Perspectives on Science Excursions with Steve Pieper
James P. Vary, Iowa State University

Computational Nuclear Physics: A Symposium in Honor of Steven C. Pieper
October 11, 2019

U.S. DEPARTMENT OF ENERGY | Office of Science

SciDAC
Scientific Discovery through Advanced Computing

NUCLEI
Nuclear Computational Low-Energy Initiative

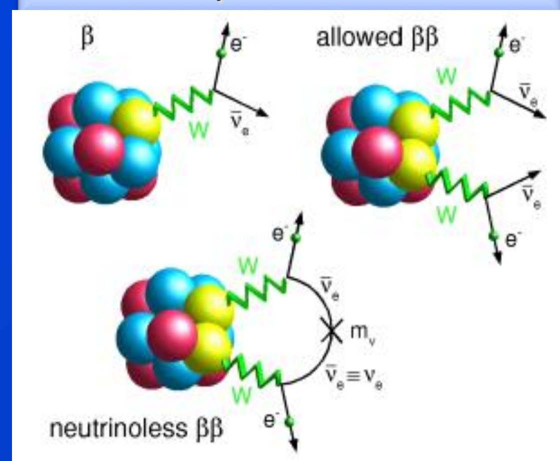
U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

The Overarching Questions

- How did visible matter come into being and how does it evolve?
- How does subatomic matter organize itself and what phenomena emerge?
- Are the fundamental interactions that are basic to the structure of matter fully understood?
- How can the knowledge and technological progress provided by nuclear physics best be used to benefit society?

- NRC Decadal Study

Topical Collaboration on Neutrinos and Fundamental Symmetries



LENPIC

Perspectives

Theme 1

Challenging Fundamental Physics Problems motivate cutting edge Computational Physics

Theme 2

Advancing the field of Nuclear Physics through collaborations and community service

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.

Successful *ab initio* quantum many-body approaches ($A \geq 6$)

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

Meson Exchg interactions

Hamiltonian matrix in basis function space
No Core Configuration Interaction (**NCSM/NCFC**)

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

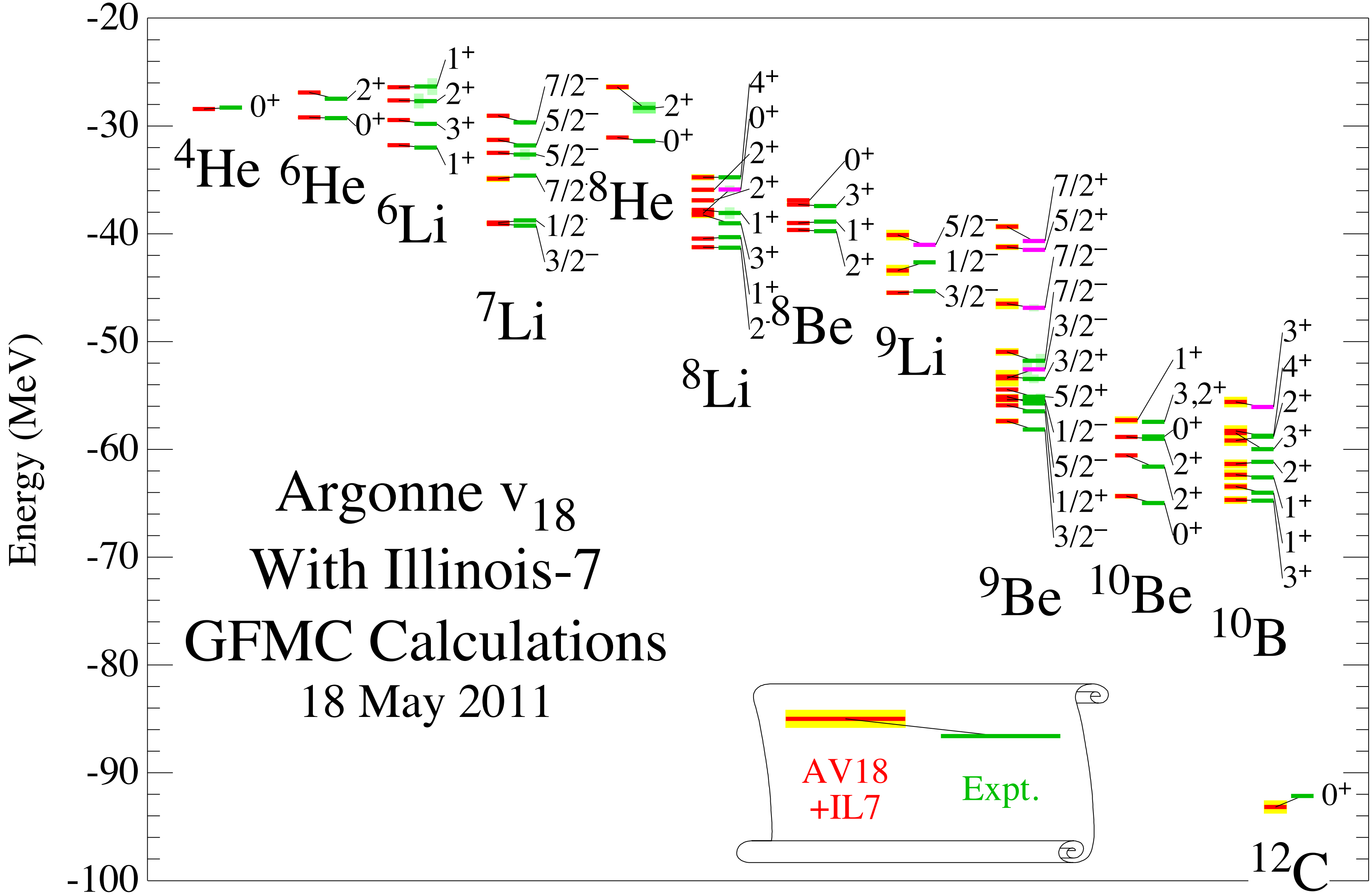
Lattice Nuclear Chiral EFT, MB Greens Function,
MB Perturbation Theory, . . . approaches

Chiral EFT interactions

Comments

All work to preserve and exploit symmetries
Extensions of each to scattering/reactions have emerged
They have different advantages and limitations

REPRODUCTION OF NUCLEAR LEVELS



AV18+IL7 reproduces ~50 levels (+ ~60 isobaric analogs) up to ^{12}C with rms error ~0.6 MeV
We have motivated or supported experimental work in almost all these nuclei

Slide provided by Steve Pieper

No-Core Configuration Interaction calculations

Barrett, Navrátil, Vary, *Ab initio no-core shell model*, PPNP69, 131 (2013)

Given a Hamiltonian operator

$$\hat{\mathbf{H}} = \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2\,m\,A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

solve the eigenvalue problem for wavefunction of A nucleons

$$\hat{\mathbf{H}}\,\Psi(r_1,\ldots,r_A) = \lambda\,\Psi(r_1,\ldots,r_A)$$

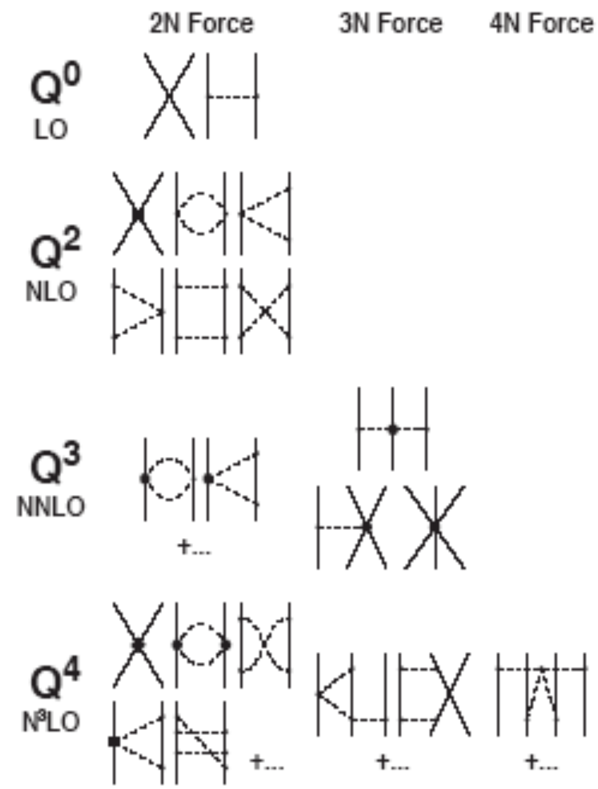
- Expand eigenstates in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Diagonalize Hamiltonian matrix $H_{ij} = \langle\Phi_j|\hat{\mathbf{H}}|\Phi_i\rangle$
- No Core Full Configuration (NCFC) – All A nucleons treated equally
- Complete basis $\longrightarrow$ exact result
- In practice
  - truncate basis
  - study behavior of observables as function of truncation

Nuclear interaction

Nuclear potential not well-known,

though in principle calculable from QCD

$$\hat{\mathbf{H}} = \hat{\mathbf{T}}_{\text{rel}} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$



In practice, alphabet of realistic potentials

- Argonne potentials: AV8′, AV18
  - plus Urbana 3NF (UIX)
  - plus Illinois 3NF (IL7)
- Bonn potentials
- Chiral NN interactions - e.g. LENPIC
  - plus chiral 3NF, ideally to the same order
- JISP16
- Daejeon16
- . . .

Major development during the past decade:
High-precision ab initio calculations now used to "discover" the correct strong NN+NNN interaction

Consistent strong and electroweak interactions from Chiral EFT

Low
Energy
Nuclear
Physics
International
Collaboration

LENPIC

J. Golak, R. Skibinski, K. Tolponicki, H. Witala

E. Epelbaum, H. Krebs

A. Nogga

R. Furnstahl

S. Binder, A. Calci, K. Hebeler, J. Langhammer, R. Roth

P. Maris, J. Vary

H. Kamada

U.-G Meissner

Current Focus

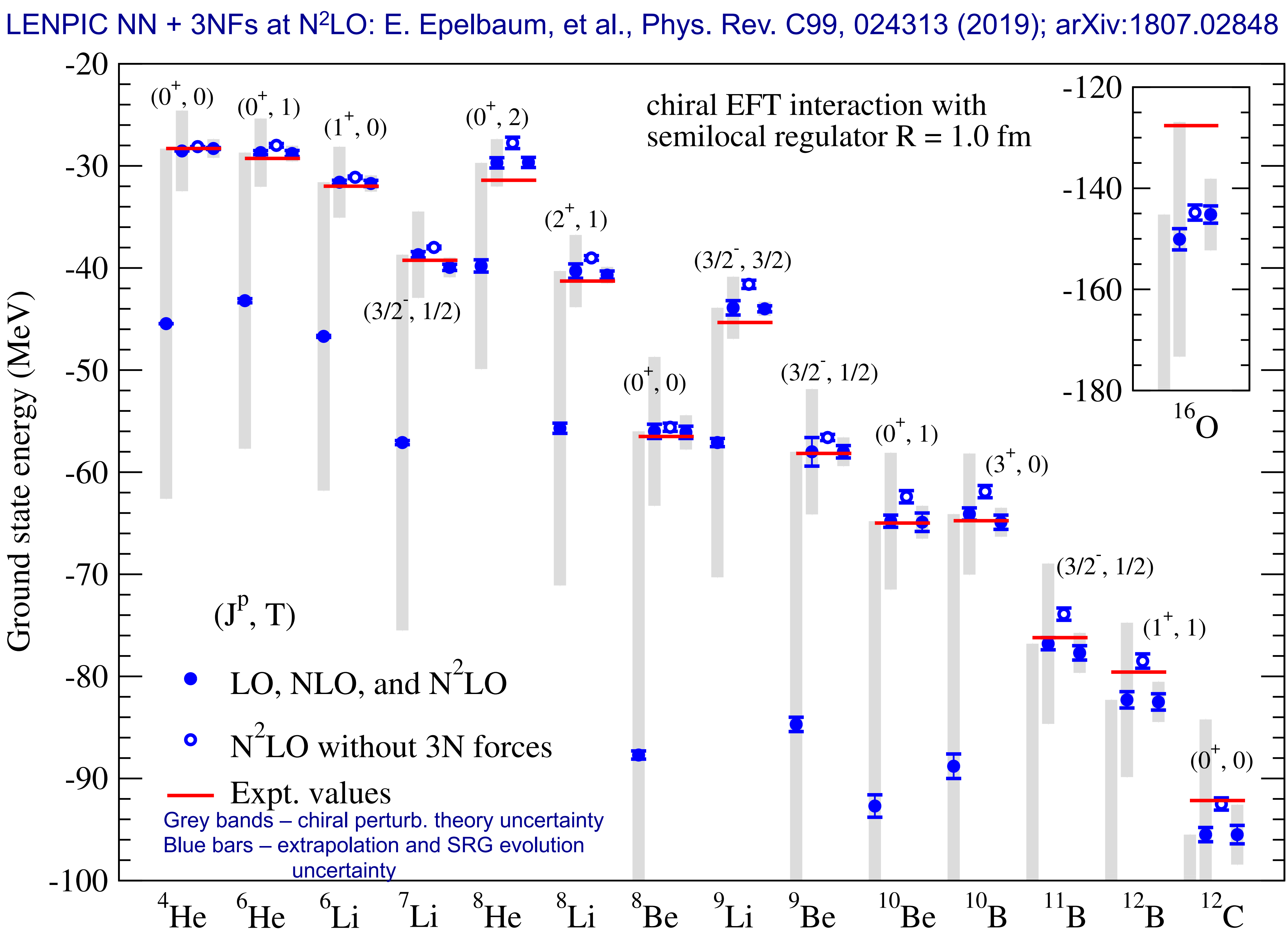
Introduce momentum space regulators to facilitate gauge invariance

Extensive studies of the NN, 3N systems: scattering, moments, form factors . . .

Light nuclei: magnetic moments, GT, $M\lambda$ and $E\lambda$ transitions with operators consistent through N3LO

Medium weight nuclei with coupled cluster

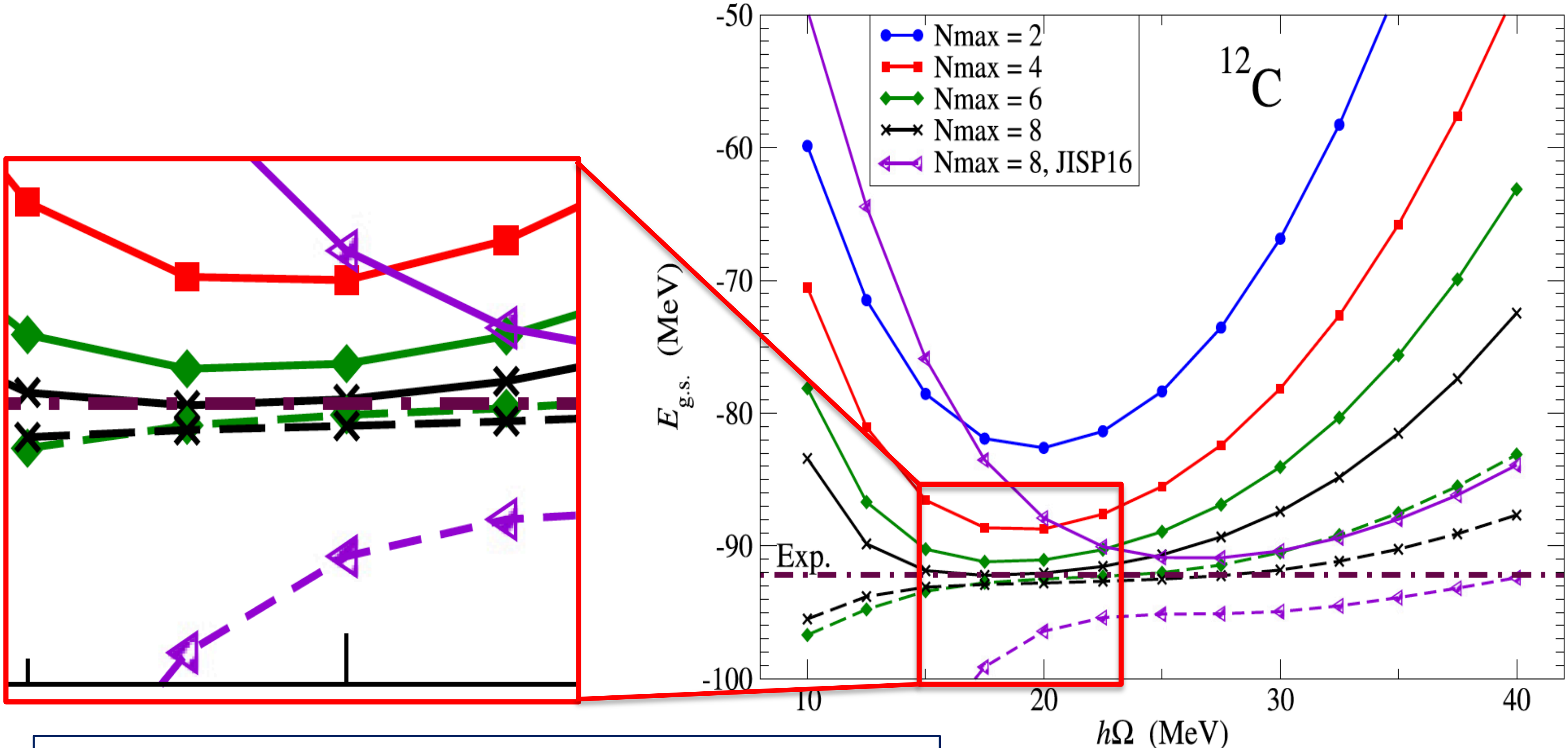
Longer term – sd-shell and pf-shell (V_{eff})


LENPIC NN + 3NFs at N2LO: E. Epelbaum, et al., Phys. Rev. C99, 024313 (2019); arXiv:1807.02848
Ground state energy (MeV)
chiral EFT interaction with semilocal regulator R = 1.0 fm
(Jp, T)
LO, NLO, and N2LO
N2LO without 3N forces
Expt. values
Grey bands – chiral perturb. theory uncertainty
Blue bars – extrapolation and SRG evolution uncertainty
(0+, 0)
(0+, 1)
(1+, 0)
(3/2-, 1/2)
(0+, 2)
(2+, 1)
(0+, 0)
(3/2-, 3/2)
(3/2-, 1/2)
(0+, 1)
(3+, 0)
(3/2-, 1/2)
(1+, 1)
(0+, 0)
4He
6He
6Li
7Li
8He
8Li
8Be
9Li
9Be
10Be
10B
11B
12B
12C
16O
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180

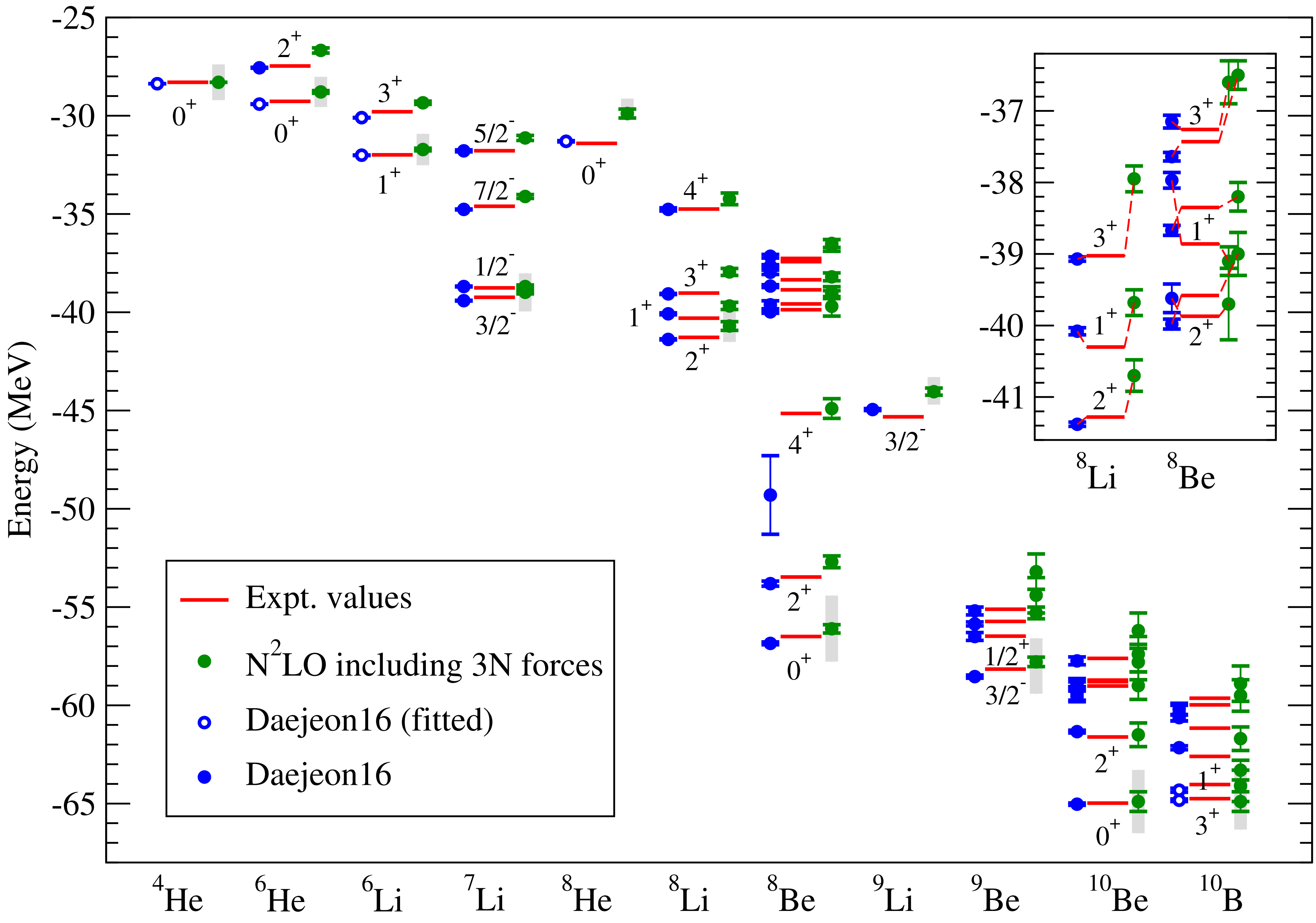
Daejeon16 NN interaction

Based on SRG evolution of Entem-Machleidt "500" chiral N3LO to $\lambda = 1.5\ \mathrm{fm}^{-1}$ followed by Phase-Equivalent Transformations (PETs) to fit selected properties of light nuclei.

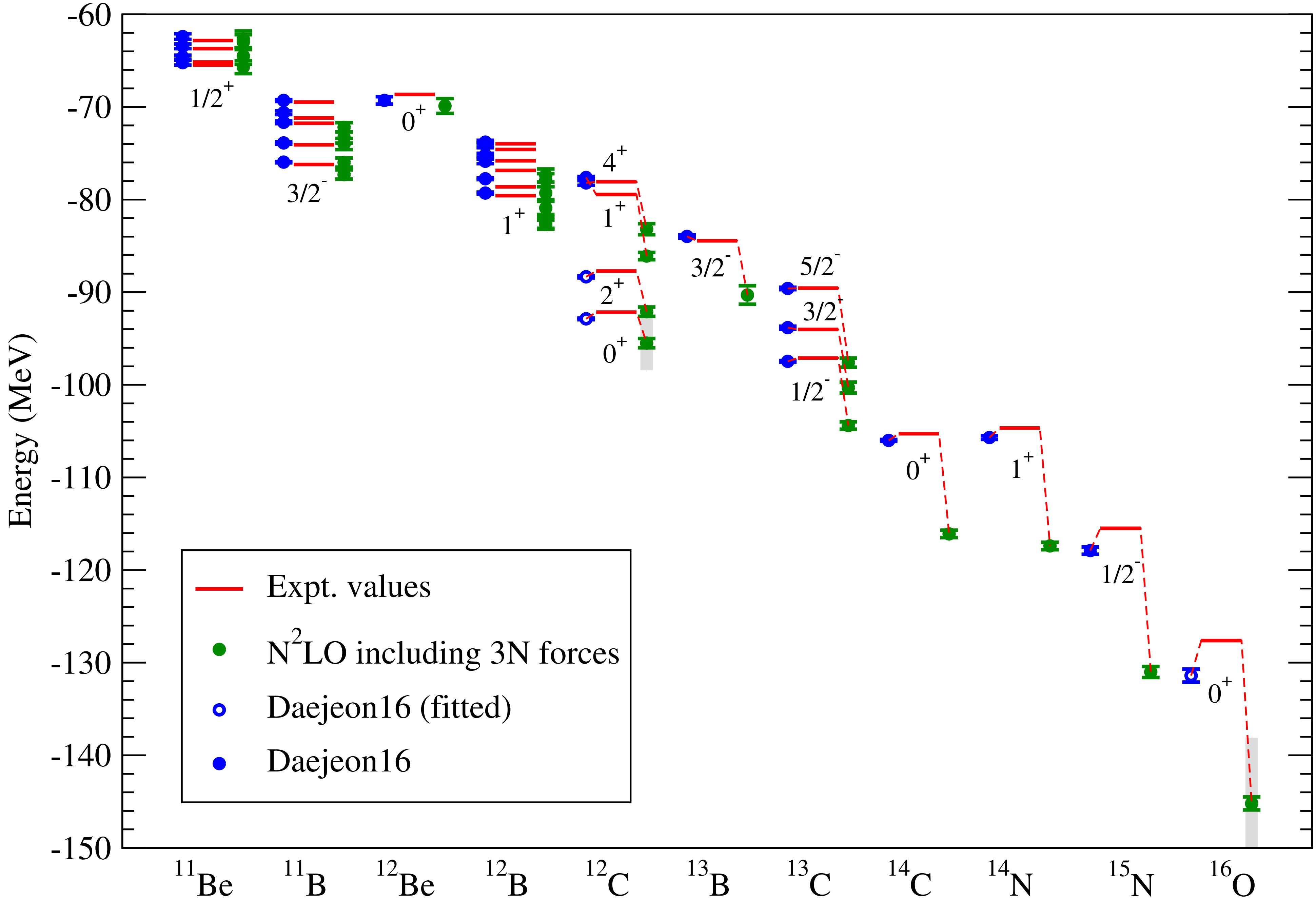
A.M. Shirokov, I.J. Shin, Y. Kim, M. Sosonkina, P. Maris and J.P. Vary, "N3LO NN interaction adjusted to light nuclei in ab exitu approach," Phys. Letts. B 761, 87 (2016); arXiv: 1605.00413



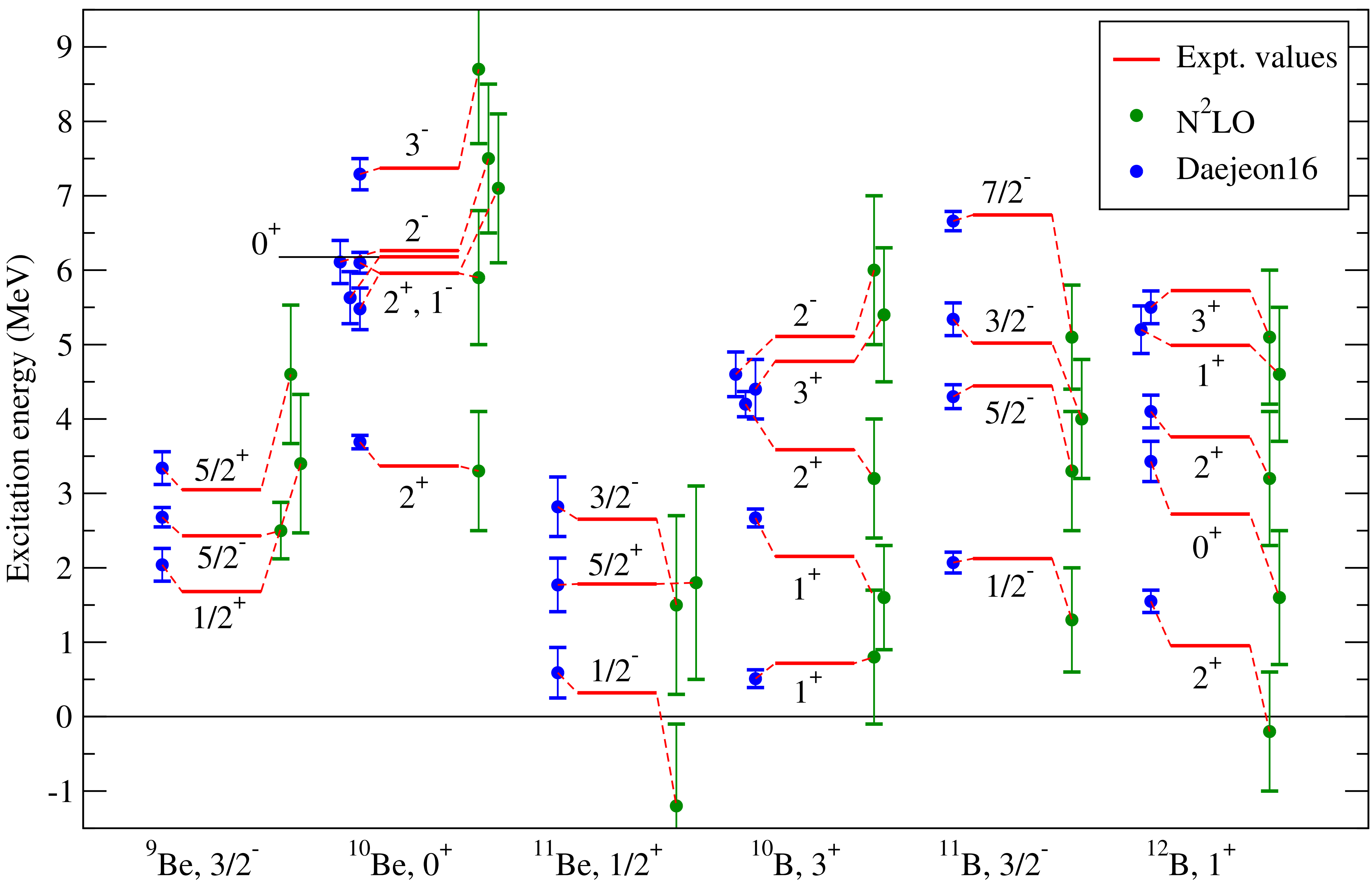
GS radius also agrees with experiment to within 1%



P. Maris, I.J. Shin and J.P. Vary, NTSE2018 Proceedings, arXiv: 1908.00155



P. Maris, I.J. Shin and J.P. Vary, NTSE2018 Proceedings, arXiv: 1908.00155



P. Maris, I.J. Shin and J.P. Vary, NTSE2018 Proceedings, arXiv: 1908.00155

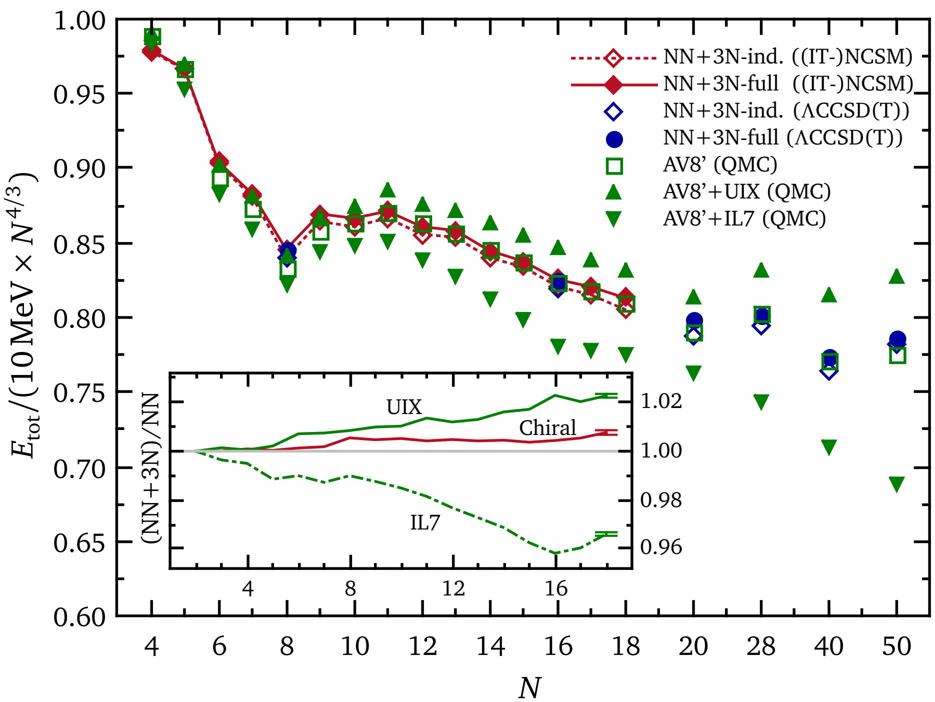
Ab initio Extreme Neutron Matter

Objectives

- Predict properties of neutron-rich systems which relate to exotic nuclei and nuclear astrophysics
- Determine how well high-precision phenomenological strong interactions compare with effective field theory based on QCD
- Produce accurate predictions with quantified uncertainties

Impact

- Improve nuclear energy density functionals used in extensive applications such as fission calculations
- Demonstrate the predictive power of *ab initio* nuclear theory for exotic nuclei with quantified uncertainties
- Guide future experiments at DOE-sponsored rare isotope production facilities



Comparison of ground state energies of systems with N neutrons trapped in a harmonic oscillator with strength 10 MeV. Solid red diamonds and blue dots signify new results with two-nucleon (NN) plus three-nucleon (3N) interactions derived from chiral effective field theory related to QCD. Inset displays the ratio of NN+3N to NN alone for the different interactions. Note that with increasing N, the chiral predictions lie between results from different high-precision phenomenological interactions, i.e. between AV8'+UIX and AV8'+IL7.

Accomplishments

1. Demonstrates predictive power of *ab initio* nuclear structure theory.
2. Provides results for next generation nuclear energy density functionals
3. Leads to improved predictions for astrophysical reactions
4. Demonstrates that the role of three-nucleon (3N) interactions in extreme neutron systems is significantly weaker than predicted from high-precision phenomemological interactions

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NUCLEI Nuclear Computational Low-Energy Initiative

References: H. Potter, S. Fischer, P. Maris, J.P. Vary, S. Binder, A. Calci, J. Langhammer and R.Roth, Phys. Lett. B739, 445 (2014); P. Maris, J.P. Vary, S. Gandolfi, J. Carlson, S.C. Pieper, Phys. Rev. C87, 054318 (2013);

Contact: jvary@iastate.edu

2014-2016 INCITE Closeout Report Highlight

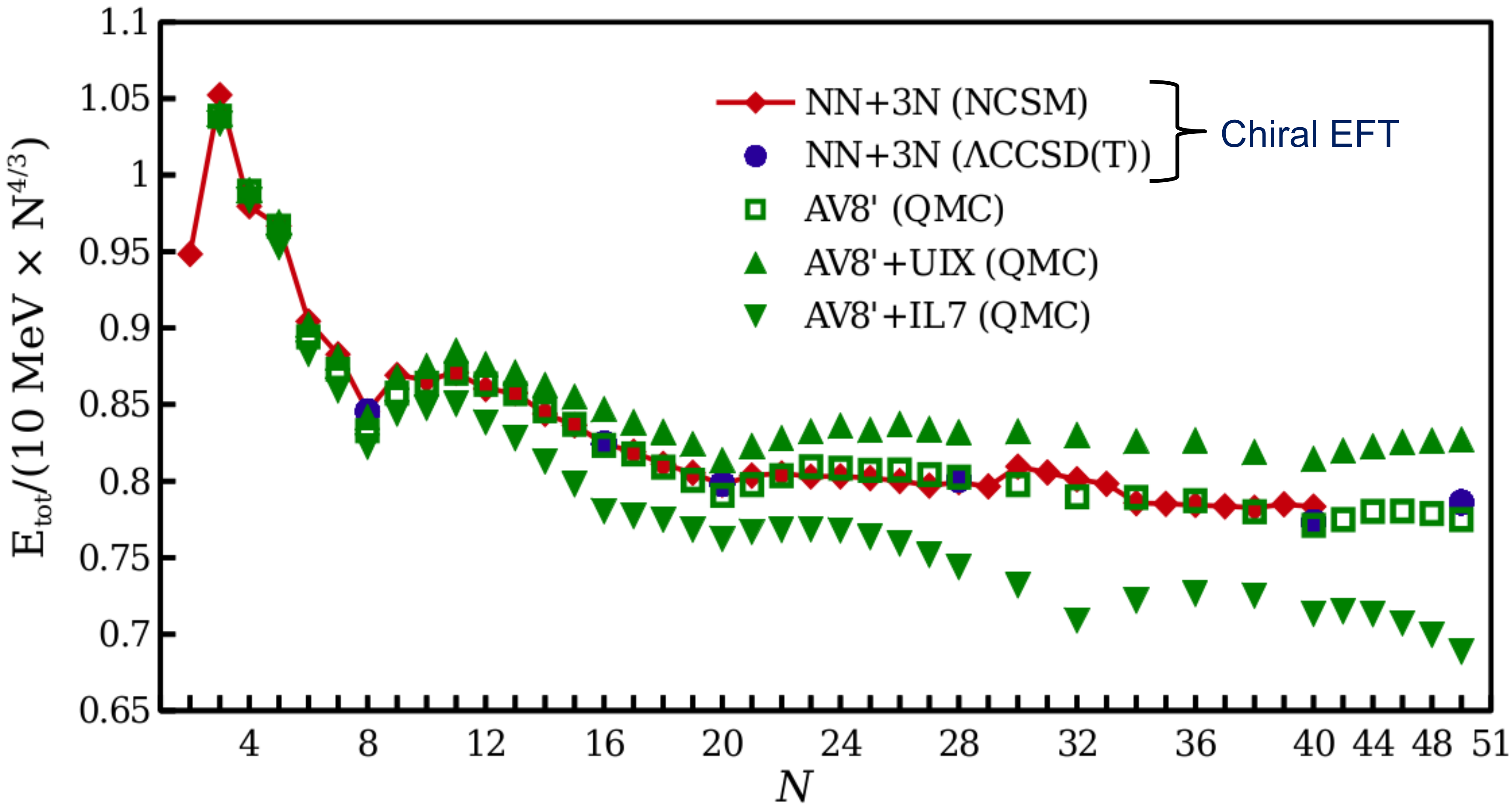


Fig. 6 Scaled ground state energies for neutron drop systems when confined to a harmonic oscillator trap with strength 10 MeV. The results are obtained with NN + 3N interactions from chiral Effective Field Theory (those labeled "NN+3N") and compared with results from meson exchange interactions using other methods (P. Maris et al., Phys. Rev. C 87, 054318 (2013)). These results help quantify the uncertainty due to interaction dependence. NCSM results (labeled "NCSM") are obtained on Titan using the GPUs for decoupling transformations of the 3N interaction from a compressed coupled angular momentum and isospin basis to an m-scheme basis that is employed in MFDn. Results from coupled-cluster calculations using the same interaction are labeled "ΛCCSD(T)".

P. Maris, J.P. Vary, S. Gandolfi, J. Carlson, S.C. Pieper, Phys. Rev. C87, 054318 (2013);
H. Potter, S. Fischer, P. Maris, J.P. Vary, S. Binder, A. Calci, J. Langhammer and R.Roth, Phys. Lett. B739, 445 (2014)

Table 5 Compare ^{8}Li observables using different MB methods and interactions

Comparison of ^{8}Li observables between experiment [155,160,161] and theory. The OLS results with Chiral $NN + NNN$ are calculated in the NCSM at $\hbar\Omega = 13$ MeV up through $N_{\max} = 8$ as reported in Ref. [153]. The SRG results ($\alpha = 0.08$) with Chiral $NN + NNN$ for $N_{\max} = 8$; 10 are calculated at $\hbar\Omega = 16$ MeV in the IT-NCSM as reported in Ref. [158]. Results up through $N_{\max} = 12$ with JISP16 [107–109] are obtained in the NCFC approach as reported in Ref. [159]. The table uses the same units as in Table 4. AV18/IL2 results are obtained in the GFMC approach as reported in Refs. [1,2] and do not include meson-exchange corrections for the magnetic moment; CD-Bonn ("CD-B") and INOY results are from Refs. [136,163], and were calculated at $N_{\max} = 12$ and $\hbar\Omega = 12$ and 16 MeV respectively for CD-Bonn and INOY, with the INOY g.s. energy extrapolated to the infinite basis space. See caption to Table 4. For the JISP16 results, the energies are obtained from extrapolations to the infinite basis space, the magnetic dipole observables are nearly converged and the RMS point-proton radius and electric quadrupole observables are evaluated at $\hbar\Omega = 12.5$ MeV.

^{8}Li	Expt.	Chiral $NN + NNN$ Okubo–Lee–Suzuki	Chiral $NN + NNN$ SRG(0.08) $N_{\max} = 8$; 10	AV18/IL2	JISP16	INOY	CD-B
$E_b(2^+)$	41.277	39.95(69)	39.90(1) ; 40.79(10)	41.9(2)	40.3(2)	41.3(5)	35.82
$\langle r_{pp}^2\rangle^{1/2}$	2.21(6)	2.09		2.09(1)	2.1	2.01	2.17
$E_x(1_1^+1)$	0.981	1.00 (16;03)	1.027(2) ; 0.985(6)	1.4(3)	1.5(2)	1.26	0.86
$E_x(3_1^+1)$	2.255(3)	2.75 (16;09)	2.608(3) ; 2.599(7)	2.5(3)	2.8(1)	2.87	3.02
$E_x(0_1^+1)$	–	4.01 (84;20)	3.842(15) ; 3.537(40)			4.22	2.48
$E_x(1_2^+1)$	3.210	4.73 (84;21)	4.632(16) ; 4.283(44)			4.90	3.25
$E_x(2_2^+1)$	–	4.78 (44;12)	4.603(7) ; 4.443(23)			5.11	3.98
$E_x(2_3^+1)$	–	5.94 (37;20)				6.07	5.29
$E_x(1_3^+1)$	5.400	6.09 (70;22)				6.76	5.02
$E_x(4_1^+1)$	6.53(20)	7.45 (36;15)		7.2(3)	7.0(3)	7.40	6.69
$E_x(3_2^+1)$	–	8.24 (50;22)				8.92	7.57
$E_x(0_1^+2)$	10.822	11.77 (27;29)				12.05	10.90
$Q(2^+)$	3.27(6)	2.65	2.73(1) ; 2.79(1)	3.2(1)	2.6	2.55	2.78
$Q(1^+)$	–	1.08	1.12(1) ; 1.12(1)		1.2		
$Q(3^+)$	–	−1.97	−1.92(1); −1.94(2)		−2.0		
$Q(4^+)$	–	−3.01			−3.4		
$\mu(2^+)$	1.654	1.49	–	1.65(1)	1.3(1)	1.42	1.24
$\mu(1^+)$	–	−2.27			−2.2(2)		
$\mu(3^+)$	–	2.13			2.0(1)		
$\mu(4^+)$	–	1.86			1.84(1)		
B(E2;1$^+$)	–	1.19			1.9		
B(E2;3$^+$)	–	3.70			4.6		
B(E2;4$^+$)	–	1.21			1.9		
B(M1;1$^+$)	5.0(16)	4.13	4.15(1) ; 4.14(1)		3.7(2)	4.56	4.39
B(M1;3$^+$)	0.52(23)	0.33	0.31(1) ; 0.30(1)		0.25(5)		

Continuing on Theme 1

VOLUME 90, NUMBER 25 PHYSICAL REVIEW LETTERS week ending 27 JUNE 2003

Can Modern Nuclear Hamiltonians Tolerate a Bound Tetraneutron?

Steven C. Pieper*
Physics Division, Argonne National Laboratory, Argonne, Illinois 60439, USA
(Received 18 February 2003; published 27 June 2003)

Conclusion: No bound state but a resonance at ~ 2 MeV is reasonable

PRL **117,** 182502 (2016) PHYSICAL REVIEW LETTERS week ending 28 OCTOBER 2016

Prediction for a Four-Neutron Resonance

A. M. Shirokov,[1,2,3,*] G. Papadimitriou,[4,†] A. I. Mazur,[3] I. A. Mazur,[3] R. Roth,[5] and J. P. Vary[2,‡]
[1]*Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow 119991, Russia*
[2]*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011-3160, USA*
[3]*Pacific National University, 136 Tikhookeanskaya Street, Khabarovsk 680035, Russia*
[4]*Nuclear and Chemical Science Division, Lawrence Livermore National Laboratory, Livermore, California 94551, USA*
[5]*Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany*
(Received 20 July 2016; revised manuscript received 9 September 2016; published 28 October 2016)

Conclusion: No bound state but a resonance at E ~ 0.8 MeV and width of ~ 1.4 MeV

Moving to Theme 2

Joint supercomputing efforts and joint funding proposals

2009	Scientific Grand Challenges Report
2007 - 2019	INCITE (several proposals)
2007 – 2012	SciDAC/UNEDF
2012 – 2022	SciDAC/NUCLEI

Failed joint proposal

2016 Early Science on Aurora

Steve’s observation about the reviews:
“The only negative seems to be lack of portability to GPU's which never made a lot of sense to me in a proposal for a machine with no GPUs.”

Computational Nuclear Physics

Comput

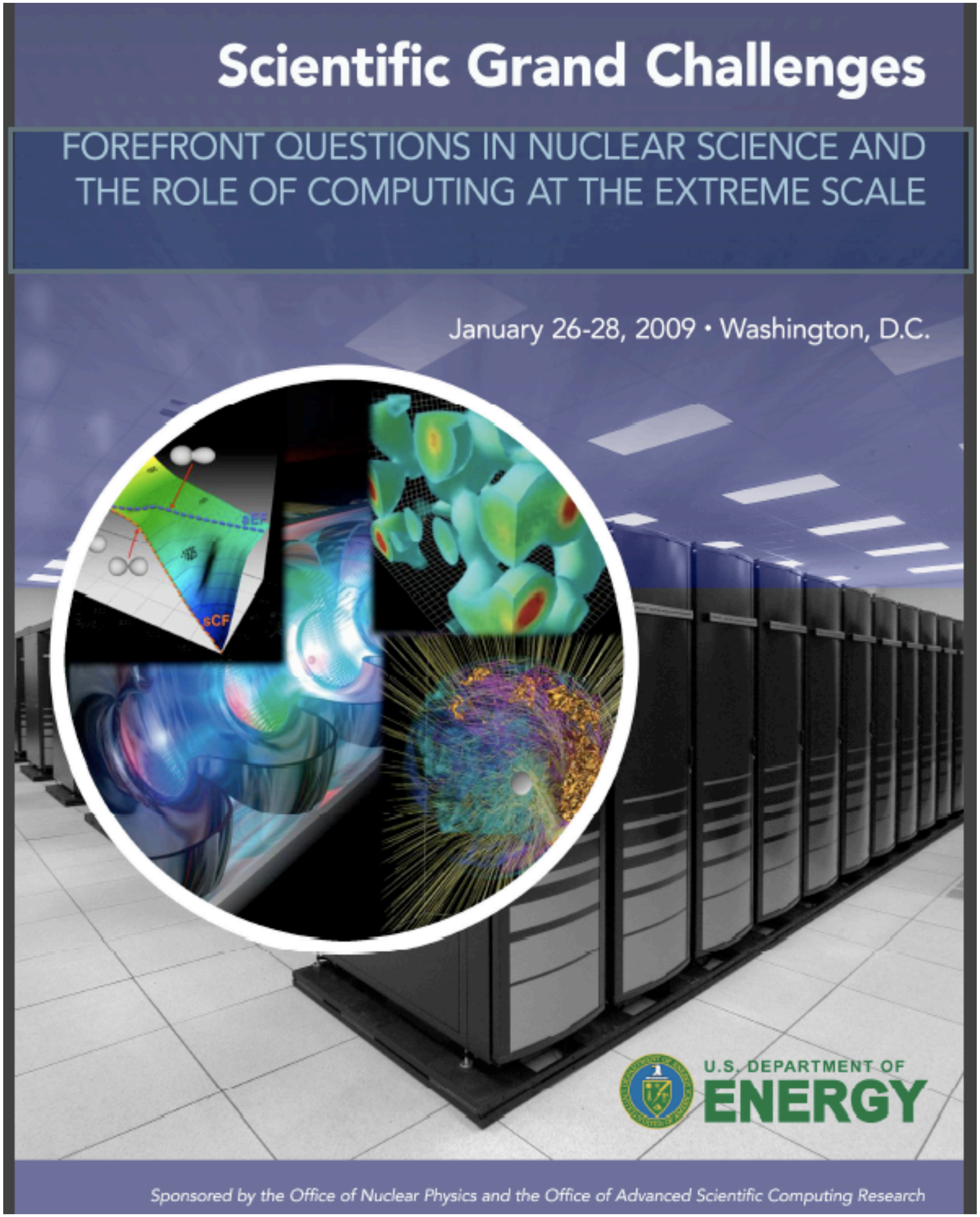
SciDAC-2 UNEDF
SciDAC-3&4 NUCLEI

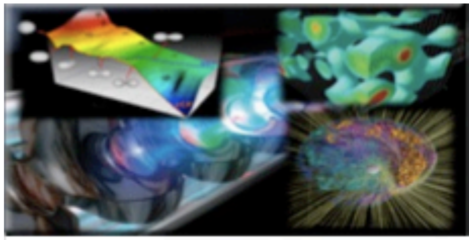
High Performance Computing provides answer ***her***
experiment nor analytic theory c
hence, it becomes the third leg supporting th ***cs***

National Academy Report
(2012)

From M. Savage

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





Forefront Questions in Nuclear Science and the Role of High Performance Computing

January 26-28, 2009 · Washington, D.C.

Nuclear Structure and Nuclear Reactions

James Vary, Iowa State

Steven Pieper, ANL

January 28, 2009

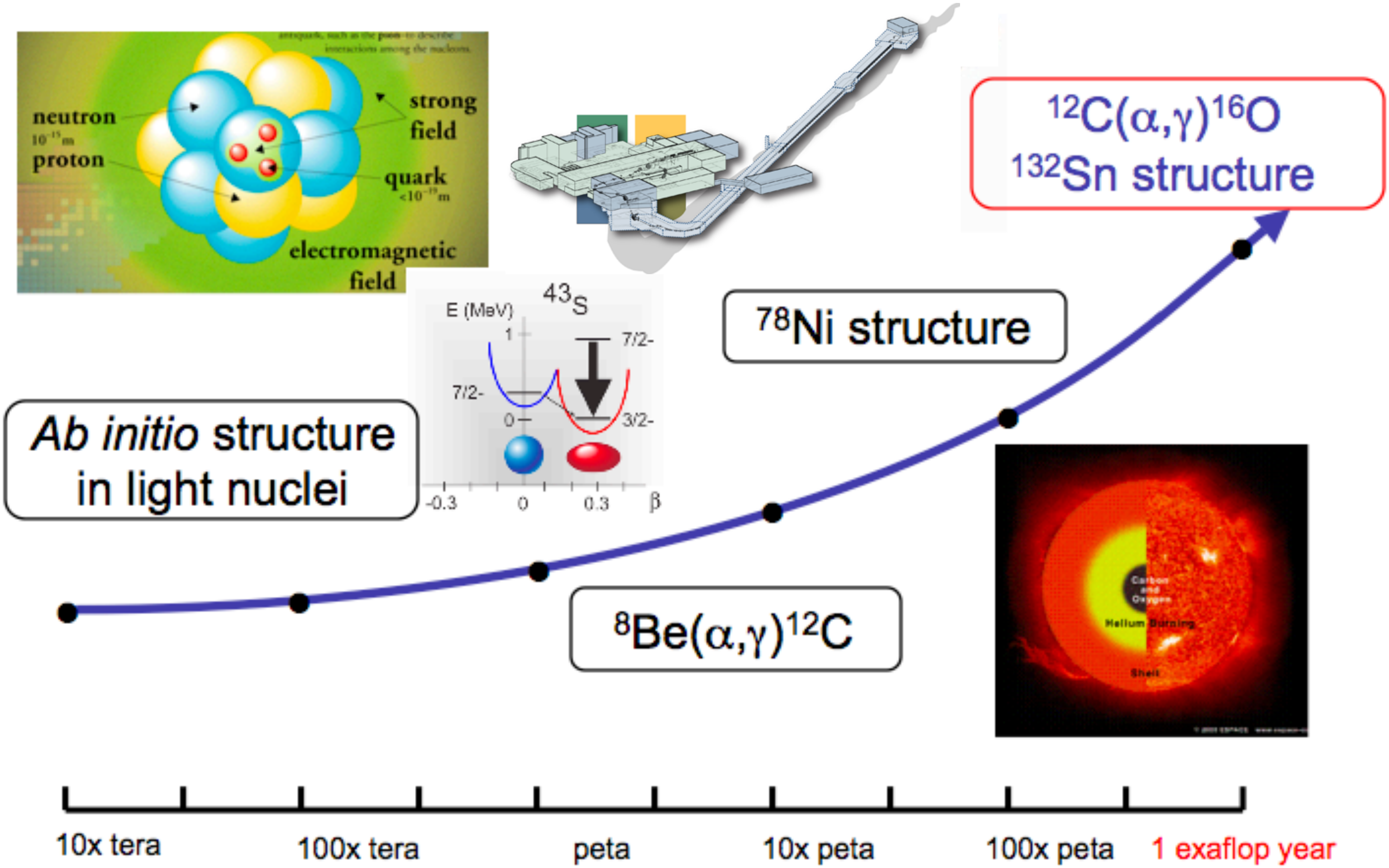
Plenary Morning Session

NUCLEAR STRUCTURE AND NUCLEAR REACTIONS

Co-Leads: James P. Vary, Iowa State University
Steven C. Pieper, Argonne National Laboratory

INTRODUCTION AND CURRENT STATUS

Atomic nuclei are the essence of the visible universe. Formed in the big bang or in cataclysmic astrophysical explosions, atomic nuclei are a crucial and intriguing part of the world. The basic features of atomic nuclei were understood in terms of the nuclear shell model in the 1963 Nobel Prize winning research of Eugene Paul Wigner, Maria Goeppert-Mayer, and J. Hans de Jensen. Since then, extensive experimental programs have yielded a detailed knowledge of the nucleon-nucleon interaction. This crucial experimental information will be augmented through studies of quantum chromodynamics (QCD) (see section on Cold QCD and Nuclear Forces). More refined descriptions of nuclei and greater predictive power require understanding nuclear structure and reactions in terms of the underlying interactions. Accurate solutions of these strongly interacting quantum many-body problems will yield new insight into the structure of nuclei and the ability to calculate processes that are difficult or impossible to measure experimentally.



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
8Be(α,γ)12C
78Ni structure
12C(α,γ)16O
132Sn structure
10x tera
100x tera
peta
10x peta
100x peta
1 exaflop year

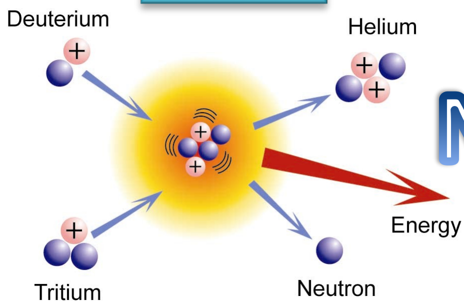
NUclear Computational Low-Energy Initiative

SciDAC Scientific Discovery through Advanced Computing

(2012-2019)

LENP facilities

fusion



NIF

TJNAF

FRIB

Validated Nuclear Interactions

Chiral EFT
Ab-initio

Optimization
Model validation
Uncertainty Quantification

Structure and Reactions: Light and Medium Nuclei

Ab-initio
GFMC
NCSM
CC
RGM

Load balancing
Eigensolvers
Nonlinear solvers
Model validation
Uncertainty Quantification

Neutron drops

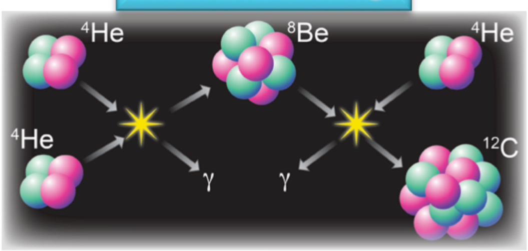
EOS
Correlations

Structure and Reactions: Heavy Nuclei

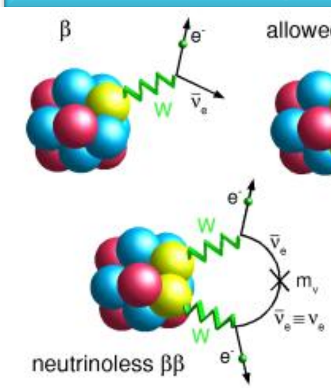
DFT
TDDFT

Load balancing
Optimization
Model validation
Uncertainty Quantification
Eigensolvers
Nonlinear solvers
Multiresolution analysis

Stellar burning



Neutrinos and Fundamental Symmetries

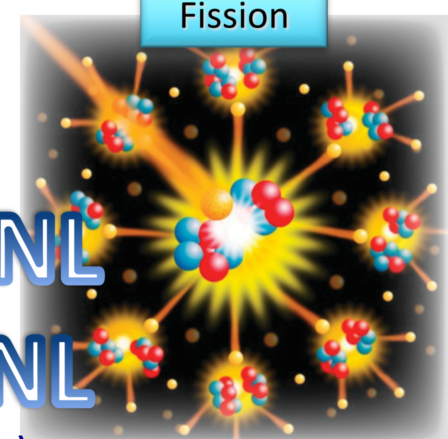


SNS

Majorana

Neutron Stars

Fission

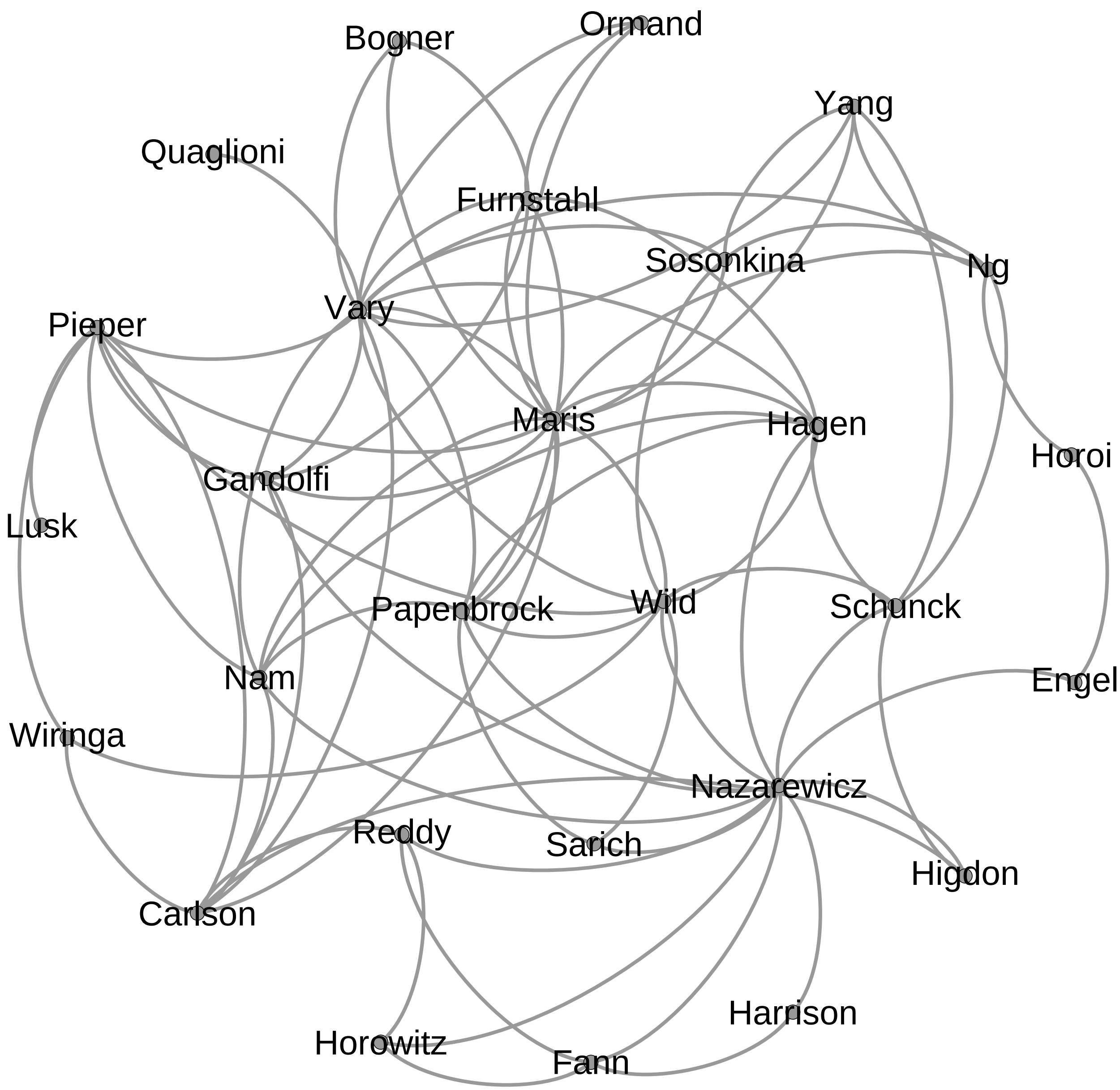


LANL

LLNL

computingnuclei.org (adapted from Gaute Hagen)

Everyone is connected in the SciDAC NUCLEI Network



Graphic by Rusty Lusk

How NUCLEI competes for INCITE resources: Workflow of NUCLEI efforts within INCITE

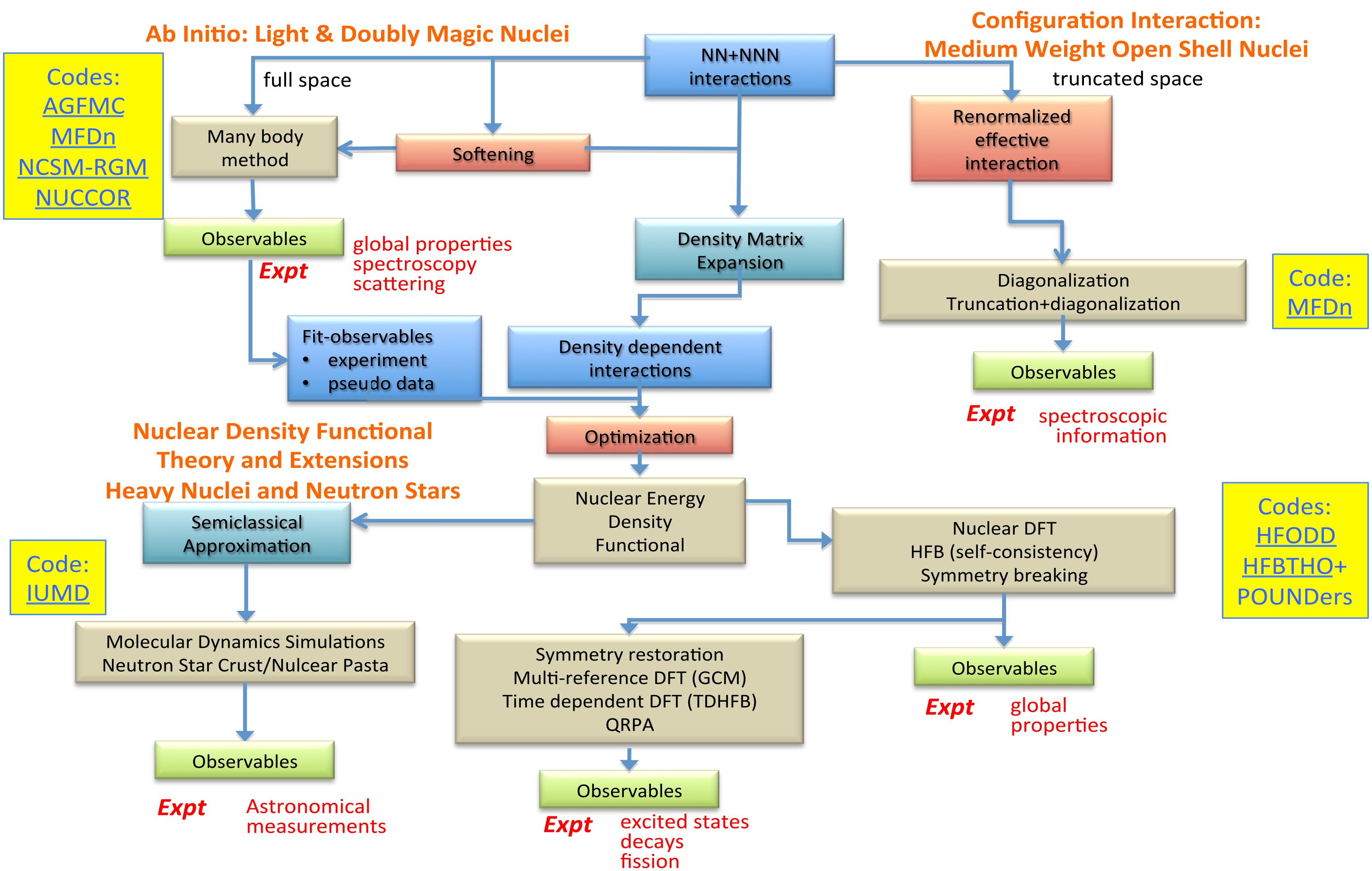


Table I. Primary applications used for INCITE production runs

Application	Production Run Sizes	Resource	Motif			Programming
			Dense Linear Alg.	Sparse Linear Alg.	Monte Carlo	Languages Libraries
AGFMC: Argonne Green's function Monte Carlo	260K cores @ 10 hrs	Mira			X	F90, MPI, OpenMP, ADLB
MFDn: Many-fermion dynamics – nuclear	360K cores @ 2 hrs 500K cores @ 1.5 hrs	Mira		X		F90, MPI, OpenMP, BLAS/LAPACK
NUCCOR: Nuclear coupled-cluster - Oak Ridge, m-scheme & spherical	100K cores @ 5 hrs (1 nucleus, multiple parameters)	Titan		X		F90, MPI, OpenMP, BLAS/LAPACK
DFTNESS: Density functional theory, mean-field methods	100K cores @ 10 hrs (entire mass table, fission barriers)	Titan	X			F90, MPI, OpenMP BLAS/LAPACK,BLACS, ScaLAPACK, ADIOS
MADNESS: Schrödinger, Lippman-Schwinger, DFT, TDSE/TDDFT, scattering	40K cores @ 12 hrs (extreme asymmetric functions)	Titan Mira	X	X		C++, MPI, pthreads BLAS, LAPACK, elemental, TBB
NCSM_RGM: Resonating group method for scattering; TRDENS support code	98K cores @ 8 hrs 48K cores @ 12 hrs	Titan	X	X		MPI, OpenMP
IUMD: Molecular Dynamics, nucleonic matter	2K GPUs @ 12 hrs	Titan				F2003, MPI, OpenMP, PGI CUDA Fortran
NLEFT: Nuclear lattice effective field theory	40K cores @ 6 hrs 2K GPUs @ 6 hrs	Titan			X	F90, MPI, OpenMP BLAS/LAPACK, PGI CUDA Fortran

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

Type: Renewal
Title: "Nuclear Structure and Nuclear Reactions"

Principal Investigator: James Vary, Iowa State University
Co-Investigator: Joseph Carlson, Los Alamos National Laboratory
Gaute Hagen, Oak Ridge National Laboratory
Pieter Maris, Iowa State University
Hai Ah Nam, Oak Ridge National Laboratory
Petr Navratil, TRIUMF
Witold Nazarewicz, University of Tennessee, Knoxville
Steven Pieper, Argonne National Laboratory
Nicolas Schunck, Lawrence Livermore National Laboratory

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation: **204,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (100,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (104,000,000 processor hours)

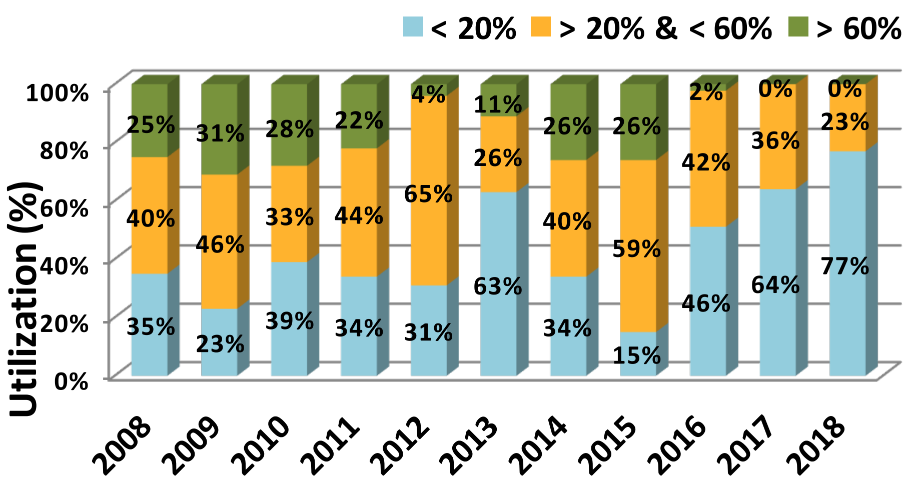
2015 Top awards by size of award
Rank and millions of cpu hours

1. 280 – Lattice QCD
2. 270 – Plasma Physics
3. **204 – Nuclear Physics**
4. (tie) 200 – Quantum Chemistry
4. (tie) 200 – Climate Science

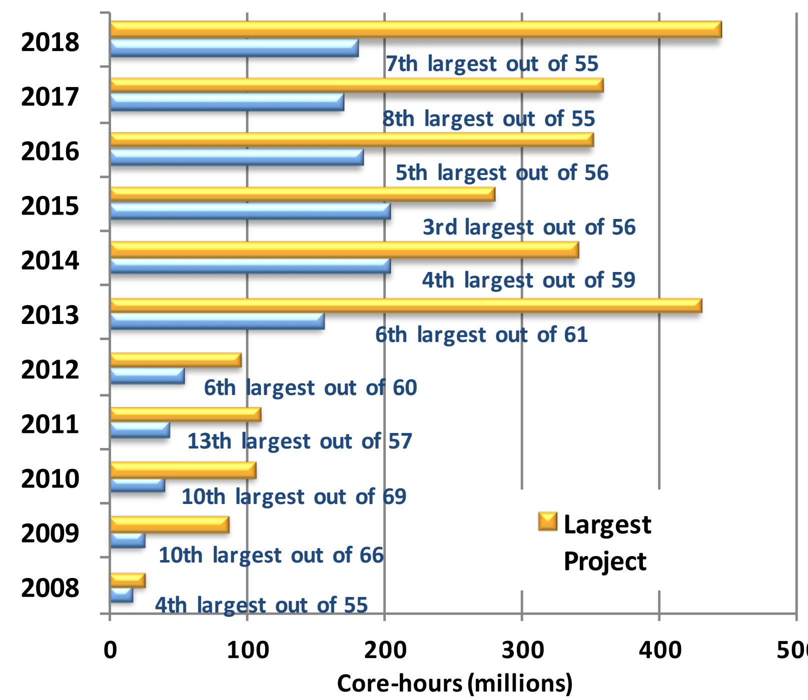
+ 51 more awards

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 the long lifetime of C-14
  - *Ab-initio* calculations of ^{78}Ni and ^{100}Sn
  - Improved energy-density functionals
  - Quantified the limits of nuclear existence



INCITE Allocation Trends 2008 – 2018



Contacts: G. Hagen, hageng@ornl.gov

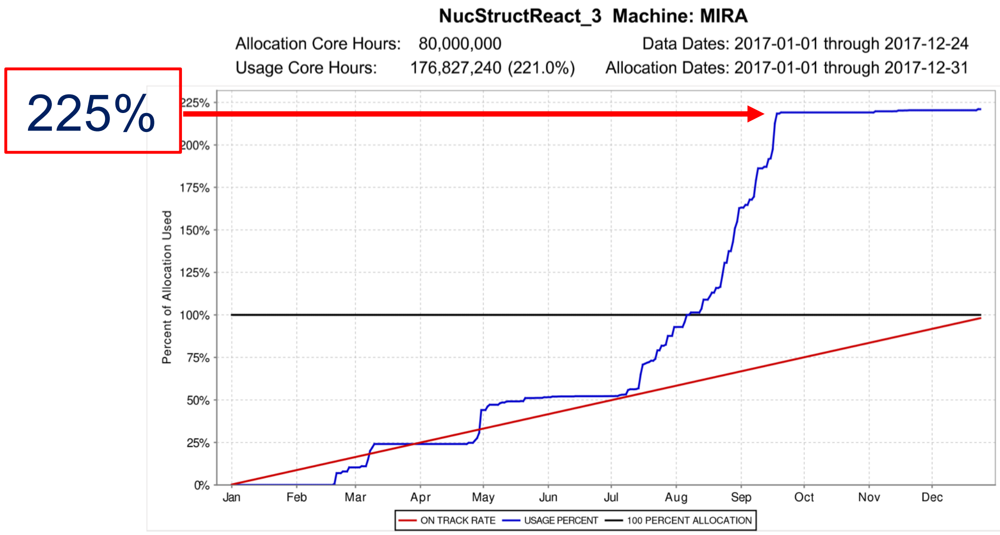
U.S. DEPARTMENT OF ENERGY

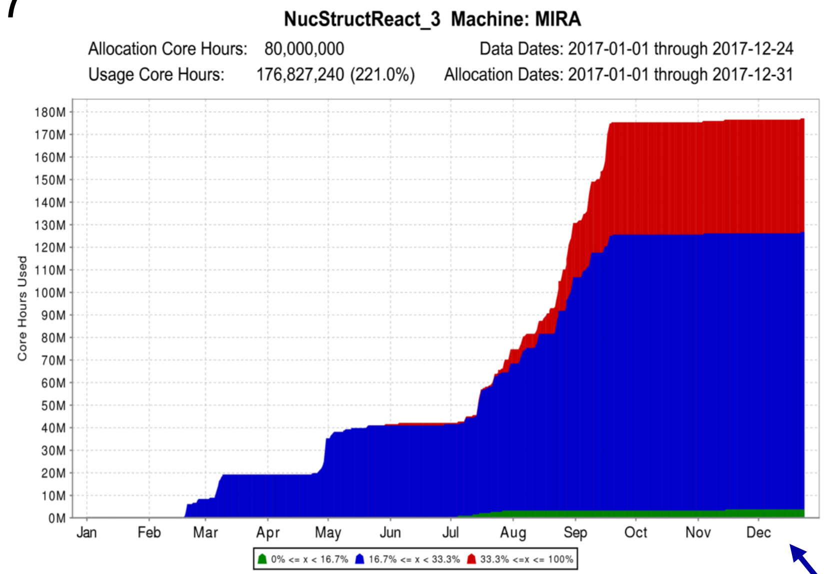
UNEDF

NUCLEI Nuclear Computational Low-Energy Initiative

Successful INCITE proposals and MIRA utilization

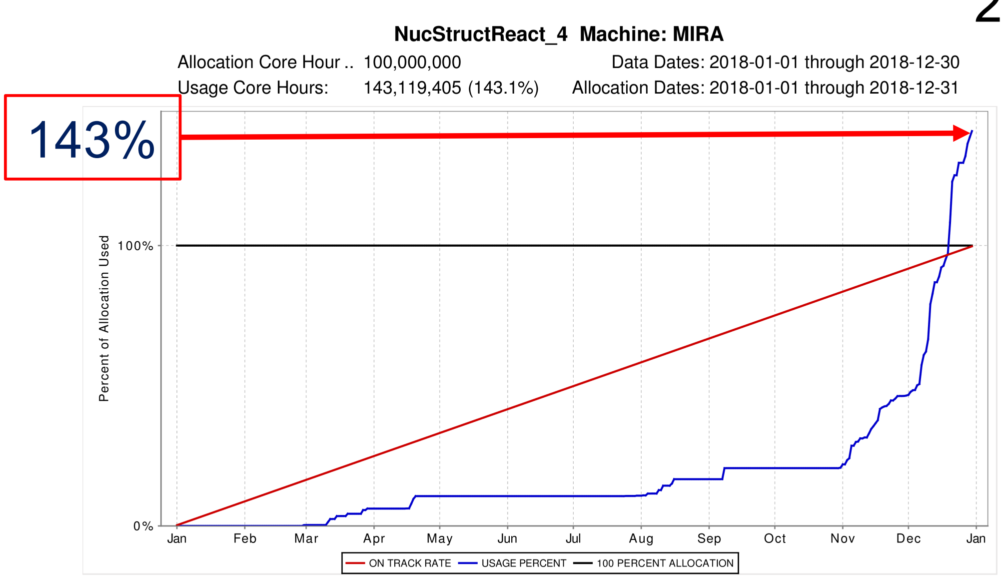
2017

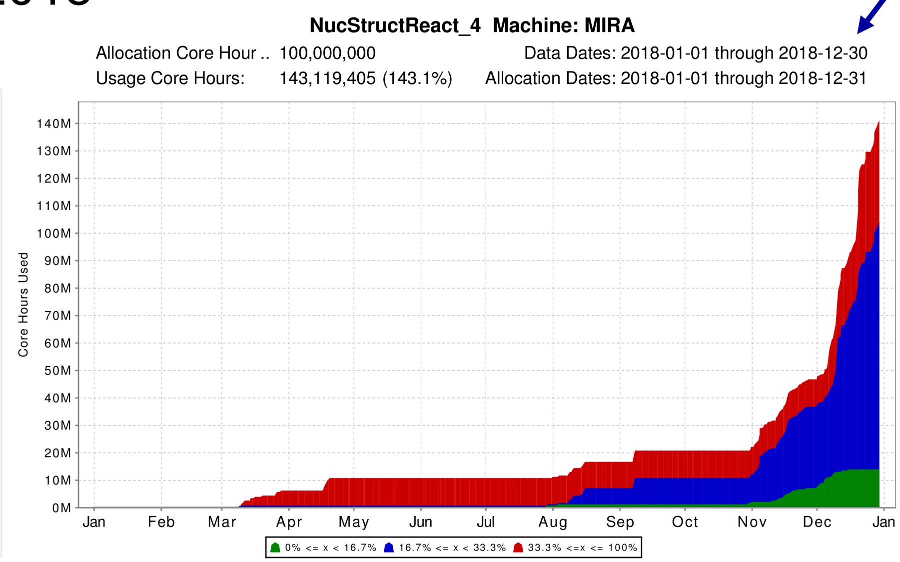




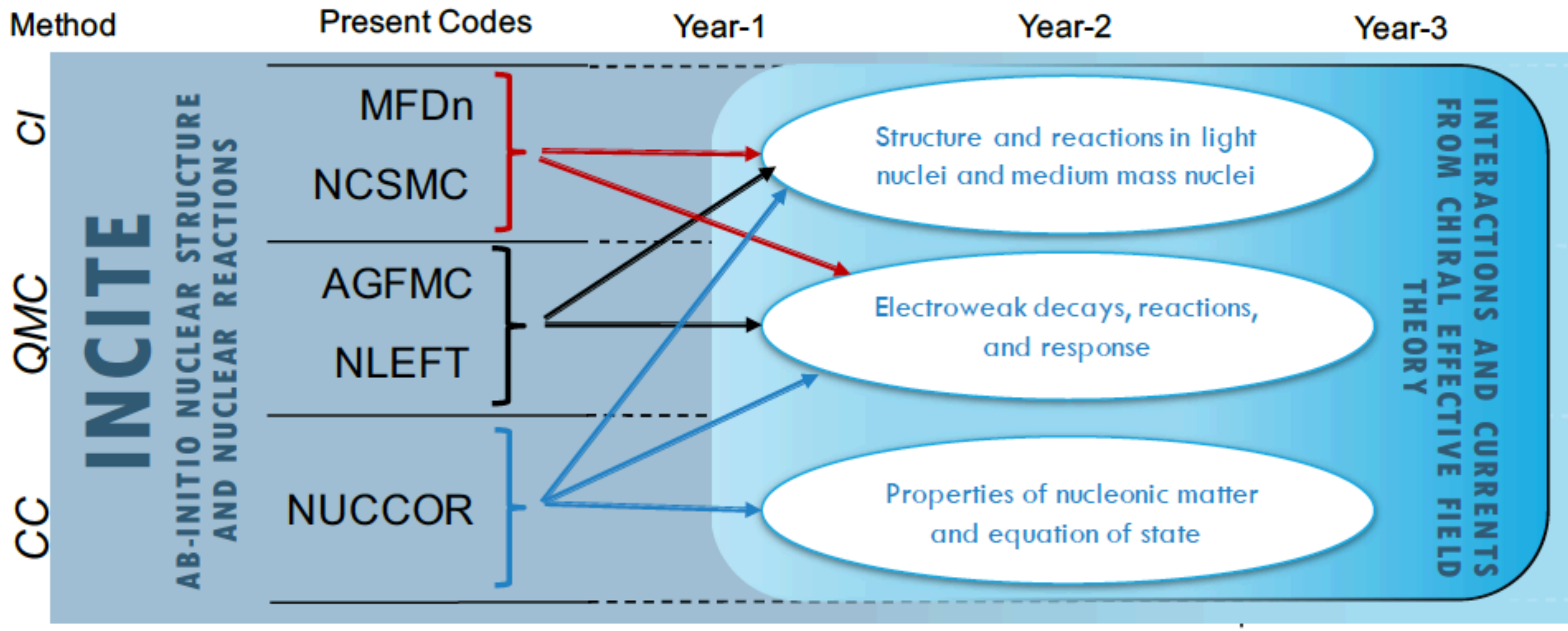
by job size

2018





INCITE 2019-2021 requested allocation



Number of Node Hours Requested if fully supported: 3.5M node hours on Titan, 3.5M node hours on Mira, 1405K node hours on Summit, and 4750K node hours on Theta over three years.

Number of Node Hours Requested if partially supported: 2.7M node hours on Titan, 3.5M node hours on Mira, 1177K node hours on Summit, and 3600K node hours on Theta over three years (see priorities in milestone tables).

Amount of Storage Requested: 243 TB of online mass storage and 587 TB of offline mass storage.

Closing Perspectives

We can all be proud of Steve Pieper's outstanding scientific achievements.

Personally, I also admired his first-rate scientific acumen, his unwavering ethical standards and his dedicated efforts to advance the entire field of Nuclear Physics on mulitiple fronts. **Thank you Steve!**