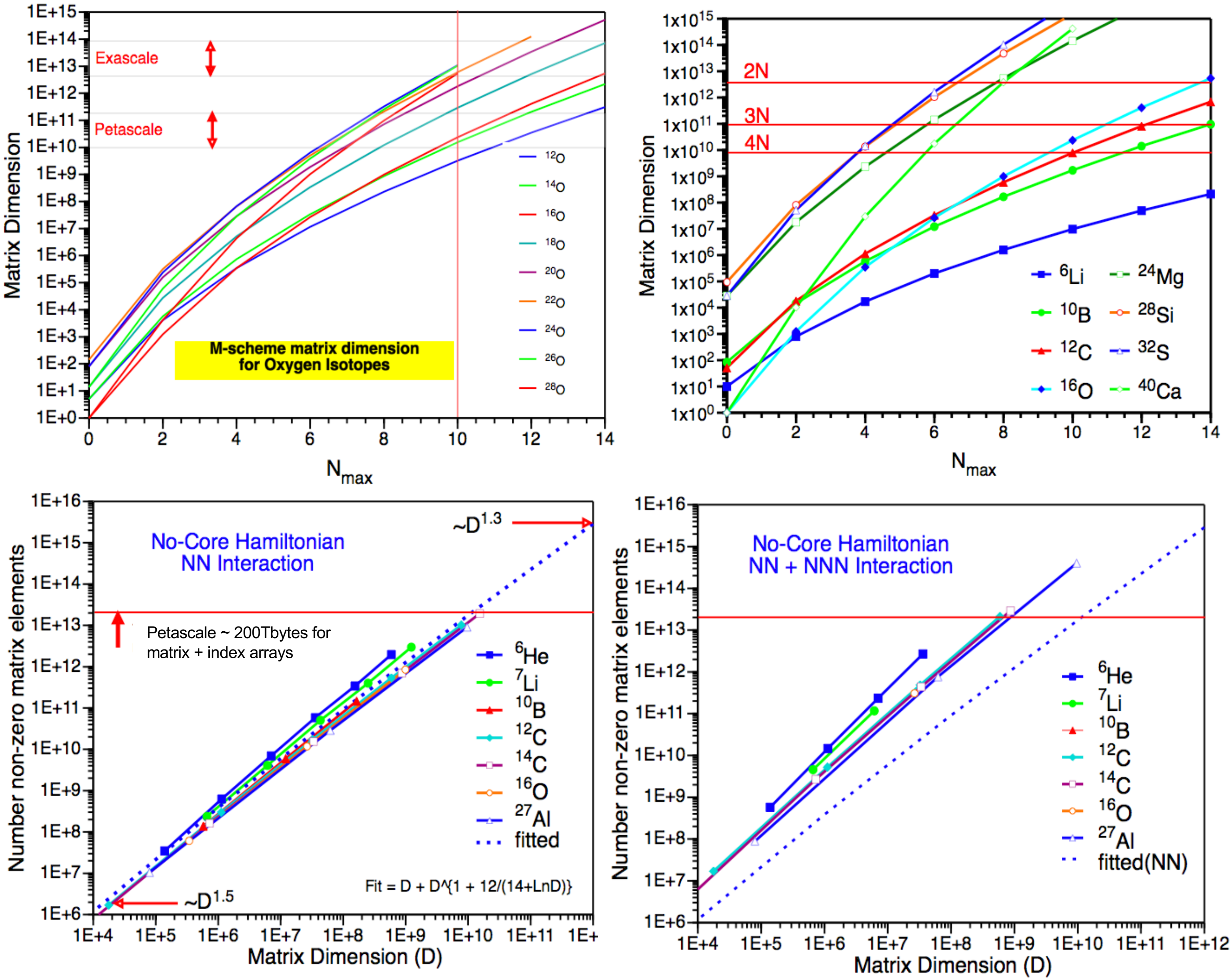
χ-symmetry breaking scale: $\Lambda_\chi \approx 1$ GeV/c $\approx \frac{2\pi}{r} \Rightarrow r \approx 1$ fm



Within χPT 2π-NNN Low Energy Constants (LEC) are related to the NN-interaction LECs $\{c_i\}$.

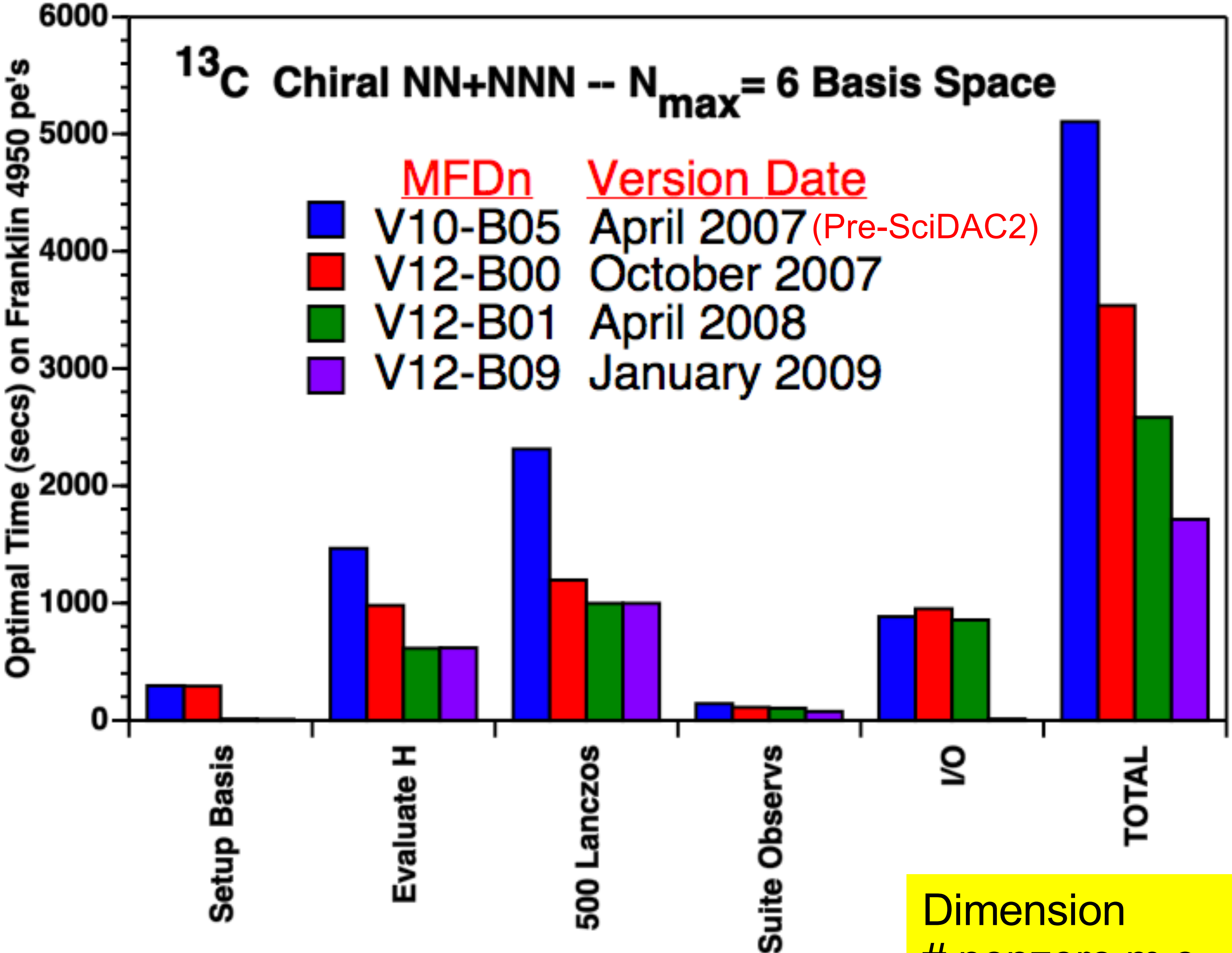
LECs fit to A = 3 & 4 ground states

R. Machleidt & D. R. Entem, Phys. Rept. 503, 1 (2011)



J.P. Vary, P. Maris, E. Ng, C. Yang and M. Sosonkina, Journal of Physics: Conference Series **180**, 012083 (2009)

Improvements to Many Fermion Dynamics - nuclear (MFDn) under SciDAC2/UNEDF

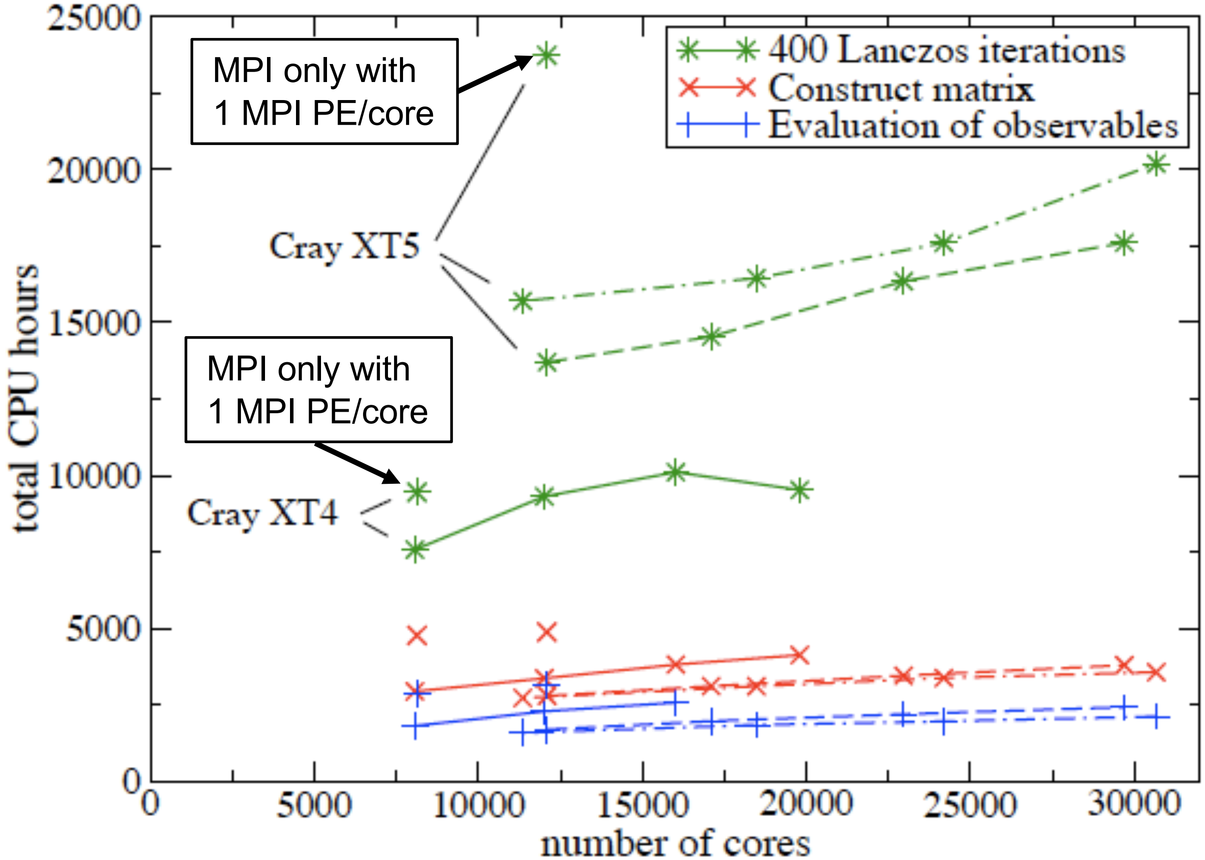


J.P. Vary, P. Maris, E. Ng, C. Yang and M. Sosonkina,
Journal of Physics: Conference Series **180**, 012083 (2009)

Dimension	38×10^{6}
# nonzero m.e.	56×10^{10}
Input 3b m.e.	3 Gbytes

Hybrid MPI/OpenMP more efficient as problem size grows

^{14}N, $N_{\max} = 8$, 2-body interactions, on Franklin (XT4) and Jaguar (XT5)



solid: hybrid OMP/MPI
1 MPI PE per node
with 4 threads (XT4)

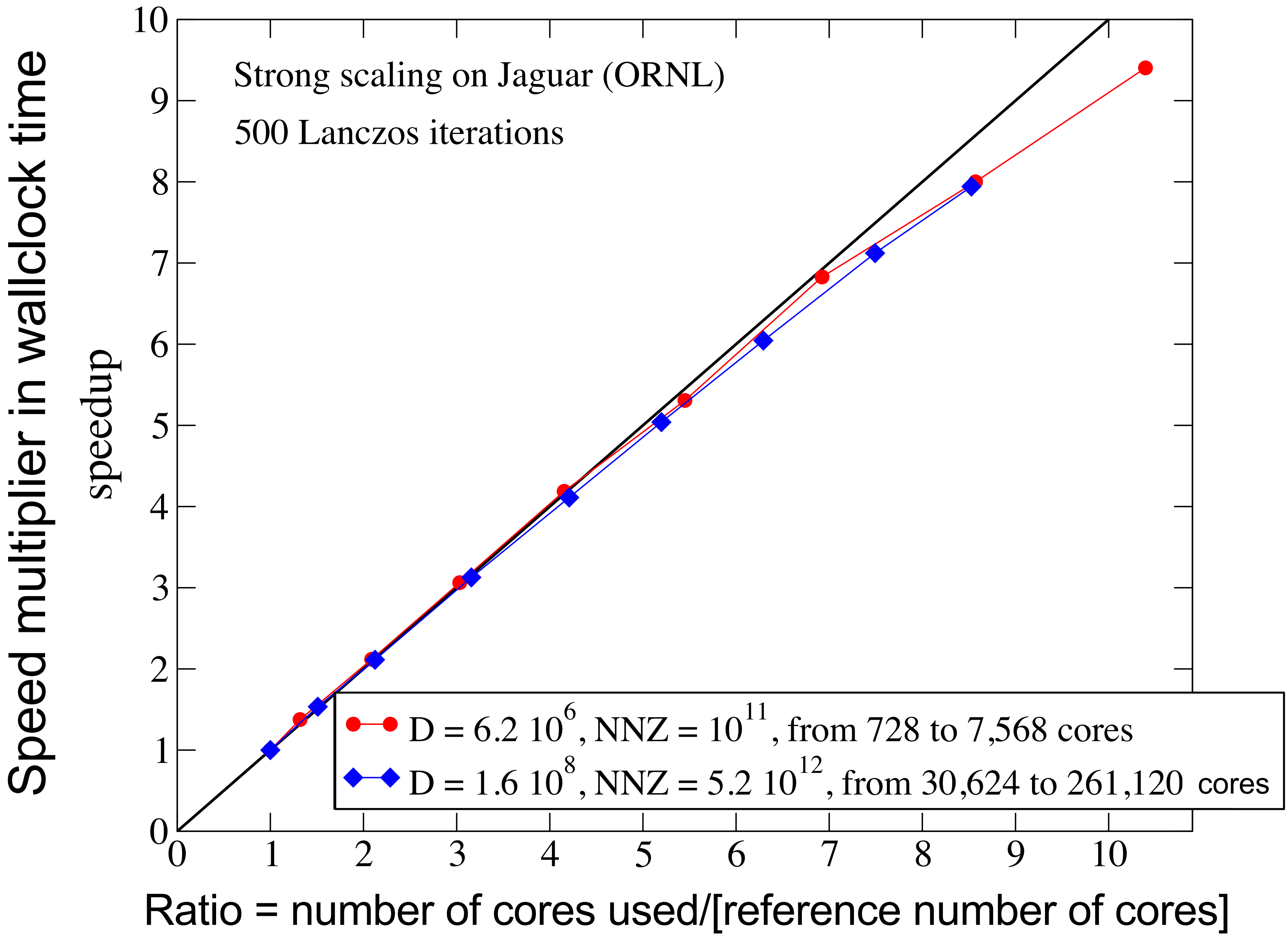
dashed: hybrid OMP/MPI
1 MPI PE per NUMA node
with 6 threads (XT5)

dot-dashed: hybrid OMP/MPI
1 MPI PE per compute node
with 12 threads (XT5)

dimension $1.1 \cdot 10^9$
nonzero m.e. $1 \cdot 10^{12}$
memory for matrix: 8 TB

P. Maris, M. Sosonkina, J.P. Vary, E.G. Ng and C. Yang, ICCS 2010, Procedia Computer Science 1, 97 (2012)

Quantifying our advances in algorithms, applied math and computer science



Metrics for MFDn Improvements within SciDAC2/UNEDF

Success in Competitions

(1) INCITE awards for the entire project and beyond
(2) Jaguar Early Science award for the ^{14}C project (30 Million CPU hrs)

Scientific Results

16 refereed publications for MFDn developments & applications
with joint physics, computer science and applied math authors

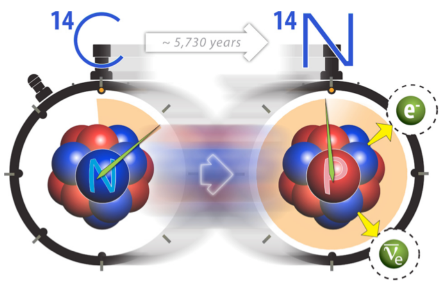
Key Achievement: Solved the 14C life-time mystery

PRL 106, 202502 (2011) PHYSICAL REVIEW LETTERS week ending 20 MAY 2011

Origin of the Anomalous Long Lifetime of ^{14}C

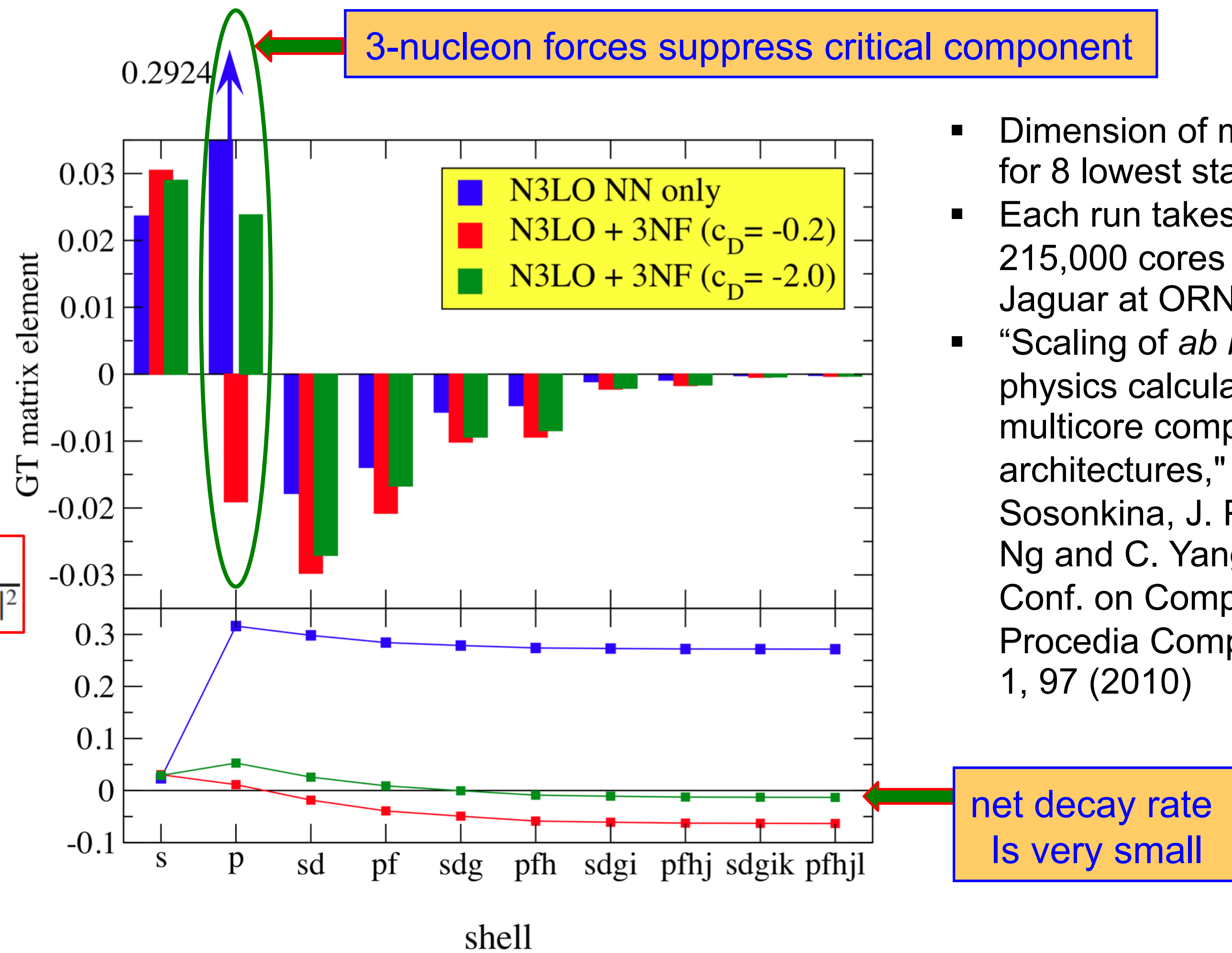
P. Maris,[1] J.P. Vary,[1] P. Navrátil,[2,3] W.E. Ormand,[3,4] H. Nam,[5] and D.J. Dean[5]

- Solves the puzzle of the long but useful lifetime of ^{14}C
- Establishes a major role for strong 3-nucleon forces in nuclei
- Strengthens foundation for guiding DOE-supported experiments



$$T_{1/2} = \frac{1}{f(Z, E_0)} \frac{2\pi^3\hbar^7 \ln 2}{m_e^5 c^4 G_V^2} \frac{1}{g_A^2 |M_{GT}|^2}$$

$$M_{GT} = \sum_k \langle \Psi_f || \sigma(k)\tau_+(k) || \Psi_i \rangle$$



- Dimension of matrix solved for 8 lowest states ~ 1×10^9
- Each run takes ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL
- "Scaling of *ab initio* nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97 (2010)

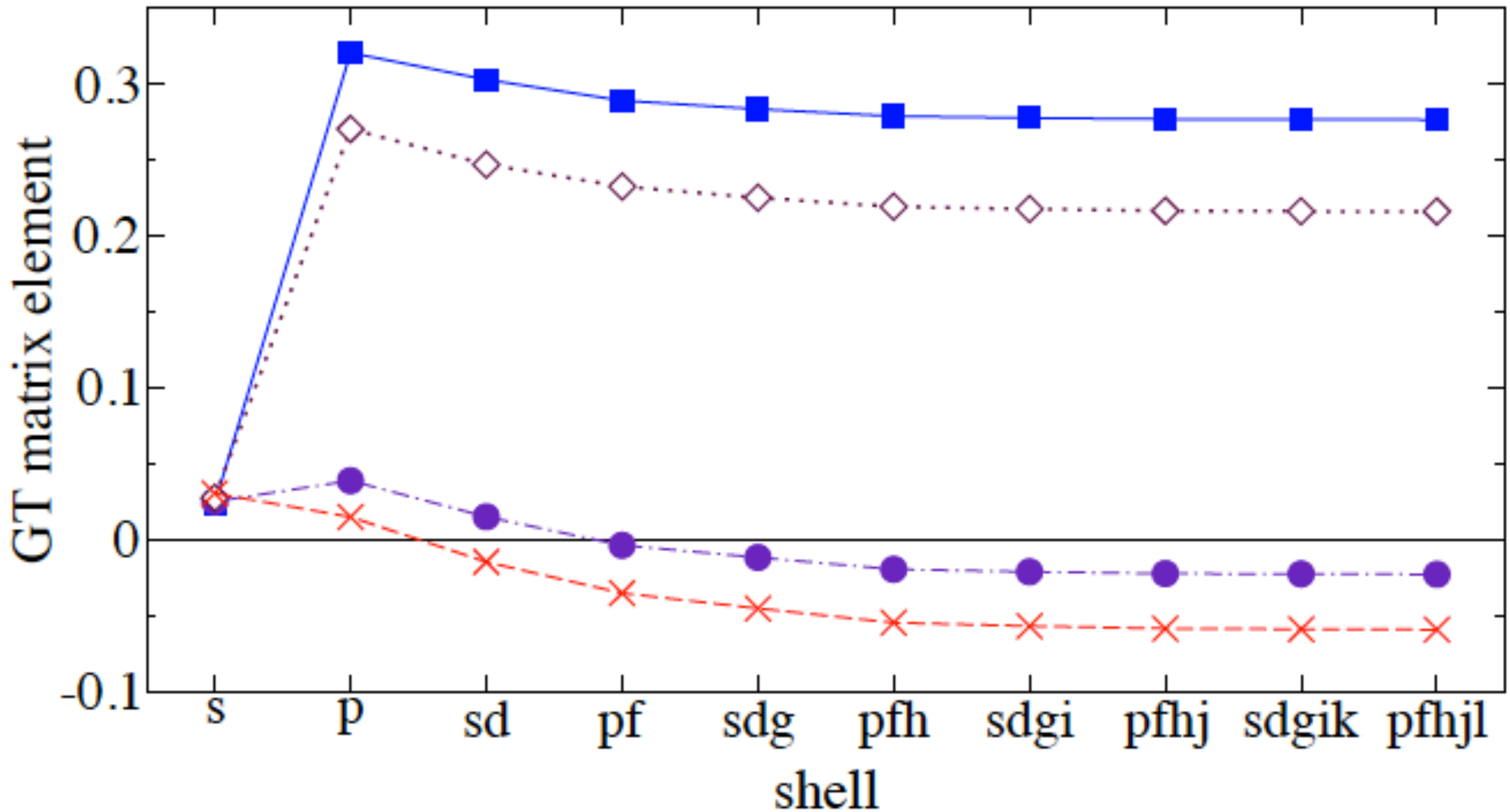


Figure 10. MGT between the ground states of ^{14}N and ^{14}C, using the ^{14}N wavefunction obtained with 3NF, but the ^{14}C wavefunction obtained without 3NF (purple •), and vice versa (maroon ◇). For comparison, we also include the results with (red cross X) and without (blue ■) 3NF for both wavefunctions.

P. Maris, J. Phys. Conf. Ser. 402, 012031 (2012); arXiv:1209.6573

Conclusions

Uniqueness of SciDAC Program evident with this ^{14}C success case

- Enabled frequent meetings of multidisciplinary teams for brainstorming and problem-solving to address bottlenecks and devise/test/implement solutions
- Novel algorithm/code developments by multidisciplinary teams that provided computational readiness in competitions for critical leadership-class resources resulting in major INCITE and Early Science awards
- Generation of successful projects not previously conceived or planned within existing agendas
- 16 refereed publications in SciDAC2/UNEDF for MFDn imrovements & applications with joint physics, computer science and applied math authors
- Accelerated breakthrough: solution of a long-standing science problem – the origin of the anomalously long lifetime of ^{14}C

Backup Slides

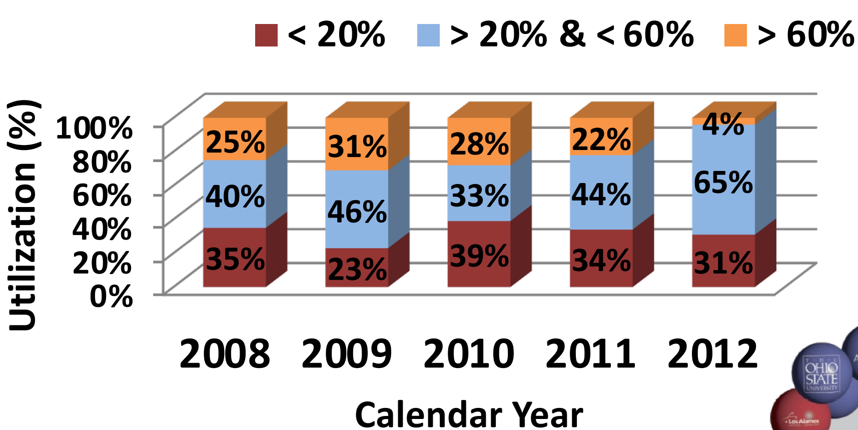
NUCLEI/UNEDF Leadership-class computing

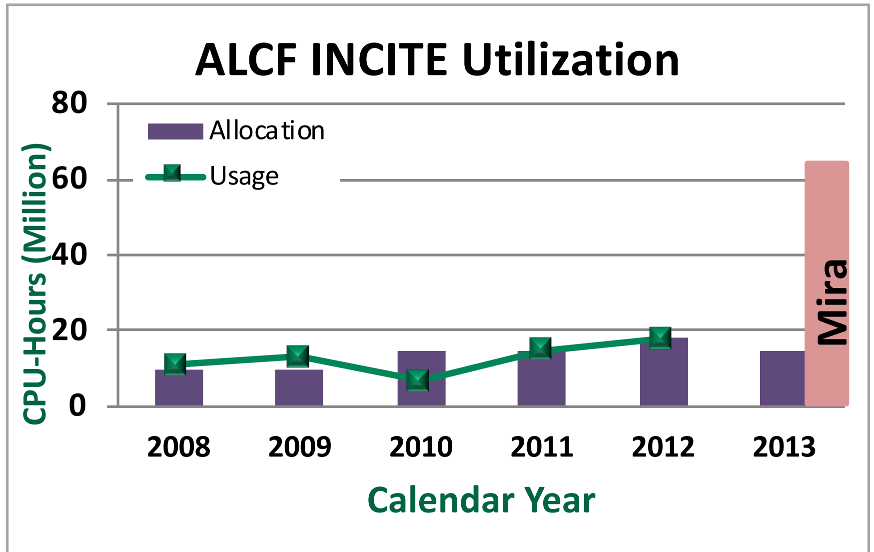
◆ SciDAC collaborations between applied mathematicians, computer scientists, and nuclear physicists lead to efficient utilization of leadership-class computing resources for nuclear physics problems

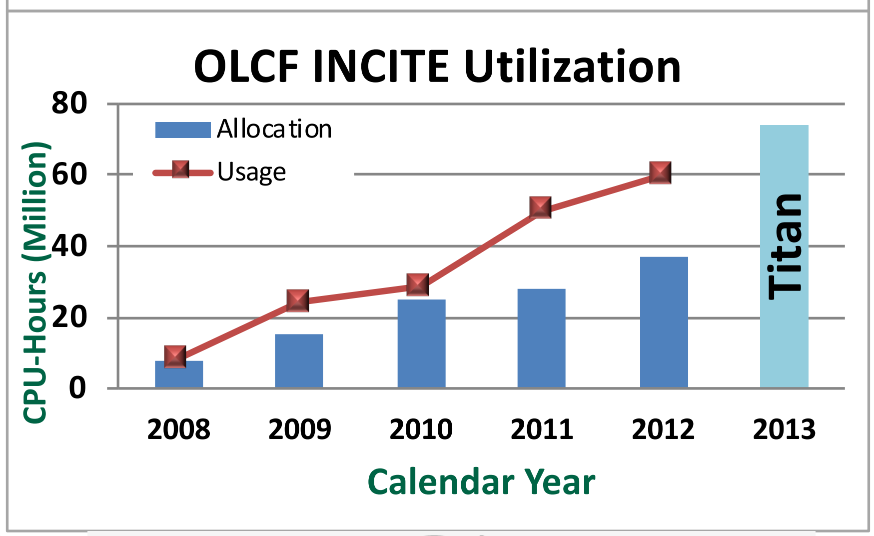
◆ Significant accomplishments in NUCLEI/UNEDF, achieved through leadership-class computing

- *Ab-initio* calculations of C-12
- Understanding of long lifetime of C-14
- *Ab-initio* calculations of Ca-54
- Improved energy-density functionals
- Quantifying the limits of nuclear existence

◆ 60% to 80% of computing resources used at leadership-class scale



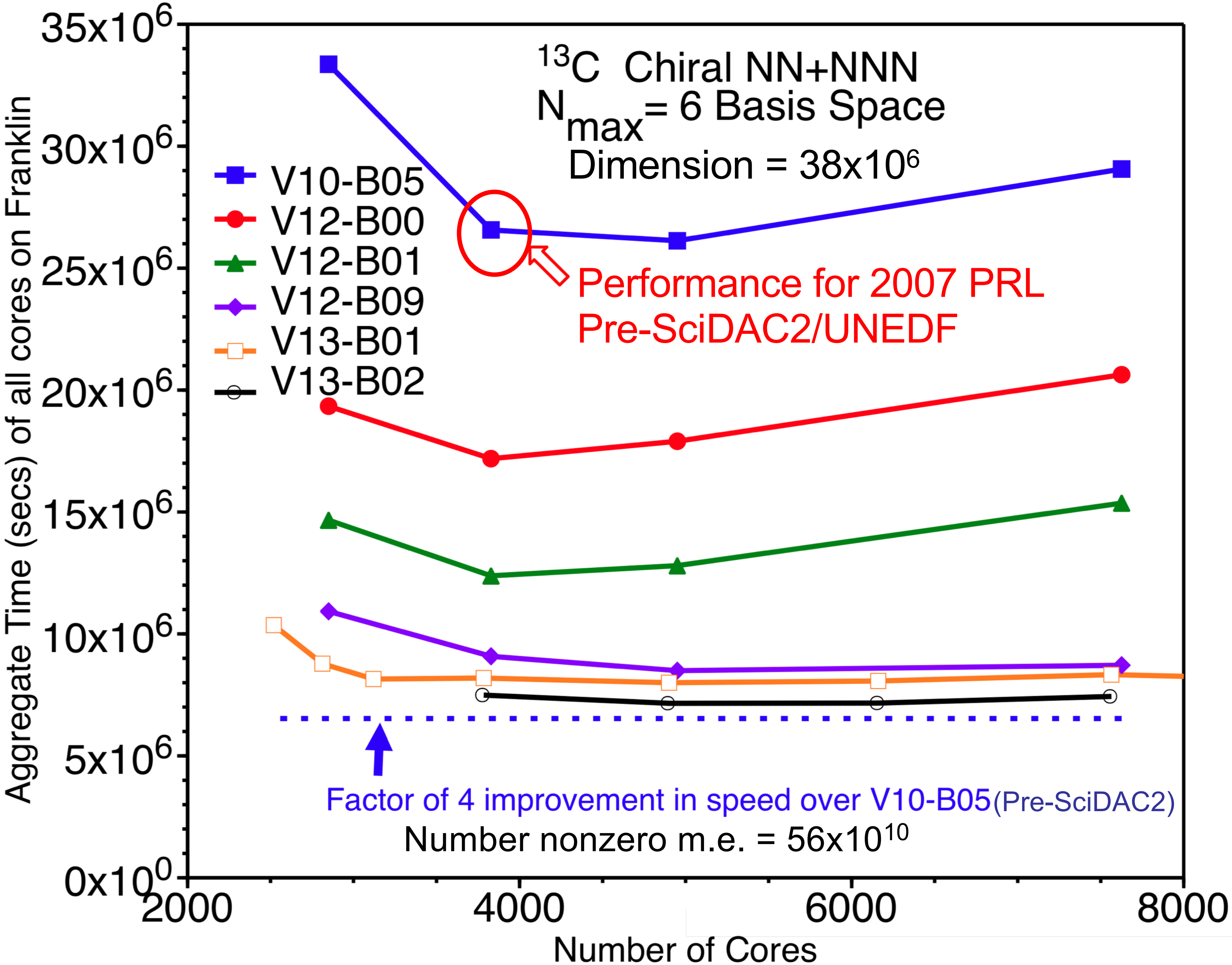




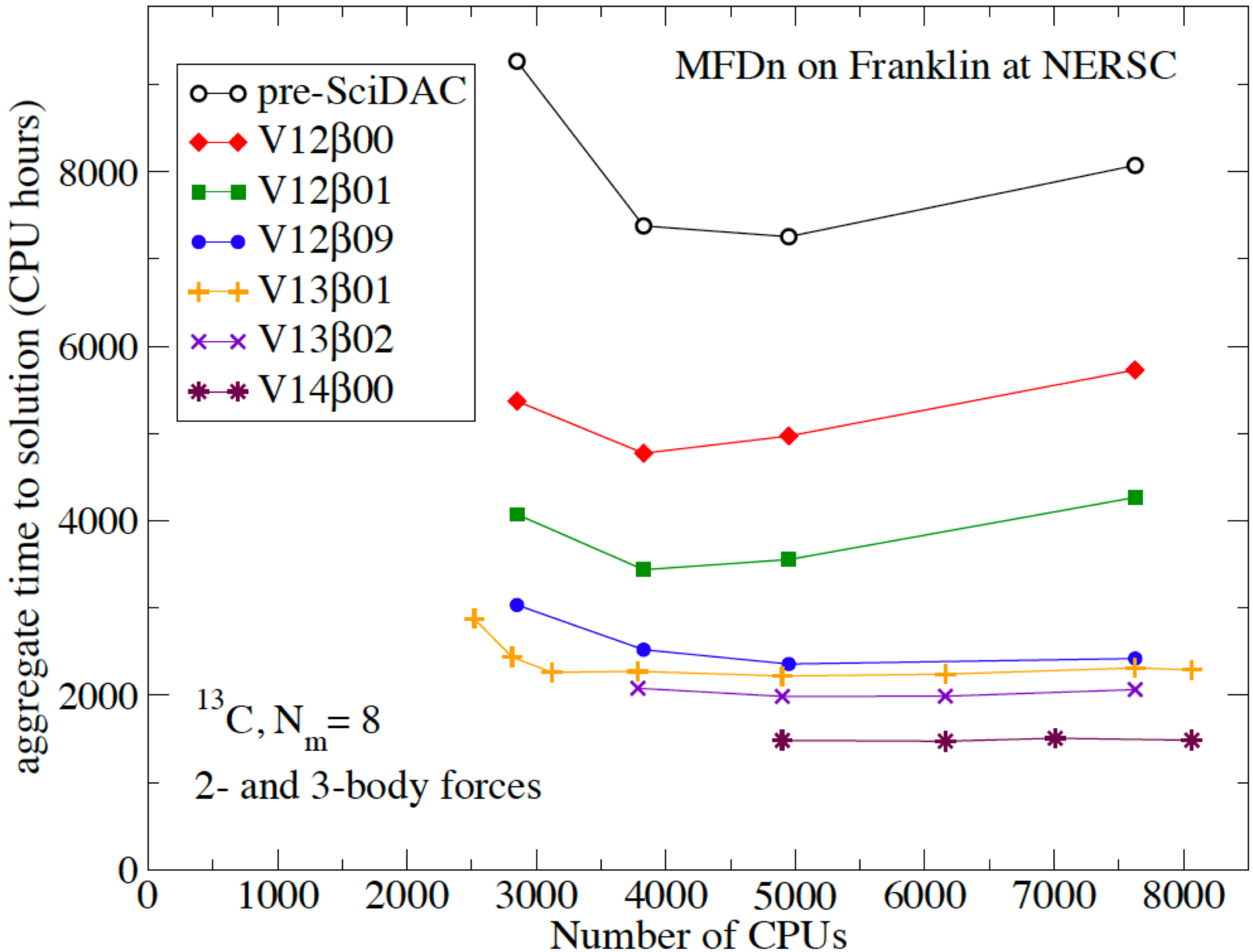
U.S. DEPARTMENT OF ENERGY

UNEDF

NUCLEI
Nuclear Computational Low-Energy Initiative



P. Maris, M. Sosonkina, J.P. Vary, E.G. Ng and C. Yang, ICCS 2010, Procedia Computer Science 1, 97 (2012)



P. Maris, Journal of Physics: Conference Series 402, 012031 (2012)

Only turn on 3NF in ^{14}C ~ no suppression

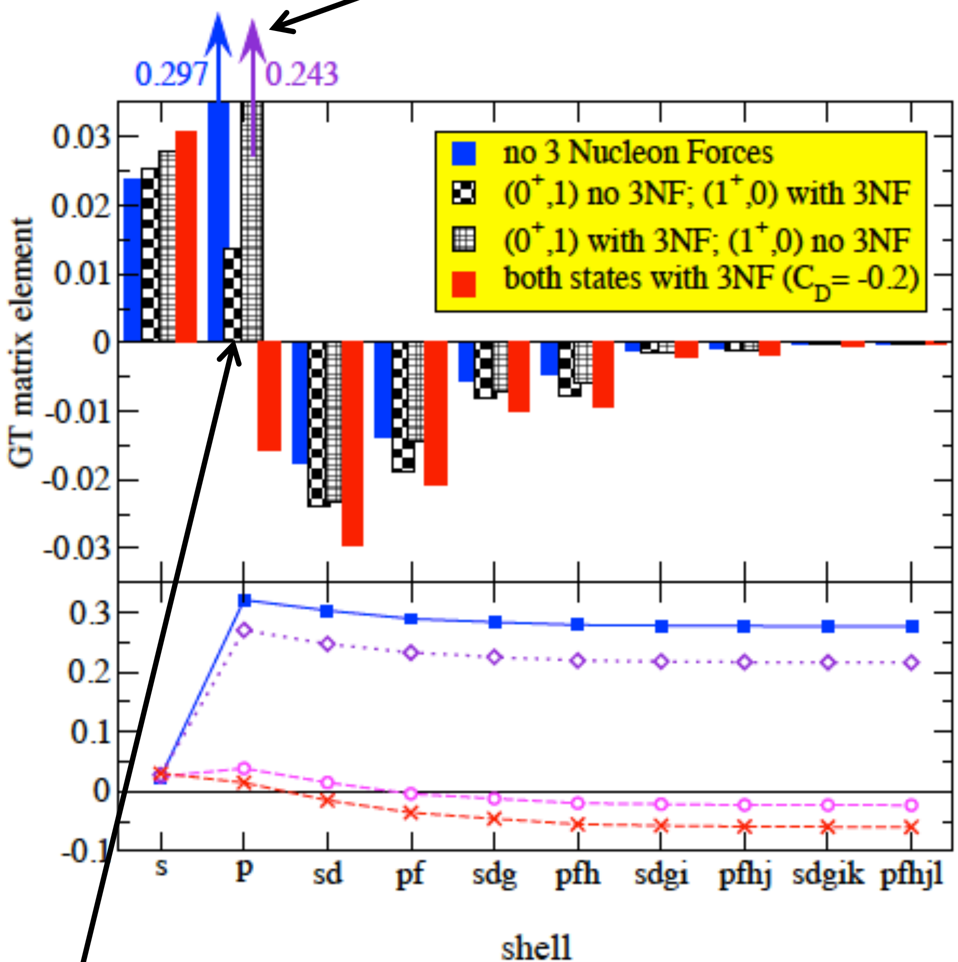


Figure 10. GT matrix element between the $(1^+, 0)$ ground state and the lowest $(0^+, 1)$ excited state of ^{14}N, using the $(1^+, 0)$ wavefunction obtained with three-body forces, but the $(0^+, 1)$ wavefunction obtained without three-body forces, and vice versa. For comparison, we also include the results with and without three-body forces for both wavefunctions.

Only turn on 3NF in ^{14}N ~ most of the suppression

P. Maris, J. Phys. Conf. Ser. 402, 012031 (2012); arXiv:1209.6573

Integration of Ab Initio Nuclear Physics Calculations with Optimization Techniques*

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Lecture Notes in Computer Science , Vol. 5101, Bubak, M.; Albada, G.D.v.; Dongarra, J.; Sloot, P.M.A. (Eds.), pp. 833 – 842 (2008)

Accelerating Configuration Interaction Calculations for Nuclear Structure

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Proceedings of the 2008 ACM/IEEE Conference on Supercomputing: Conference on High Performance Networking and Computing. IEEE Press, Piscataway, NJ, 1-12 (2008)

Recent progress in Hamiltonian light-front QCD

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P. Sternberg, E. G. Ng, C. Yang
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Proceedings of Science LC2008 (Sissa, IT), 040 (2008), 040 (2008)

Ab initio nuclear structure - the large sparse matrix eigenvalue problem

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Journal of Physics: Conference Series **180**, 012083 (2009)

Benefits of Parallel I/O in Ab Initio Nuclear Physics Calculations

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(ICCS) 2009 , Part I, (Springer Verlag, Berlin), G. Allen et al., (Eds.), LNCS 5544, 84 (2009)

Hamiltonian light-front field theory in a basis function approach

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Physical Review C 81, 035205 (2010)

Hamiltonian light-front field theory within an AdS/QCD basis

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Nuclear Physics B199, 64 (2010)

Computing Atomic Nuclei on the Cray XT5

Hai Ah Nam and David J. Dean
Oak Ridge National Laboratory
James P. Vary and Pieter Maris
Iowa State University

Proc. 51st Cray User Group Conference 2009 (www.cug.org)

International Conference on Computational Science, ICCS 2010

Scaling of ab-initio nuclear physics calculations on multicore computer architectures

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International Conference on Computer Science, ICCS 2010,
Procedia Computer Science 1, 97 (2010); Elsevier, Amsterdam

Ab-initio Hamiltonian approach to light nuclei and to quantum field theory

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Pramana Jnl of Phys. 75, 39 (2010)

Dynamic adaptations in ab-initio nuclear physics calculations on multicore computer architectures

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Proceedings of 12th IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC-11) ipdpsw, pp.1332-1339 (2011)

Large-scale Parallel Null Space Calculation for Nuclear Configuration Interaction

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2011 International Conference on High Performance Computing and Simulation (HPCS 2011), 176 (2011)

Advancing Nuclear Physics Through TOPS Solvers and Tools

E Ng[1], J Sarich[2], S M Wild[2], T Munson[2], H Aktulga[1], C Yang[1], P Maris[3], J P Vary[3], N Schunck[4], M G Bertolli[5], M Kortelainen[5,6], W Nazarewicz[5,6], T Papenbrock[5,6], M V Stoitsov[5,6]

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Proceedings of SC2011

Origin of the Anomalous Long Lifetime of ^{14}C

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Physical Review Letters 106, 202502 (2011)

Article in New Scientist (selected passages)

Quantum quirk makes carbon dating possible

15 July 2011 by **David Shiga**
Magazine issue 2821. **Subscribe and save**

RADIOCARBON dating relies on carbon-14 to decode an object's age, but the isotope has steadfastly refused to divulge the key to its own unusual longevity. The answer, it seems, lies in the bizarre rules of quantum physics.

The near-perfect cancellation means carbon-14 has a low probability of decay, giving it its unusual lifetime. "One can now say confidently that the problem is solved," says Jeremy Holt of the Technical University Munich, Germany.