Computational Nuclear Physics: Key to Discovery Opportunities

James P. Vary
Iowa State University

Computational Nuclear Physics

Comput

SciDAC-2 UNEDF
SciDAC-3 NUCLEI

High Performance Computing provides answer ... ther experiment nor analytic theory c ... hence, it becomes the third leg supporting th ... cs

National Academy Report (2012)

From M. Savage

Fundamental questions of nuclear physics => discovery potential

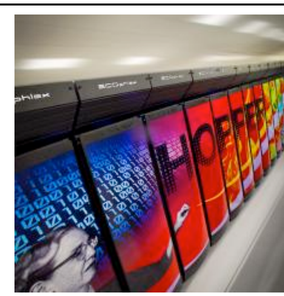
- What controls nuclear saturation?
- How shell and collective properties emerge from the underlying theory?
- What are the properties of nuclei with extreme neutron/proton ratios?
- Can we predict useful cross sections that cannot be measured?
- Can nuclei provide precision tests of the fundamental laws of nature?
- Can we solve QCD to describe hadronic structures and interactions?

U.S. DEPARTMENT OF ENERGY | Office of Science

NSF National Science Foundation WHERE DISCOVERIES BEGIN

SciDAC Scientific Discovery through Advanced Computing

Office of Science INCITE Advancing America's Science and Industrial Competitiveness

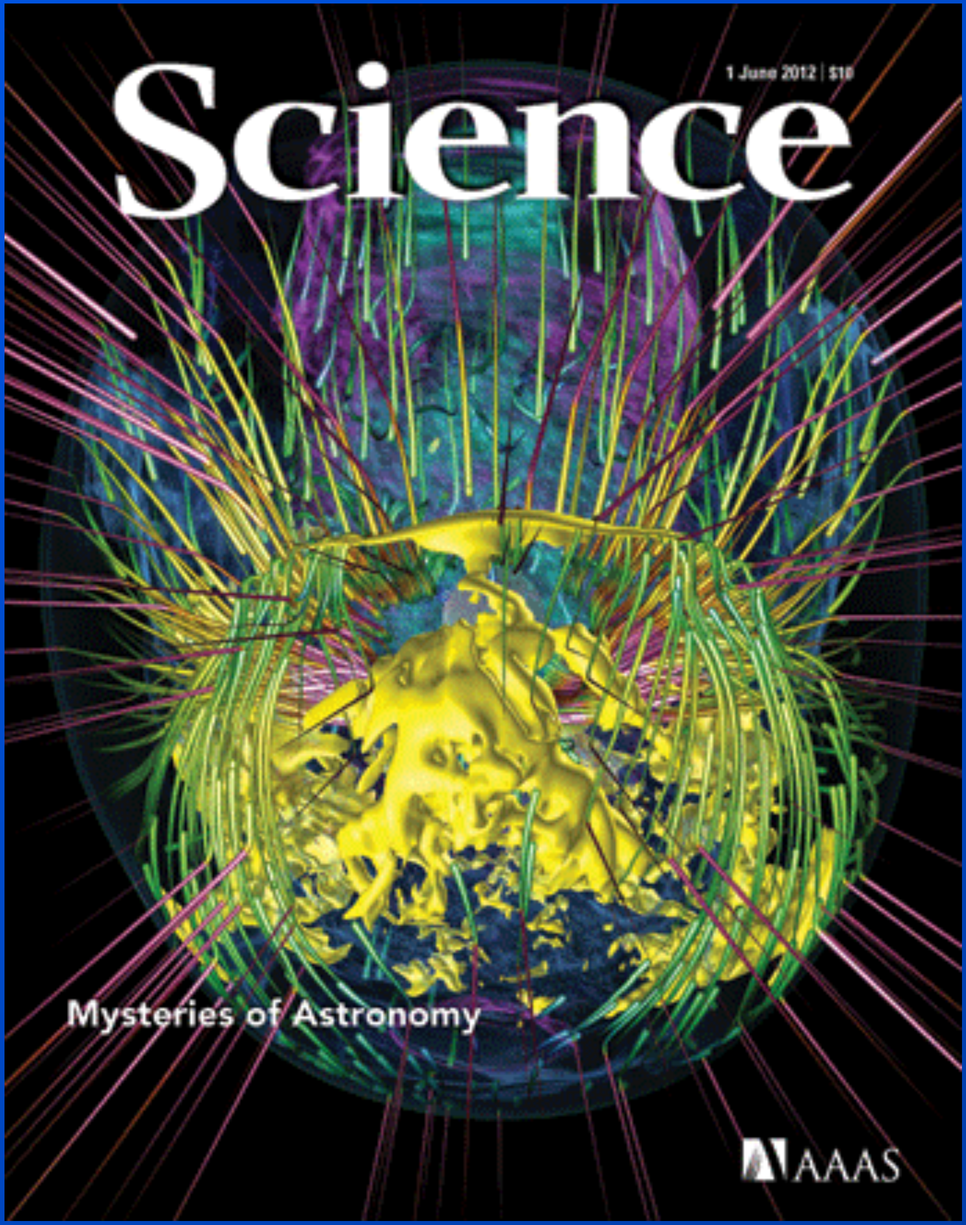


+ K-super.
+ Blue Waters
+ Lomonosov
+ Tachyon-II

What is computational nuclear physics?

Problem Statement
Hardware & Resource Assessments
Algorithms
Software
Generate Results & Analysis
-> Problem Solution

Core-collapse supernova simulation – Science, 1 June 2012



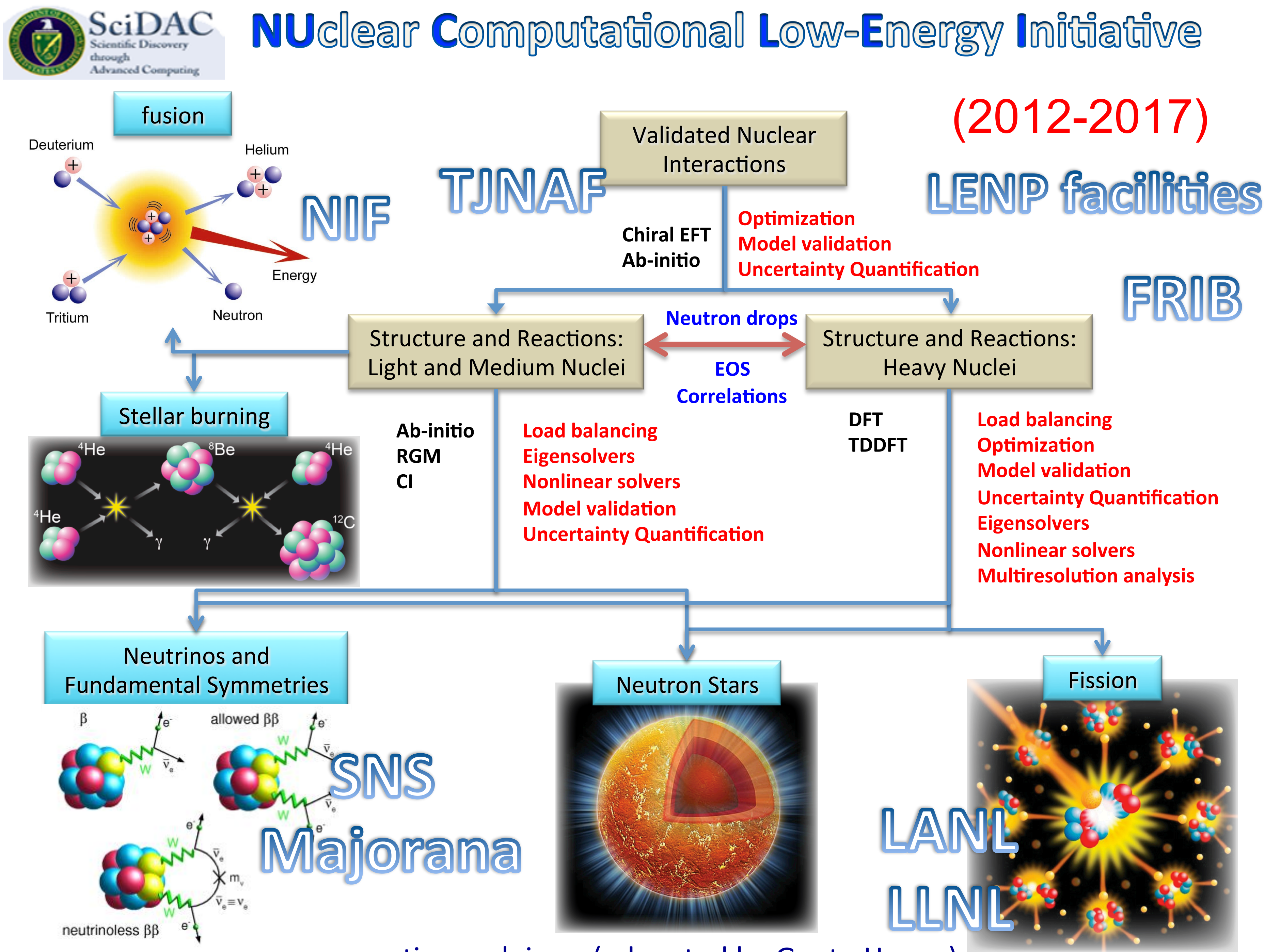
Supercomputers play an essential role in understanding nature

Nobel Prizes for Computational Science

2011 Accelerating Universe (Perlmutter, Riess, Schmidt) – implicit
1999 Electroweak renormalization (‘t Hooft, Veltman)
1985 Shake and Bake Algorithm - quantum chemistry (Hauptman, Karle)
1982 Critical Phenomena - Renormalization Group (Ken Wilson) - implicit

Ab initio nuclear theory is an example of computational physics.
Physical Review Letters published within *ab initio* nuclear theory alone:
~80 through 2012

NUclear Computational Low-Energy Initiative



computingnuclei.org (adapeted by Gaute Hagen)

Overarching Problem

Main hypothesis

If the Standard Model is correct, we should be able to accurately describe all nuclear processes

Long-term goal

Use all fundamental interactions
including yet-to-be-discovered interactions
to construct a model
for the evolution of the entire universe

Purpose of this International Conference

Current progress with theory
and supercomputer simulations

Problem statement for
Quantum Hamiltonian Physics:
Solve the non-relativistic quantum
many-body problem
with strong interactions

Note: Light front Hamiltonian and
non-relativistic nuclear Hamiltonian
problems present similar challenges

Hamiltonian framework of Light-Front Quantum Field Theory has similarities and differences with the non-relativistic quantum many-body problem

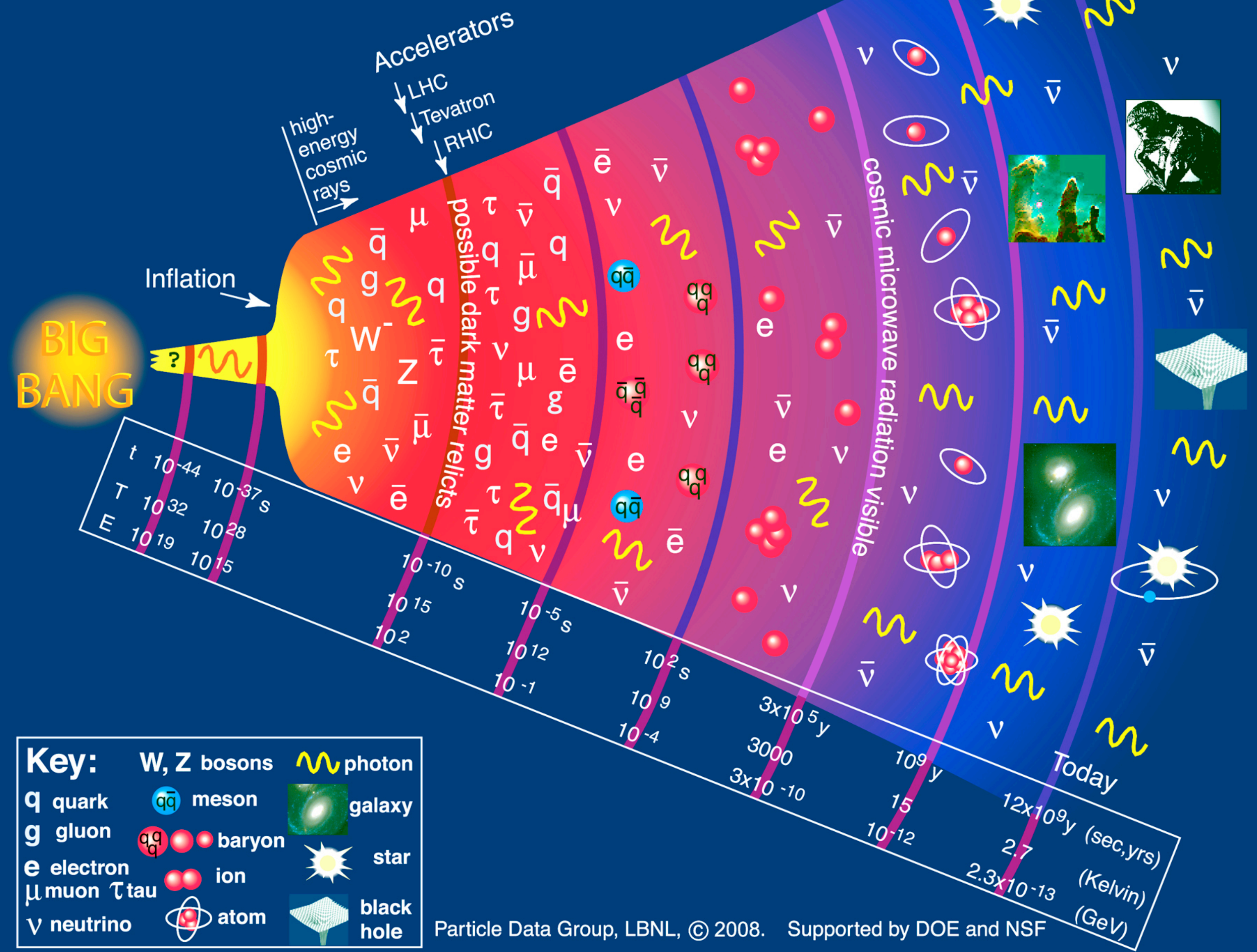
QCD bound state problems:	Nuclear many-body problems:
➢ relativistic;	➢ non-relativistic;
➢ QCD (+ *effective interaction*†);	➢ effective interaction;
➢ strong coupling;	➢ strong coupling;
➢ intrinsically many-body;	➢ many-body by definition;
➢ renormalization;	➢ *renormalization*†;

† *optional*

Yang Li, NTSE-2013

Nuclear and Particle Physics address critical problems in our understanding of the

History of the Universe



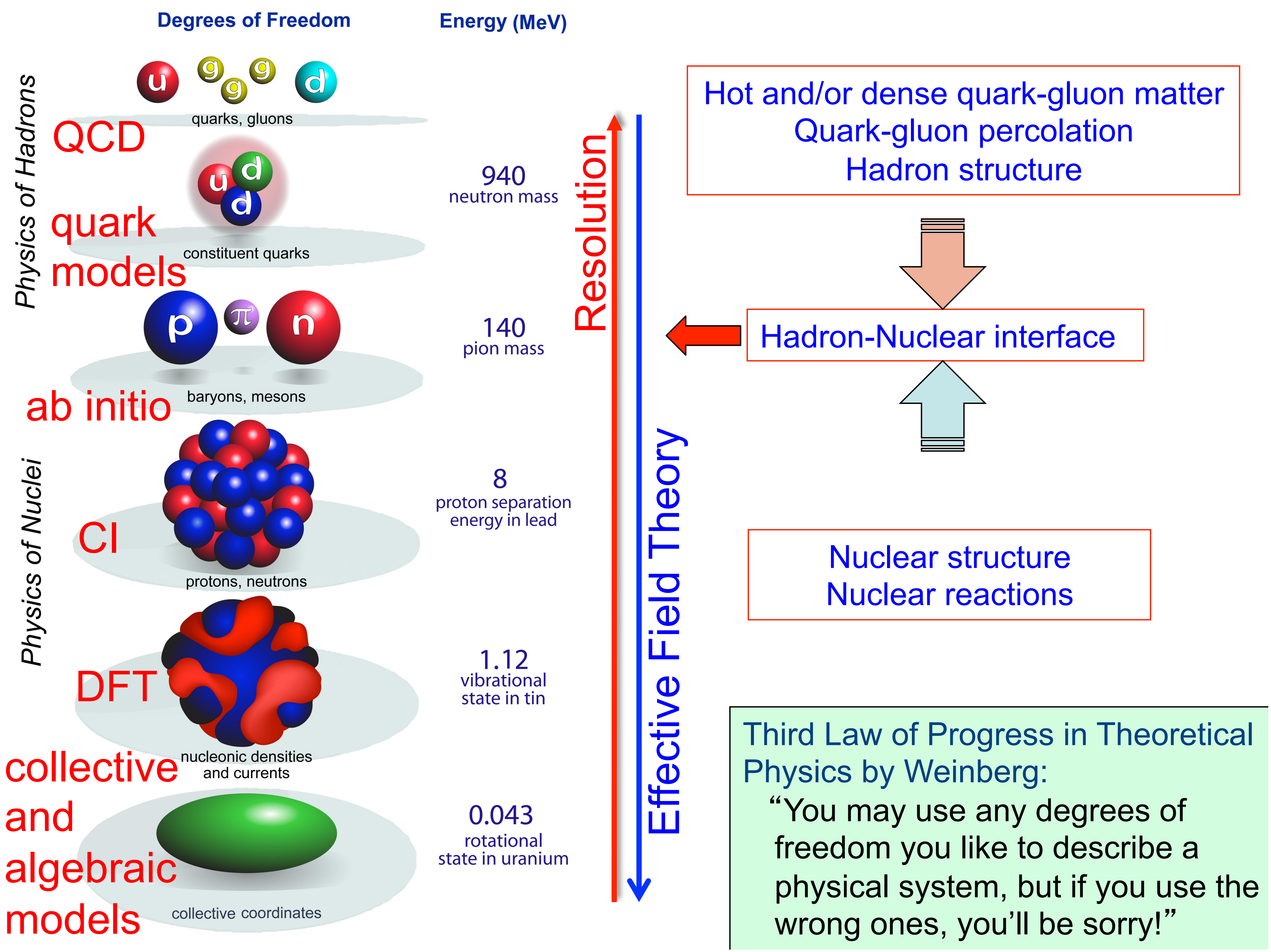
Particle Data Group, LBNL, © 2008. Supported by DOE and NSF

Going to the scale of the nucleus – can we accurately describe and predict nuclear processes governing supernovae and governing exotic decays such as neutrinoless double beta-decay, as examples?

Standard Model is the current starting point
for describing the nuclear processes
that brought the universe to the present time
and can provide fusion energy for the future

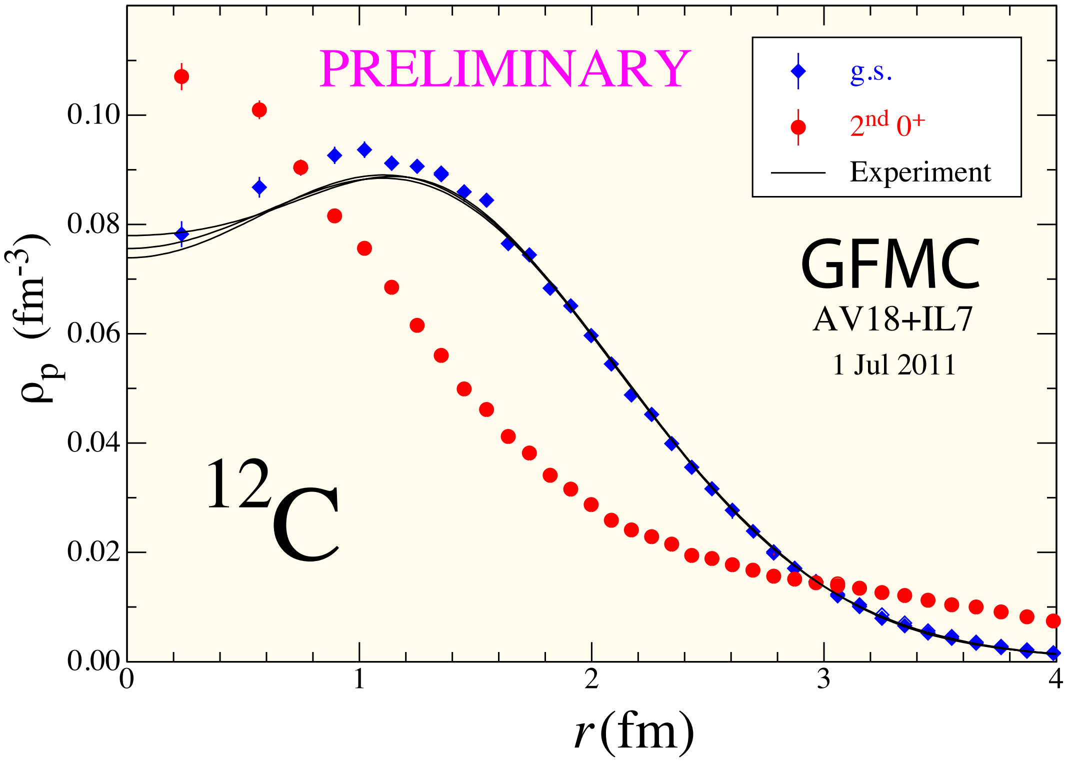
This starting point defines our “ab initio”
or “from the beginning” theory of the atomic nucleus

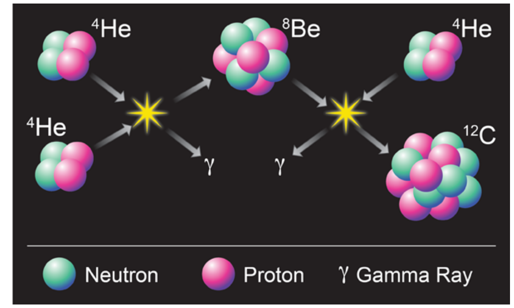
Can we successfully proceed from that starting point
to explain/predict all nuclear phenomena?

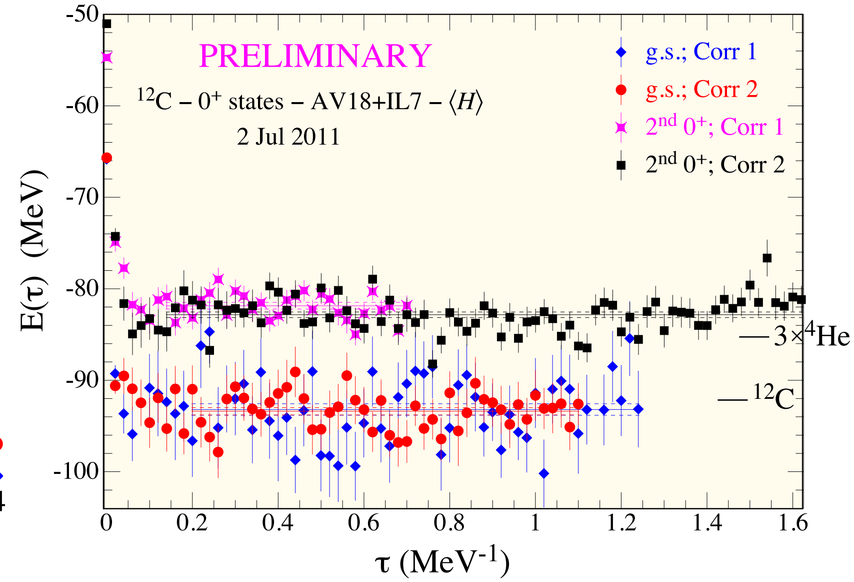

Degrees of Freedom
Energy (MeV)
Physics of Hadrons
Physics of Nuclei
QCD
quark models
ab initio
CI
DFT
collective and algebraic models
quarks, gluons
constituent quarks
baryons, mesons
protons, neutrons
nucleonic densities and currents
collective coordinates
940
neutron mass
140
pion mass
8
proton separation energy in lead
1.12
vibrational state in tin
0.043
rotational state in uranium
Resolution
Effective Field Theory
Hot and/or dense quark-gluon matter
Quark-gluon percolation
Hadron structure
Hadron-Nuclear interface
Nuclear structure
Nuclear reactions
Third Law of Progress in Theoretical Physics by Weinberg:
"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

Examples: Ab Initio

^{12}C in GFMC: Pieper et al.







The ADLB (Asynchronous Dynamic Load-Balancing) version of GFMC was used to make calculations of ^{12}C with a complete Hamiltonian (two- and three-nucleon potential AV18+IL7) on 32,000 processors of the Argonne BGP. These are believed to be the best converged ab initio calculations of ^{12}C ever made. The computed binding energy is 93.5(6) MeV compared to the experimental value of 92.16 MeV and the point rms radius is 2.35 fm vs 2.33 from experiment.

Lattice spacing 1.97 fm

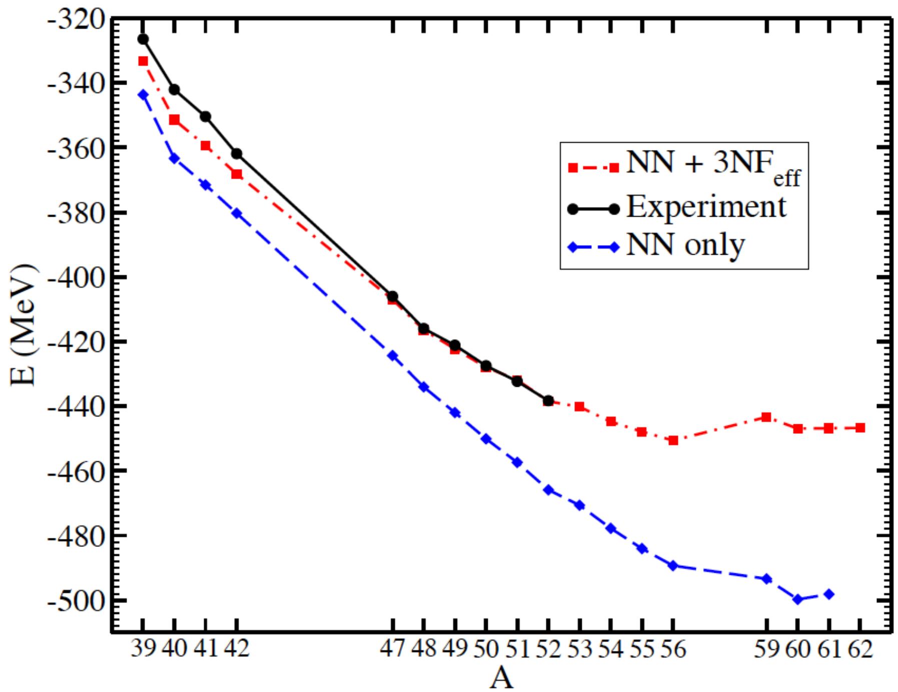
Epelbaum et al., Phys. Rev. Lett. 106, 192501 (2011)

TABLE II. Lattice results for the low-lying excited states of ^{12}C. For comparison the experimentally observed energies are shown. All energies are in units of MeV.

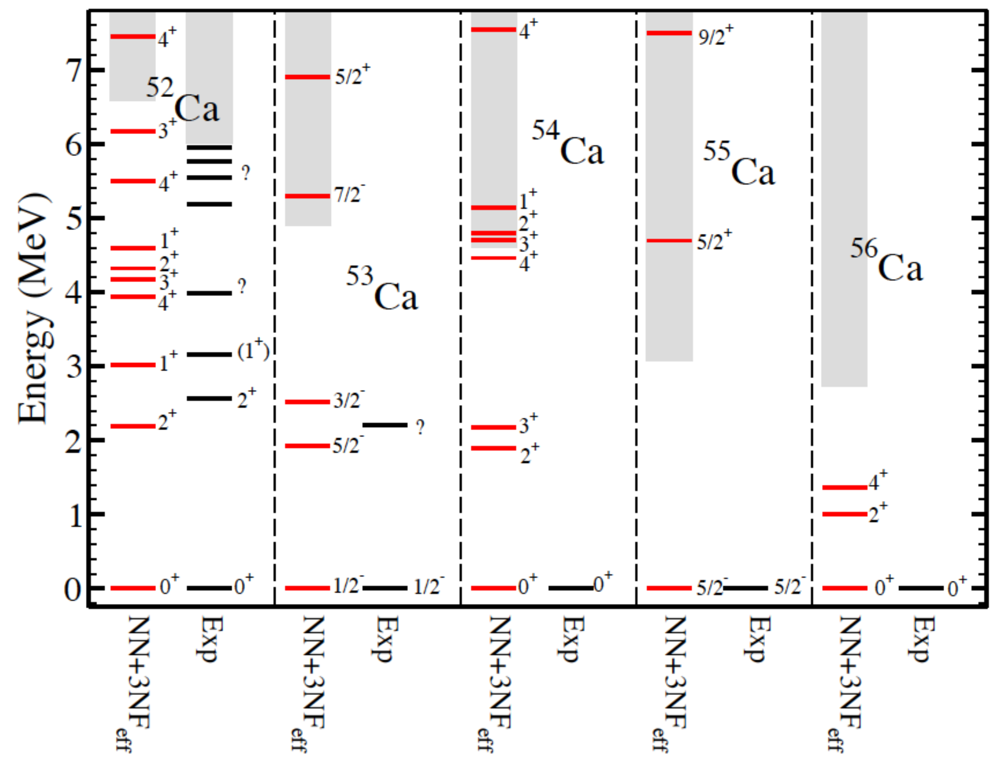
	0_2^+	$2_1^+, J_z = 0$	$2_1^+, J_z = 2$
LO $[O(Q^0)]$	−94(2)	−92(2)	−89(2)
NLO $[O(Q^2)]$	−82(3)	−87(3)	−85(3)
IB + EM $[O(Q^2)]$	−74(3)	−80(3)	−78(3)
NNLO $[O(Q^3)]$	−85(3)	−88(3)	−90(4)
Experiment	−84.51	−87.72	

Coupled-cluster method

description of medium-mass open nuclear systems



G. Hagen et al., arXiv:1204.3612 (2012)

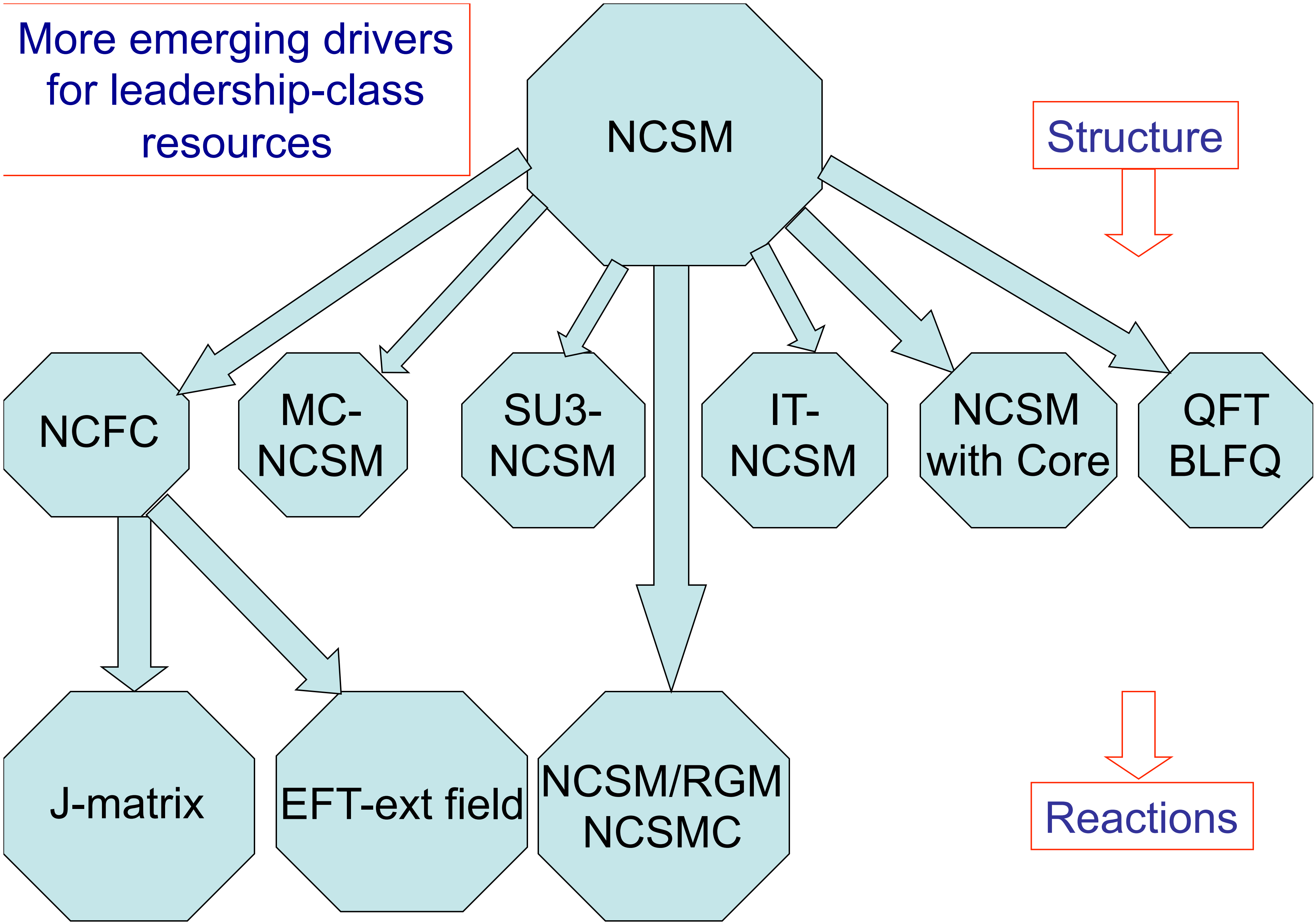


	^{53}Ca		^{55}Ca		^{61}Ca	
J^π	Re[E]	Γ	Re[E]	Γ	Re[E]	Γ
$5/2^+$	1.99	1.97	1.63	1.33	1.14	0.62
$9/2^+$	4.75	0.28	4.43	0.23	2.19	0.02

½$^+$ virtual state

- Strong coupling to continuum for neutron rich calcium isotopes
- Level ordering of states in the *gds* shell is contrary to naïve shell model picture

More emerging drivers for leadership-class resources



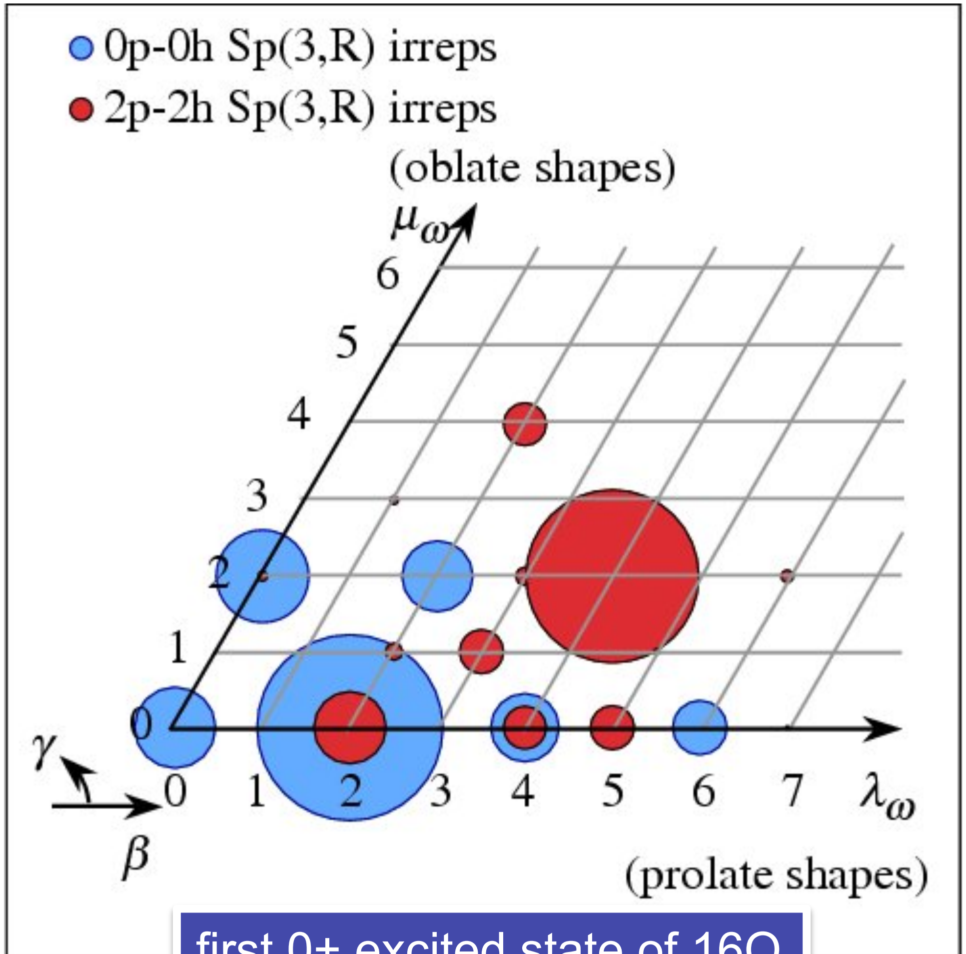
J.P. Vary, May 15, 2013

Ab initio symplectic no-core shell model

T Dytrych, K D Sviratcheva, J P Draayer, C Bahri, and J P Vary. J. Phys. G 35, 123101 (2008)

Symplectic Sp(3,R) symmetry-adapted basis

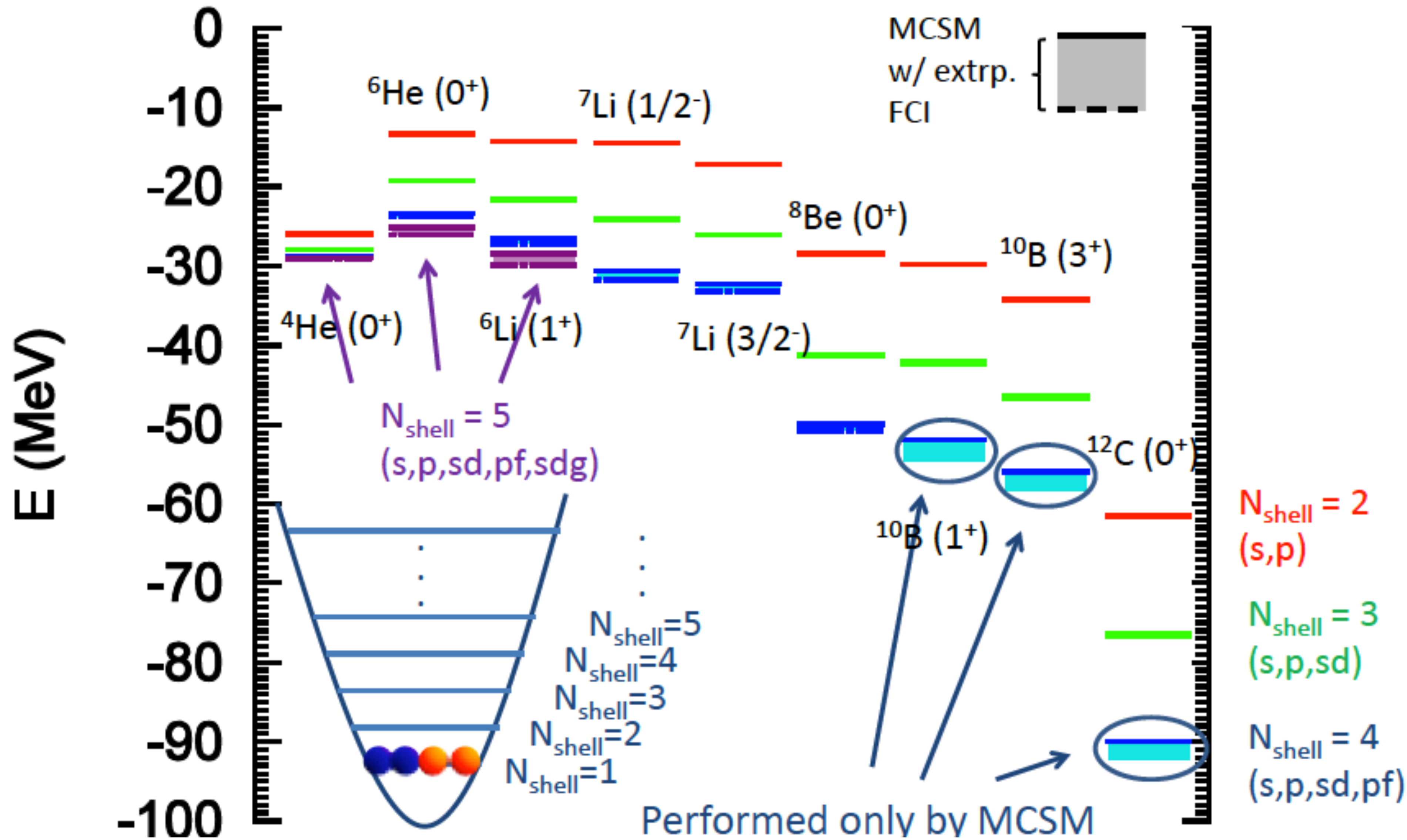
G. Rosensteel and D.J. Rowe, Phys. Rev. Lett. 38, 10 (1977)



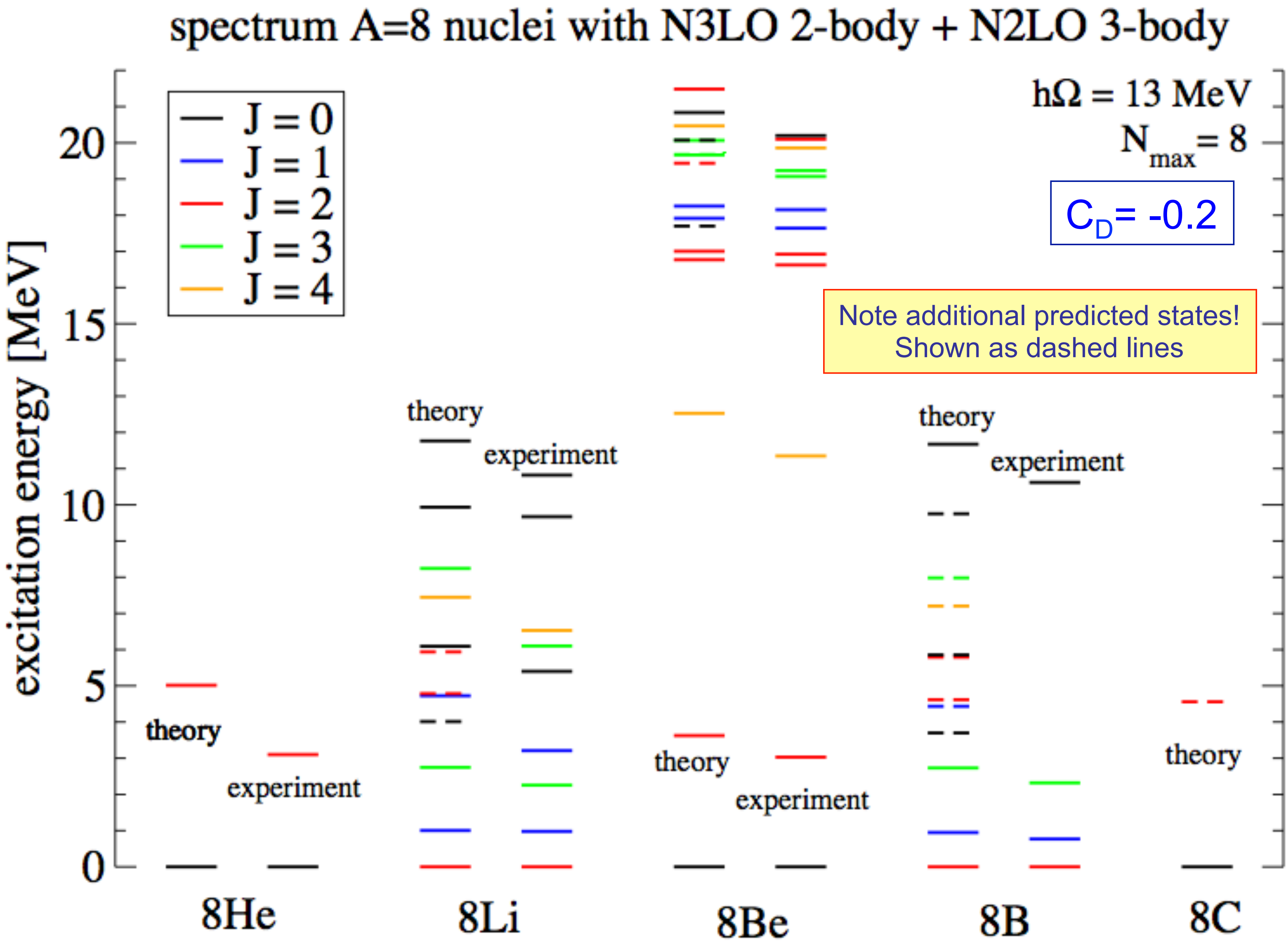
first 0+ excited state of 16O

- Effective truncation scheme
- Very promising approach for cluster states

Energies of the Light Nuclei



T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno and J.P. Vary, Phys. Rev. C 86, 054301 (2012); arXiv:1204.1755



P. Maris, J. P. Vary and P. Navratil, Phys. Rev. C87, 014327 (2013); arXiv 1205.5686

No Core CI calculations for light nuclei with chiral 2- and 3-body forces

Pieter Maris[1], H Metin Aktulga[2], Sven Binder[3], Angelo Calci[3], Ümit V Çatalyürek[4,5], Joachim Langhammer[3], Esmond Ng[2], Erik Saule[4], Robert Roth[3], James P Vary[1] and Chao Yang[2]

CCP-2012 proceedings (to appear).

Renormalization scale invariance & agreement with experiment

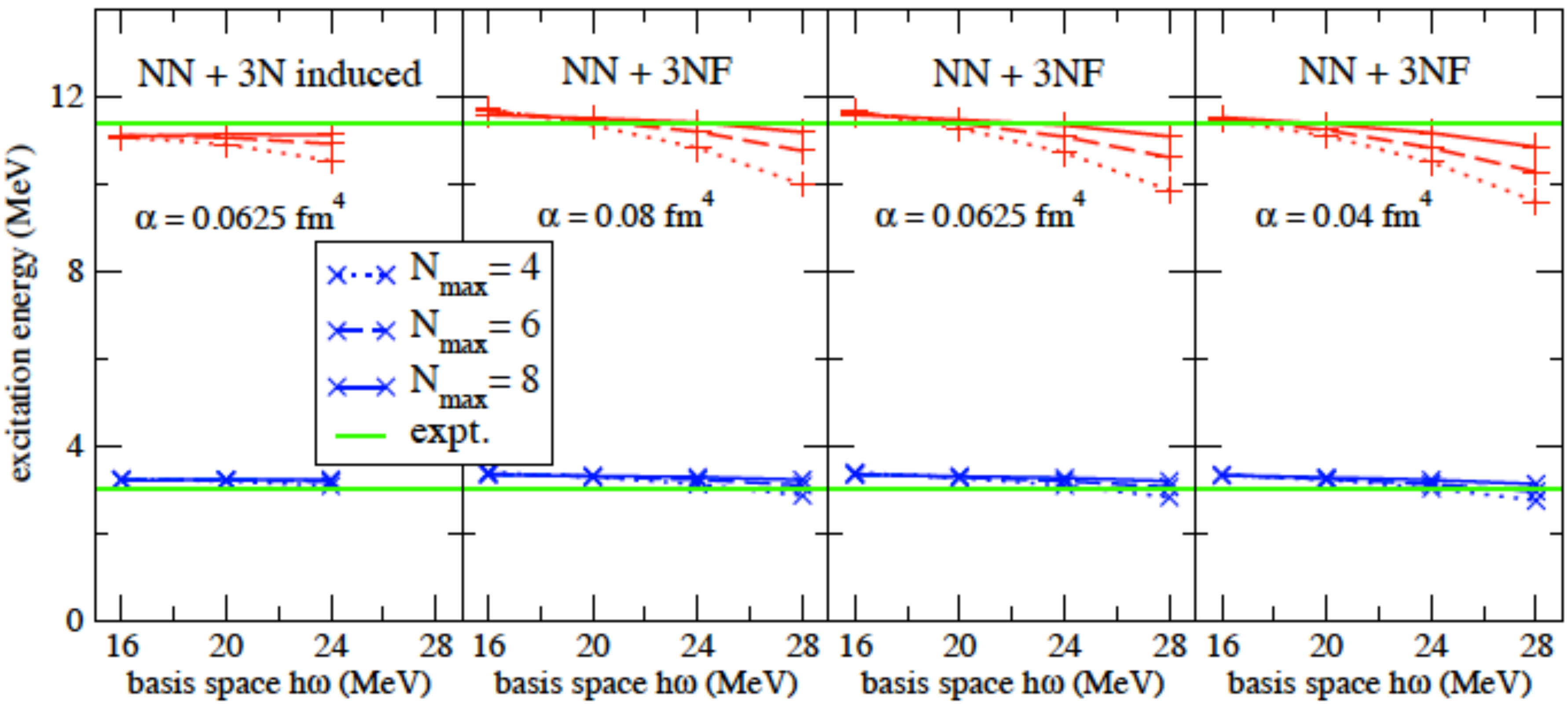


Figure 5. Excitation energies of the 2^+ (blue crosses) and 4^+ states (red plusses) for ^{8}Be with SRG evolved chiral N^{3}LO 2NF plus induced 3NF at $\alpha = 0.0625$ fm^4 (left-most panel) and with SRG evolved chiral N^{3}LO 2NF plus chiral N^{2}LO 3NF. Experimental values are indicated by the horizontal green lines.

Physics Letters B 719 (2013) 179–184

ELSEVIER

Contents lists available at SciVerse ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

Emergence of rotational bands in *ab initio* no-core configuration interaction calculations of light nuclei

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[a] Department of Physics, University of Notre Dame, Notre Dame, IN 46556-5670, USA
[b] Department of Physics and Astronomy, Iowa State University, Ames, IA 50011-3160, USA

Black line: Yrast band in collective model fit
Red line: excited band in collective model fit

Both natural and unnatural parity bands identified
Employed JISP16 interaction; N_{max} = 10 - 7

K=1/2 bands include Coriolis decoupling parameter:

$$E(J) = E_0 + A\left[J(J+1) + a(-)^{J+1/2}\left(J+\frac{1}{2}\right)\right],$$

$$Q(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} Q_0,$$

$$B(E2; J_i \to J_f) = \frac{5}{16\pi}(J_i K 20 | J_f K)^2 (eQ_0)^2$$

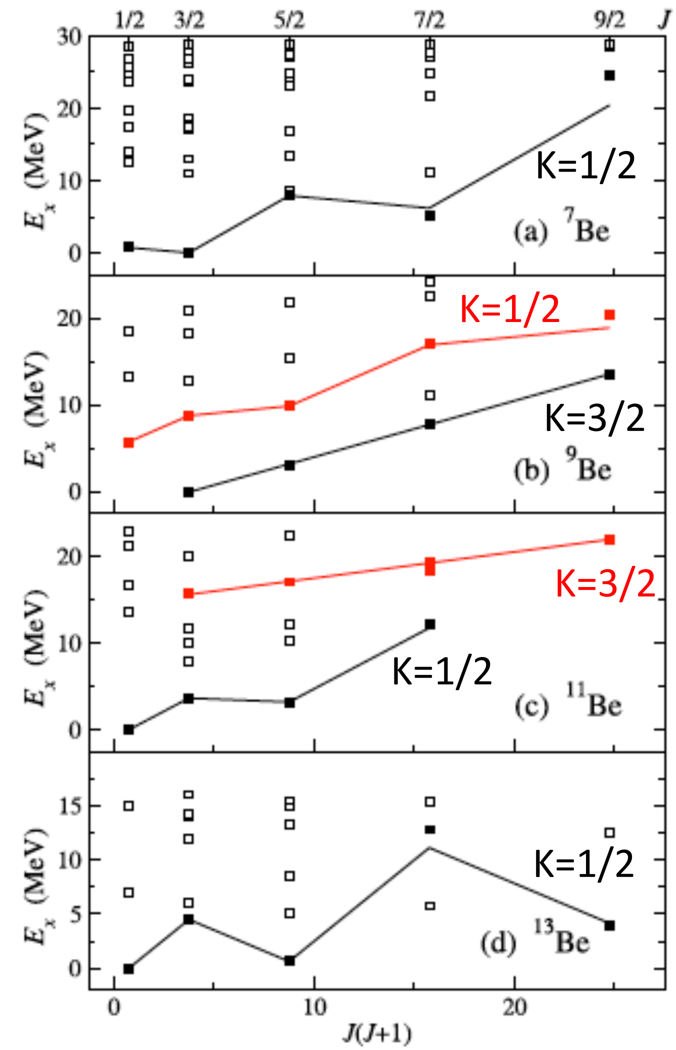


Fig. 1. Excitation energies obtained for states in the *natural* parity spaces of the odd-mass Be isotopes: (a) ^{7}Be, (b) ^{9}Be, (c) ^{11}Be, and (d) ^{13}Be. Energies are plotted with respect to $J(J+1)$ to facilitate identification of rotational energy patterns, while the J values themselves are indicated at top. Filled symbols indicate candidate rotational bandmembers (black for yrast states and red for excited states, in the web version of this Letter). The lines indicate the corresponding best fits for rotational energies. Where quadrupole transition strengths indicate significant two-state mixing (see text), more than one state of a given J is indicated as a bandmember.

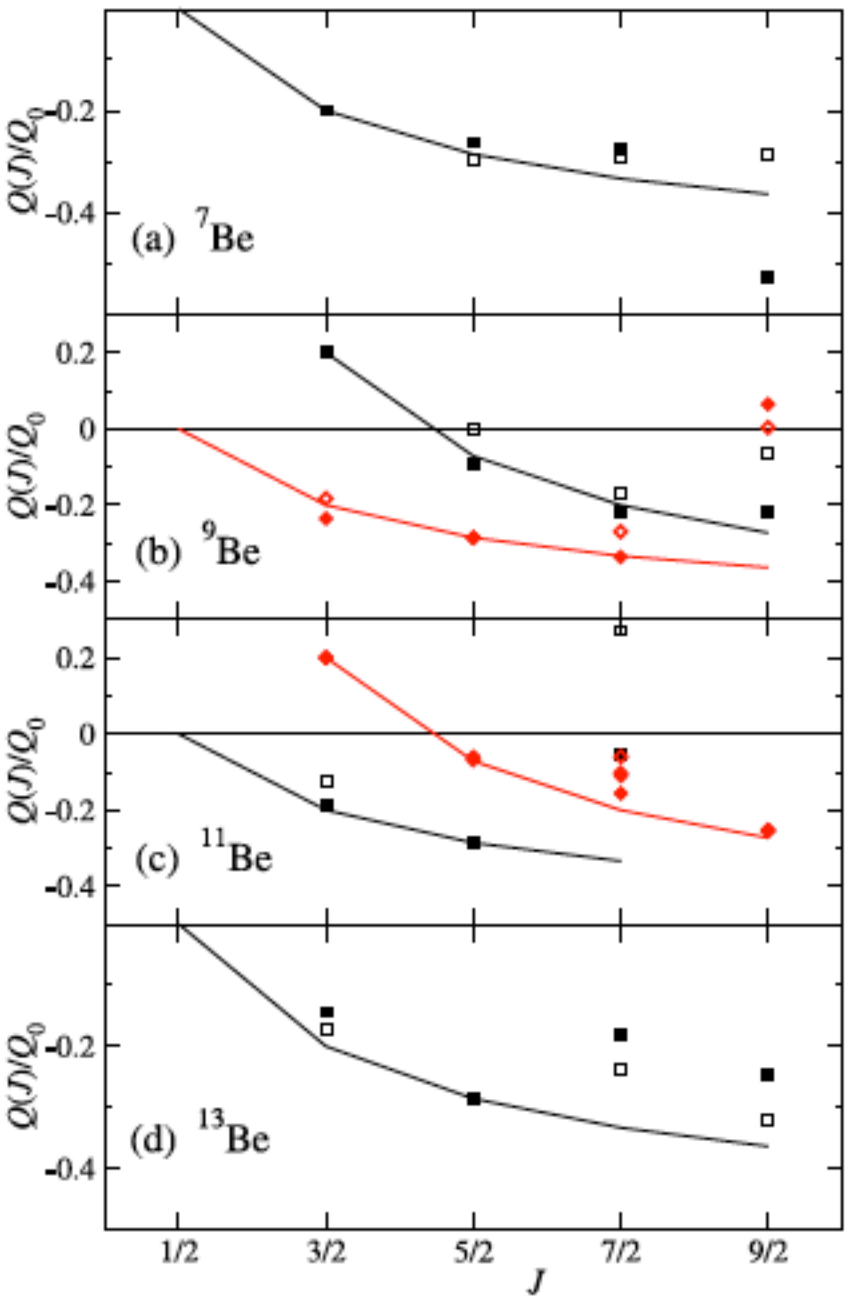
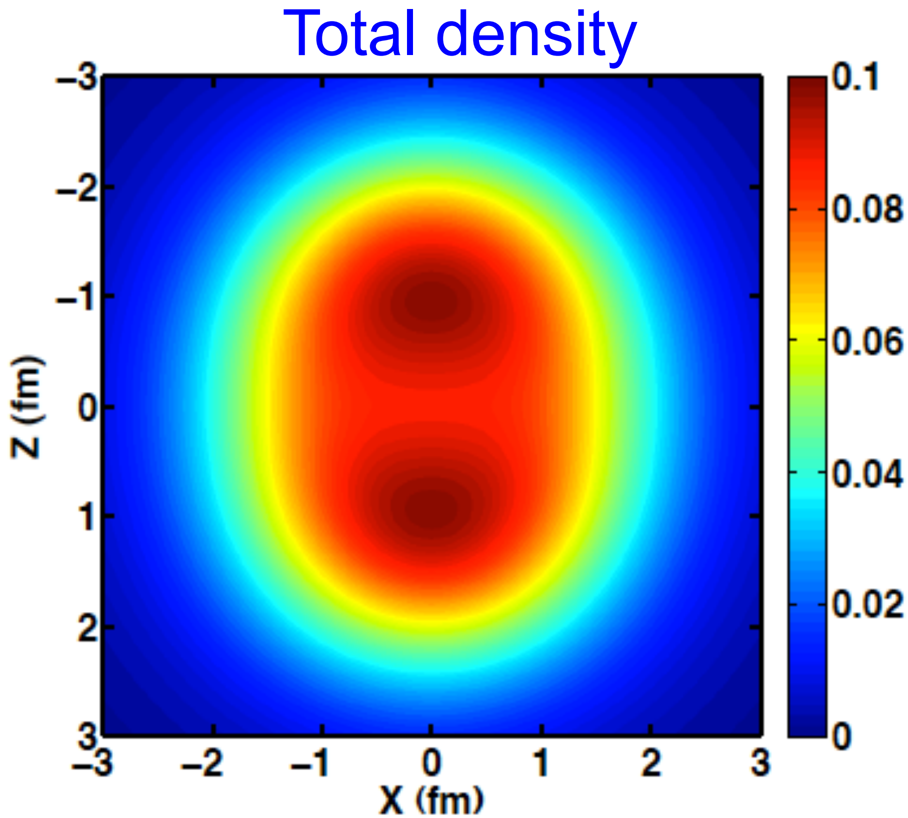


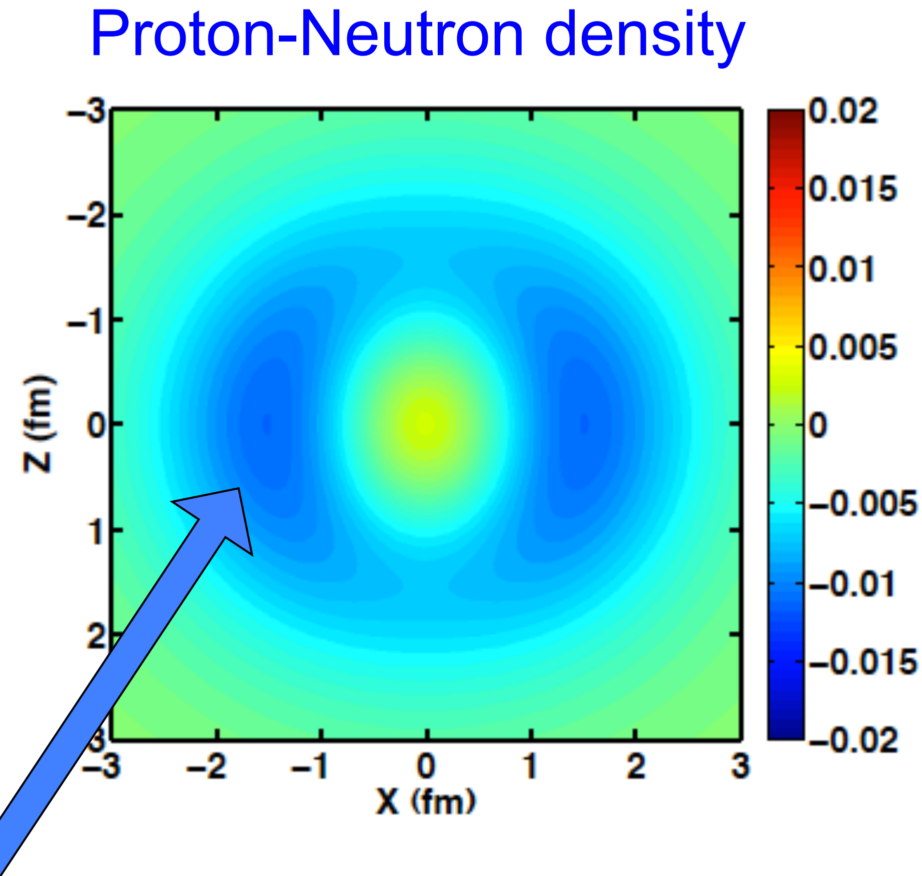
Fig. 3. Quadrupole moments calculated for candidate bandmembers in the *natural* parity spaces of the odd-mass Be isotopes: (a) ^{7}Be, (b) ^{9}Be, (c) ^{11}Be, and (d) ^{13}Be. The states are as identified in Fig. 1 and are shown as black squares for yrast states or red diamonds for excited states (color in the web version of this Letter). Filled symbols indicate proton quadrupole moments, and open symbols indicate neutron quadrupole moments. The curves indicate the theoretical values for a $K = 1/2$ or $K = 3/2$ rotational band, as appropriate, given by (4). Quadrupole moments are normalized to Q_0, which is defined by either the $J = 3/2$ or $J = 5/2$ bandmember (see text).

Note:
Although Q, B(E2) are slowly converging, the ratios within a rotational band appear remarkably stable

M.A. Caprio, P. Maris and J.P. Vary, Phys. Lett. B 719, 179 (2013)

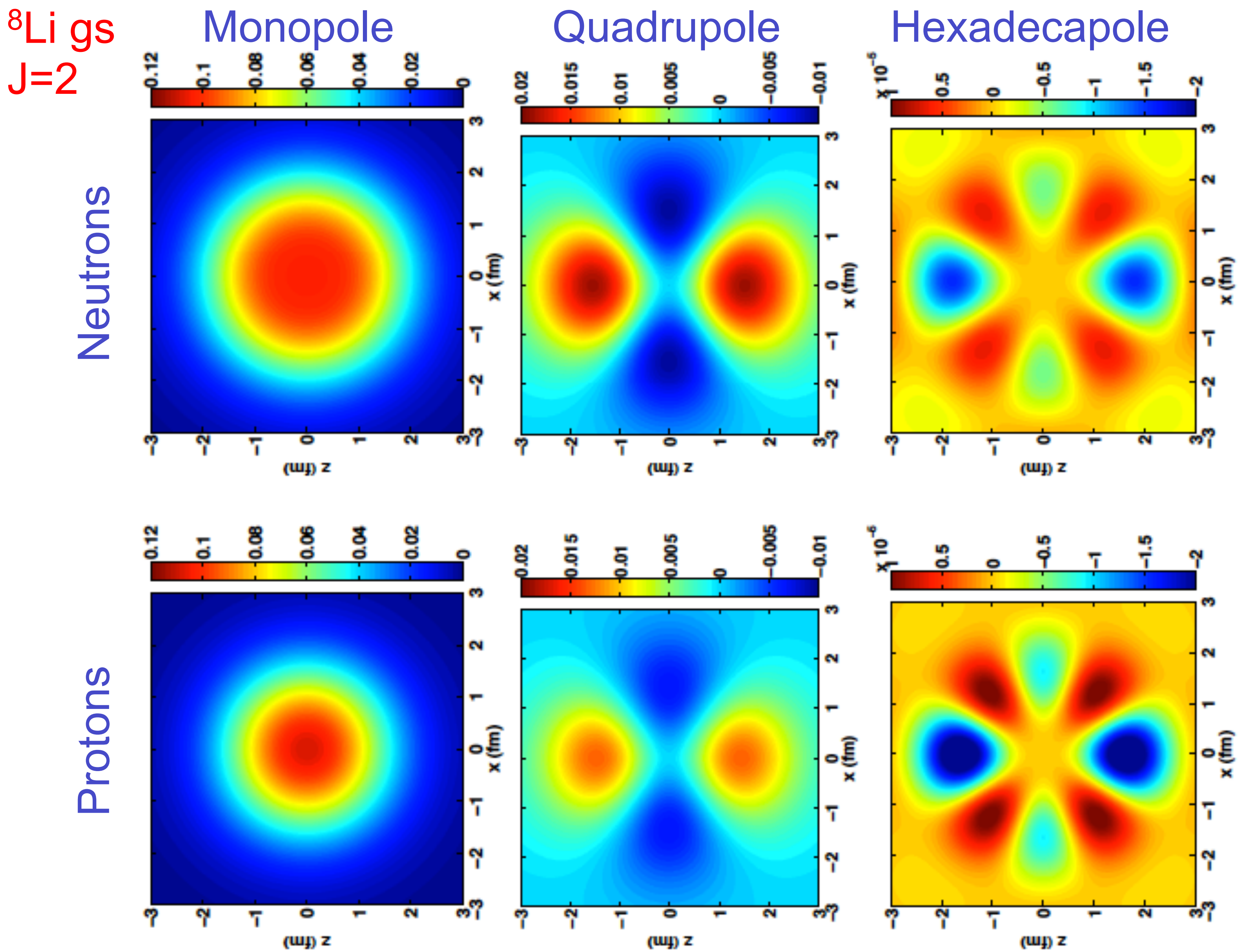
9Be Translationally invariant gs density
Full 3D densities = rotate around the vertical axis





Shows that one neutron provides a “ring” cloud around two alpha clusters binding them together

C. Cockrell, J.P. Vary, P. Maris, Phys. Rev. C 86, 034325 (2012); arXiv:1201.0724;
C. Cockrell, PhD, Iowa State University


^{8}Li gs
J=2
Monopole
Quadrupole
Hexadecapole
Neutrons
Protons
z (fm)
x (fm)
x 10^{-6}

Theory published PRC: Feb. 4, 2010

Physics Letters B 692 (2010) 307–311

Experiment published: Aug. 3, 2010

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

First observation of ^{14}F

V.Z. Goldberg [a,*], B.T. Roeder [a], G.V. Rogachev [b], G.G. Chubarian [a], E.D. Johnson [b], C. Fu [c], A.A. Alharbi [a,1], M.L. Avila [b], A. Banu [a], M. McCleskey [a], J.P. Mitchell [b], E. Simmons [a], G. Tabacaru [a], L. Trache [a], R.E. Tribble [a]

[a] Cyclotron Institute, Texas A&M University, College Station, TX 77843-3366, USA
[b] Department of Physics, Florida State University, Tallahassee, FL 32306-4350, USA
[c] Indiana University, Bloomington, IN 47408, USA

ab initio predictions in close agreement with experiment

TAMU Cyclotron Institute

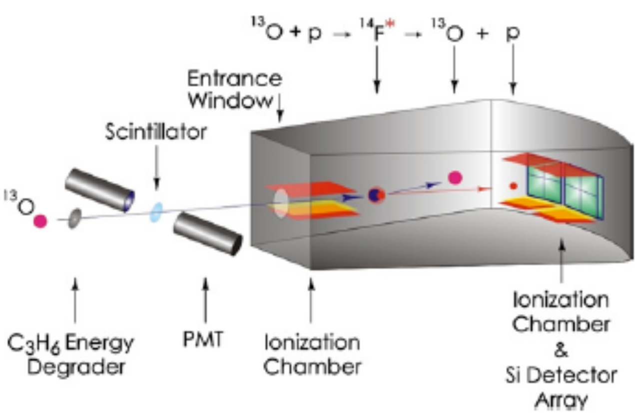


Fig. 1. (Color online.) The setup for the ^{14}F experiment. The "gray box" is the scattering chamber. See explanation in the text.

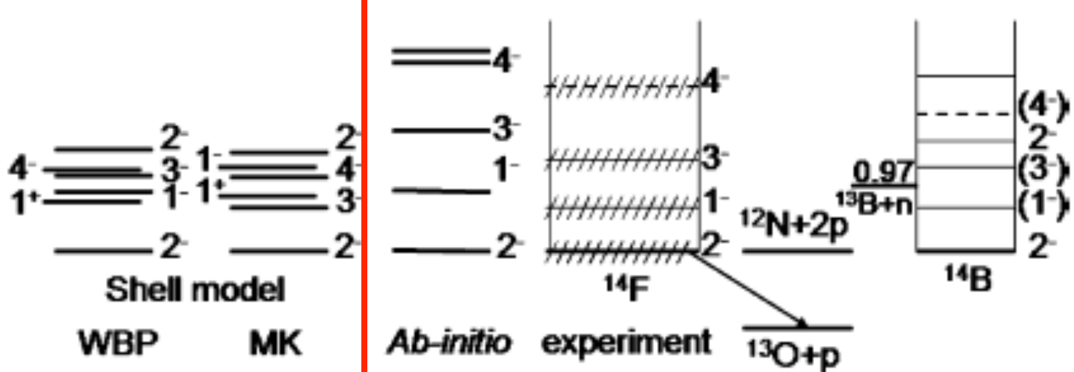


Fig. 6. ^{14}F level scheme from this work compared with shell-model calculations, *ab-initio* calculations [3] and the ^{14}B level scheme [16]. The shell model calculations were performed with the WBP [21] and MK [22] residual interactions using the code COSMO [23].

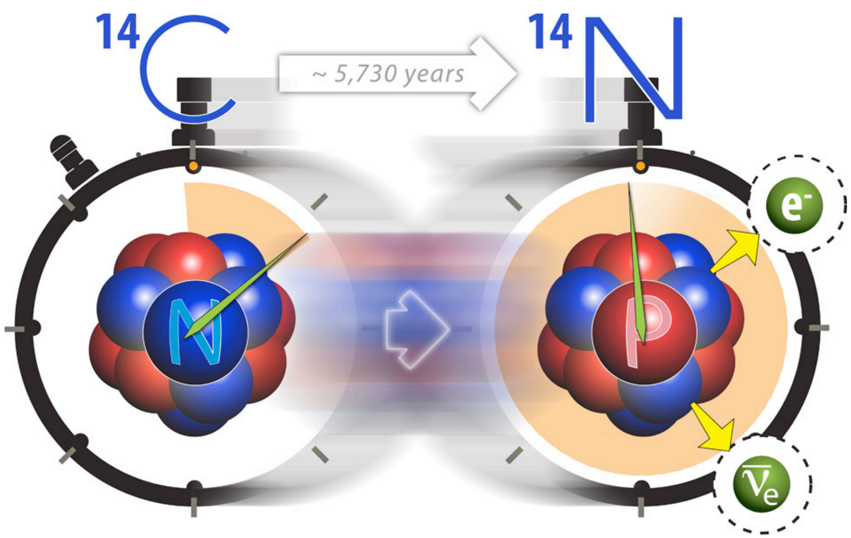
"Anomalous Long Lifetime of Carbon-14"

Objectives

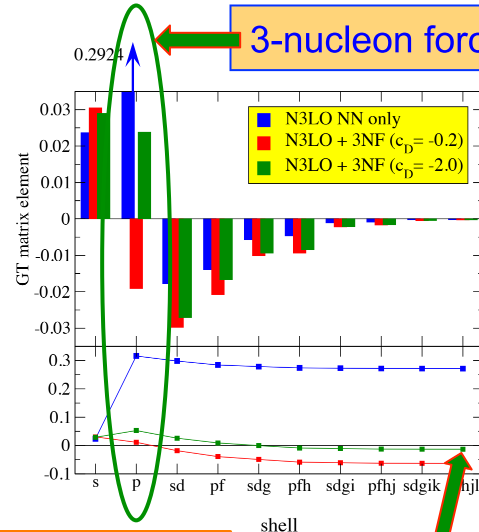
- Solve the puzzle of the long but useful lifetime of ^{14}C
- Determine the microscopic origin of the suppressed β-decay rate

Impact

- Establishes a major role for strong 3-nucleon forces in nuclei
- Verifies accuracy of *ab initio* microscopic nuclear theory
- Provides foundation for guiding DOE-supported experiments



3-nucleon forces suppress critical component



net decay rate
Is very small

- Dimension of matrix solved for 8 lowest states ~ 1x10^9
- Solution 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)

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]

U.S. DEPARTMENT OF ENERGY | Office of Science

INCITE Advancing America's Science and Industrial Competitiveness

IOWA STATE UNIVERSITY

TRIUMF

UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

NNSA

OAK RIDGE NATIONAL LABORATORY
Managed by UT-Battelle for the Department of Energy

Ab initio nuclear reactions

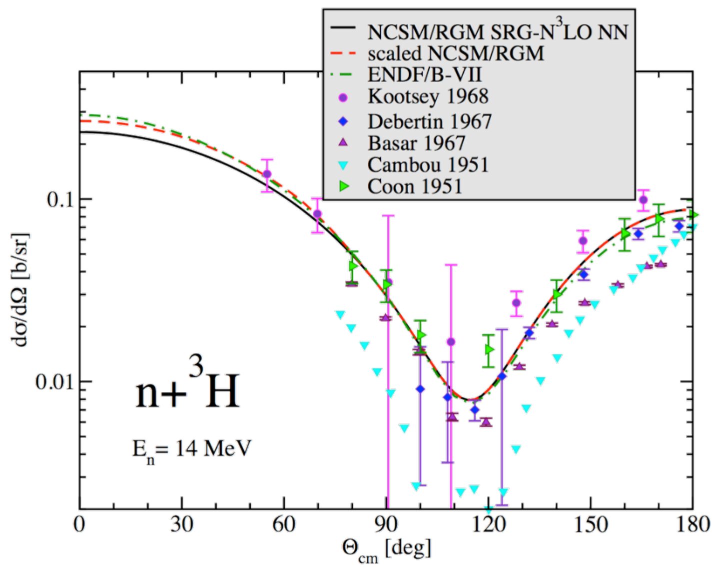
Objectives

- Arrive at a fundamental understanding of nuclear properties from a unified theoretical standpoint rooted in the fundamental forces among nucleons
- Develop theoretical foundations for an accurate description of reactions between light ions in a thermonuclear environment

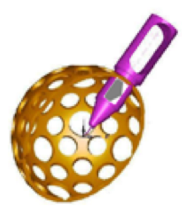
Impact

- Computational tools for addressing fusion reactions that power stars and Earth-based fusion facilities such as the National Ignition Facility (NIF)
- Provide research community with accurate evaluations and uncertainties for nuclear astrophysics and fusion diagnostic

Ab initio theory reduces uncertainty due to conflicting data



- The *n*-^{3}H elastic cross section for 14 MeV neutrons, important for understanding how the fuel is assembled in an implosion at NIF, was not known precisely enough. Nuclear theory was asked to help.
- Delivered evaluated data with required 5% uncertainty and successfully compared to measurements using an Inertial Confinement Facility
- *"Ab initio theory* of light-ion reactions", by P. Navrátil, S. Quaglioni, and R. Roth, J. Phys. Conf. Ser. **312**, 082002 (2011)
- ``First measurements of the differential cross sections for the elastic n-^{2}H and n-^{3}H scattering at 14.1 MeV using an Inertial Confinement Facility", by J.A. Frenje *et al.,* Phys. Rev. Lett. **107,** 122502 (2011)



http://physics.aps.org/synopsis-for/10.1103/PhysRevLett.107.122502

UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

Extrapolating to the infinite matrix limit
i.e. to the “continuum limit”

Results with both IR and UV extrapolations

References:
S.A. Coon, M.I. Avetian, M.K.G. Kruse, U. van Kolck, P. Maris, and J.P. Vary, Phys. Rev. C 86, 054002 (2012); arXiv: 1205.3230
R.J. Furnstahl, G. Hagen, T. Papenbrock, Phys. Rev. C 86 (2012) 031301
E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary, submitted to PRC; arXiv: 1302:5473

Convergence and Uncertainty Assessments: Recent Highlight

Convergence properties of *ab initio* calculations of light nuclei in a harmonic oscillator basis

Phys. Rev. C 86, 054002 (2012); arXiv:1205.3230

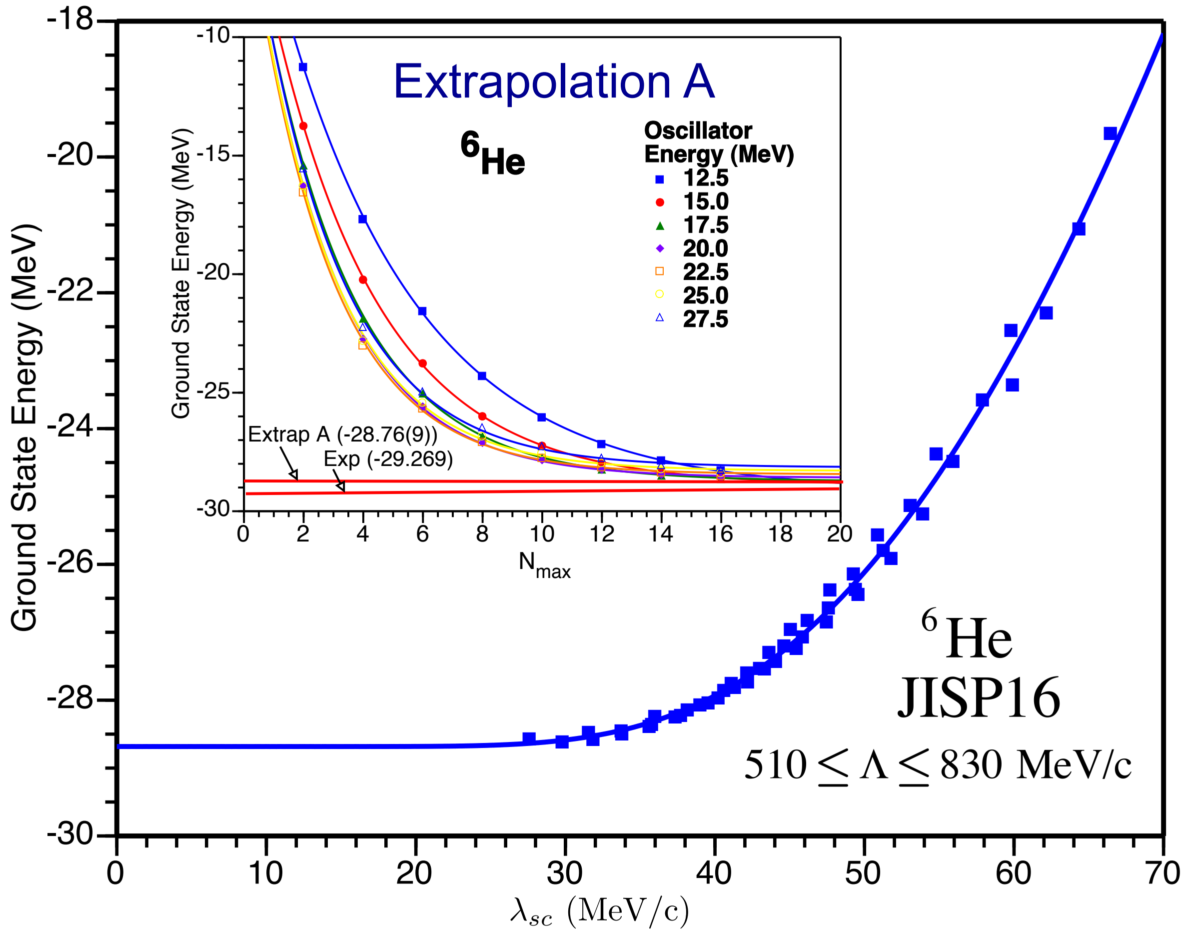
S. A. Coon[a], M. I. Avetian[a], M. K. G. Kruse[a], U. van Kolck[a,b], P. Maris[c], J. P. Vary[c]

UV regulator:

$$\Lambda = \sqrt{(N + 3/2) m\hbar\Omega}$$

IR regulator:

$$\lambda_{sc} = \sqrt{\frac{m\hbar\Omega}{(N + 3/2)}}$$



Combined IR and UV extrapolation: HO-basis regulator definitions

	Ref. 1	Ref. 2	Ref. 3
UV: Λ	$\sqrt{(N+3/2)m\hbar\Omega}$	$\sqrt{2(N+3/2)m\hbar\Omega}$	$\sqrt{2(N+3/2)m\hbar\Omega}$
IR: λ	$\sqrt{\frac{m\hbar\Omega}{(N+3/2)}}$	$\sqrt{\frac{m\hbar\Omega}{2(N+3/2)}}$	$\sqrt{\frac{m\hbar\Omega}{2(N+3/2)}}$
N (p-shell)	$N_{max} + 1$	$N_{max} + 2$	$N_{max} + 3$

$$E(\Lambda,\lambda) \approx E_\infty + B_0 e^{-2\Lambda^2/B_1^2} + B_2 e^{-2k_\infty/\lambda}$$

[1]S.A. Coon, M.I. Avetian, M.K.G. Kruse, U. van Kolck, P. Maris, and J.P. Vary, Phys. Rev. C 86, 054002 (2012); arXiv: 1205.3230

[2]R.J. Furnstahl, G. Hagen, T. Papenbrock, Phys. Rev. C 86 (2012) 031301

[3]E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary, submitted to PRC; arXiv: 1302:5473

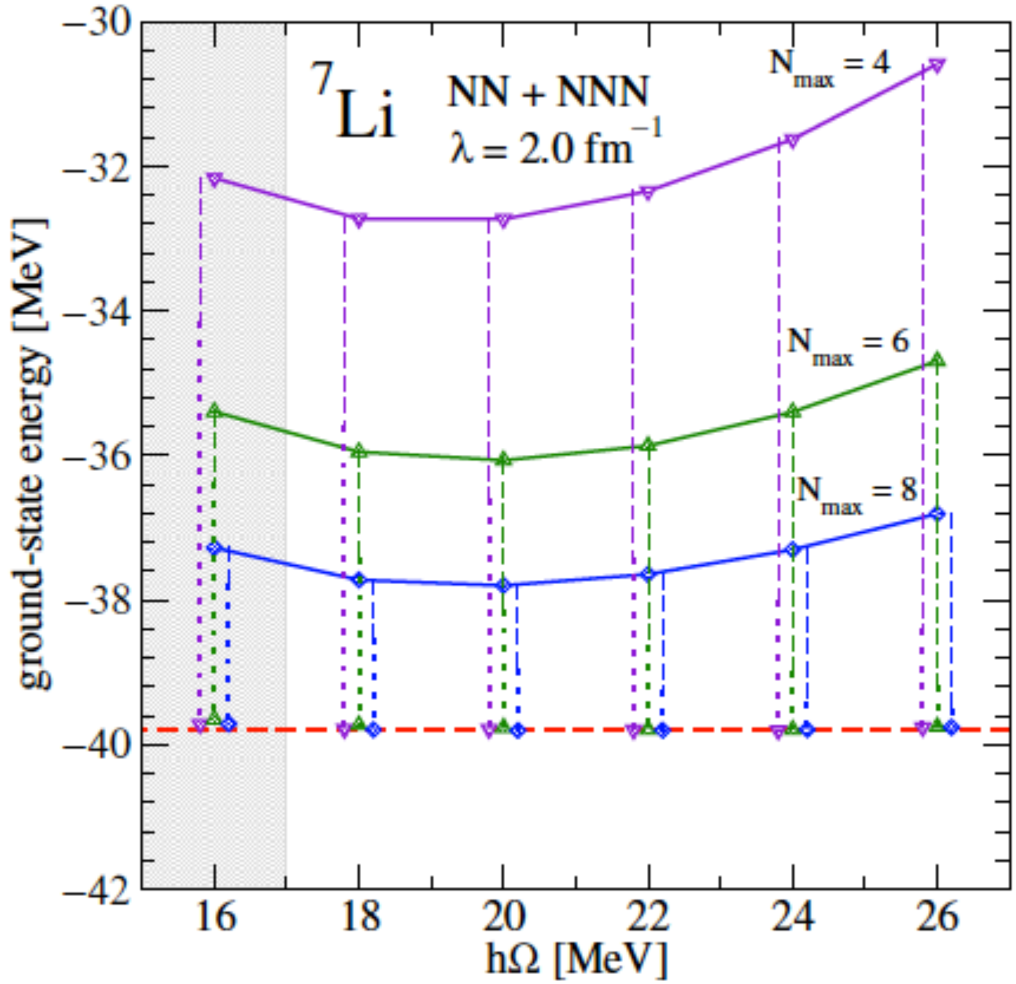
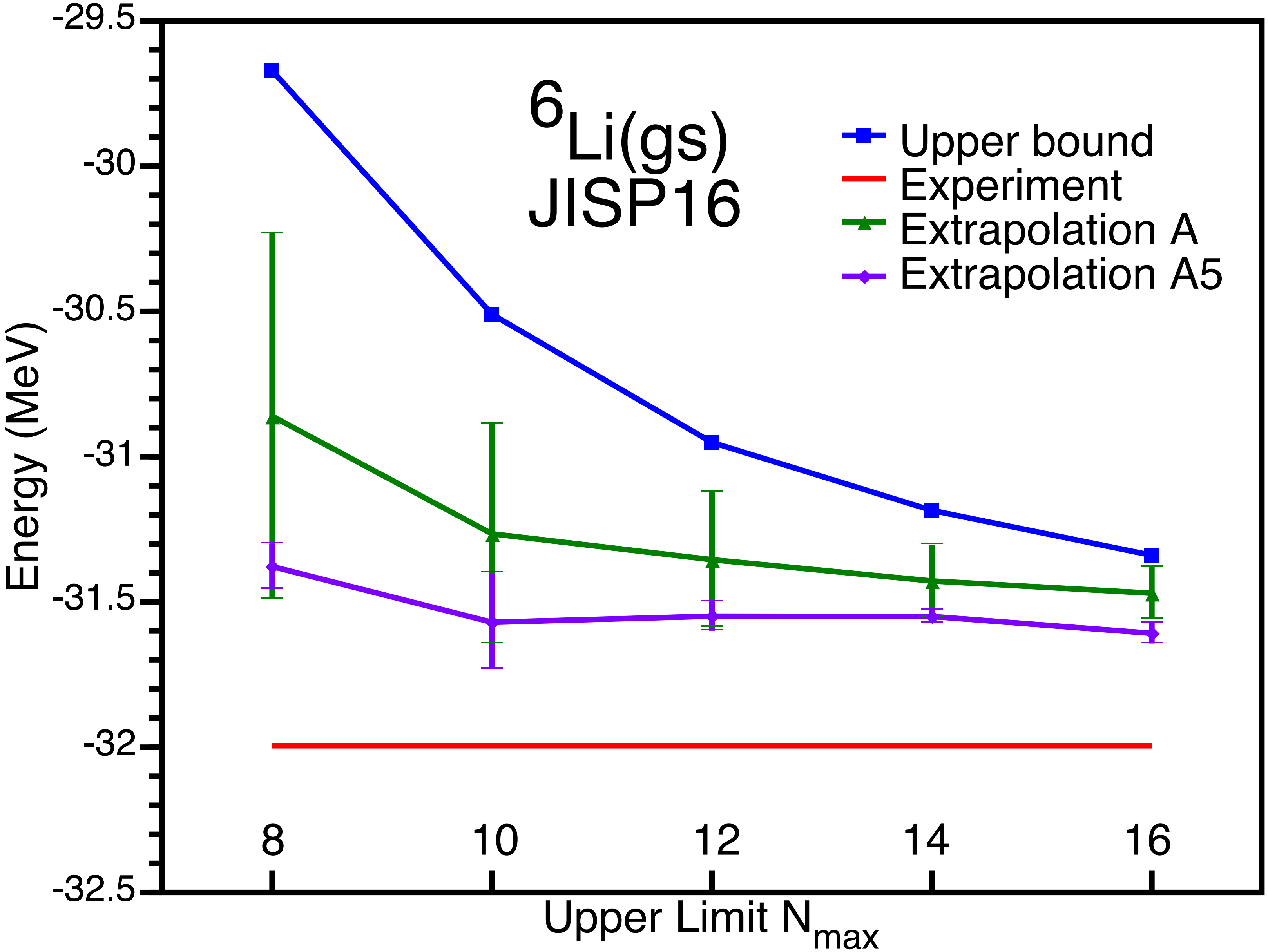
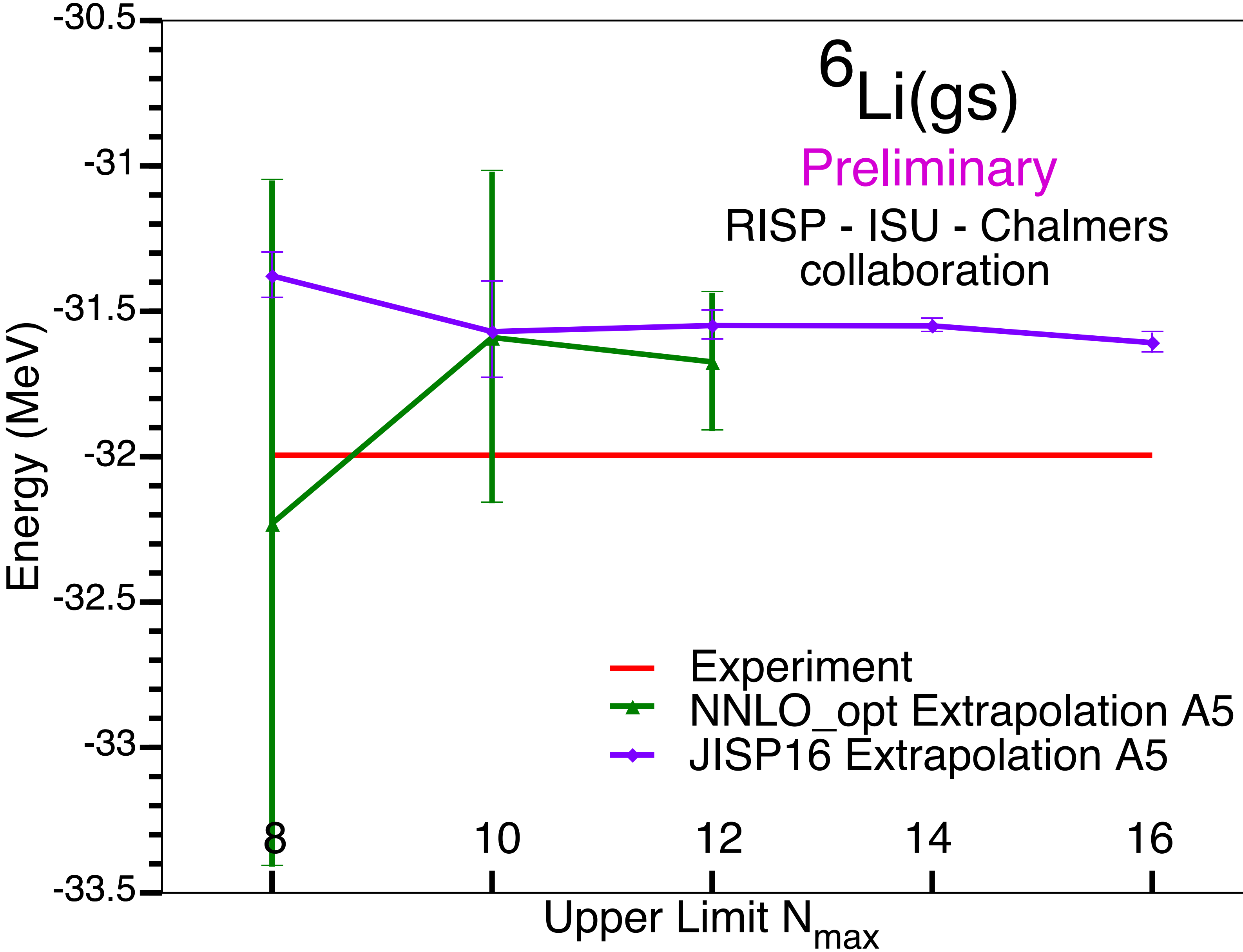


FIG. 17. (color online) Ground-state energy of ^{7}Li for the NN+NNN evolved Hamiltonians at $\lambda = 2.0\,\text{fm}^{-1}$, with IR (vertical dashed) and UV (vertical dotted) corrections from Eq. (5) that add to predicted E_∞ values (points near the horizontal dashed line, which is the global E_∞).

E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary, Phys. Rev. C. 87, 054312 (2013); arXiv: 1302:5473



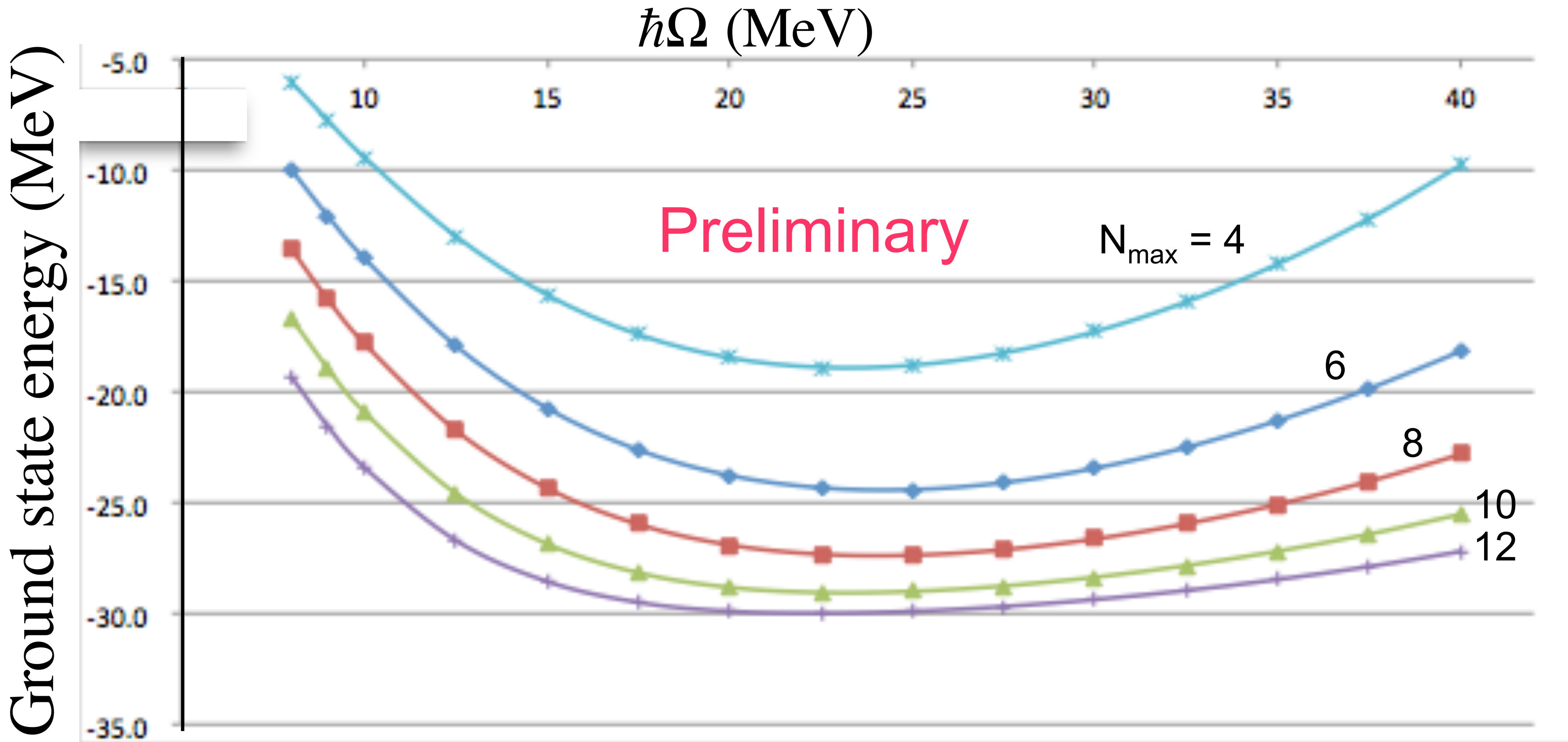
6Li(gs)
JISP16
Upper bound
Experiment
Extrapolation A
Extrapolation A5
Energy (MeV)
-29.5
-30
-30.5
-31
-31.5
-32
-32.5
8
10
12
14
16
Upper Limit Nmax



^{6}Li(gs)
Preliminary
RISP - ISU - Chalmers collaboration
Energy (MeV)
-30.5
-31
-31.5
-32
-32.5
-33
-33.5
8
10
12
14
16
Upper Limit N_{max}
Experiment
NNLO_opt Extrapolation A5
JISP16 Extrapolation A5

^{6}Li with NNLO_opt

RISP – ISU – Chalmers Collaboration



Basis Light Front Quantization (BLFQ)
Framework with discovery potential

Physics drivers:
Spin content of the proton
Exotic meson states around 4 Gev (X, Y, Z, . . .)
In-medium propagation & energy loss of jets, charmonia, . . .
Strong, time-dependent external field physics applications

Initial applications and test cases

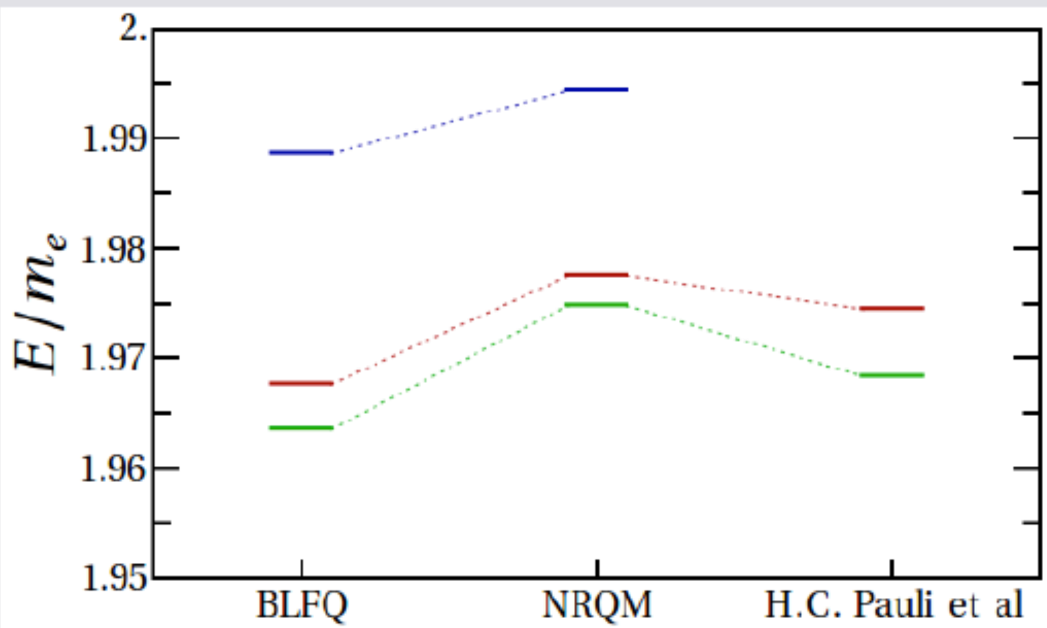
$\alpha = 0.3$

Hyperfine Splitting

$$M_t = 2 - \frac{\alpha^2}{4}\left(1 - \frac{1}{48}\alpha^2\right)$$

$$M_s = 2 - \frac{\alpha^2}{4}\left(1 + \frac{63}{48}\alpha^2\right)$$

$$\varepsilon \equiv 2\frac{\mu^2}{b^2}$$

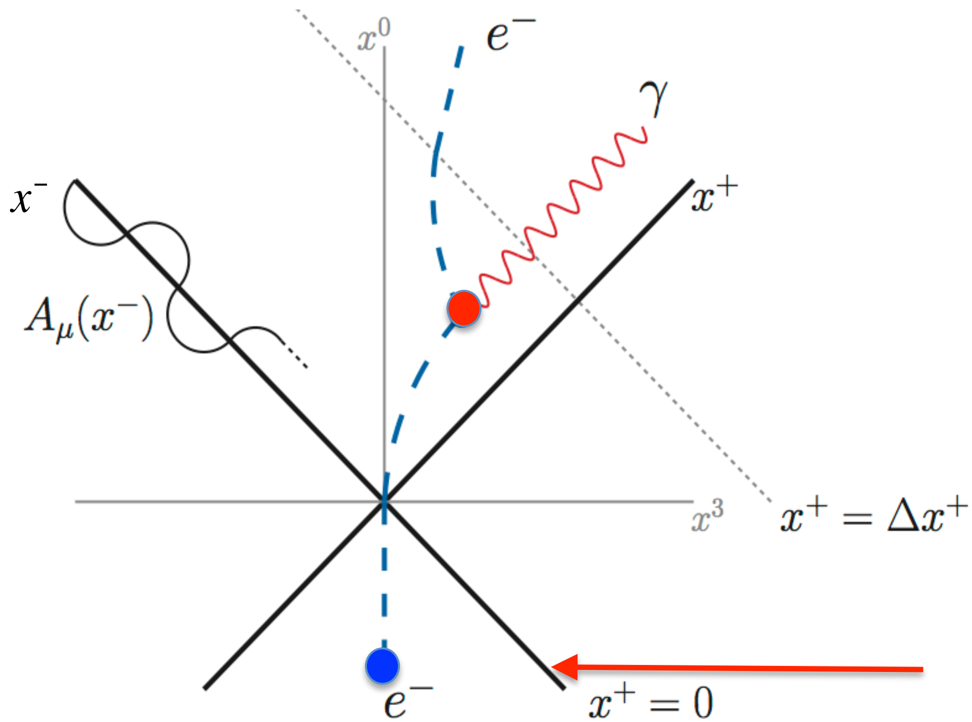


PRD 45 2968

Paul Wiecki

tBLFQ: Nonlinear Compton Scattering

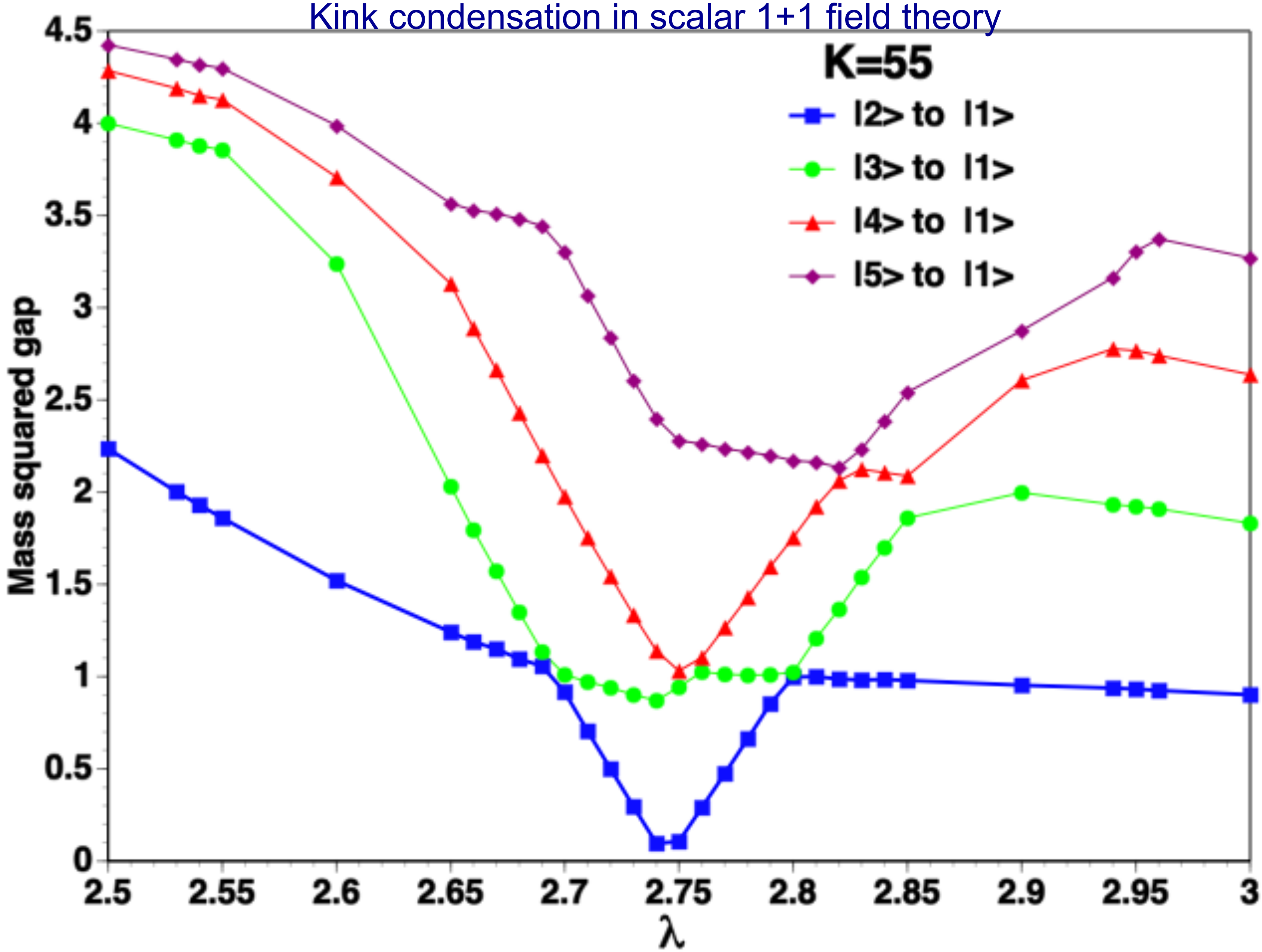
- Space-time structure



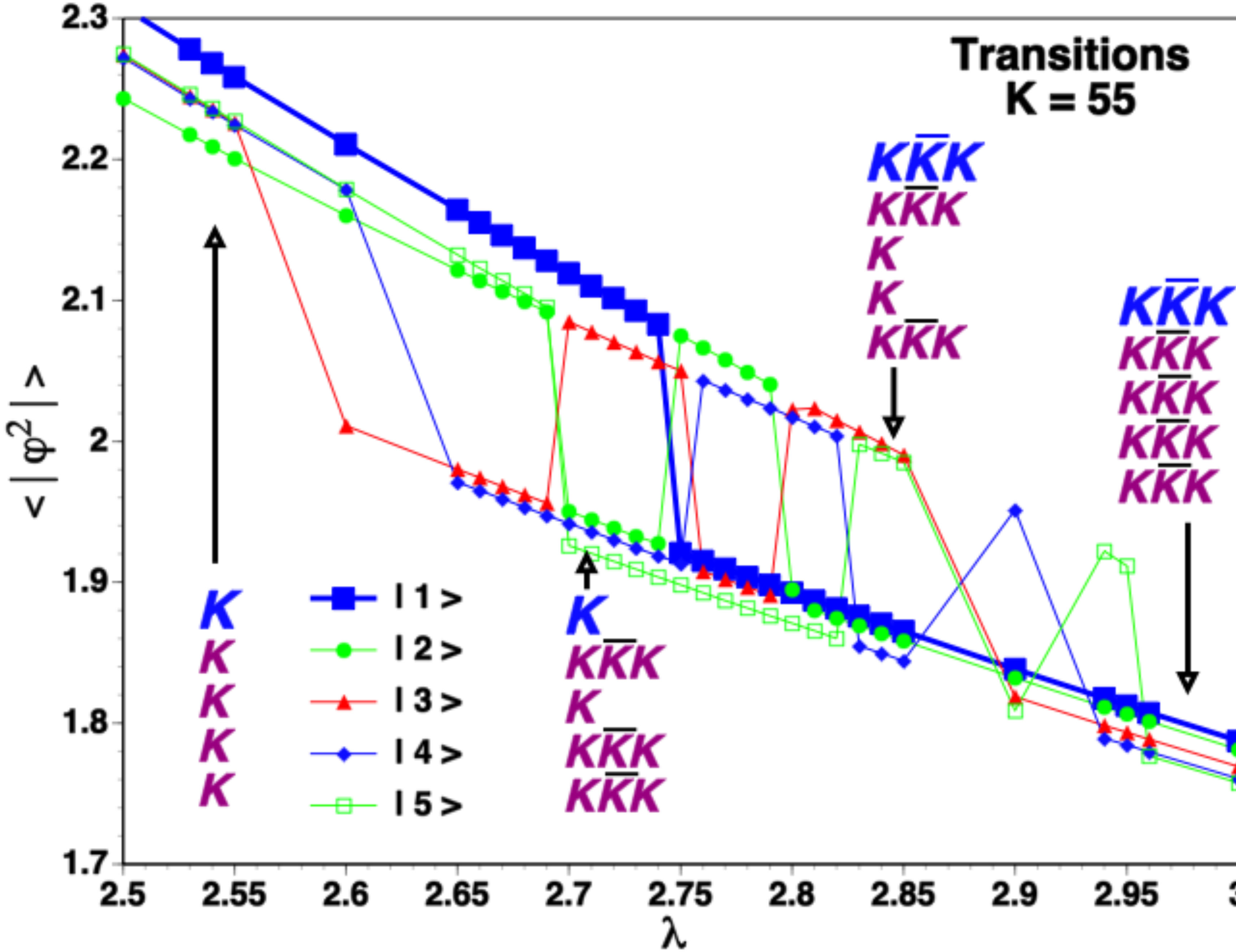
- Two effects: acceleration and radiation

Xingbo Zhao

Spontaneous symmetry breaking in LF quantized Hamiltonian approach
Kink condensation in scalar 1+1 field theory

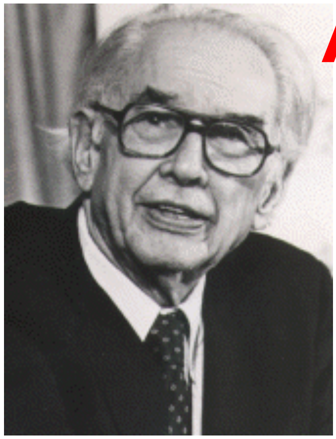


D. Chakrabarti, A. Harindranath and J.P. Vary, *Phys. Rev. D* **71**, 125012(2005); hep-th/05104094.

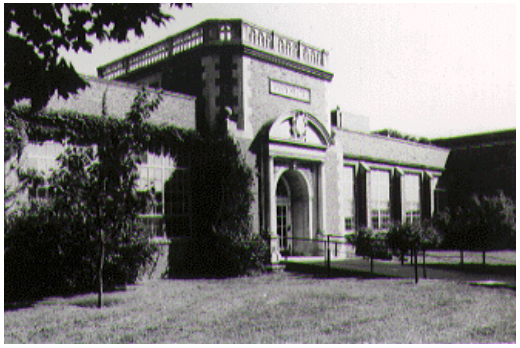


D. Chakrabarti, A. Harindranath and J.P. Vary, *Phys. Rev. D* **71**, 125012(2005); hep-th/05104094.

Atanasoff-Berry Computer (ABC)



John Vincent Atanasoff
1983 photo

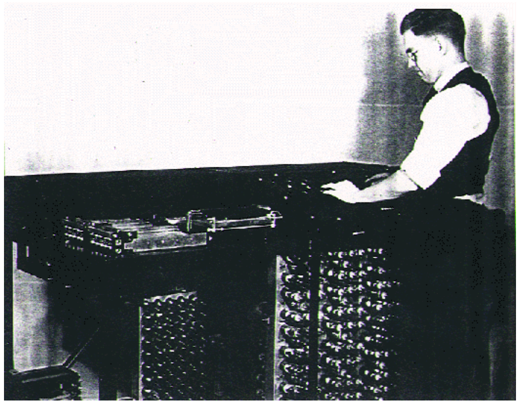


Clifford Berry
1962 photo

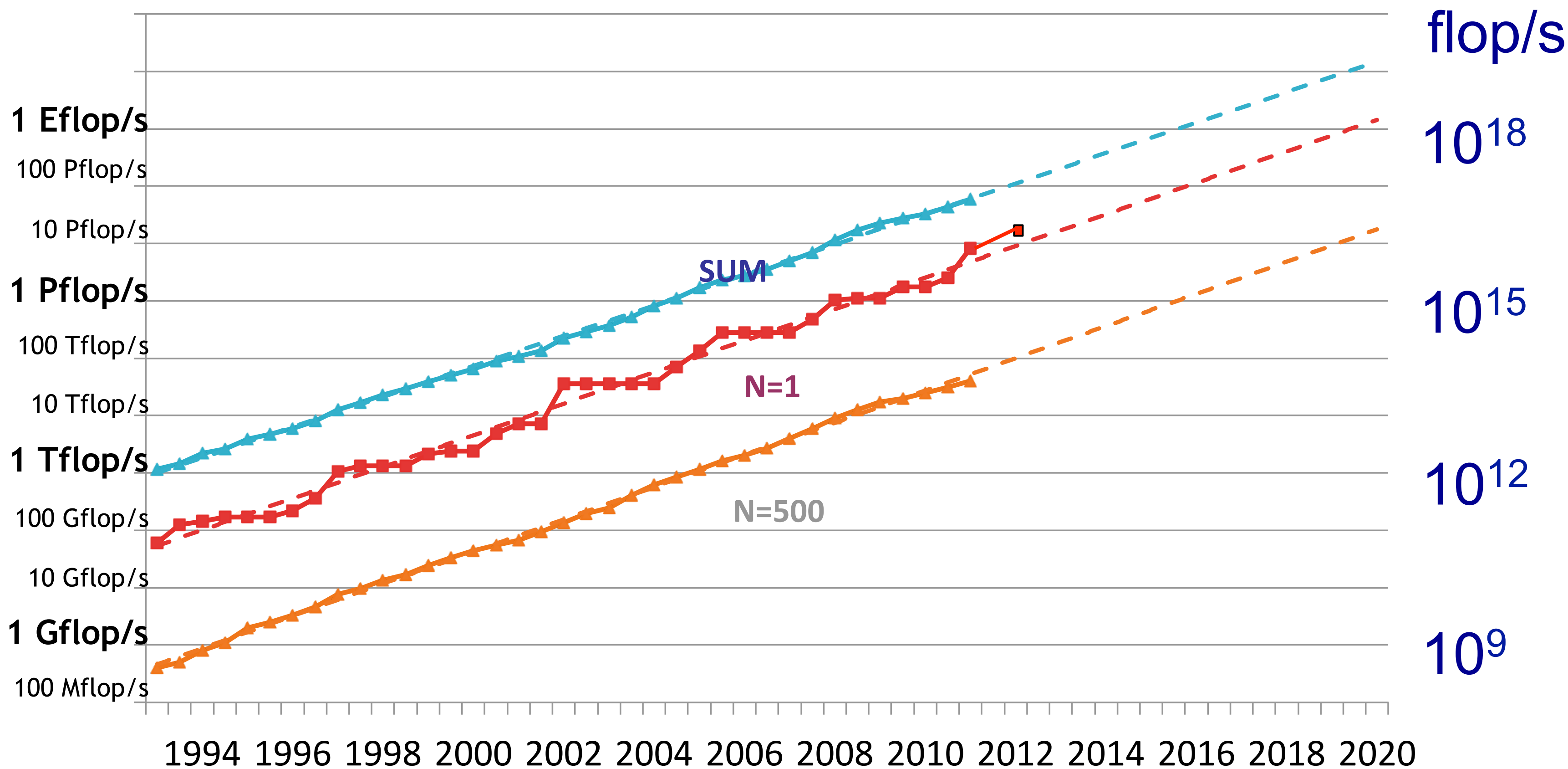
- 1939 - Iowa State Physics Professor Atanasoff invents the electronic digital computer based on binary mathematics with stored program and data along with punch card input. Atanasoff and graduate student Clifford Berry construct the ABC and use ABC to solve simultaneous linear equations
- 1997 - Replica completed and demonstrated in public

1990 - Atanasoff awarded the National Medal of Technology by President George W. Bush

1942 photo of Clifford Berry and the ABC



Projected Performance Development



1 floating point operation (flop)

$$
\begin{array}{r}
8.4917523 \times 10^{8} \\
\times\ 5.0261744 \times 10^{7} \\
\hline
4.2681028 \times 10^{16}
\end{array}
$$

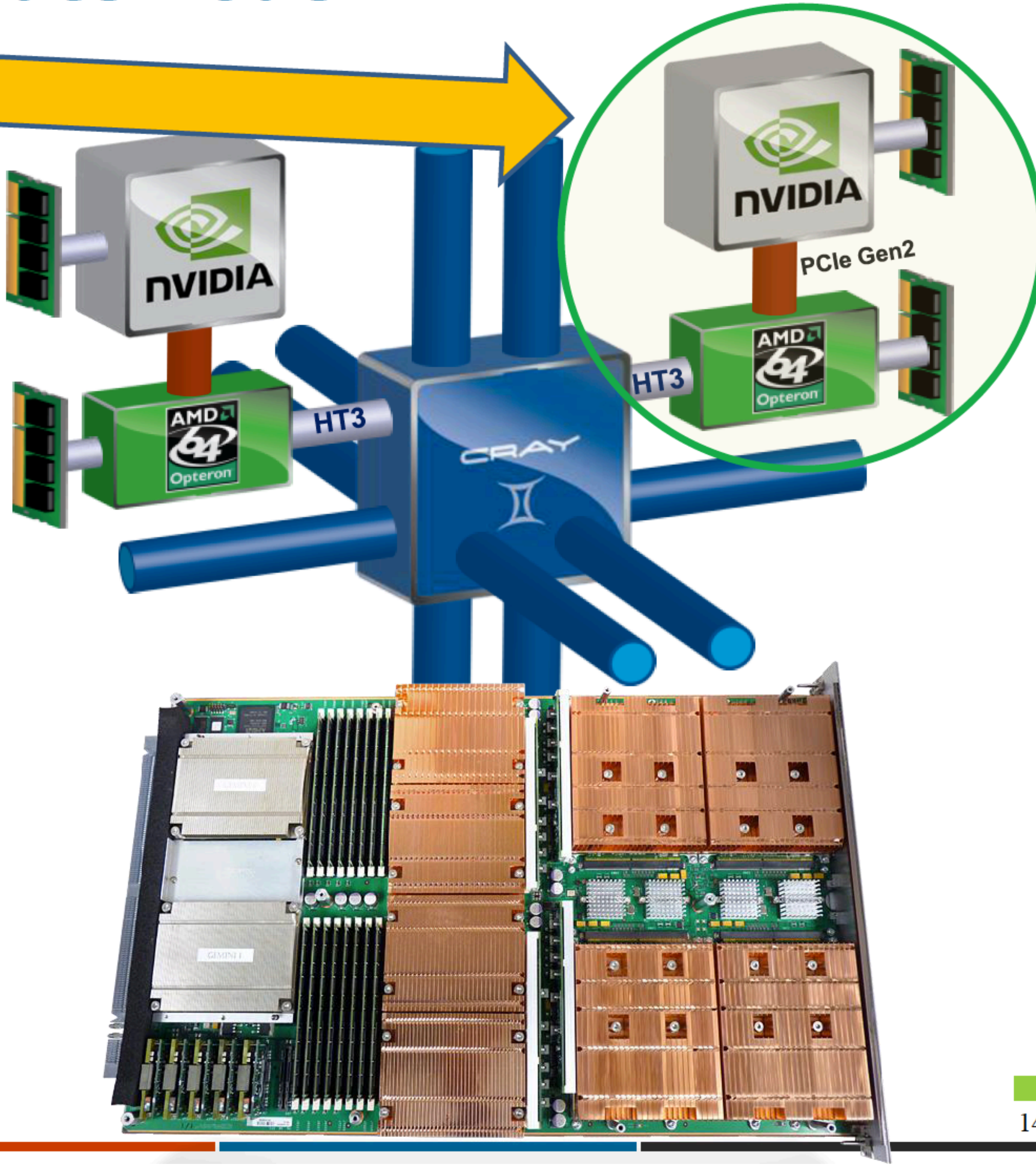
Newest “Top 500” list
November 12, 2012

TOP10 November 2012

1	Titan - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x
2	Sequoia - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom
3	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect
4	Mira - BlueGene/Q, Power BQC 16C 1.60GHz, Custom
5	JUQUEEN - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect
6	SuperMUC - iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR
7	Stampede - PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi
8	Tianhe-1A - NUDT YH MPP, Xeon X5670 6C 2.93 GHz, NVIDIA 2050
9	Fermi - BlueGene/Q, Power BQC 16C 1.60GHz, Custom
10	DARPA Trial Subset - Power 775, POWER7 8C 3.836GHz, Custom Interconnect

Cray XK6 compute node

XK6 Compute Node Characteristics
AMD Opteron 6200 "Interlagos" 16 core processor @ 2.2GHz
Tesla M2090 "Fermi" @ 665 GF with 6GB GDDR5 memory
Host Memory 32GB 1600 MHz DDR3
Gemini High Speed Interconnect
Upgradeable to NVIDIA's next generation "Kepler" processor in 2012
Four compute nodes per XK6 blade. 24 blades per rack



INCITE
U.S. DEPARTMENT OF ENERGY
LEADERSHIP COMPUTING

INCITE resources: Mira at ALCF

- *Mira* - Blue Gene/Q System
  - 48K nodes / 768K cores
  - 786 TB of memory
  - Peak flop rate: 10 PF
- Storage
  - ~35 PB capacity, 240GB/s bandwidth (GPFS)
  - Disk storage upgrade planned in 2015
    - Double capacity and bandwidth
- New Visualization Systems
  - Initial system in 2012
  - Advanced visualization system in 2014
    - State-of-the-art server cluster with latest GPU accelerators
    - Provisioned with the best available parallel analysis and visualization software

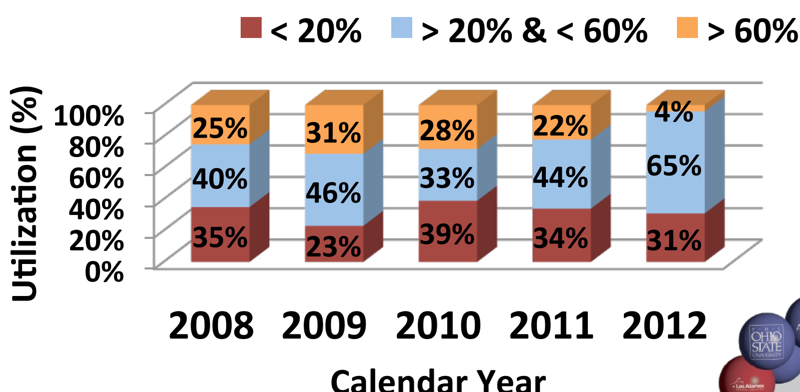
NUCLEI/UNEDF Leadership-class computing

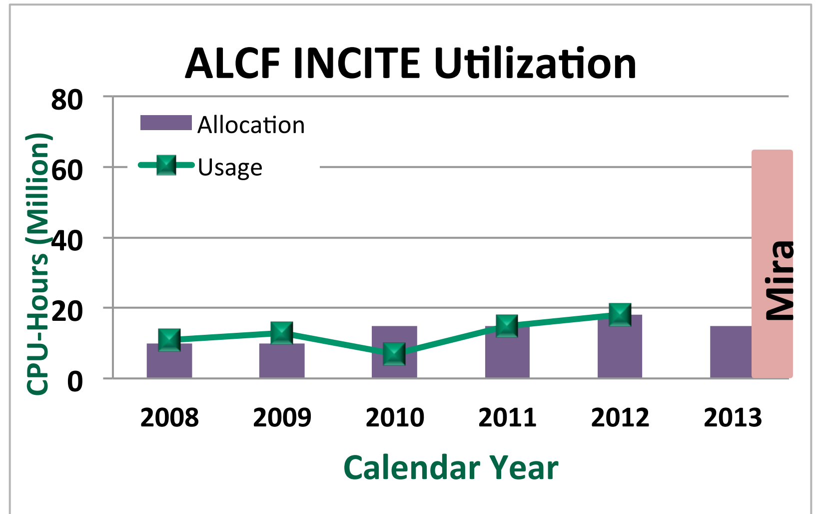
◆ SciDAC collaborations between applied mathematicians, computer scientists, and nuclear physicists lead to efficient utilization of leadership-class computing resources for nuclear physics problems

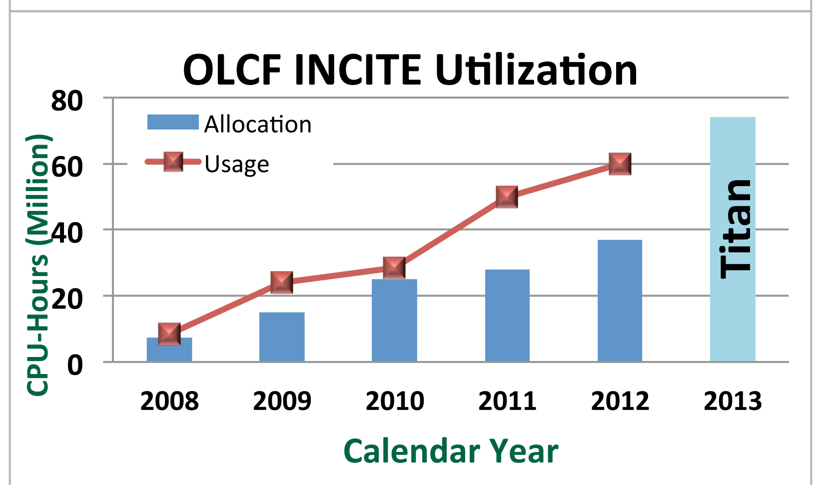
◆ Significant accomplishments in NUCLEI/UNEDF, achieved through leadership-class computing

- ➢Ab-initio calculations of C-12
- ➢Understanding of long lifetime of C-14
- ➢Microscopic calculations of select medium-mass nuclei
- ➢Improved energy-density functionals

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







U.S. DEPARTMENT OF ENERGY

UNEDF

NUCLEI

Nuclear Computational Low-Energy Initiative

- Hardware advances: Moore's Law
- Theory/Algorithms/Software advances: Doubles Moore's Law

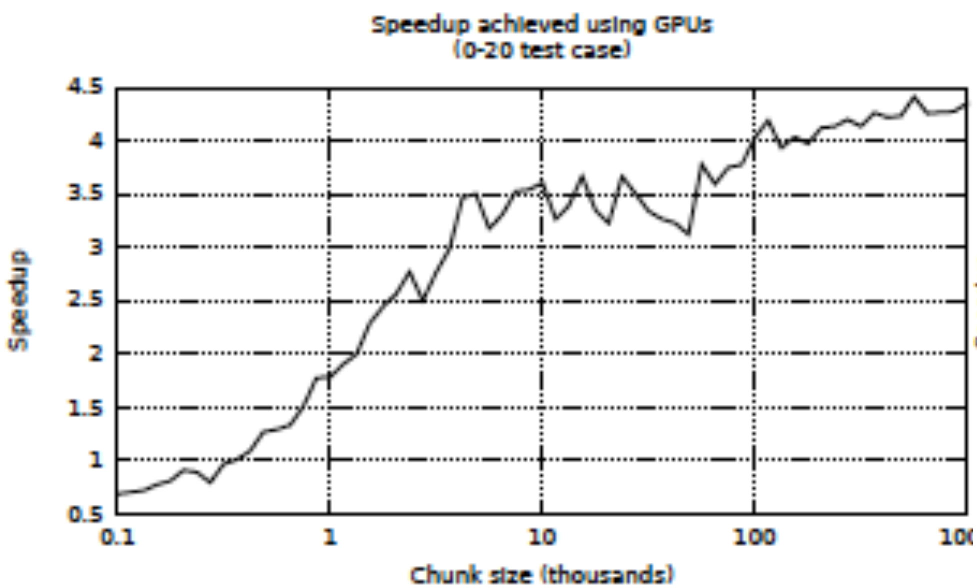
Discovery potential increases geometrically

Leveraging GPUs in Ab Initio Nuclear Physics Calculations

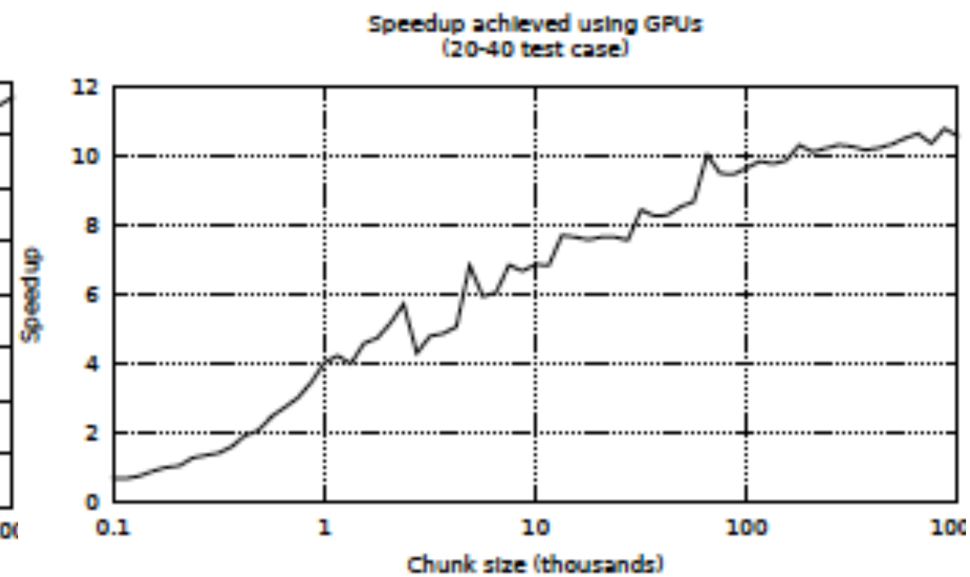
Dossay Oryspayev[*], Hugh Potter[†], Pieter Maris[†], Masha Sosonkina[*‡], James P. Vary[†], Sven Binder[§],
Angelo Calci[§], Joachim Langhammer[§], and Robert Roth[§]

accepted by IEEE conference PDSEC-13, March 2013

Decouple NNN interaction matrix elements from JT-scheme to m-scheme



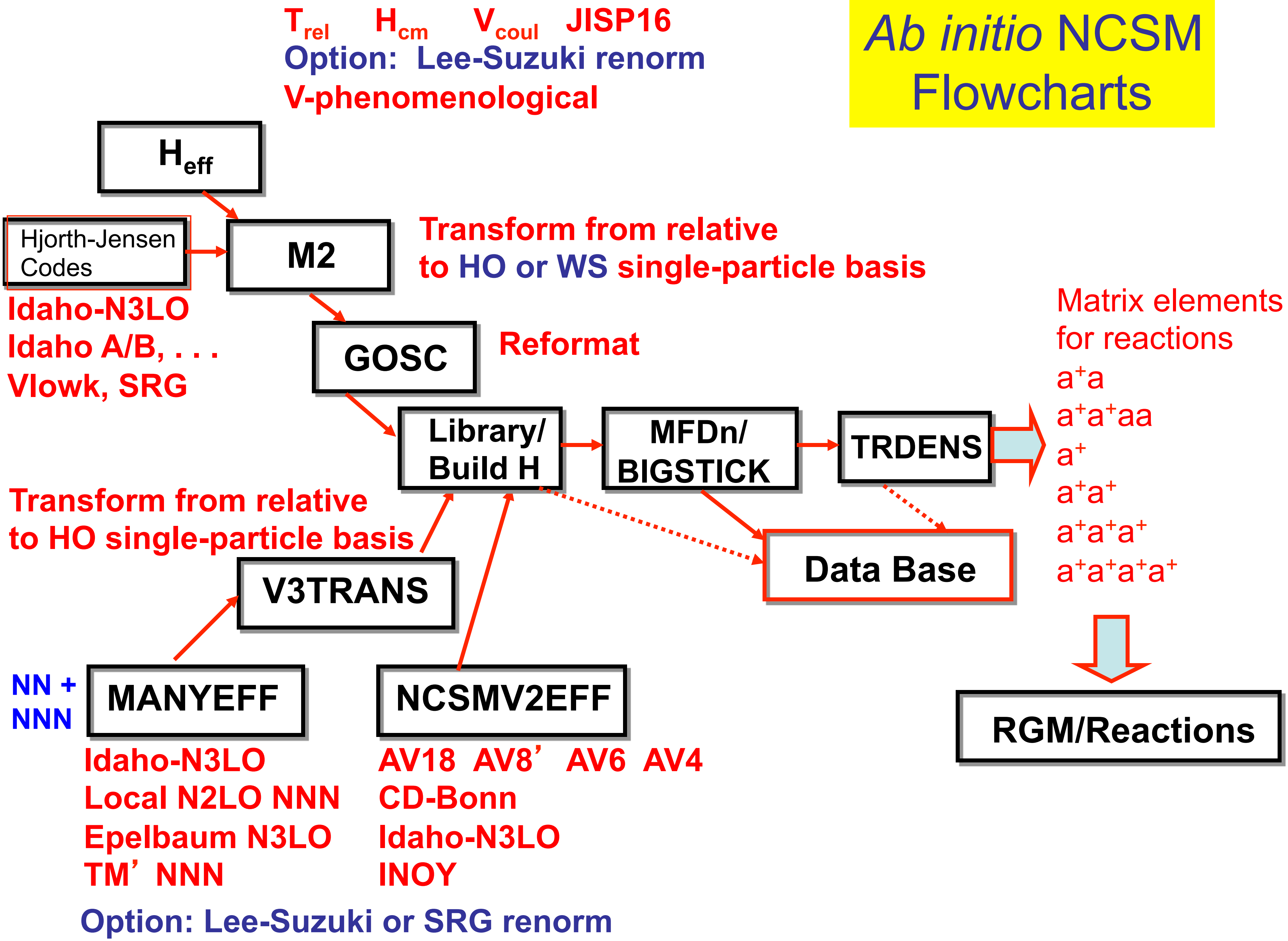
(a) 0-20 test case



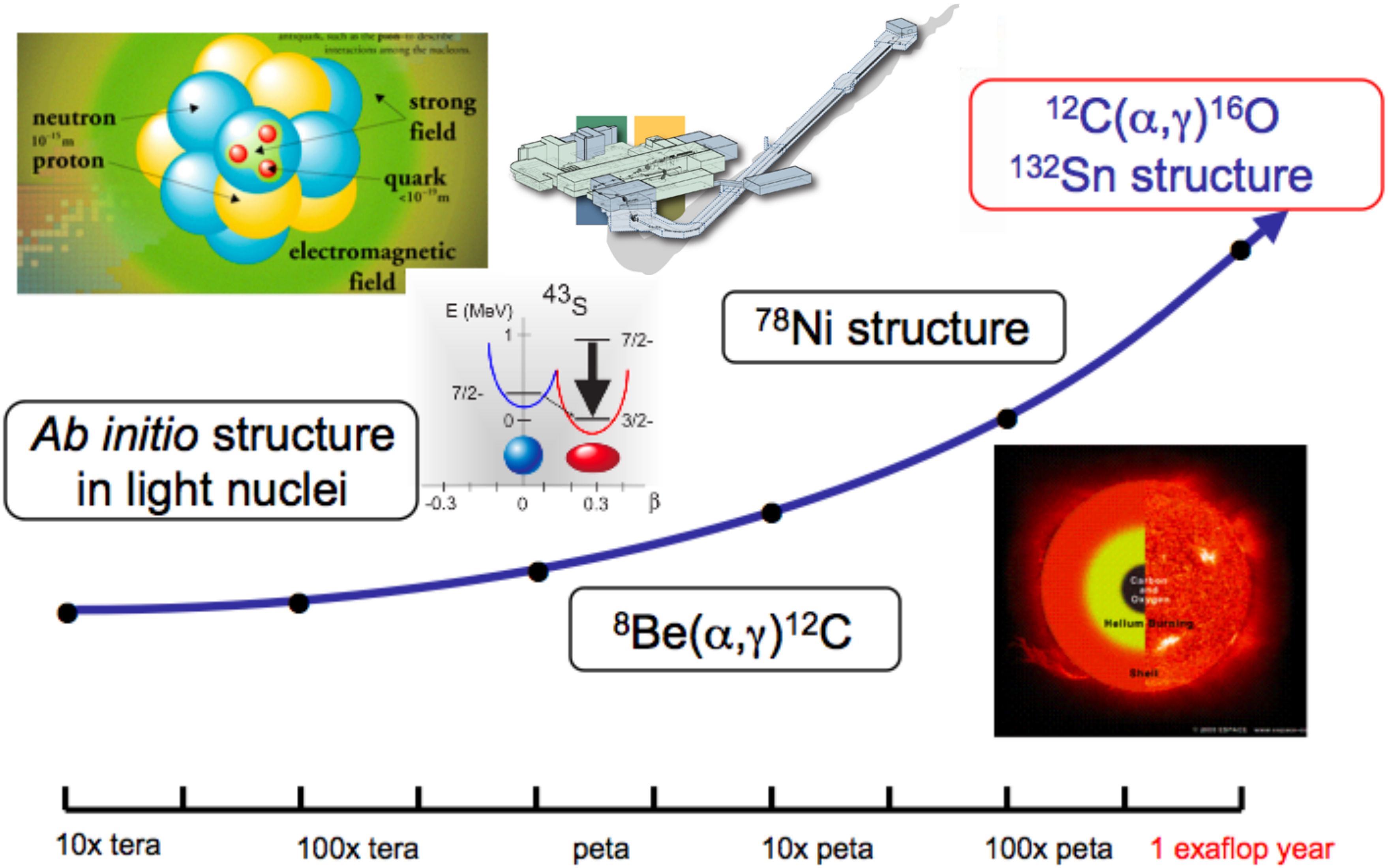
(b) 20-40 test case

The bigger the workload transferred to the GPU, the greater the gain up to a limit

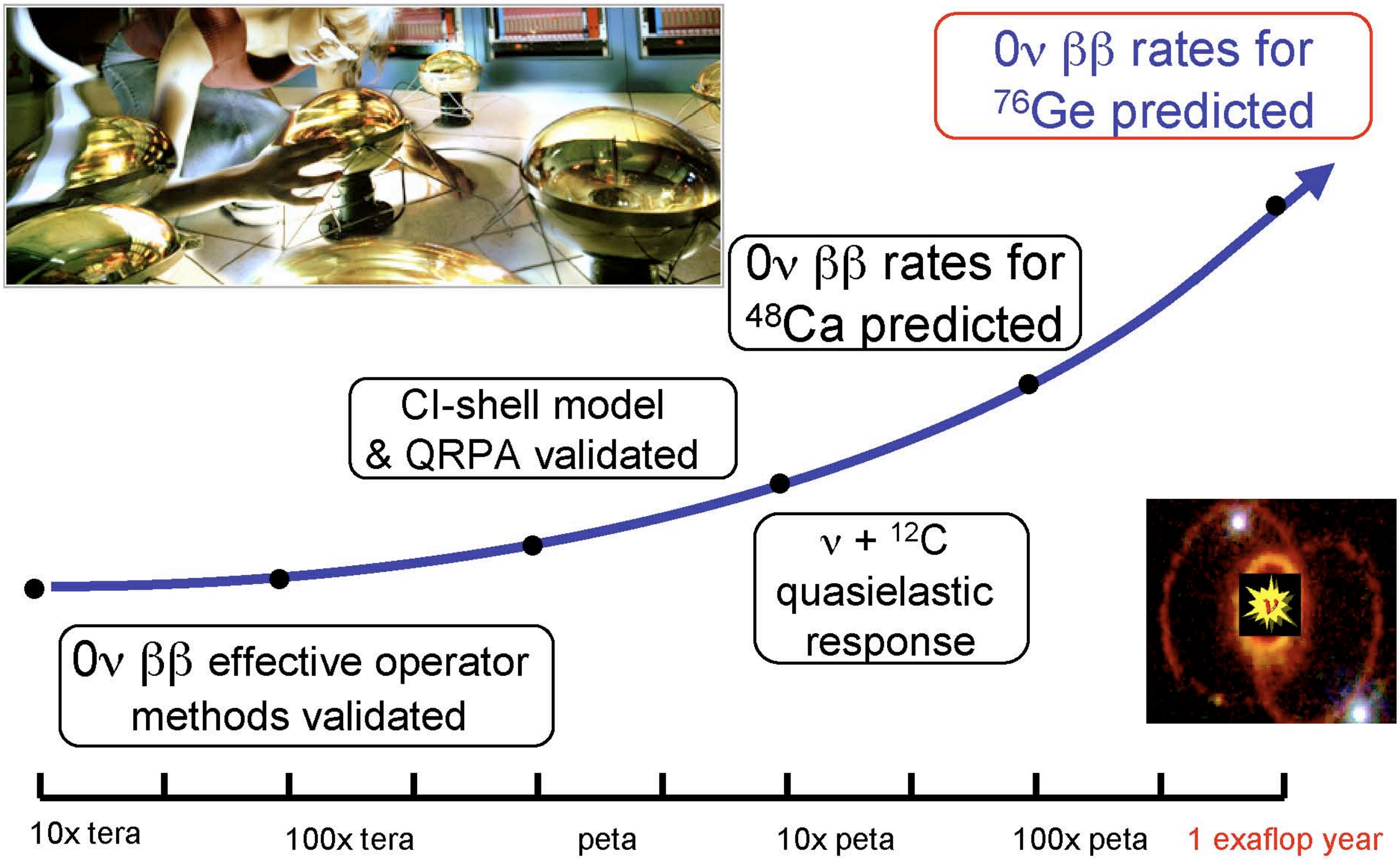
Ab initio NCSM Flowcharts



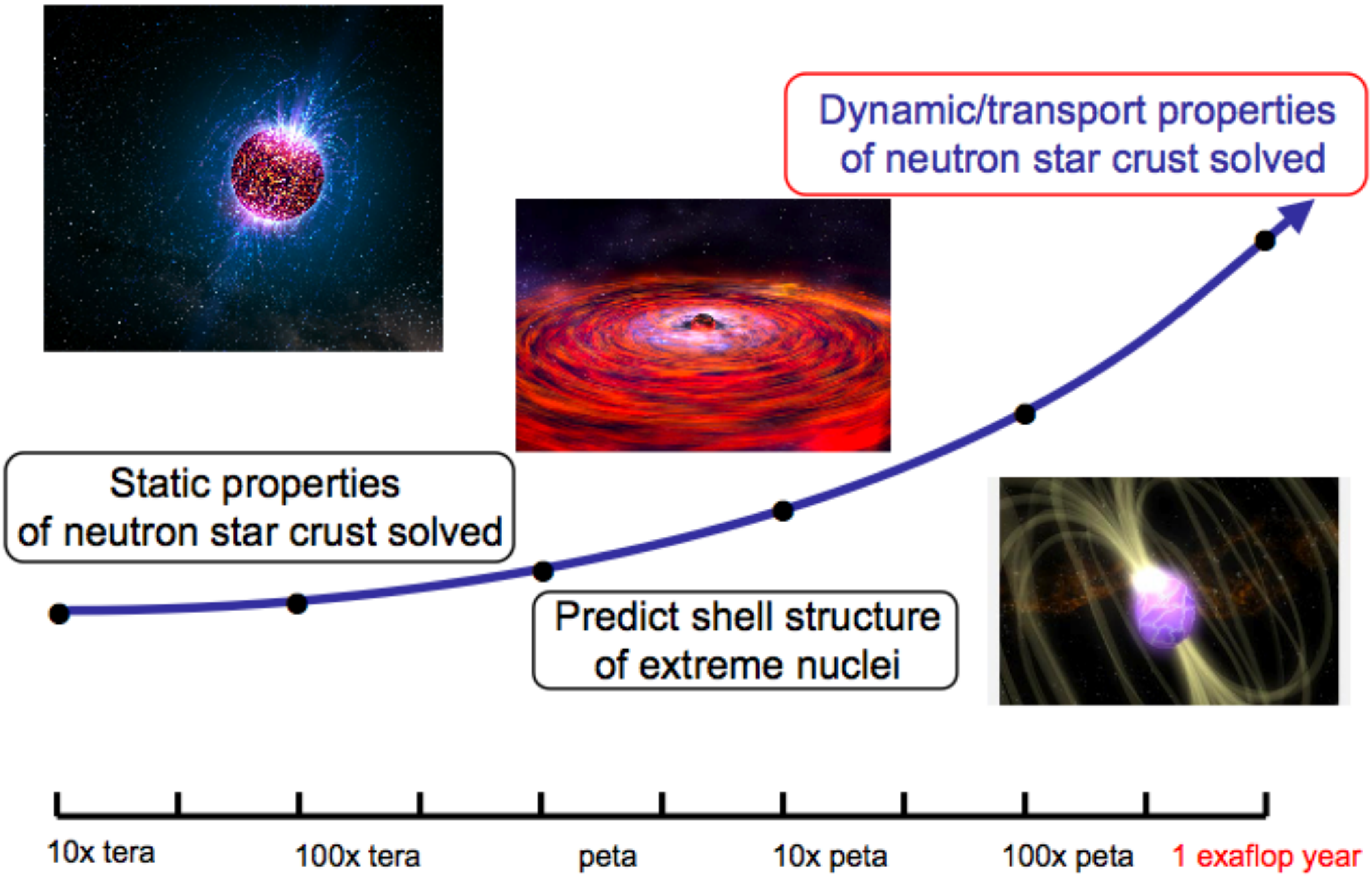
Selected science and technology “drivers” for high-performance computing



neutron
proton
strong field
quark
electromagnetic field
43S
E (MeV)
1
7/2-
0
7/2-
3/2-
-0.3
0
0.3
β
Ab initio structure in light nuclei
78Ni structure
12C(α,γ)16O
132Sn structure
8Be(α,γ)12C
Helium Burning
Shell
10x tera
100x tera
peta
10x peta
100x peta
1 exaflop year



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

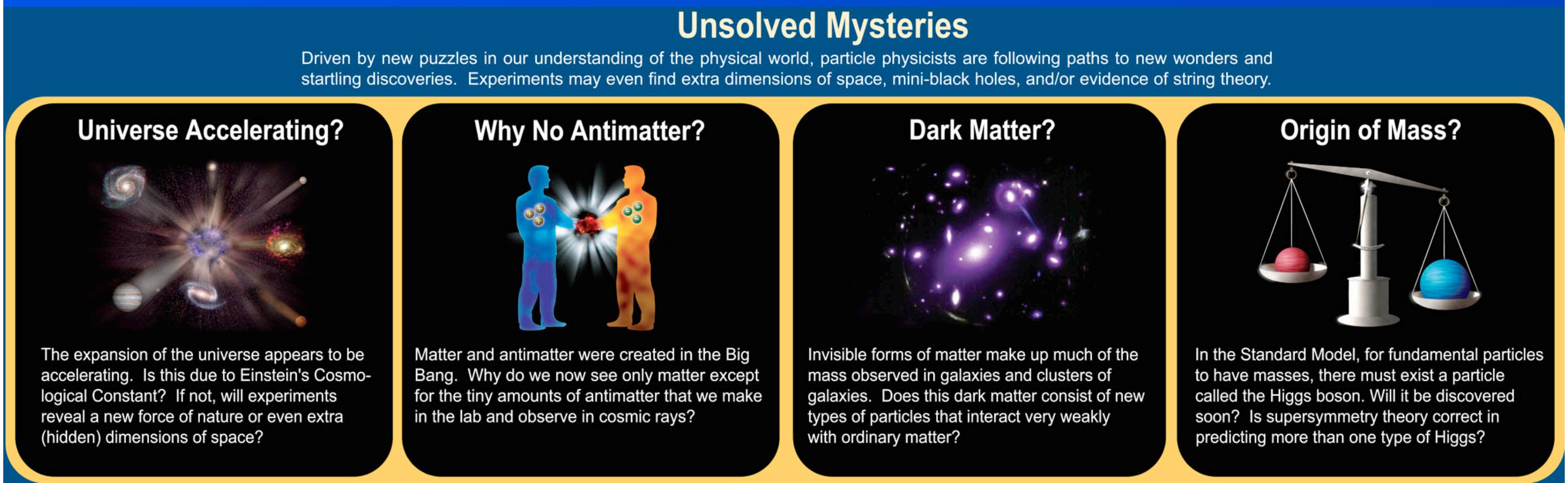


Dynamic/transport properties of neutron star crust solved
Static properties of neutron star crust solved
Predict shell structure of extreme nuclei
10x tera
100x tera
peta
10x peta
100x peta
1 exaflop year

Many outstanding nuclear physics
puzzles and discoveries remain

Clustering phenomena
Origin of the successful nuclear shell model
Nuclear reactions and breakup
Astrophysical r/p processes & drip lines
Predictive theory of fission
Existence/stability of superheavy nuclei
Physics beyond the Standard Model
Possible lepton number violation
Spin content of the proton
+ Many More!

Are there more than four interactions in nature?
Is there evidence that the Standard Model is incomplete?



<u>We are looking for astonishing new discoveries</u>

Supersymmetry

Extra dimensions (string theory)

Multiple universes

- - - - - - - - - -

- A third rate theory forbids
- A second rate theory explains after the fact
- A first rate theory predicts

- M. Lomonosov

Status report from the conference

We are developing successful *predictive* theory
with wide applicability
and the supercomputer simulations to exploit that theory

Many recent insights obtained from ab initio NCSM/NCFC:

Collective modes in light nuclei accessible with ab initio approach
3NFs continue to play an important role in many observables
Neutron drop results show (sub)shell closures
IR and UV convergence in HO basis (Coon et al., Papenbrock et al.)
Alternative basis spaces poised to relieve IR shortcomings of HO basis
Alternative MB methods poised to access clustering, halo physics regions
Computer Science and Applied Math collaborations invaluable
Generous allocations of computer resources essential to progress

Recent Collaborators

United States

- ISU: Pieter Maris, Alina Negoita, Chase Cockrell, Hugh Potter
- LLNL: Erich Ormand, Tom Luu, Eric Jurgenson, Michael Kruse
- ORNL/UT: David Dean, Hai Ah Nam, Markus Kortelainen, Witek Nazarewicz, Gaute Hagen,Thomas Papenbrock
- OSU: Dick Furnstahl, Kai Hebeler, students
- MSU: Scott Bogner, Heiko Hergert
- Notre Dame: Mark Caprio
- ANL: Harry Lee, Steve Pieper, Fritz Coester
- LANL: Joe Carlson, Stefano Gandolfi
- UA: Bruce Barrett, Sid A. Coon, Bira van Kolck, Matthew Avetian, Alexander Lisetskiy
- LSU: Jerry Draayer, Tomas Dytrych, Kristina Sviratcheva, Chairul Bahri
- UW: Martin Savage

International

- Canada: Petr Navratil
- Russia: Andrey Shirokov, Alexander Mazur, Eugene Mazur, Sergey Zaytsev, Vasily Kulikov
- Sweden: Christian Forssen, Jimmy Rotureau
- Japan: Takashi Abe, Takaharu Otsuka, Yutaka Utsuno, Noritaka Shimizu
- Germany: Achim Schwenk, Robert Roth, Javier Menendez, students
- South Korea: Youngman Kim, Ik Jae Shin
- Turkey: Erdal Dikman

Computer Science/ Applied Math

- ODU/Ames Lab: Masha Sosonkina, Dossay Oryspayev
- LBNL: Esmond Ng, Chao Yang, Hasan Metin Aktulga
- ANL: Stefan Wild, Rusty Lusk
- OSU: Umit Catalyurek, Eric Saule

Quantum Field Theory

- ISU: Xingbo Zhao, Pieter Maris, Paul Wiecki, Yang Li, Kirill Tuchin, John Spence
- Stanford: Stan Brodsky
- Penn State: Heli Honkanen
- Russia: Vladimir Karmanov
- Germany: Hans-Juergen Pirner
- Costa Rica: Guy de Teramond
- India: Avaroth Harindranath, Usha Kulshreshtha, Daya Kulshreshtha, Asmita Mukherjee, Dipankar Chakrabarti, Ravi Manohar

Thank you for your participation here
and for all the warm wishes!

I welcome your questions!