Ab initio Nuclear Theory:
the SINP-ISU Collaboration

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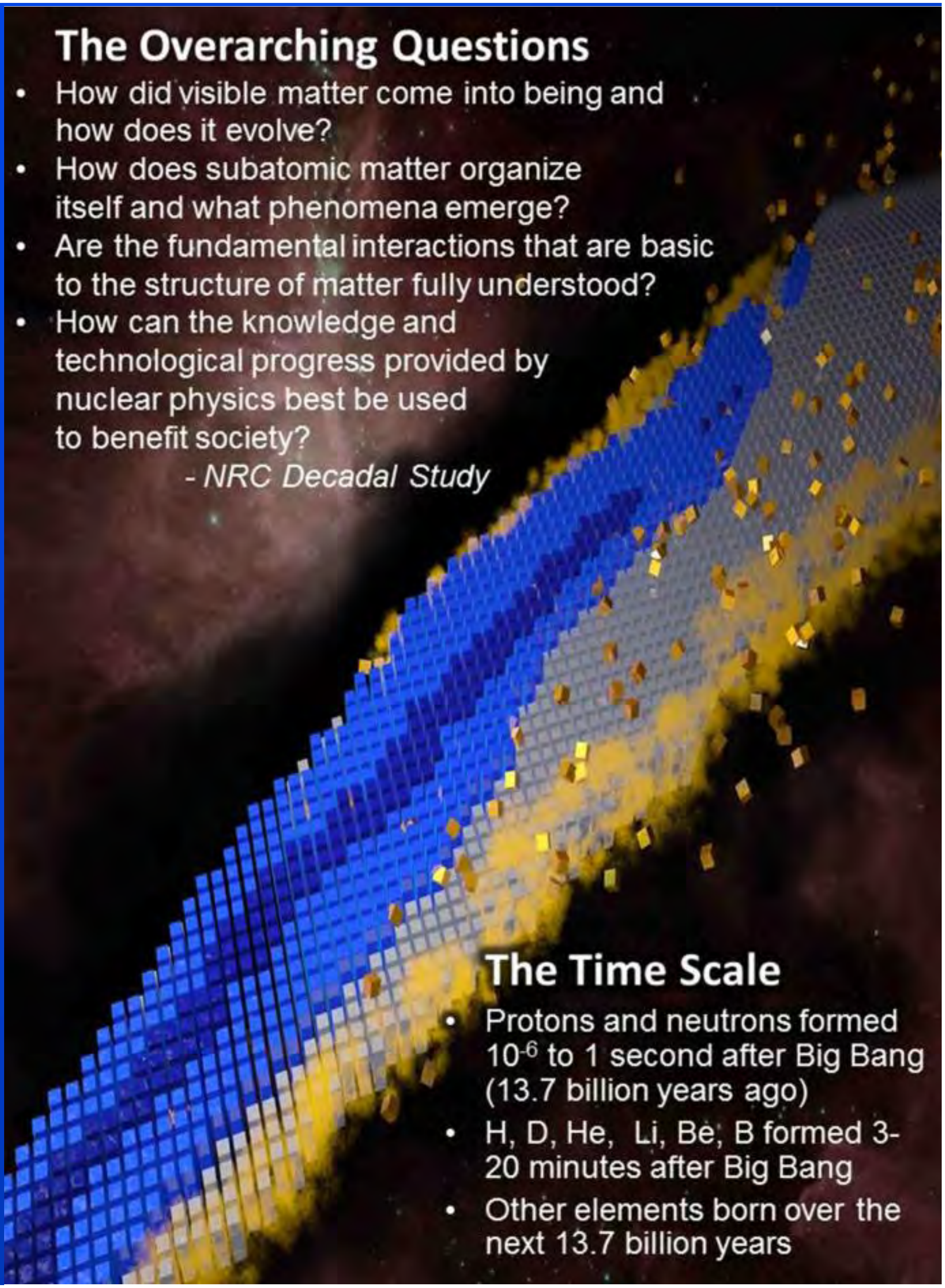
(SINP)
Lomonosov Moscow
State University

Jubilee Symposium
Moscow, February 15, 2021



Focus of the SINP-ISU Collaboration

Frontier Problem: Understanding the atomic nucleus from first principles

Nearly all of the visible matter in the universe is made of atomic nuclei, yet we do not know how the fundamental laws of physics govern their basic properties such as their binding energy, their size and their reactions.

Given our physics “first principles”, i.e. knowledge of the microscopic forces, relativity and quantum mechanics, we aim to calculate these basic properties and test for agreement with experimental measurements. This is also called “ab initio” (from the beginning) theoretical physics.

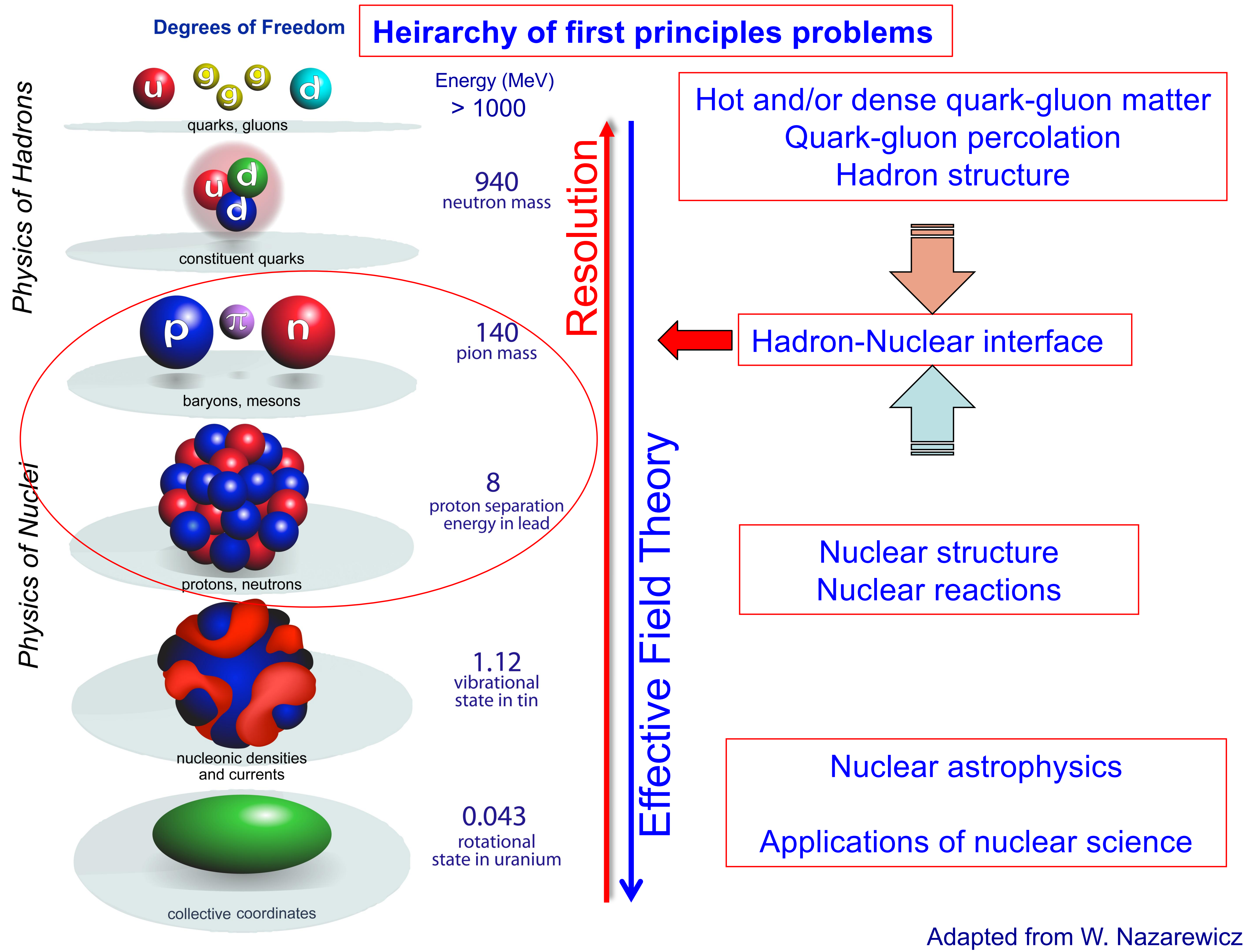
When we are successful, we can claim to understand the atomic nucleus from first principles. Any discrepancies would point to the exciting prospect for the discovery of new physics which is expected and needed to help explain outstanding puzzles such as dark matter and dark energy.

This is a frontier physics problem requiring the most advanced theoretical and computational methods.

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 nuclear phenomena and use
discrepancies with experiment to reveal new physics?



Heirarchy of first principles problems
Degrees of Freedom
Physics of Hadrons
Physics of Nuclei
u g g g d
quarks, gluons
Energy (MeV)
> 1000
u d d
constituent quarks
940
neutron mass
p π n
baryons, mesons
140
pion mass
protons, neutrons
8
proton separation energy in lead
nucleonic densities and currents
1.12
vibrational state in tin
collective coordinates
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
Nuclear astrophysics
Applications of nuclear science
Adapted from W. Nazarewicz

Short History of the SINP – ISU Collaboration in Theoretical Physics

In 1995, a delegation from ISU, led by the University Provost, visits Lomonosov Moscow State University to sign cooperation agreements under the auspices of the International Institute of Theoretical and Applied Physics (IITAP) at ISU.

In 1995 Profs. Edward Boos and Victor Savrin visit ISU under IITAP auspices to plan for collaborations between SINP and ISU faculty. This leads to an agreement for scientific exchanges that is later formalized and continues to the present day.

In 1997 Prof. Andrey Shirokov visits ISU with support from IITAP to work with ISU Profs. Derek Pursey and Thomas Weber. A productive collaboration emerges with several exchange visits and scientific papers.

In 1998 Prof. Shirokov begins collaboration with Profs. Thomas Weber, Derek Pursey, James Vary and Alexander I. Mazur (Khabarovsk) addressing *ab initio* nuclear structure and reactions. The first joint publication is in 2000 and it leads to the successful development of the JISP16 NN interaction published in 2007 now with 196 citations on INSPIRE, 289 citations on Google Scholar.

Beginning in 2012, six successful Nuclear Theory in the Supercomputing Era (NTSE) International Conferences organized. The next NTSE meeting is scheduled for 2021 or 2022 in Roorkee, India.

SINP-ISU collaboration has grown to include many additional scientists from Russia, United States, Korea, China, France and other countries.

AGREEMENT

on scientific coperation
between
D. V. Skobeltsyn Institute of Nuclear Physics,
M. V. Lomonosov Moscow State University, Russia
and
Department of Physics and Astronomy,
Iowa State University, USA

D. V. Skobeltsyn Institute of Nuclear Physics, M. V. Lomonosov Moscow State University, Russia and Department of Physics and Astronomy, Iowa State University, USA, hereinafter referred to as the Parties, conscious of their aspirations to extend international cooperation and having common intentions in the field of scientific research, have agreed on the following basic principles of cooperation:

Section 1.

The purpose of the Agreement is to promote cooperation in the area of science between the two Parties in fields of mutual interest.

Section 2.

For the realization of these objectives both Parties agree:

- to promote establishment of scientific cooperation in nuclear physics and related fields;
- to render mutual assistance in raising the scientific qualifications of the academic staff;
- to promote the exchange of publications and documentation on current research;
- to organize bilateral joint symposia, workshops and conferences;
- to implement joint research programs and projects in areas of mutual interest and to promote collaborative studies and publications.

Section 3.

Both Parties agree that the best forms of cooperation are through direct scientist-to-scientist initiative and connections in a given field, based on personal and departmental interests, and in a form that is most suitable to these parties.

Section 4.

All scientists of both Parties can take part in the exchange on the basis of individual invitations, which the Parties send to each other.

The Party inviting or receiving researchers of the other Party bears the expenses of their stay in the receiving University as agreed upon by the Parties according to the conditions adopted in the receiving University.

The sending Party pays transport expenses of the participants of the exchange from one country to the other.

The number of invitations and duration of visits will depend in each case on the financial resource available to each Party.

Medical insurance to participants of the exchange will be covered on conditions accepted in the receiving University.

Section 5.

The Parties agree that the scientific cooperation between them will be implemented on the basis of the Working Programs signed by representatives of both Parties after coordination of conditions, topics and participants of scientific cooperation.

Section 6.

Should one of the two Parties wish to broaden the sphere of academic contacts in the other country so as to involve other institutions, each Party may agree to act as an intermediary in promoting such contacts and cooperation.

Section 7.

The Parties are entitled to propose amendments to be made to the current Agreement. In order to become effective the amendments must be recognized by both Parties in a joint Protocol or Memorandum.

Section 8.

The Agreement has been prepared in two original copies in Russian and English, all being equally authentic.

Section 9.

The Agreement comes into force on the date of signature and is valid for a period of 5 (five) years, unless one Party notifies the other in writing of its wish to terminate the Agreement at least ninety days prior to the termination date.

On behalf of
D. V. Skobeltsyn Institute of Nuclear Physics,
M. V. Lomonosov Moscow State University,
1(2), Leninskie gory, Moscow 119991,
Russia

____

Prof. M. I. Panasyuk, Director

Date: ____________________

On behalf of
Department of Physics and Astronomy,
Iowa State University,
Ames, IA, 50011, USA

____

Prof. Frank Krennrich, Department Chair

Date: ________________

Formally registered on March 25, 2016

Key collaborative papers ordered by their citation counts [InSPIRE,Google]

1. A.M. Shirokov, et al., Phys. Lett. B 644 (2007). [196,289]
2. P. Maris, J.P. Vary and A.M. Shirokov, Phys. Rev. C 79 (2009) [161,242]
3. A.M. Shirokov, et al., Phys. Rev. C70 (2004) [76,144]
4. A.M. Shirokov, et al., Phys. Lett. B 621 (2005) [72,125]
5. P. Maris, A.M. Shirokov and J.P. Vary, Phys. Rev. C 81 (2010) [61,88]
6. A.M. Shirokov, et al., Phys. Lett. B 761 (2016) [47,69]
7. A.M. Shirokov, et l., Phys. Rev. Lett. 117 (2016) [46,62]
8. E. Dikmen, et al., Phys. Rev. C 91 (2015) [36,44]
9. A.M. Shirokov, et al., Phys. Rev. C 94 (2016) [25,42]
10. A.M. Shirokov, et al., Phys. Rev. C 79 (2009) [25,38]
11. G.A. Negoita, et al., Phys. Rev. C 99 (2019) [16, 18]

+ ~30 more publications including conference proceedings

JISP16+Apps: **1**, 2, 3, 4, 5, 7, 8, 10
Daejeon16+Apps: **6**, 11
Scattering theory: **9**, 10, & To be published

5 – Prediction of Fluorine-14 (USDOE highlight slide)
7 – Prediction of the tetraneutron (USDOE highlight slide)
11 – Deep Learning & ab initio theory (USDOE highlight slide)
To be published: Helium-7 resonances

Phenomeological NN interaction: JISP16

"JISP16" is the **J**-matrix **I**nverse **S**cattering **P**otential tuned up to Oxygen **16**

- Constructed to reproduce np scattering data
- Finite rank seperable potential in H.O. representation
- Nonlocal NN-only potential
- Use Phase-Equivalent Transformations (PET) to tune off-shell interaction to
  - binding energy of ^{3}H and ^{4}He
  - low-lying states of ^{6}Li (JISP6, precursor to JISP16)
  - binding energy of ^{16}O

ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

Physics Letters B 644 (2007) 33–37

PHYSICS LETTERS B

www.elsevier.com/locate/physletb

Realistic nuclear Hamiltonian: Ab exitu approach

A.M. Shirokov [a,b,*], J.P. Vary [b,c,d], A.I. Mazur [e], T.A. Weber [b]

"Proton-Dripping Fluorine-14"

DOE/ASCR/NP – Computational Science Highlight

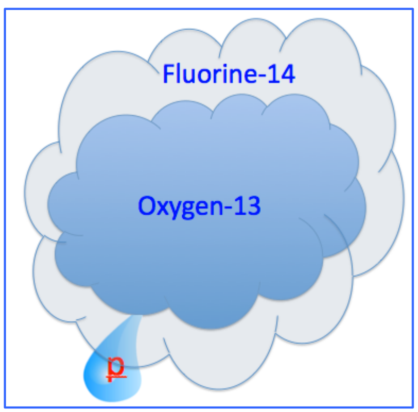
Objectives

- **Apply *ab initio* microscopic nuclear theory's predictive power to major test case**

Impact

- **Deliver robust predictions important for improved energy sources**
- **Provide important guidance for DOE-supported experiments**
- **Compare with new experiment to improve theory of strong interactions**

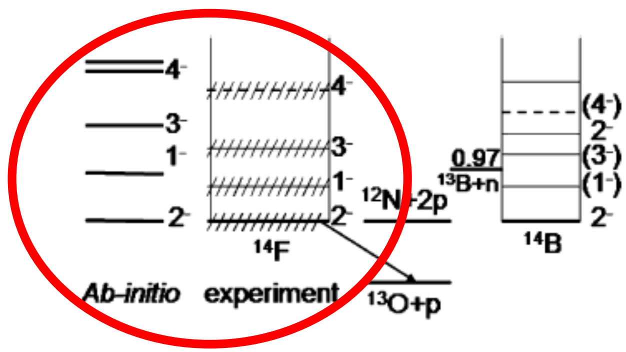
P. Maris, A.M. Shirokov, and J.P. Vary, Phys. Rev. C 81, 021301(R), **Feb. 2010**, uses JISP16 to predict ^{14}F lives a short life in specified states (the "Ab-initio" ladder in the red oval) and decays to Oxygen-13 by emitting a proton.



$^{13}O + p \rightarrow {}^{14}F^{*} \rightarrow {}^{13}O + p$

Experiment validates our published predictions!

V.Z. Goldberg et al., "First observation of 14F", Phys. Lett. B 692, 307 (**August 2010**).



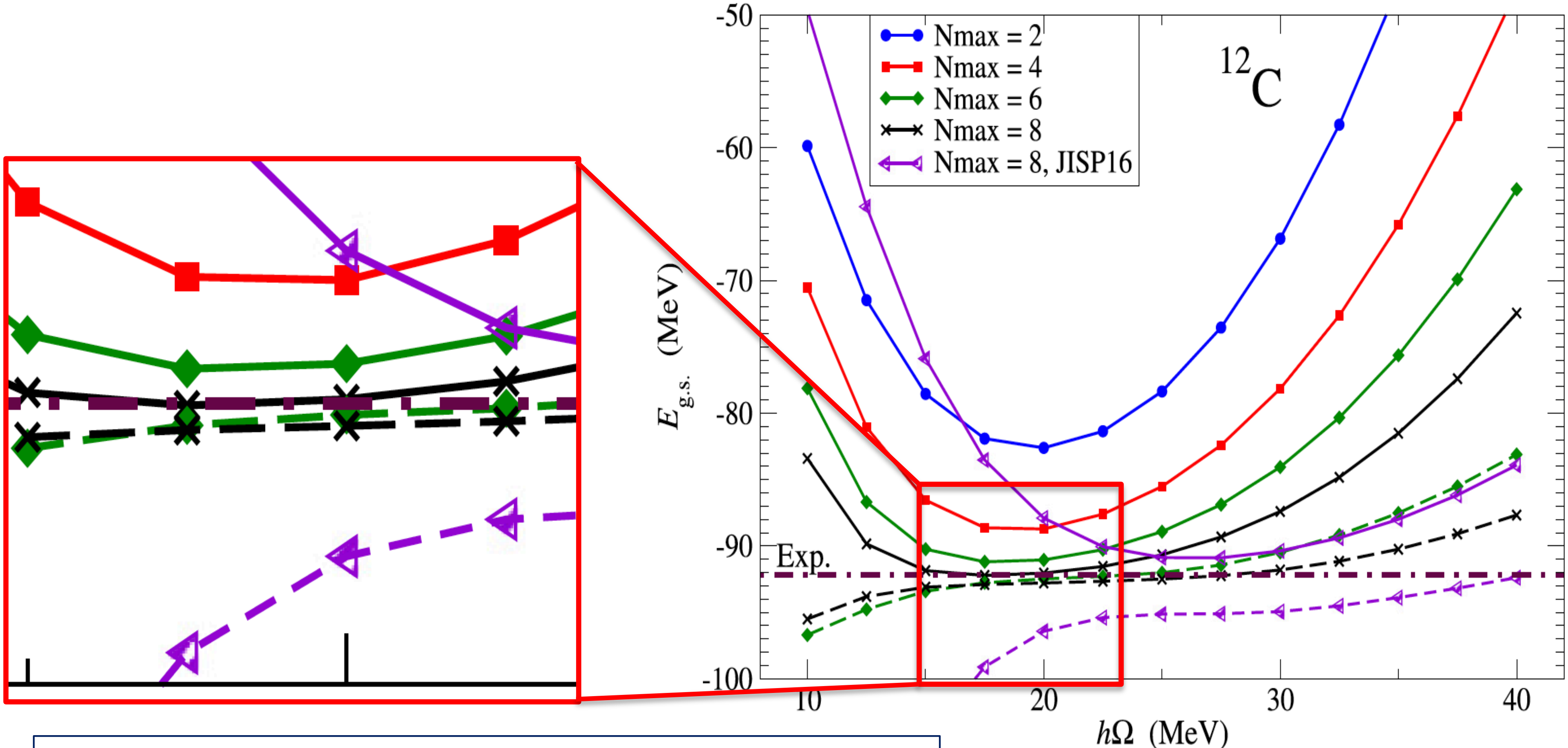
Progress

- Dimension of matrix solved for 14 lowest states ~ $2x10^9$
- Solution takes ~ 2.5 hours on 30,000 cores (Cray XT4 Jaguar at ORNL)
- P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, "Scaling of ab-initio nuclear physics calculations on multicore computer architectures", 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97, May 2010.

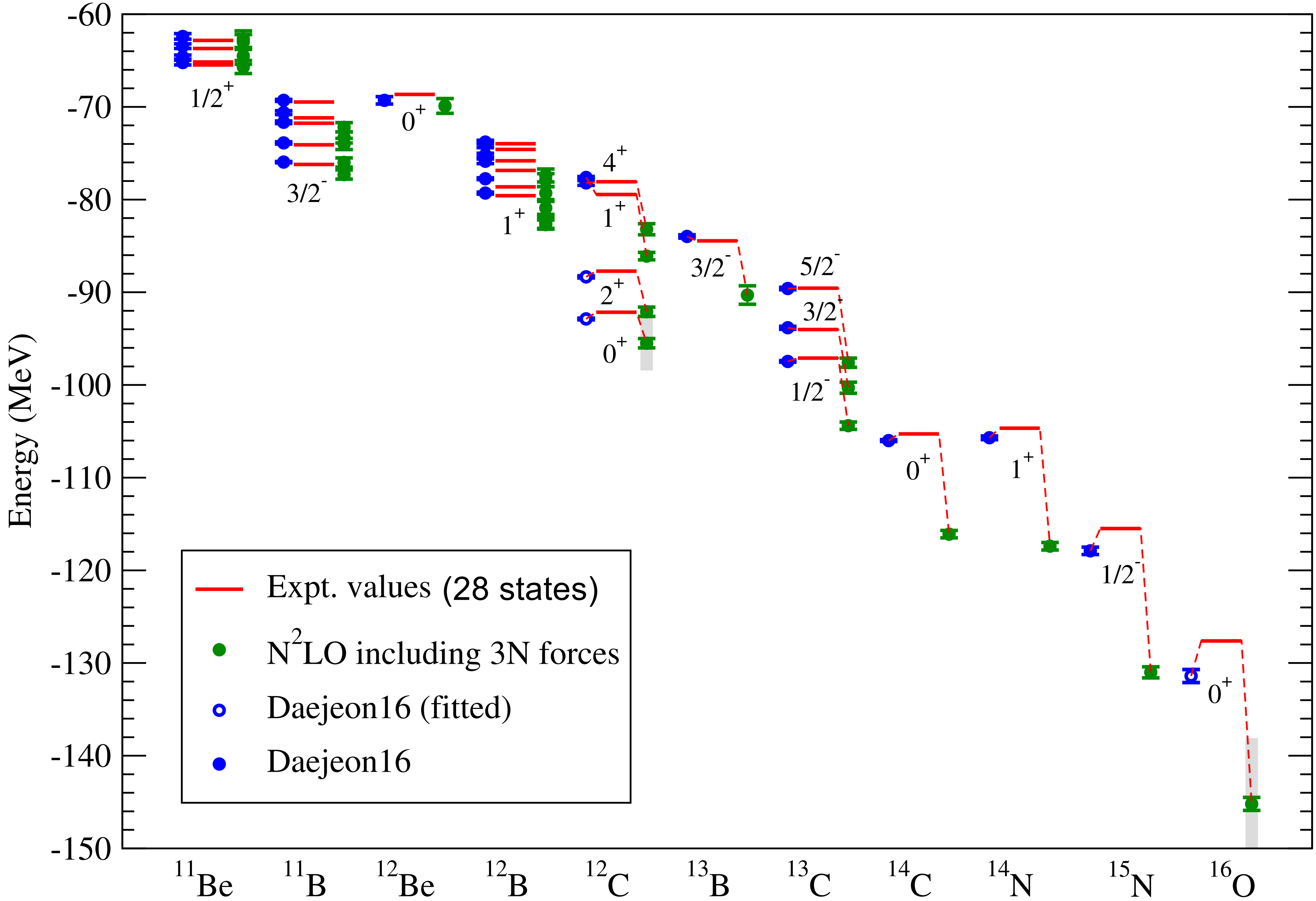
Daejeon16 NN interaction

Based on SRG evolution of Entem-Machleidt “500” chiral N3LO to $\lambda = 1.5\ \text{fm}^{-1}$ 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

General idea of the HORSE formalism

"Harmonic Oscillator Representation of Scattering Equations"

$$T \;+\; V$$

NCSM with:
$\lambda(N,\hbar\Omega)$ & $\Lambda(N,\hbar\Omega)$

Infinite set of algebraic equations in HO basis of relative motion:

$$\sum_{n'=0}^{N}\left(T^{l}_{nn'}+V^{l}_{nn'}-\delta_{nn'}E\right)a_{n'l}(E)=0. \qquad n\le N-1$$

Matching condition at $n = N$

$$\sum_{n'=0}^{N}\left(T^{l}_{Nn'}+V^{l}_{Nn'}-\delta_{Nn'}E\right)a_{n'l}(E)+T^{l}_{N,N+1}a_{N+1,l}(E)=0. \quad n\le N-1$$

Then for $n\ge N+1$

$$\sum_{n'=0}^{\infty}\left(T^{l}_{nn'}-\delta_{nn'}E\right)a_{n'l}(E)=0, \text{ which produces:}$$

$$T^{l}_{n,n-1}a_{n-1,l}(E)+\left(T^{l}_{nn}-E\right)a_{nl}(E)+T^{l}_{n,n+1}a_{n+1,l}(E)=0.$$

"think outside the box"=> T

Arises as a natural extension of NCSM where both potential and kinetic energies are truncated

This is an exactly solvable algebraic problem!

Single-State HORSE (SS-HORSE)

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

$$(H-E)^{-1}_{nn'} \equiv -G_{nn'} = \sum_{\lambda'=0}^{N} \frac{\langle n|\lambda'\rangle\langle\lambda'|n'\rangle}{E_{\lambda'} - E}$$

← Standard HORSE

$$\tan\delta(E) = -\frac{S_{Nl}(E) - G_{NN} T^{l}_{N,N+1} S_{N+1,l}(E)}{C_{Nl}(E) - G_{NN} T^{l}_{N,N+1} C_{N+1,l}(E)}.$$ Also, S-matrix = S(G_{NN})

Suppose $E = E_{\lambda'}$ ← Single-State HORSE

$$\tan\delta(E_\lambda) = \frac{S_{N+1,l}(E_\lambda)}{C_{N+1,l}(E_\lambda)} = (-1)^l q^{2l+1} \Gamma(-l+\tfrac{1}{2}) \frac{L^{l+1/2}_{(N-l)/2}(q^2)}{\Phi(-\tfrac{N}{2}-\tfrac{l}{2}-\tfrac{1}{2}, -l+\tfrac{1}{2}; q^2)}$$

where $L^{l+1/2}_{(N-l)/2}$ are associated Laguerre polynomials, Φ are confluent hypergeometric functions and $q = \sqrt{\dfrac{2E_\lambda}{\hbar\Omega}}$.

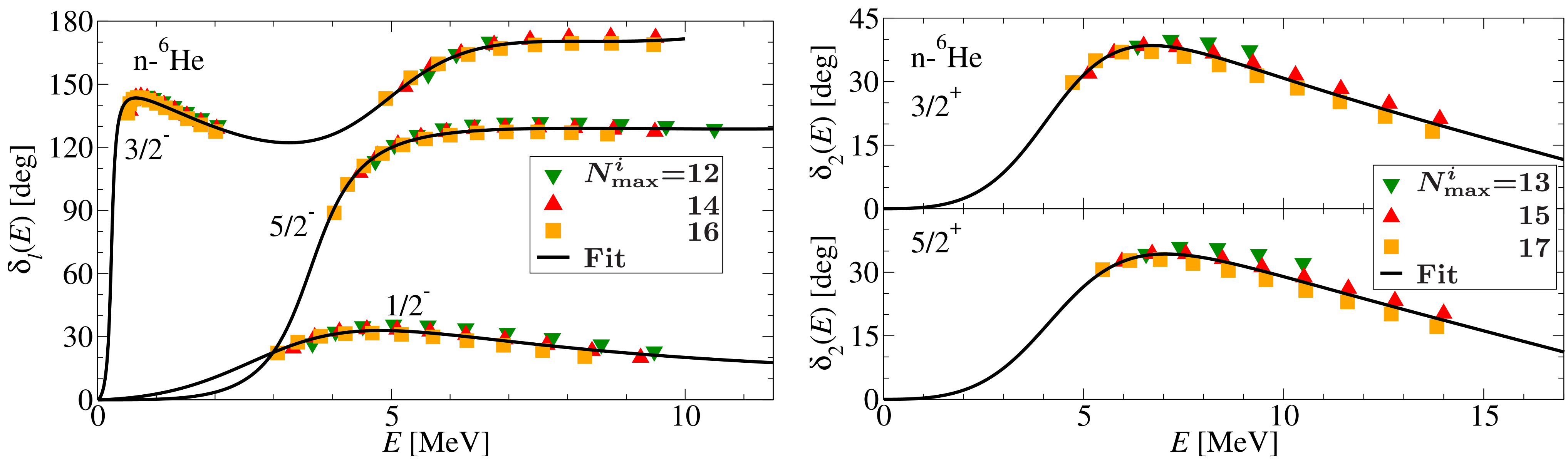
E_λ are (obtained from) eigenvalues of the NCSM (for given $\hbar\Omega$ and N_{max}). Once a scattering channel is defined (sets the continuum energy scale) the phase shift is calculated. Analog of Lüscher's method for a plane-wave basis.

A.M. Shirokov, A.I. Mazur, I.A. Mazur and J.P. Vary, PRC 94, 064320 (2016); arXiv:1608.05885

Resonances in Exotic ^{7}He Nucleus within the No-Core Shell Model

I. A. Mazur,[1,2] A. M. Shirokov,[2,3,4] I. J. Shin,[5] A. I. Mazur,[2] Y. Kim,[5] P. Maris,[4] and J. P. Vary[4]

arXiv: 2001.08898



Once the converged phase shifts are obtained via SS-HORSE, proceed to analyze:
Phase shifts -> S-matrix -> complex poles of the S-matrix

Use the spread of the phase shifts to determine resonance uncertainties.

Experiments: stripping/pickup reactions, IAS studies, one neutron knockout from ^{8}He

SS-HORSE (Daejeon16) agrees with Experiment, GSM and NCSMC for two resonances

TABLE II: Energies E_r (relative to the $n+{}^6$He threshold) and widths of resonant states in ^{7}He nucleus. Our estimate of the uncertainties of the quoted results are presented in parentheses. The available results of the GSM calculations [24] in the *psdf* valence space and of the NCSMC calculations [25, 26] with SRG-evolved N^{3}LO chiral NN force together with experimental data are shown for comparison. All values are in MeV.

		This work	GSM	NCSMC	Experiment		
						[20]	
	E_r^1	0.24(6)	0.39	0.71		0.430(3)	
$3/2^-$	Γ^1	0.11(2)	0.178	0.30		0.182(5)	
	E_r^2	4.9(3)					
	Γ^2	3.1(3)					
					[21]	[22]	[23]
$1/2^-$	E_r	2.7(4)		2.39	3.0(5)	3.5	1.0(1)
	Γ	4.3(3)		2.89	2	10	0.75(8)
						[19]	
$5/2^-$	E_r	3.63(18)	3.47(2)	3.13		3.36(9)	
	Γ	1.36(3)	2.3(3)	1.07		1.99(17)	
$3/2^+$	E_r	4.1(3)					
	Γ	4.4(5)					
$5/2^+$	E_r	4.2(5)					
	Γ	5.0(5)					

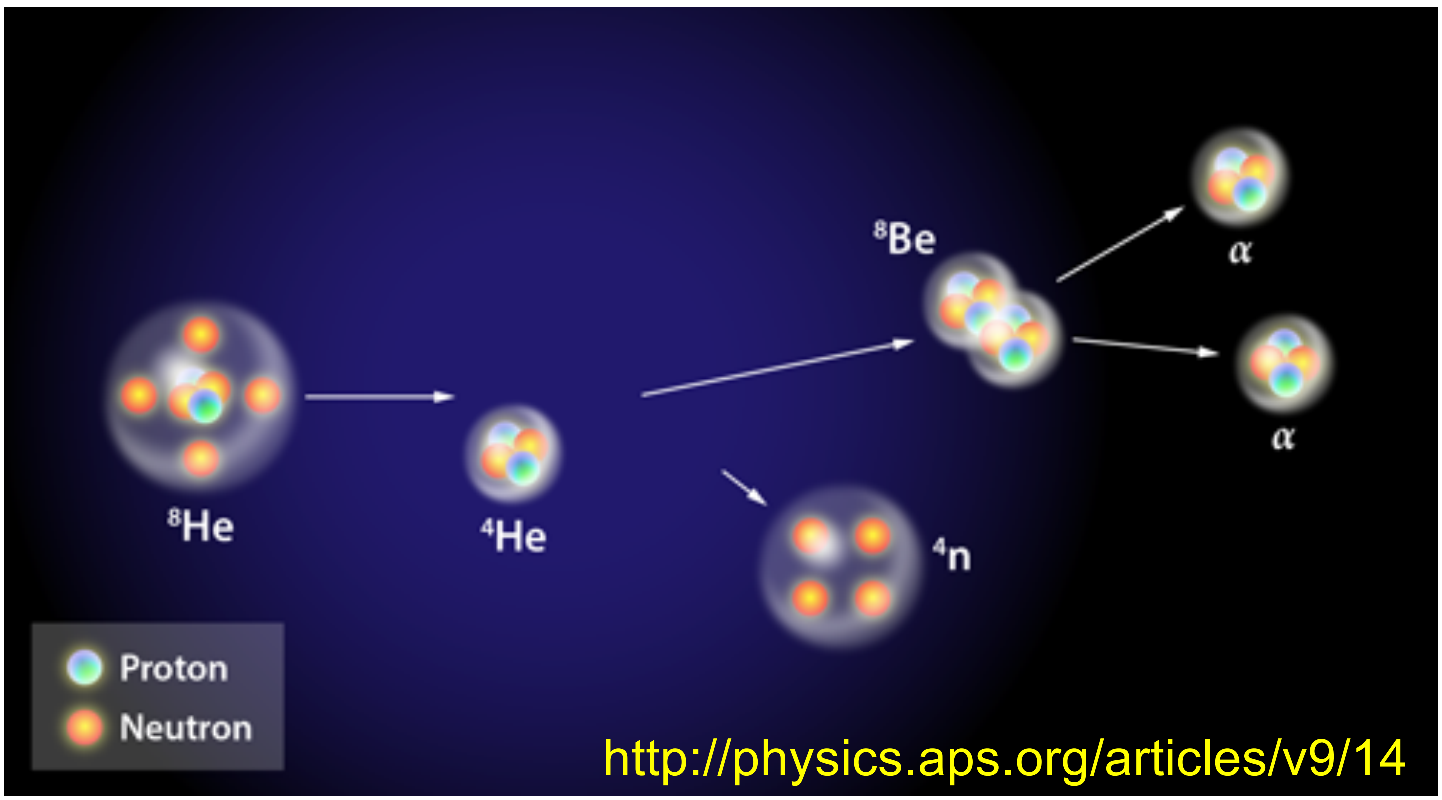
SS-HORSE (Daejeon16) predicts 4 more resonances (1/2- ~ NCSMC) that could help explain conflicting Experiments

I.A. Mazur, A.M. Shirokov, I.J. Shin, A.I. Mazur, Y. Kim, P. Maris and J.P. Vary, arXiv: 2001.08898

PHYSICAL REVIEW LETTERS

Candidate Resonant Tetraneutron State Populated by the ^{4}He(^{8}He, ^{8}Be) Reaction

K. Kisamori *et al.*
Phys. Rev. Lett. **116**, 052501 – Published 3 February 2016



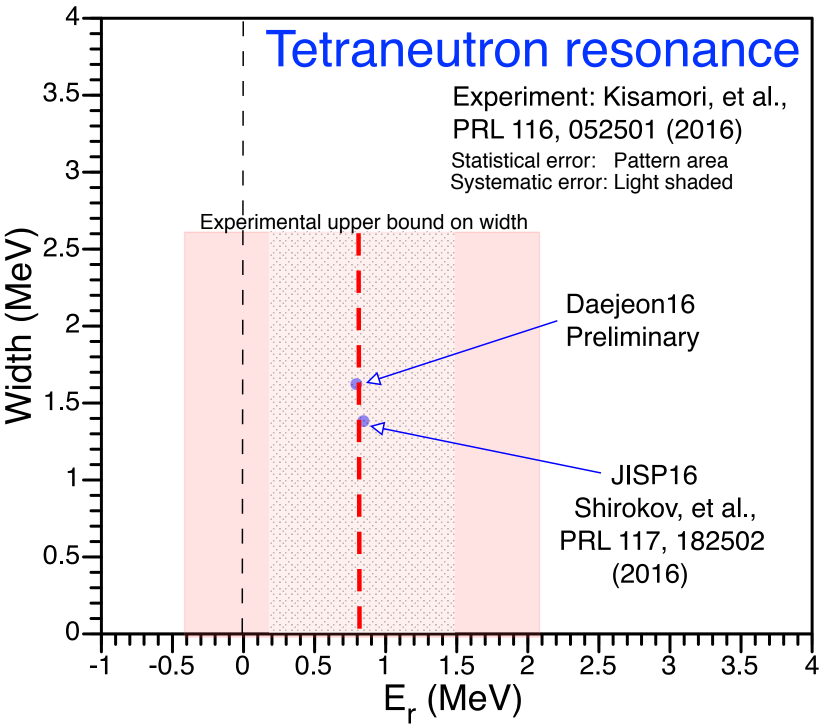
Prediction of a Tetraneutron

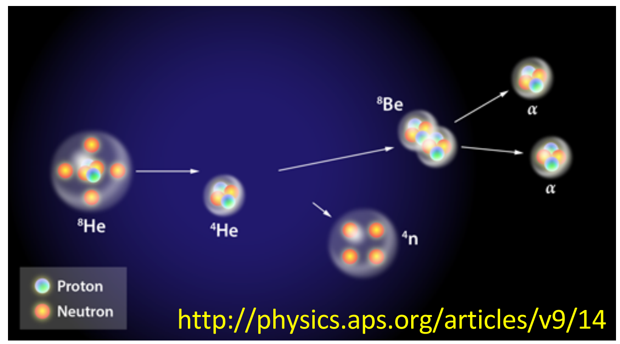
Objectives

- Predict properties of neutron-rich systems which relate to exotic nuclei and nuclear astrophysics
- Develop and apply new methods for deriving scattering properties from *ab initio* nuclear structure simulations
- Produce accurate predictions of nuclear resonances with quantified uncertainties

Impact

- Guides experimental programs searching for tetraneutron resonances
- Demonstrate the predictive power of *ab initio* nuclear theory for nuclear resonances
- Establishes foundation for precision determination of new trineutron and tetraneutron interactions





Above: illustration of the experiment by Kisamori, et al, reporting the detection of the tetraneutron. **Left**: comparison between theory and experiment for the tetraneutron resonance. The statistical and systematic errors of the experiment are shown separately with the width determined only as a upper bound. The results of the NCSM are employed in the SS-HORSE method to produce the phase shifts leading to the resonance parameters.

Accomplishments

1. Development of SS-HORSE, a new *ab initio* scattering formalism extending the No-Core Shell Model (NCSM) into the continuum
2. Demonstrated predictive power of *ab initio* nuclear theory for scattering observables
3. Provided resonance predictions for future experimental searches
4. Introduced new element to the chart of the nuclides
5. Provided a stepping-stone to possible heavier multi-neutron systems

U.S. DEPARTMENT OF ENERGY | Office of Science

NUCLEI
Nuclear Computational Low-Energy Initiative

References: A.M. Shirokov, G. Papadimitriou, A.I. Mazur, I.A. Mazur, R. Roth and J.P. Vary, Phys Rev Lett 117, 182502 (2016); A.M. Shirokov, et al, Phys Rev C 94, 064320 (2016)

Contact: jvary@iastate.edu

计算机模拟证明四中子结构存在

有助加深对中子间强核力的理解

文章来源：科技日报 刘霞　发布时间：2016-11-08　【字号： 小 中 大 】　我要分享

研究人员与四中子结构示意图

据物理学家组织网日前报道，美国爱荷华州立大学的物理学和天文学教授詹姆斯·瓦瑞和访问学者安德烈·希罗科夫领导的国际科研团队，使用复杂的超级计算机模拟，证明了曾被认为不可能存在的、由四个中子组

热点新闻

中央组织部、中国科学院联合召...

中国科学院“十三五”发展规划纲要
中科院-广东省召开院省合作领导小组会议...
中科院科技扶贫工作交流会在广西环江召开
中科院与河钢集团举行科技合作座谈会并...
“十三五”空间科学任务全面启动新闻发...

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【朝闻天下】领航十三五：大国重器——带领中国创新前进

专题推荐

How can Machine Learning (ML), a branch of Artificial Intelligence (AI), provide help for solving this Big Problem?

Answer: use results from the best, but incomplete, calculations available with today's supercomputers to train an artificial neural network (ANN) to learn the patterns of these incomplete solutions and **then use the well-trained ANN to infer the complete first principles solution.**

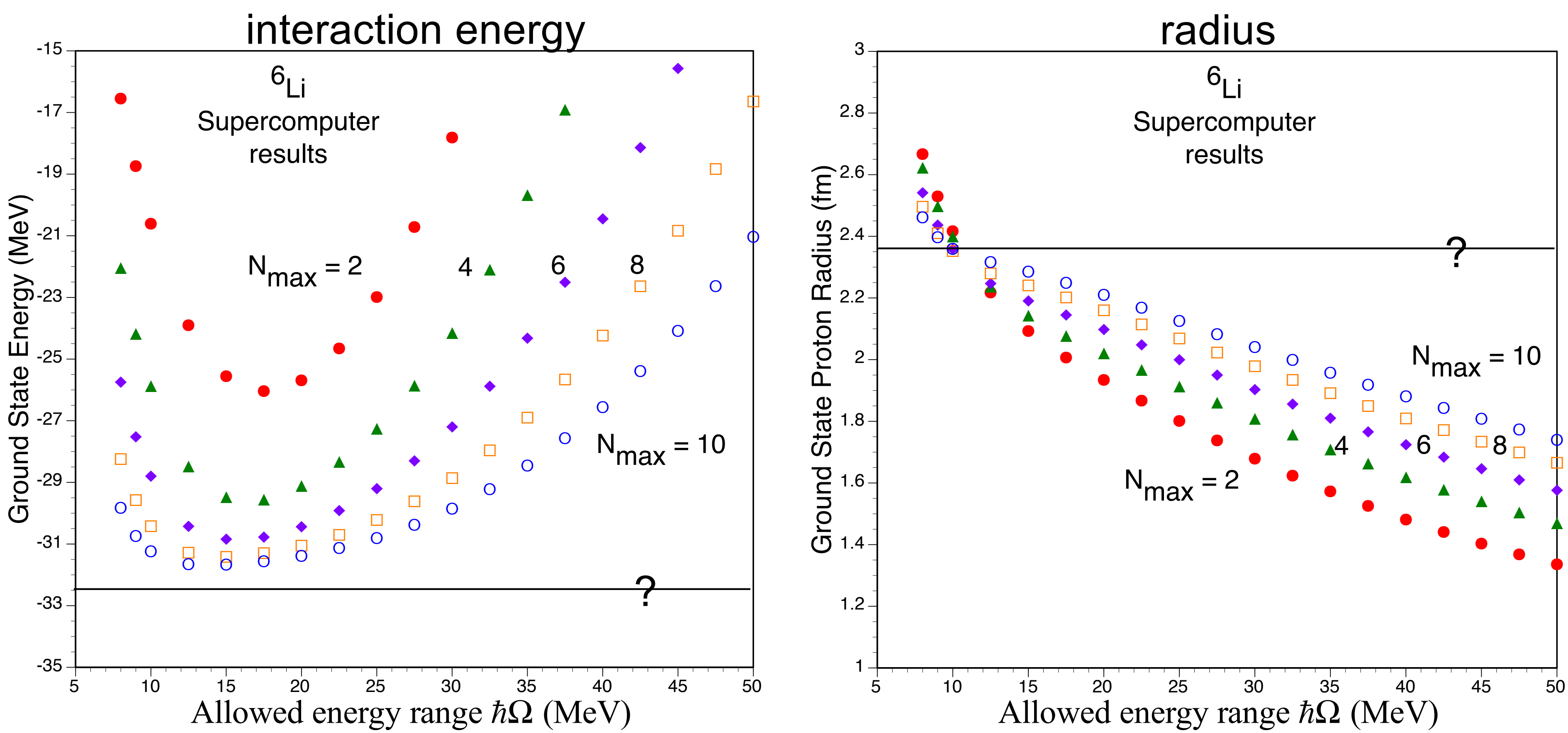
This is an example of the application of Deep Learning paradigm in AI.

The supercomputer calculations employ the interactions of the neutrons and the protons (**Daejeon16**) within the rules of quantum mechanics to solve for the binding energy and radius of an atomic nucleus. We will use the specific example of Lithium-6, or ^{6}Li, which consists of 3 protons and 3 neutrons. These supercomputer calculations are performed as a function of a cutoff in the number of allowed configurations (N_{max}) and as a function of the allowed energy range of the neutrons and protons ($[0 - N_{max}]\hbar\Omega$).

We want the ANN to learn how the supercomputer results depend on this cutoff and on this allowed energy range so that the ANN will infer the first principles results which are independent of the cutoff and independent of the allowed energy range.

Consider the goal of solving for the interaction energy and the radius of ^{6}Li. These are important test cases since available supercomputer calculations can be used to train and test the validity of an ANN for predicting the first principles results.

Results of supercomputer calculations up to N_{max} = 10 used for training/testing



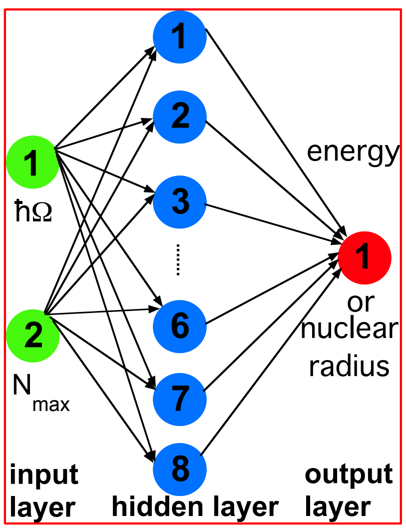
Deep Learning for Nuclear Binding Energy and Radius

Scientific Achievement

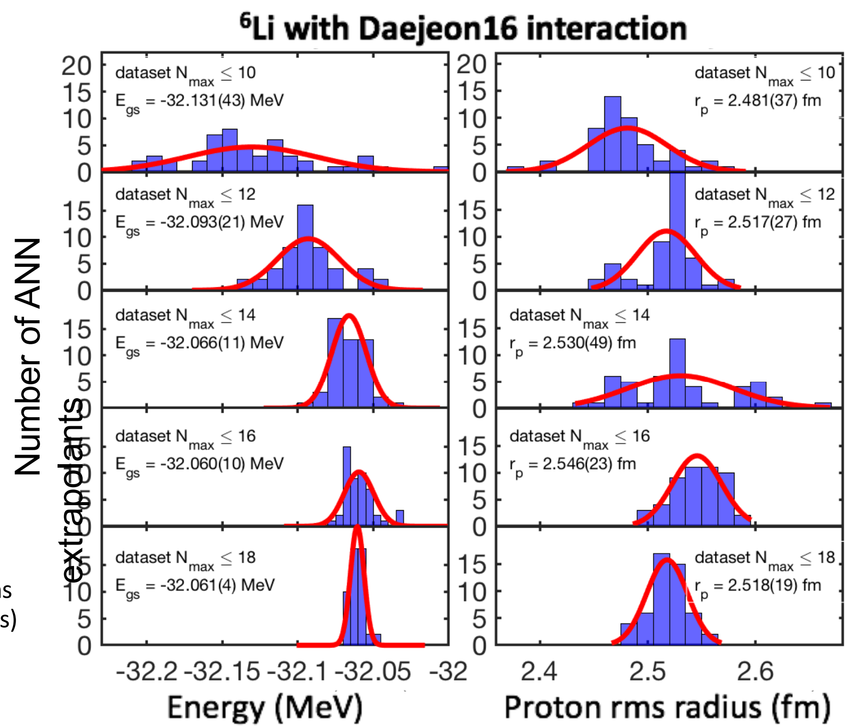
- Developed artificial neural networks (ANNs) for extending the application range of the *ab initio* No-Core Shell Model (NCSM)
- Demonstrated predictive power of ANNs for converged solutions of weakly converging simulations of the nuclear radius
- Provided a new paradigm for matching deep learning with results from high performance computing simulations

Significance and Impact

- Guides experimental programs at DOE's rare isotope facilities
- Extends the predictive power of *ab initio* nuclear theory beyond the reach of current high performance computing simulations
- Establishes foundation for deep learning tools in nuclear theory useful for a wide range of applications



Neural network **(above)** used to successfully extrapolate the ^{6}**Li** ground state energy and rms radius from modest basis spaces (N_{max} datasets) to extreme basis spaces achieving basis parameter independence (histograms of extrapolation ensembles in **right figure**).



Research Details

- Develop ANNs that extend the reach of high performance computing simulations of nuclei
- Predict properties of nuclei based on *ab initio* structure calculations in achievable basis spaces
- Produce accurate predictions of nuclear properties with quantified uncertainties using fundamental inter-nucleon interactions such as Daejeon16

Ref: G. A. Negoita, et al., Phys. Rev. C **99**, 054308 (2019); https://journals.aps.org/prc/pdf/10.1103/PhysRevC.99.054308

Contacts: jvary@iastate.edu; egng@lbl.gov

Many outstanding nuclear physics
puzzles and discoveries remain ahead
for the SINP – MSU collabortion

Clustering phenomena
Origin of the successful nuclear shell model
Nuclear reactions and breakup
Astrophysical processes & drip lines
Precision Nuclear Theory as a window on
Physics beyond the Standard Model

Congratulations to the
Skobeltsyn Institute for Nuclear Physics
on its first 75 successful years!

Thank you for your attention
I welcome your questions