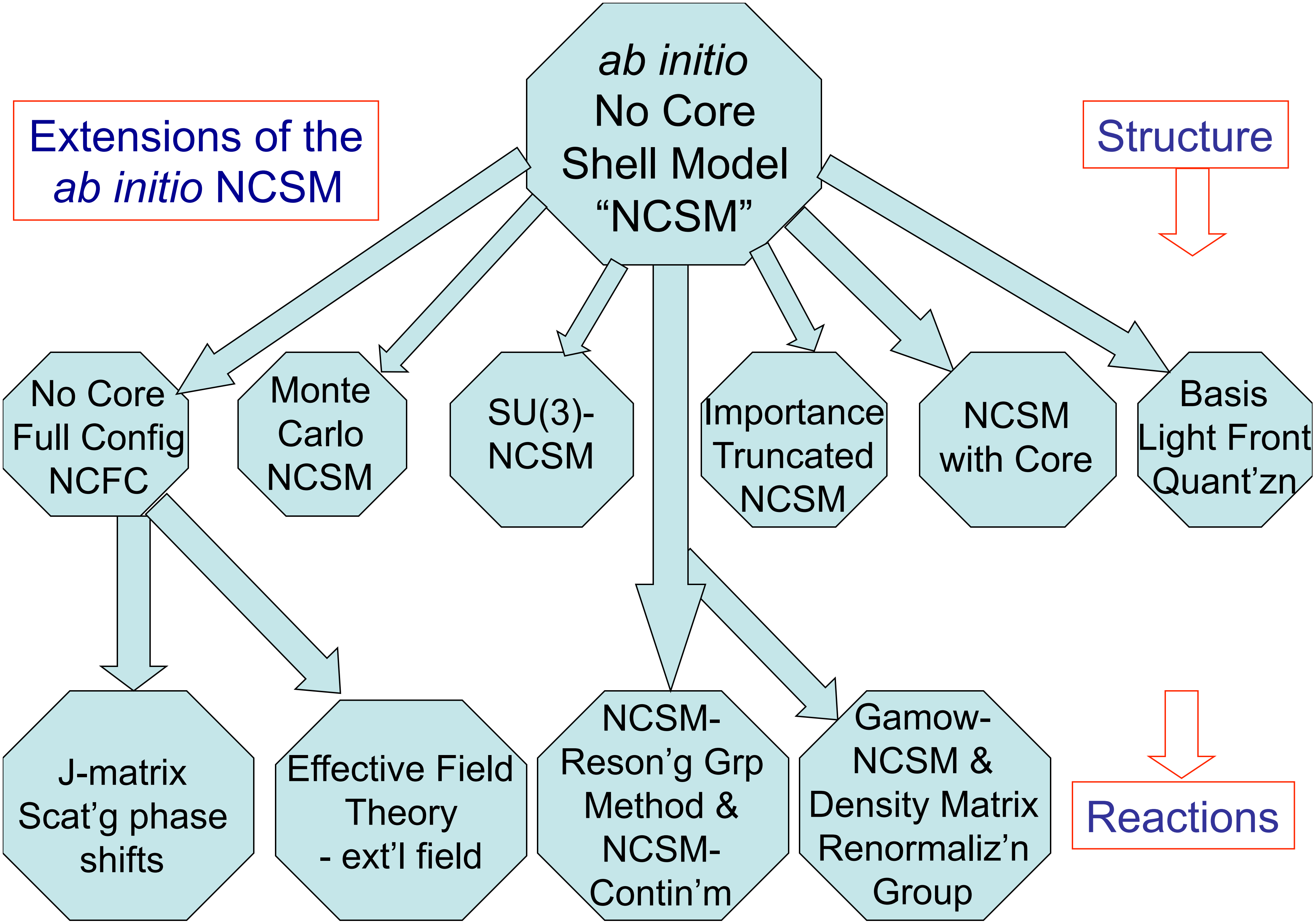
Computational Nuclear Physics Meeting
James P. Vary, Iowa State University, July 14, 2014

- **ab initio theory is entering new territory...**
  - **QCD frontier**
    nuclear structure connected systematically to QCD via chiral EFT
    and to the full Standard Model
  - **accuracy frontier**
    control uncertainties, improve convergence, inform extrapolations
  - **mass frontier**
    ab initio calculations up to heavy nuclei with quantified uncertainties
  - **open-shell frontier**
    extend to medium-mass open-shell nuclei and their excitation spectrum
  - **continuum & clustering frontier**
    include continuum & clustering effects for threshold states & nuclei
  - **reaction frontier**
    describe structure & reaction observables on the same footing

...providing a coherent theoretical framework for nuclear structure & reactions and linking it to experiment

Adapted from TRIUMF talk by Robert Roth February 2014

Extensions of the *ab initio* NCSM



ab initio
No Core
Shell Model
“NCSM”

Structure

No Core
Full Config
NCFC

Monte
Carlo
NCSM

SU(3)-
NCSM

Importance
Truncated
NCSM

NCSM
with Core

Basis
Light Front
Quant’zn

J-matrix
Scat’g phase
shifts

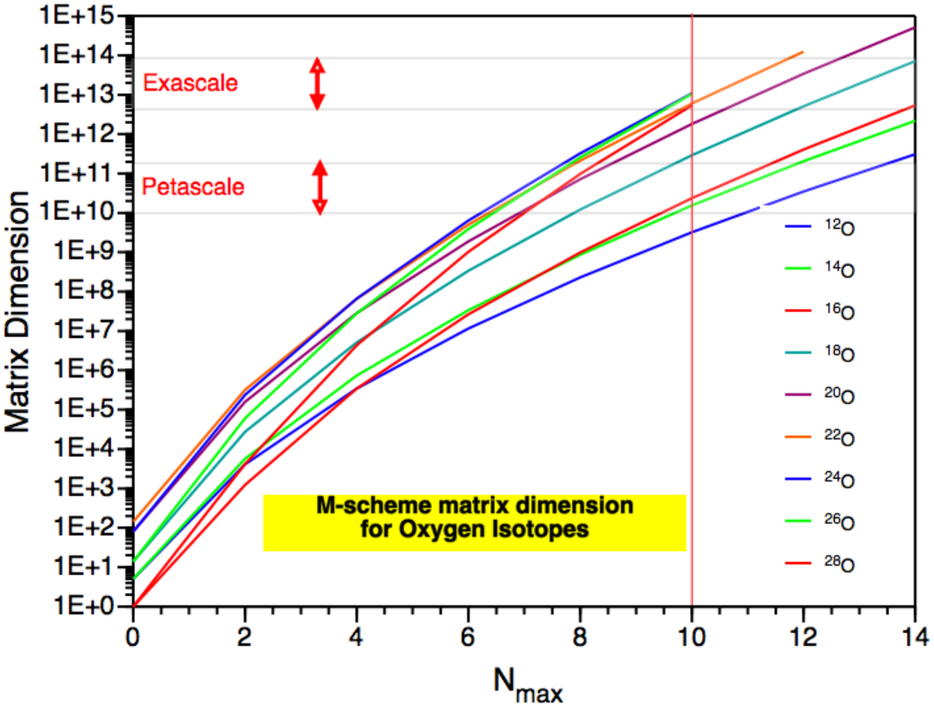
Effective Field
Theory
- ext’l field

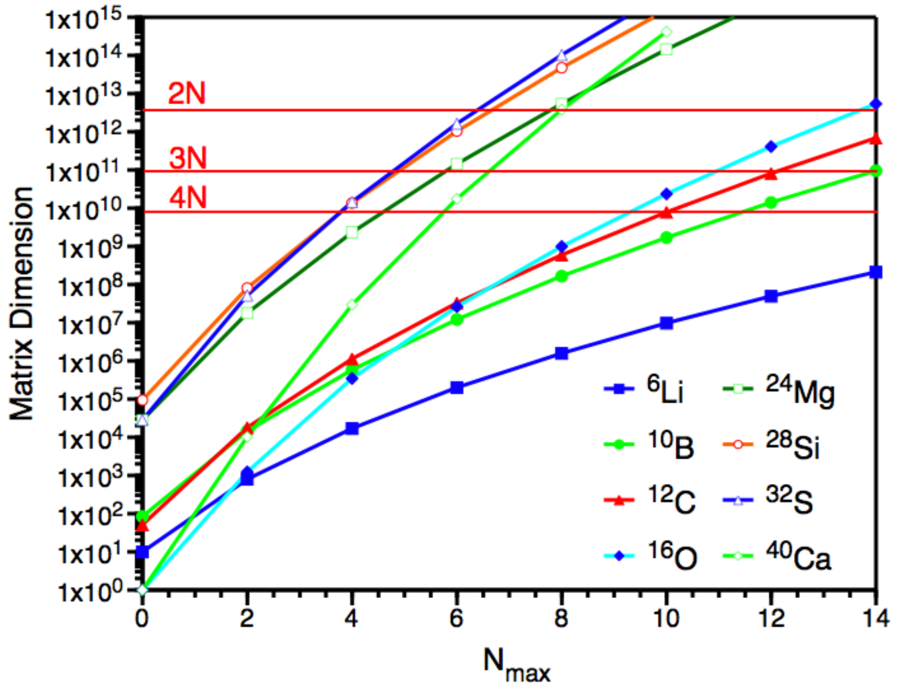
NCSM-
Reson’g Grp
Method &
NCSM-
Contin’m

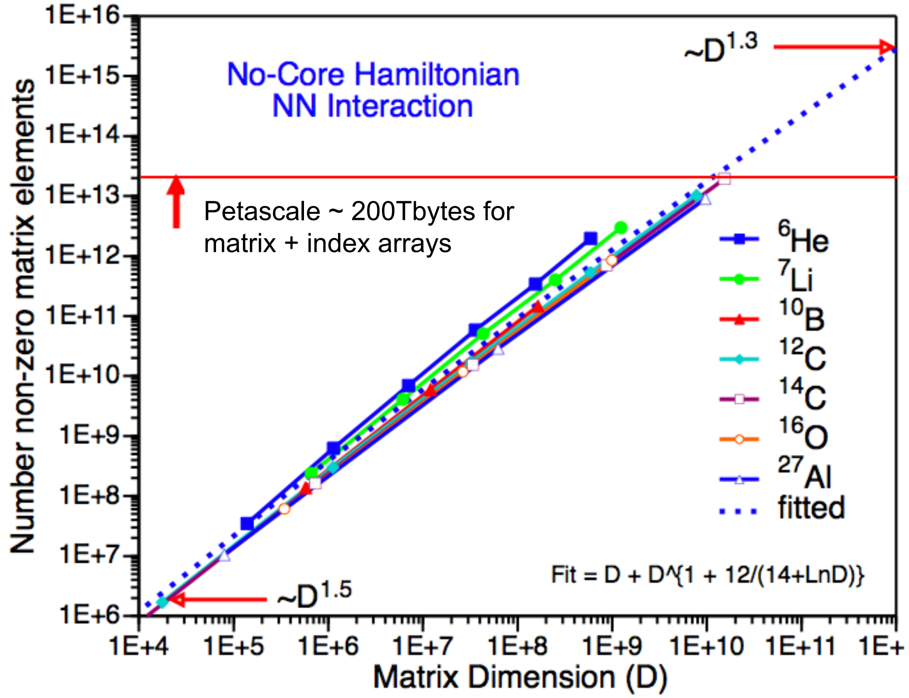
Gamow-
NCSM &
Density Matrix
Renormaliz’n
Group

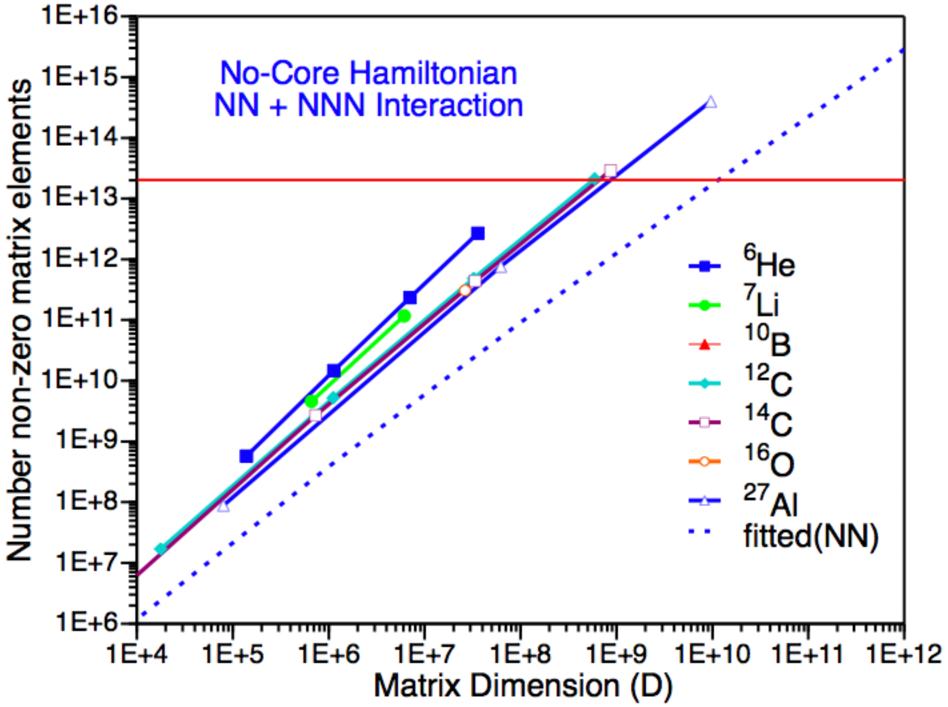
Reactions

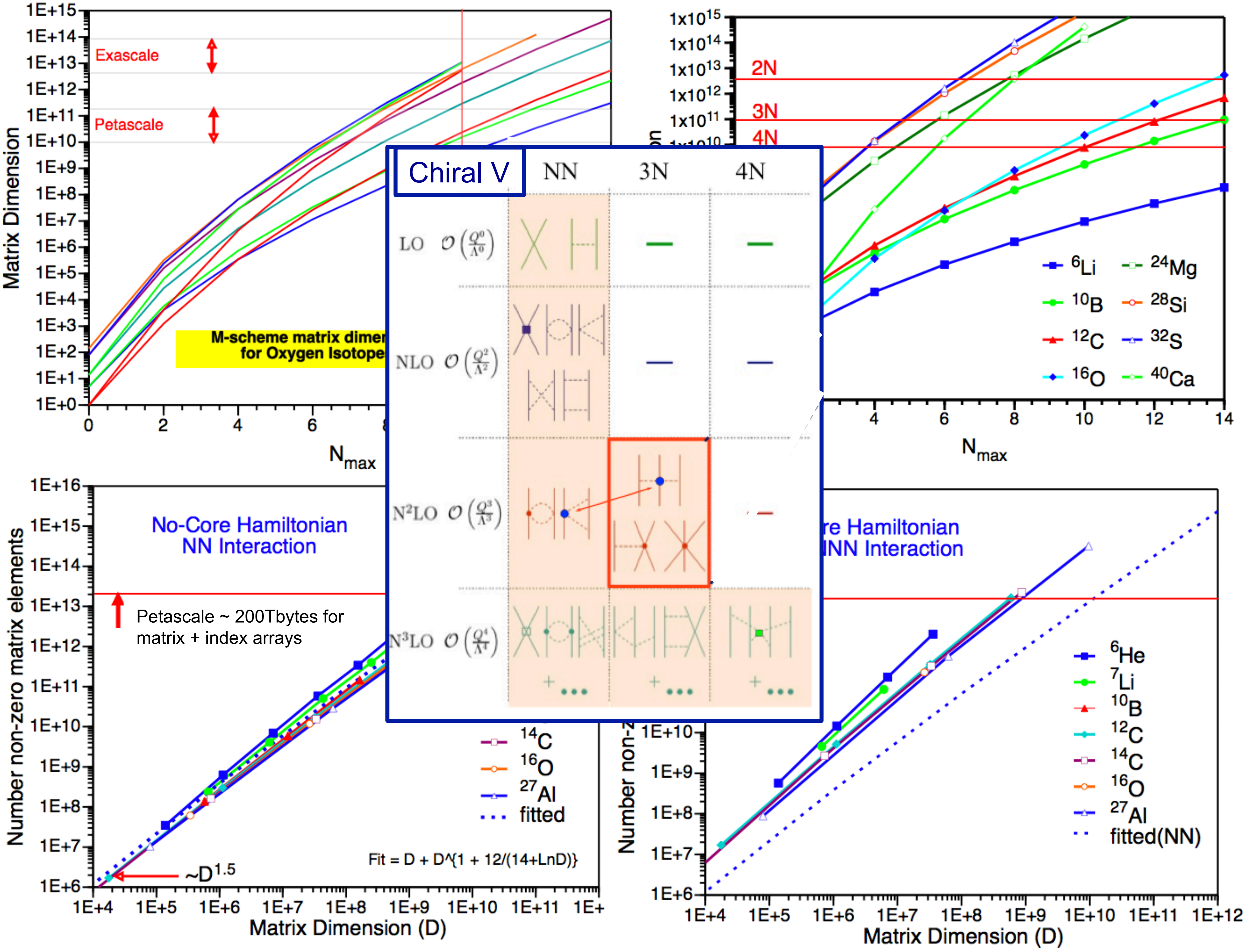
J.P. Vary, NTSE-2013 Proceedings


M-scheme matrix dimension
for Oxygen Isotopes
Exascale
Petascale
Matrix Dimension
N_{max}
1E+0
1E+1
1E+2
1E+3
1E+4
1E+5
1E+6
1E+7
1E+8
1E+9
1E+10
1E+11
1E+12
1E+13
1E+14
1E+15
0
2
4
6
8
10
12
14
^{12}O
^{14}O
^{16}O
^{18}O
^{20}O
^{22}O
^{24}O
^{26}O
^{28}O


Matrix Dimension
N_{max}
2N
3N
4N
$1x10^{0}$
$1x10^{1}$
$1x10^{2}$
$1x10^{3}$
$1x10^{4}$
$1x10^{5}$
$1x10^{6}$
$1x10^{7}$
$1x10^{8}$
$1x10^{9}$
$1x10^{10}$
$1x10^{11}$
$1x10^{12}$
$1x10^{13}$
$1x10^{14}$
$1x10^{15}$
0
2
4
6
8
10
12
14
^{6}Li
^{10}B
^{12}C
^{16}O
^{24}Mg
^{28}Si
^{32}S
^{40}Ca


No-Core Hamiltonian
NN Interaction
$\sim D^{1.3}$
Petascale ~ 200Tbytes for
matrix + index arrays
$\sim D^{1.5}$
Fit = D + D^{1 + 12/(14+LnD)}
Number non-zero matrix elements
Matrix Dimension (D)
1E+6
1E+7
1E+8
1E+9
1E+10
1E+11
1E+12
1E+13
1E+14
1E+15
1E+16
1E+4
1E+5
1E+6
1E+7
1E+8
1E+9
1E+10
1E+11
1E+
^{6}He
^{7}Li
^{10}B
^{12}C
^{14}C
^{16}O
^{27}Al
fitted


No-Core Hamiltonian
NN + NNN Interaction
Number non-zero matrix elements
Matrix Dimension (D)
1E+6
1E+7
1E+8
1E+9
1E+10
1E+11
1E+12
1E+13
1E+14
1E+15
1E+16
1E+4
1E+5
1E+6
1E+7
1E+8
1E+9
1E+10
1E+11
1E+12
^{6}He
^{7}Li
^{10}B
^{12}C
^{14}C
^{16}O
^{27}Al
fitted(NN)


Matrix Dimension
1E+15
1E+14
1E+13
1E+12
1E+11
1E+10
1E+9
1E+8
1E+7
1E+6
1E+5
1E+4
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1E+2
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M-scheme matrix dimen
for Oxygen Isotope
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$1x10^{15}$
$1x10^{14}$
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$1x10^{11}$
2N
3N
4N
^{6}Li
^{24}Mg
^{10}B
^{28}Si
^{12}C
^{32}S
^{16}O
^{40}Ca
4
6
8
10
12
14
N_{max}
Chiral V
NN
3N
4N
LO $\mathcal{O}\left(\frac{Q^0}{\Lambda^0}\right)$
NLO $\mathcal{O}\left(\frac{Q^2}{\Lambda^2}\right)$
N^{2}LO $\mathcal{O}\left(\frac{Q^3}{\Lambda^3}\right)$
N^{3}LO $\mathcal{O}\left(\frac{Q^4}{\Lambda^4}\right)$
+ ...
+ ...
+ ...
Number non-zero matrix elements
1E+16
1E+15
1E+14
1E+13
1E+12
1E+11
1E+10
1E+9
1E+8
1E+7
1E+6
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Fit = D + D^{1 + 12/(14+LnD)}
1E+4
1E+5
1E+6
1E+7
1E+8
1E+9
1E+10
1E+11
1E+
Matrix Dimension (D)
re Hamiltonian
NN Interaction
Number non-z
1E+10
1E+9
1E+8
1E+7
1E+6
^{6}He
^{7}Li
^{10}B
^{12}C
^{14}C
^{16}O
^{27}Al
fitted(NN)
1E+4
1E+5
1E+6
1E+7
1E+8
1E+9
1E+10
1E+11
1E+12
Matrix Dimension (D)

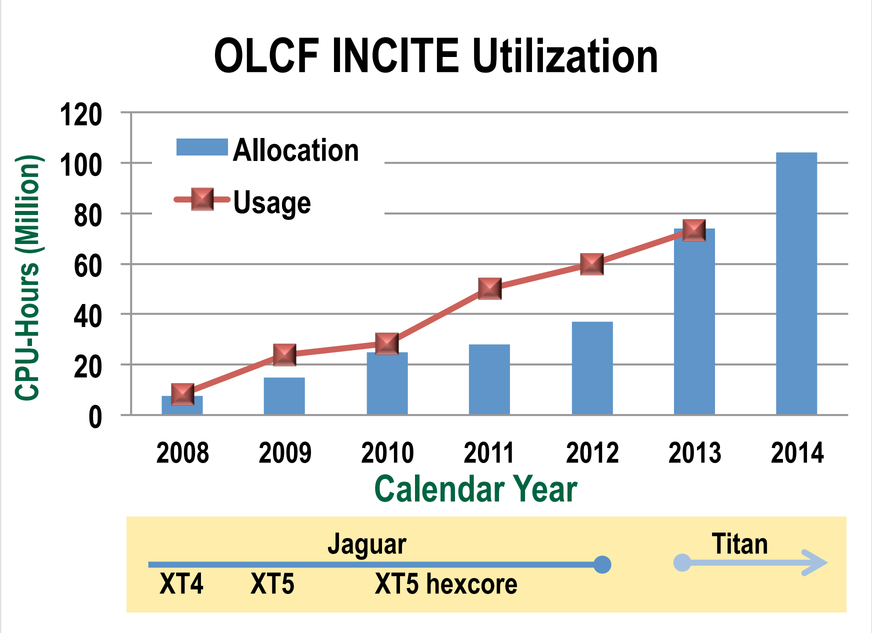
Low-energy nuclear physics & HPC

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

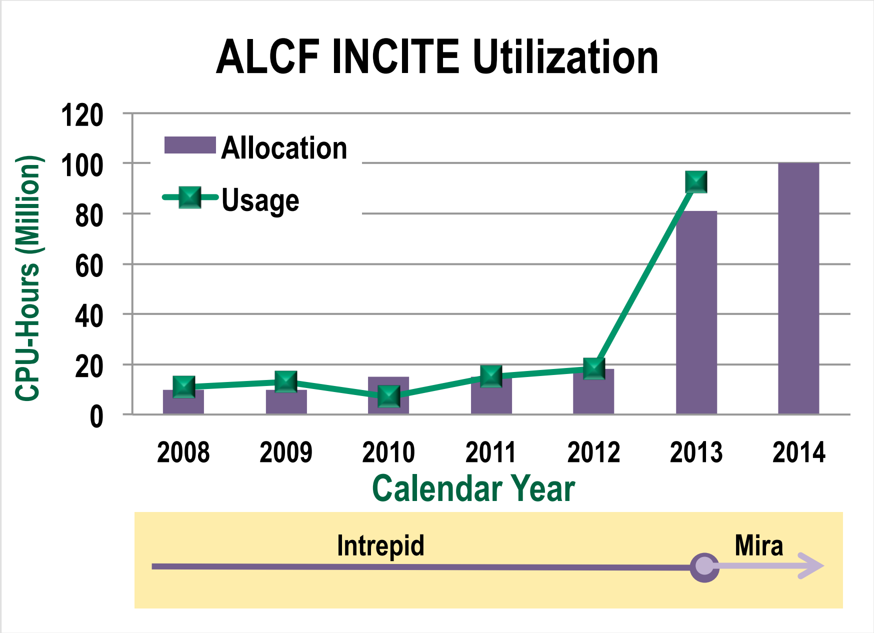
- **INCITE Awards**
  - **(2008 – 2010) PI: D. J. Dean (ORNL)**
    H. Nam (ORNL), W. Nazarewicz (UTK/ORNL), S. Pieper (ANL), J. P. Vary (ISU)
  - **(2011 – 2013) PI: J. P. Vary (ISU)**
    P. Maris (ISU), J. Carlson (LANL), H. Nam (ORNL), P. Navratil (TRIUMF), W. Nazarewicz (UTK/ORNL), S. Pieper (ANL), N. Schunck (LLNL)
  - **(2014 – 2016) PI: J. P. Vary (ISU)**
    P. Maris (ISU), J. Carlson (LANL), H. Nam, G. Hagen (ORNL), P. Navratil (TRIUMF), W. Nazarewicz (UTK/ORNL), S. Pieper (ANL), N. Schunck (LLNL)

Supports ~ 40 users

- **2 Early Science Awards**
  - **2009 – Jaguar XT5, 30 Million hours**
    Origin of the Anomalous Long Lifetime of ^{14}C
    Physical Review Letters 106, 202502 (2011)
  - **2012 – Mira, 110 Million hours**
    Ab Initio Reaction Calculations for Carbon-12
    Charge Form Factor and Sum Rules of Electromagnetic Response Functions in ^{12}C
    Physical Review Letters 111, 092501 (2013)



OLCF INCITE Utilization

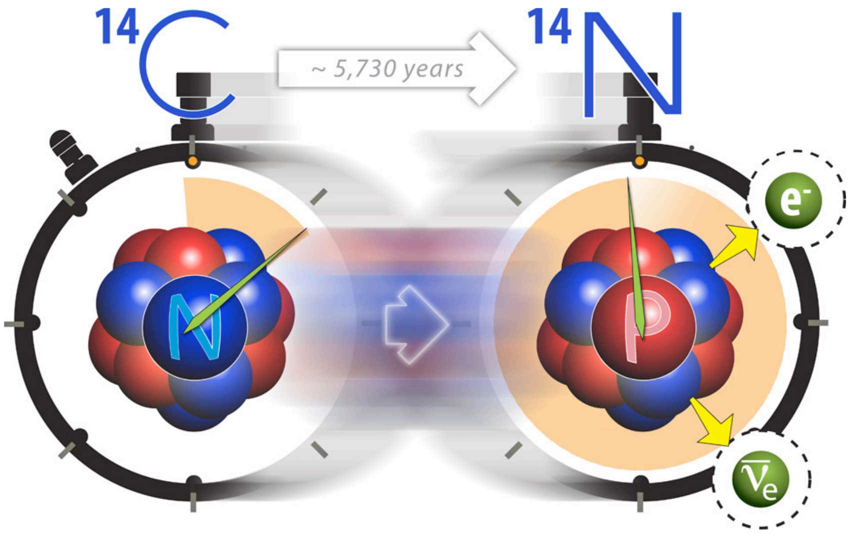


ALCF INCITE Utilization

U.S. DEPARTMENT OF ENERGY | Office of Science

"Why does Carbon-14 live so long?"

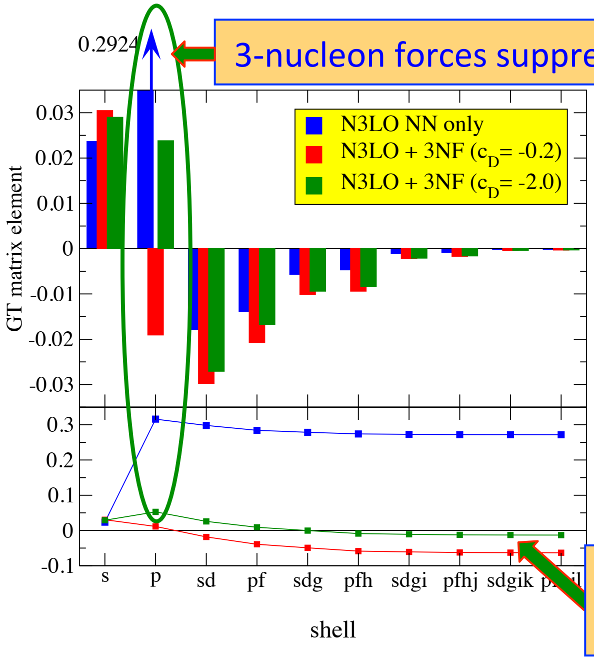
Carbon-14 dating relies on ~5,730 year half-life, but other light nuclei undergo similar beta decay with half-lives less than a day!



UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

- Members of UNEDF collaboration made microscopic nuclear structure calculations to solve the puzzle
- Used systematic chiral Hamiltonian from low-energy effective field theory of QCD
- Key feature: consistent *3-nucleon* interactions

3-nucleon forces suppress critical component compared to 2-nucleon forces only



net decay rate is very small

- Solutions of ^{14}C and ^{14}N through Hamiltonian diagonalization
- 100-fold reduction in Gamow-Teller transition matrix element

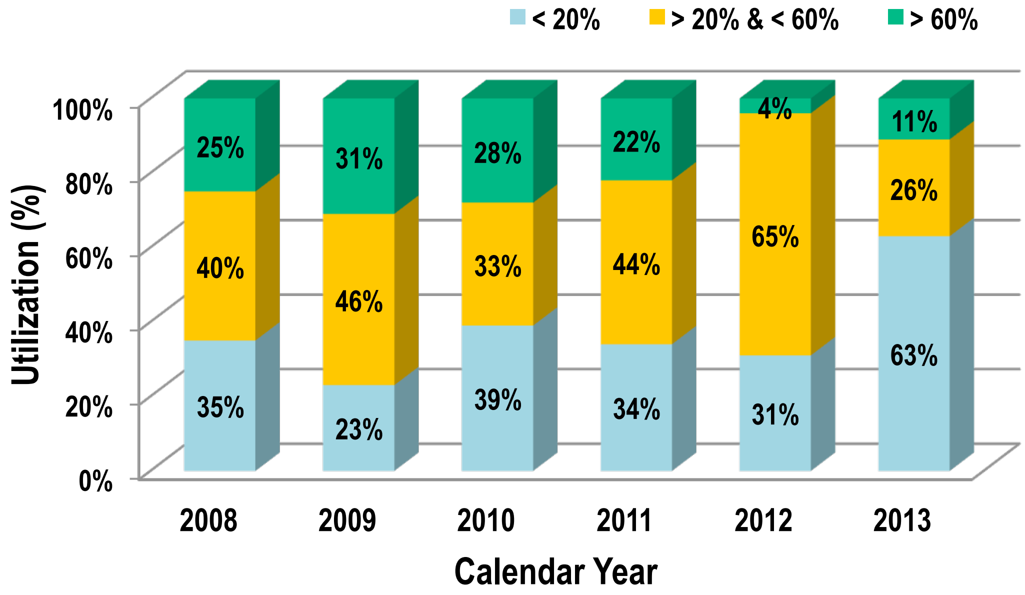
Calculations enabled by high-performance computing through INCITE program

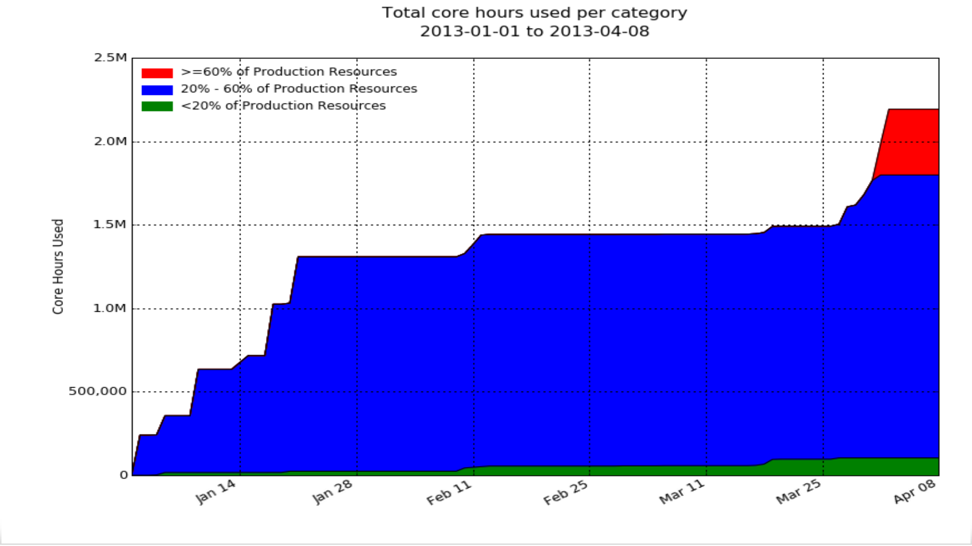
- Dimension of matrix solved for 8 lowest states: ~ 1×10^9
- Solution takes ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL

INCITE
Advancing America's Science and Industrial Competitiveness

Science ref.: Physical Review Letters **106**, 202502 (2011)
Computational ref.: Procedia Computer Science **1**, 97 (2010)

NP Utilization @ Leadership Class



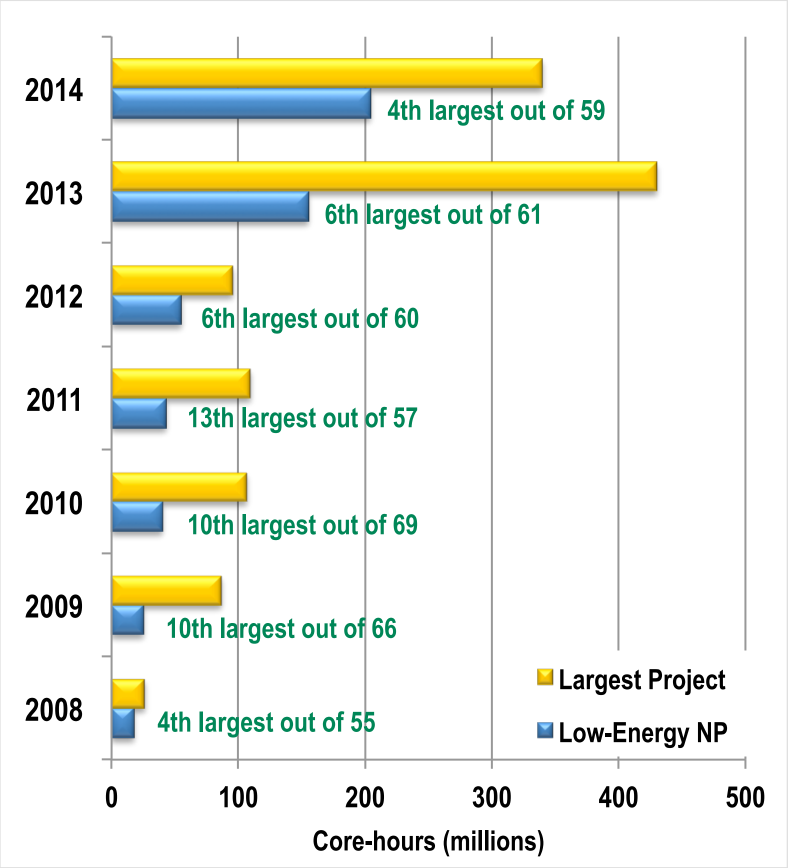


- Titan
  (18,688 nodes = 299,008 CPU-cores + 261,632 GPU-cores)
  - 20% = 3738 nodes = 59,808 CPU-cores
- Mira
  (48k nodes = 786k cores)
  - 20% = 9600 nodes = 153,600 cores

Low Energy NP Application Areas

Application	Production Run Sizes	Resource	Dense Linear Alg.	Sparse Linear Alg.	Monte Carlo
AGFMC: Argonne Green's Function Monte Carlo	262,144 cores @ 10 hrs	Mira			X
MFDn: Many Fermion Dynamics - nuclear	260K cores @ 4 hrs 500K cores @ 1.33 hrs	Titan Mira		X	
NUCCOR: Nuclear Coupled-Cluster Oak Ridge, m-scheme & spherical	100K cores @ 5 hrs (1 nucleus, multiple parameters)	Titan		X	
DFT Code Suite: Density Functional Theory, mean-field methods	100K cores @ 10 hrs (entire mass table, fission barriers)	Titan	X		
MADNESS: Schroedinger, Lippman-Schwinger and DFT	40,000 cores @ 12 hrs (extreme asymmetric functions)	Titan	X	X	
NCSM_RGM: Resonating Group Method for scattering	98,304 cores @ 8 hrs	Titan	X	X	

- Ab initio Methods (CC, GFMC, NCSM) → pushing the limits to calculate larger nuclei
- Density Functional Theory → reasonable time to solution to calculate the entire mass table



2014 Case Studies: ab initio Nuclear Structure ab initio Nuclear Reactions

	ab initio Nuclear Structure		ab initio Nuclear Reactions	
	Used at NERSC in 2013	**Needed at NERSC in 2017**	**Used at NERSC in 2013**	**Needed at NERSC in 2017**
Computational Hours	27 (mostly Edison pre-acceptance usage)	96	~12M (Edison early users)	75M
Typical number of cores* used for production runs	From 5% to full machine	From 5% to full machine	4,800 to 14,400 (3% to 10% of machine)	28,800 to 60,000 (20% to 45% of machine)
Maximum number of cores* that can be used for production runs	Full machine	Full machine	28,800 (20% of machine)	Full machine
Data read and written per run	< 1 TB	< 1 TB	<1TB	< 1TB
Maximum I/O bandwidth	Not known	Not known	Not known	Not known
Percent of runtime for I/O	< 5%	< 5%	<5%	<5%
Scratch File System space	1 TB	3 TB	1 TB	4 TB
Shared filesystem space	2 TB	8 TB	2 TB	8 TB
Archival data	5 TB	50 TB	Not used	30 TB
Memory per node	All available GB	Maximum possible GB	All available memory	All available memory
Aggregate memory	Full machine	Full machine	<38 TB	Typical: 160 TB

Adapted from Case Studies presented to NERSC May 2014:
James P. Vary, “ab initio Nuclear Structure”
http://www.nersc.gov/assets/HPC-Requirements-for-Science/NP2017/VaryNPStructureApril2014.pdf
Sofia Quaglioni, “ab initio Calculations of Nuclear Reactions and Exotic Nuclei”
http://www.nersc.gov/assets/HPC-Requirements-for-Science/NP2017/Quaglioni.pdf

BACKUP SLIDES

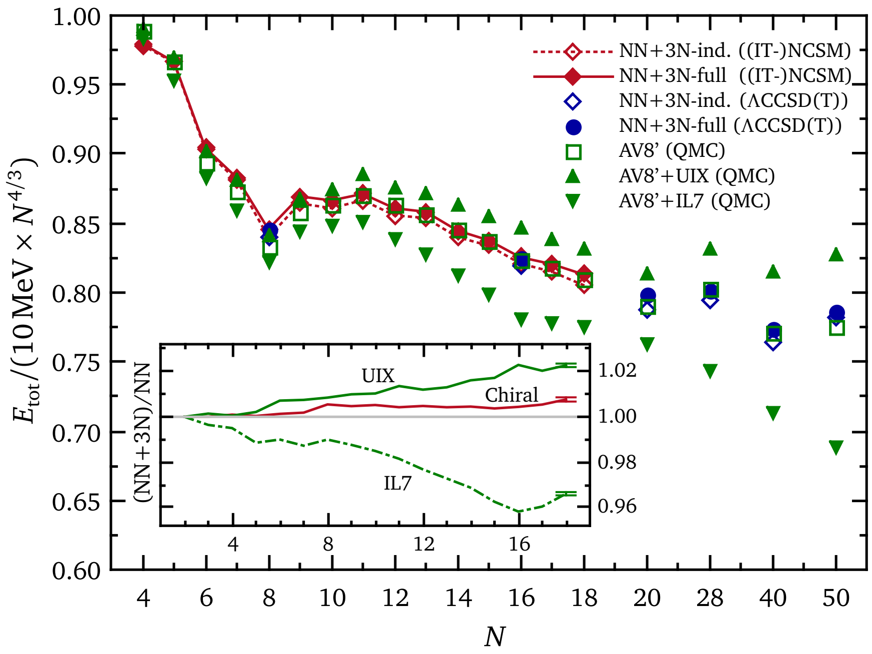
Ab initio Extreme Neutron Matter

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

U.S. DEPARTMENT OF ENERGY | Office of Science

NUCLEI
Nuclear Computational Low-Energy Initiative

References: 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, arXiv:1406.1160; Contact: jvary@iastate.edu

Calculation of three-body forces at N^3LO

Low
Energy
Nuclear
Physics
International
Collaboration

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

Goal

Calculate matrix elements of 3NF in a partial-wave decomposed form which is suitable for different few- and many-body frameworks

Challenge

Due to the large number of matrix elements, the calculation is extremely expensive.

Strategy

Develop an efficient code which allows to treat arbitrary local 3N interactions.
(Krebs and Hebeler)

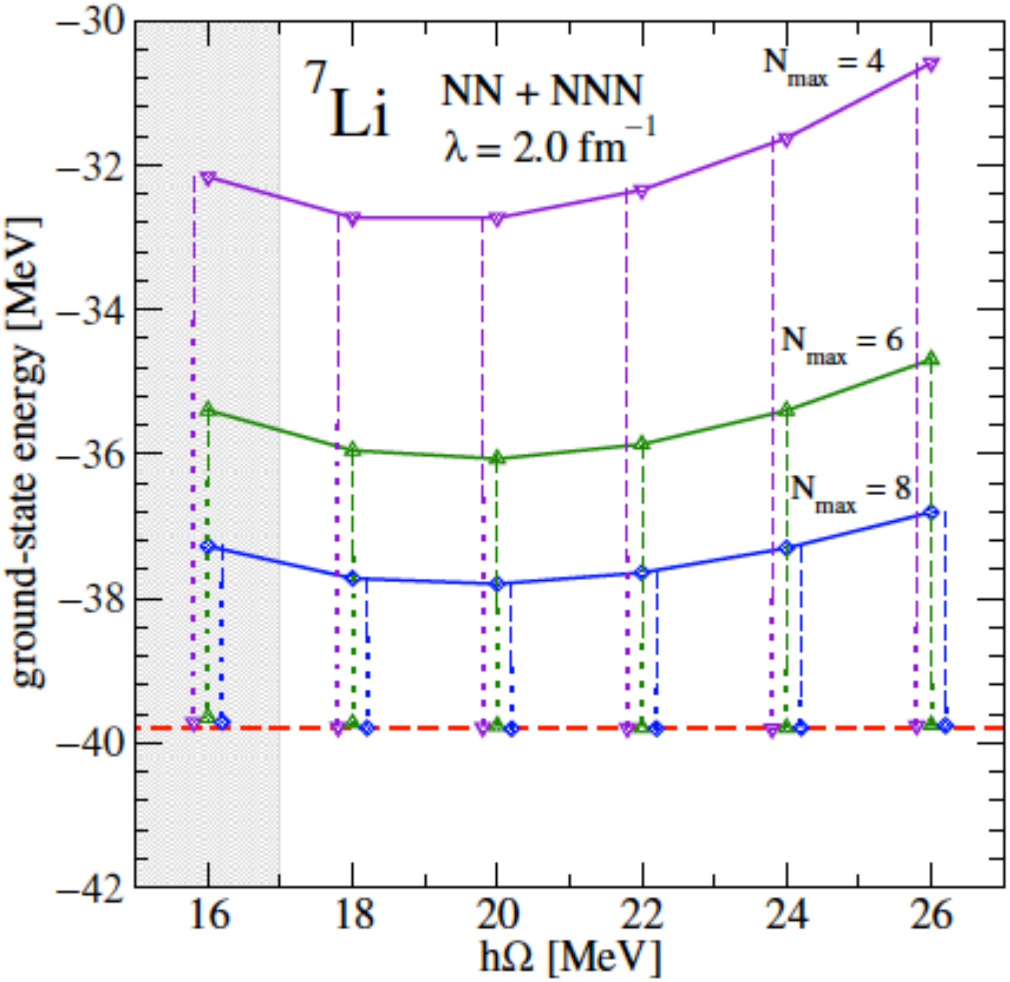


FIG. 17. (color online) Ground-state energy of ^{7}Li for the NN+NNN evolved Hamiltonians at $\lambda = 2.0\,\mathrm{fm}^{-1}$, with IR (vertical dashed) and UV (vertical dotted) corrections from Eq. (5) that add to predicted E_∞ values (points near the horizontal dashed line, which is the global E_∞).

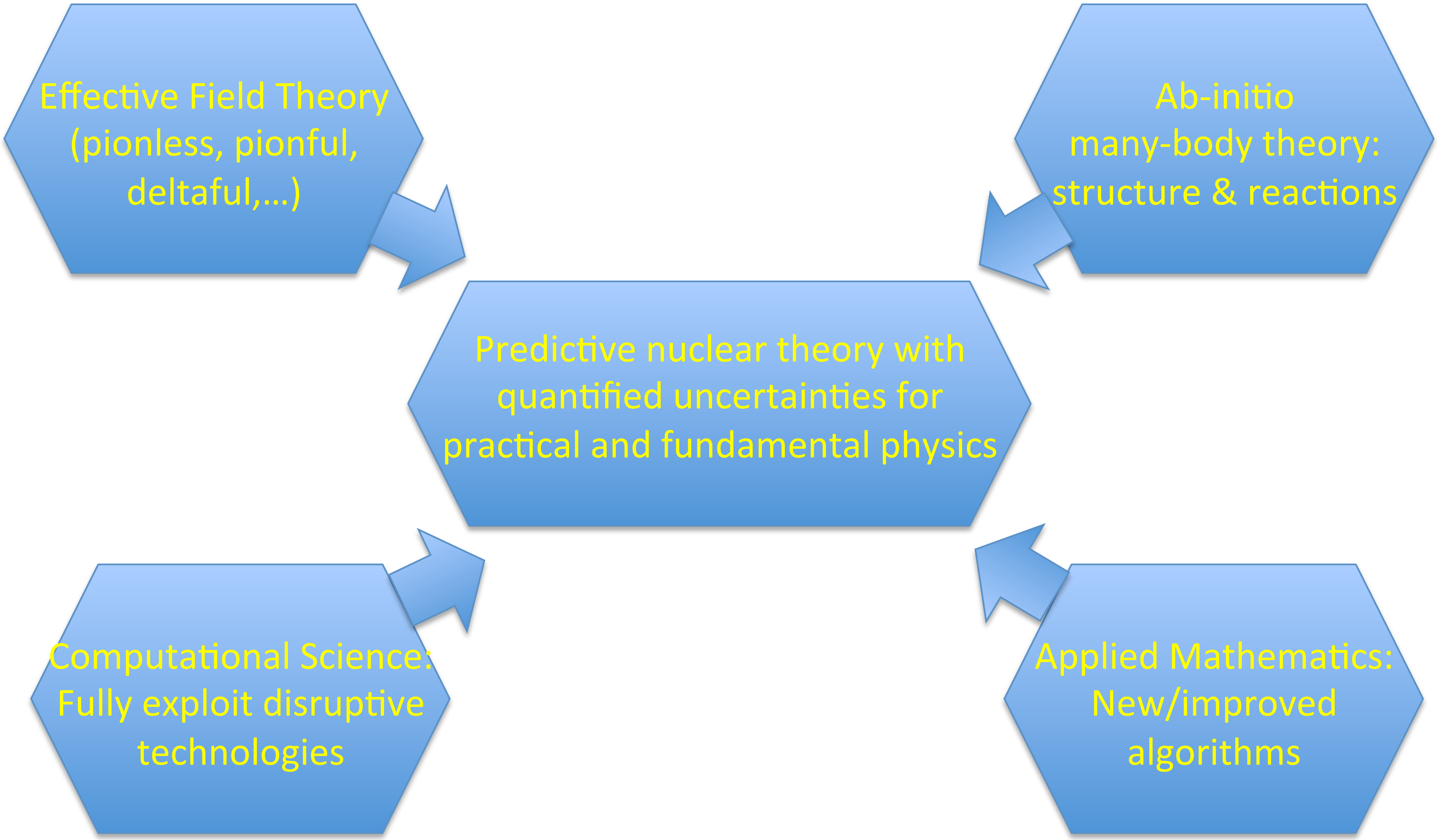
E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary, Phys. Rev. C. 87, 054312 (2013); arXiv: 1302:5473

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

Discovery potential increases geometrically

Many outstanding nuclear physics puzzles and discovery opportunities

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!



Effective Field Theory (pionless, pionful, deltaful,…)

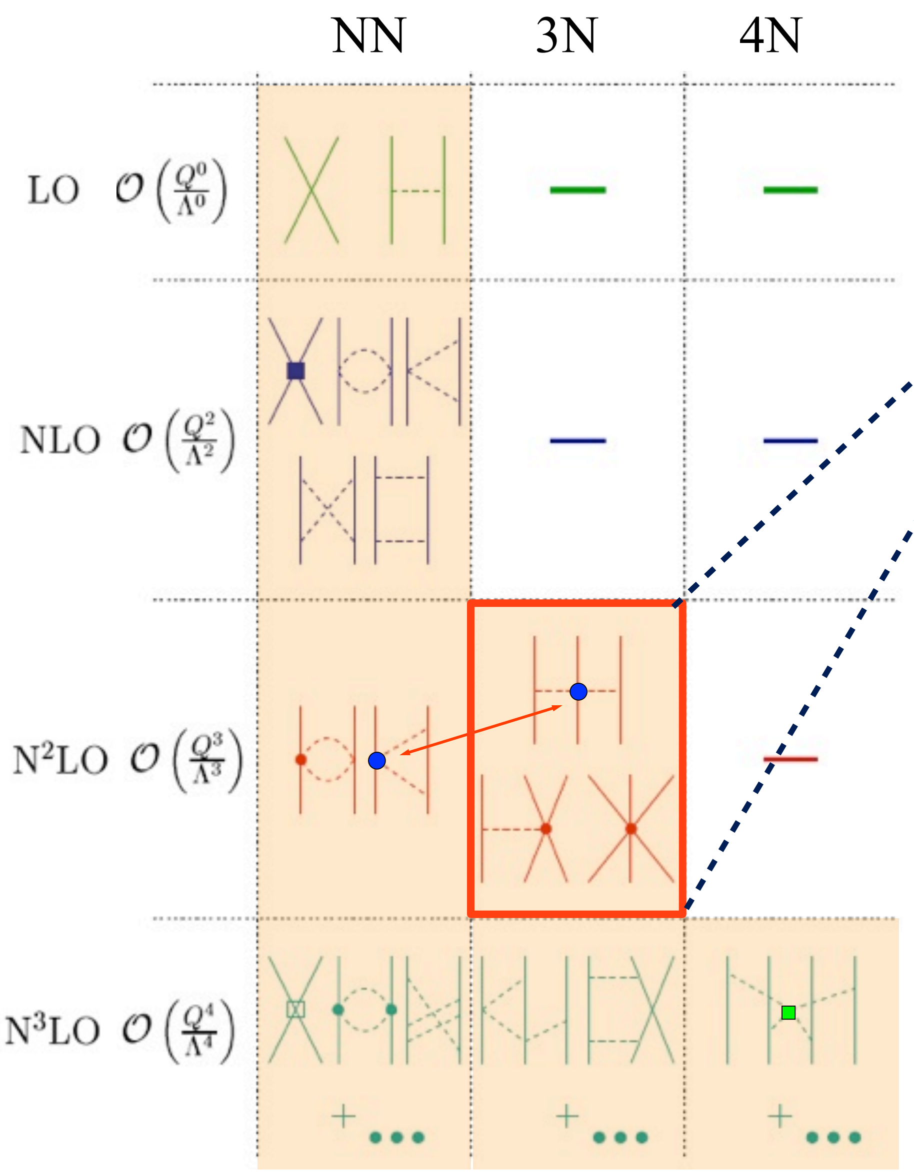
Ab-initio many-body theory: structure & reactions

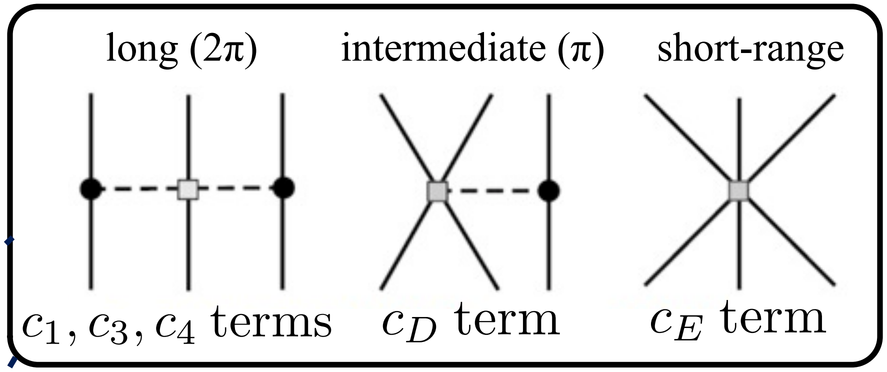
Predictive nuclear theory with quantified uncertainties for practical and fundamental physics

Computational Science: Fully exploit disruptive technologies

Applied Mathematics: New/improved algorithms

Chiral EFT for nuclear forces, leading order 3N forces





large uncertainties in coupling constants at present:

$$c_1 = -0.9^{+0.2}_{-0.5}\ ,\ c_3 = -4.7^{+1.5}_{-1.0}\ ,\ c_4 = 3.5^{+0.5}_{-0.2}$$

lead to theoretical uncertainties in many-body observables

Adapted from Kai Hebeler, ECT* workshop May 2014