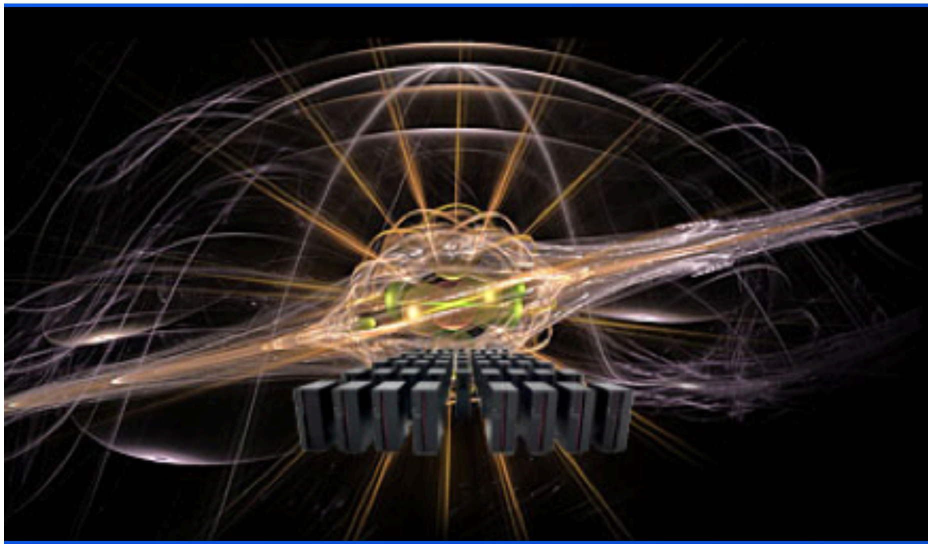


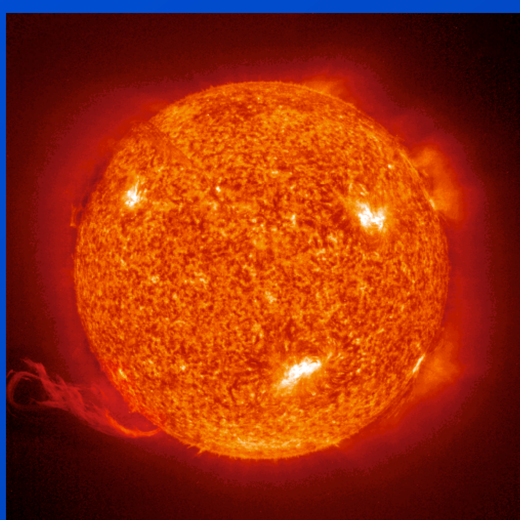
International Workshop
Nuclear Theory
in the Supercomputing Era
Pacific National University, Khabarovsk, Russia
June 18–22, 2012

New Perspectives on the Atomic Nucleus

James P. Vary
Iowa State University

Brief review of the four known interactions (or forces) in nature

Property	Gravitational Interaction	Weak Interaction (Electroweak)	Electromagnetic Interaction	Strong Interaction
Acts on:	Mass – Energy	Flavor	Electric Charge	Color Charge
Particles experiencing:	All	Quarks, Leptons	Electrically Charged	Quarks, Gluons
Particles mediating:	Graviton (not yet observed)	W^+ W^- Z^0	γ	Gluons
Strength at 10^{-18} m	10^{-41}	0.8	1	25
Strength at 3×10^{-17} m	10^{-41}	10^{-4}	1	60



These three interactions govern nuclear reactions and scattering & compose the "Standard Model" of elementary particles

Main hypothesis

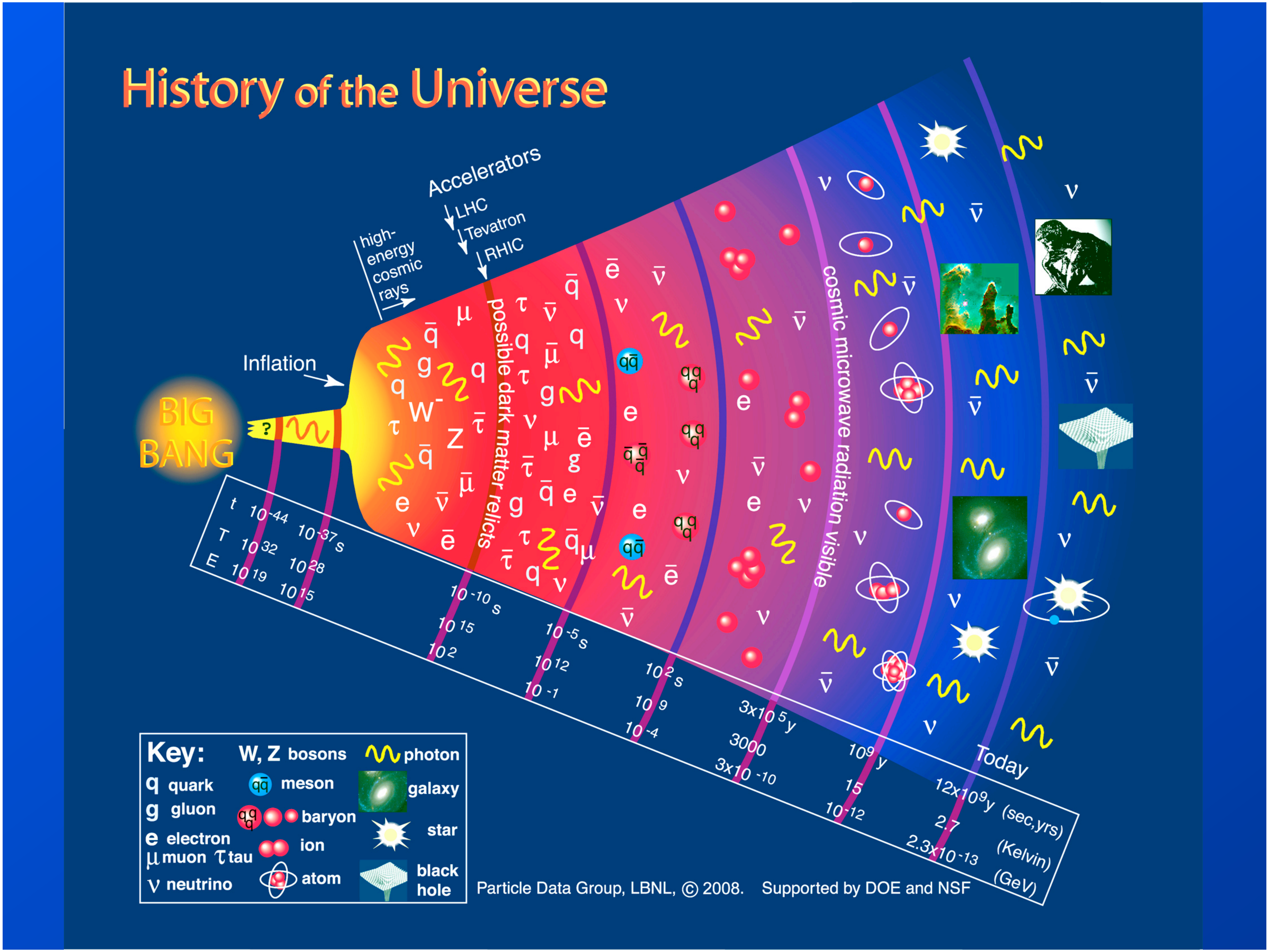
If the Standard Model is correct, we should be able to accurately describe all nuclear processes

Purpose of this International Workshop

Current progress with theory and supercomputer simulations

Long-term goal

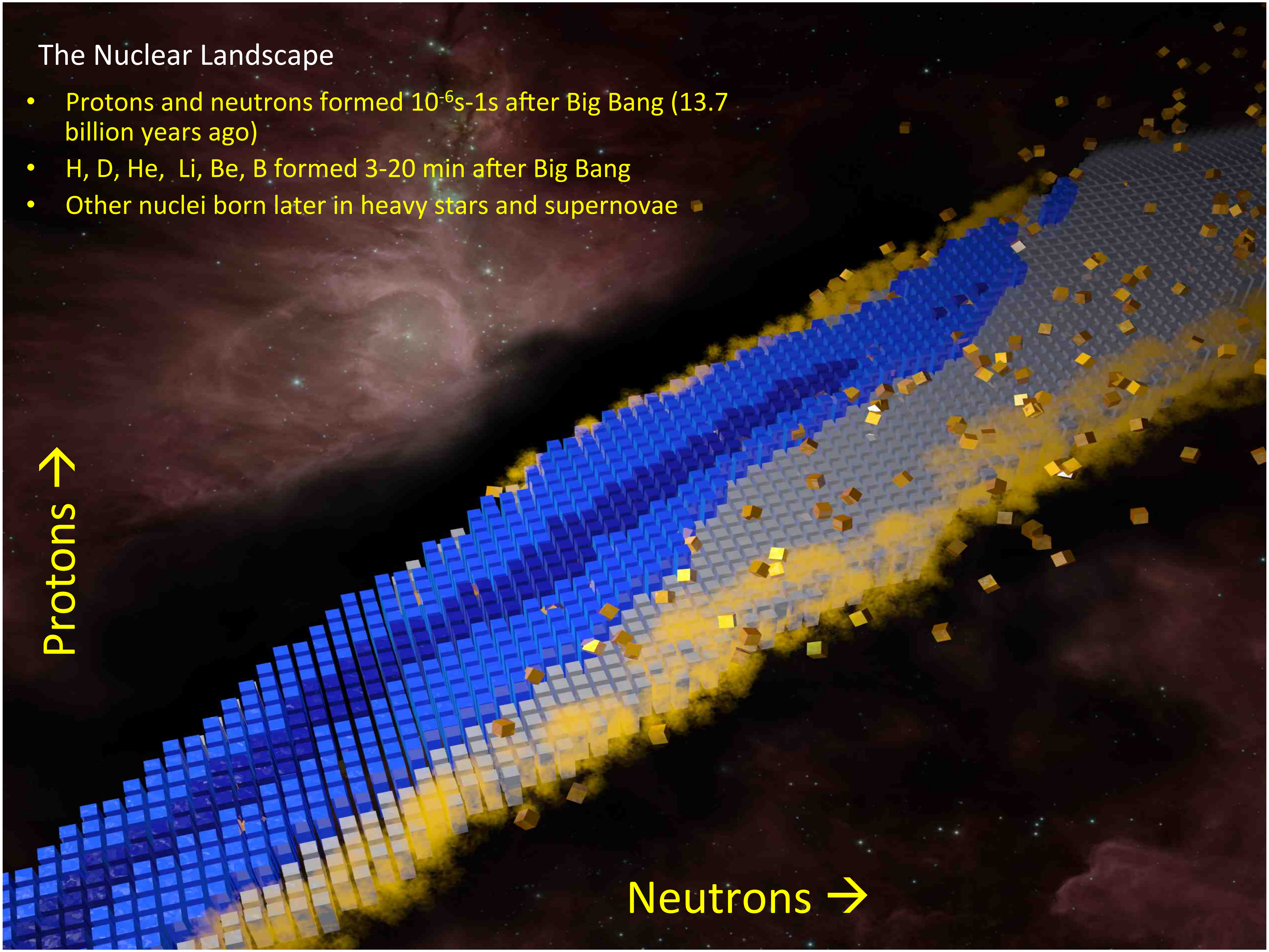
Use all fundamental interactions including yet unkown interactions to construct a model for the evolution of the entire universe



History of the Universe
Accelerators
LHC
Tevatron
RHIC
high-energy cosmic rays
Inflation
BIG BANG
possible dark matter relicts
cosmic microwave radiation visible
t 10 -44 10 -37 s
T 10 32 10 28
E 10 19 10 15
10 -10 s
10 15
10 2
10 -5 s
10 12
10 -1
10 2 s
10 9
10 -4
3x10 5 y
3000
3x10 -10
10 9 y
15
10 -12
Today
12x10 9 y (sec,yrs)
2.7 (Kelvin)
2.3x10 -13 (GeV)
Key:
q quark
g gluon
e electron
µ muon τ tau
ν neutrino
W, Z bosons
meson
baryon
ion
atom
photon
galaxy
star
black hole
Particle Data Group, LBNL, © 2008. Supported by DOE and NSF

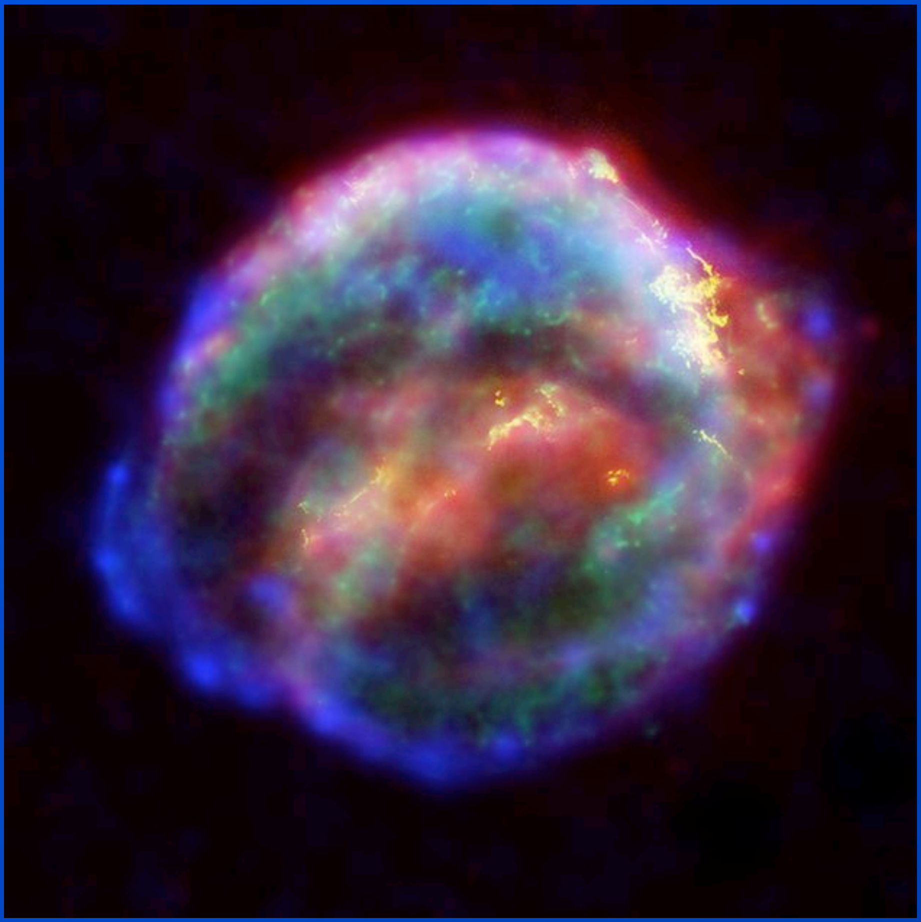
The Nuclear Landscape

- Protons and neutrons formed 10^{-6}s-1s after Big Bang (13.7 billion years ago)
- H, D, He, Li, Be, B formed 3-20 min after Big Bang
- Other nuclei born later in heavy stars and supernovae



Formation of heavy elements (A > 56) requires extreme conditions - difficult to create in laboratory experiments. Where can we find the “factory” that produces these isotopes?

Kepler's supernova (courtesy: NASA + ESA)

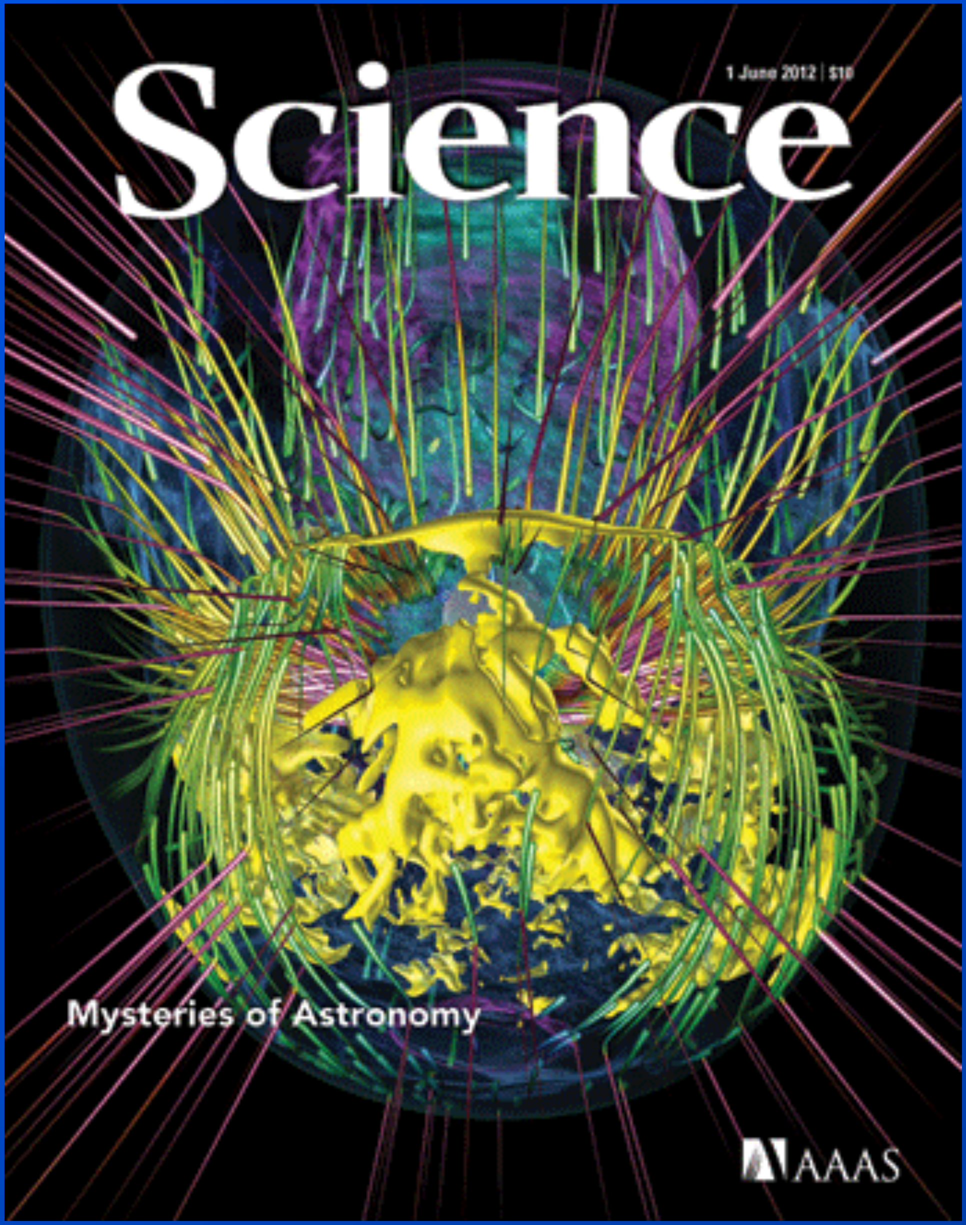


What are supernovae and why are they important?

Formation of the heavy elements - r/p processes

Nuclear equation of state governs energy release

Core-collapse supernova simulation – Science, 1 June 2012



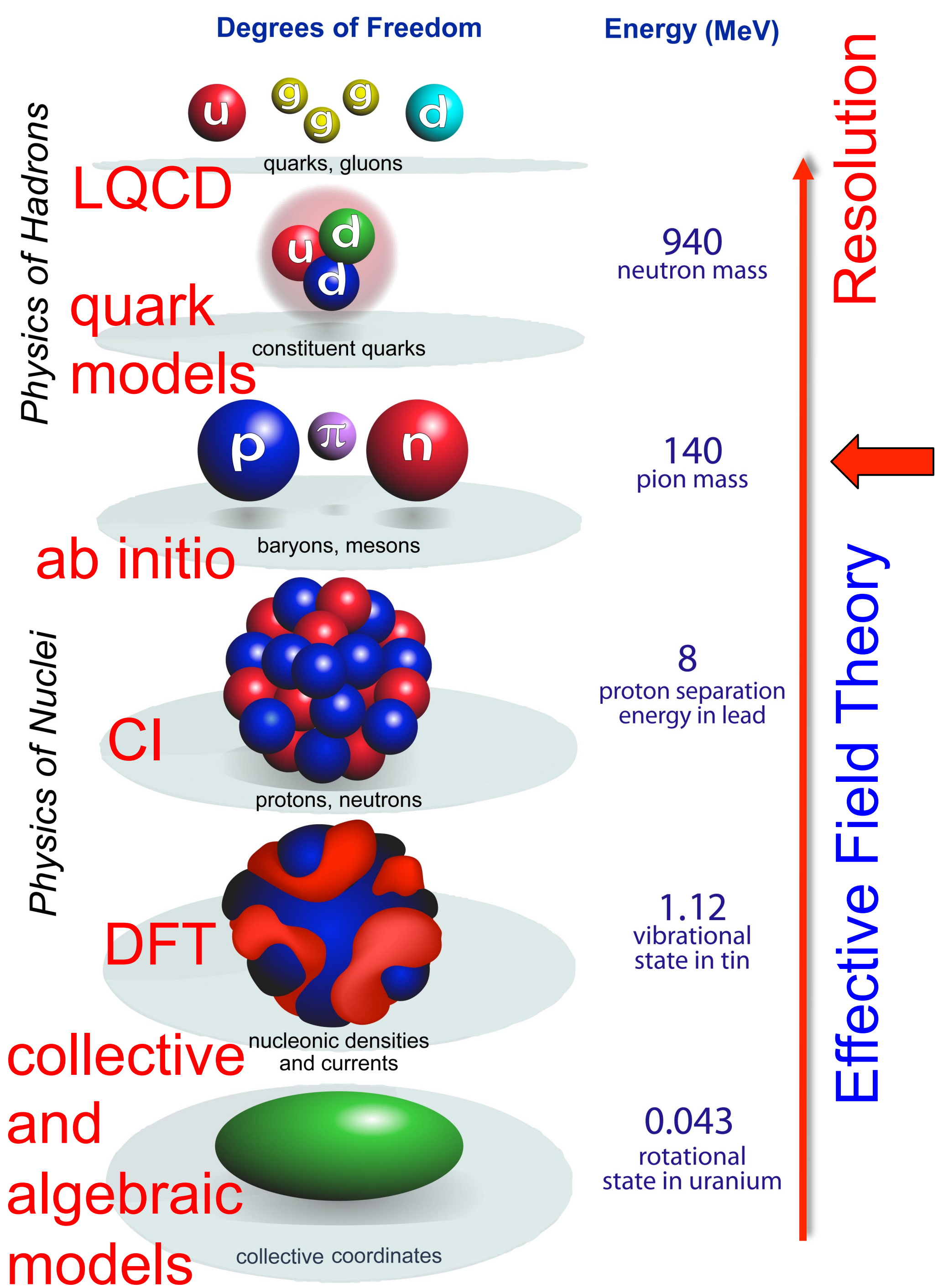
Supercomputers play an essential role in testing our theories

Going to the scale of the nucleus – can we describe and predict nuclear processes governing supernovae, for example?

Standard Model is the current starting point
for describing the nuclear processes
that brought the universe to the present time
and hold the key to 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?



Hot and dense quark-gluon matter

Hadron structure

Hadron-Nuclear interface

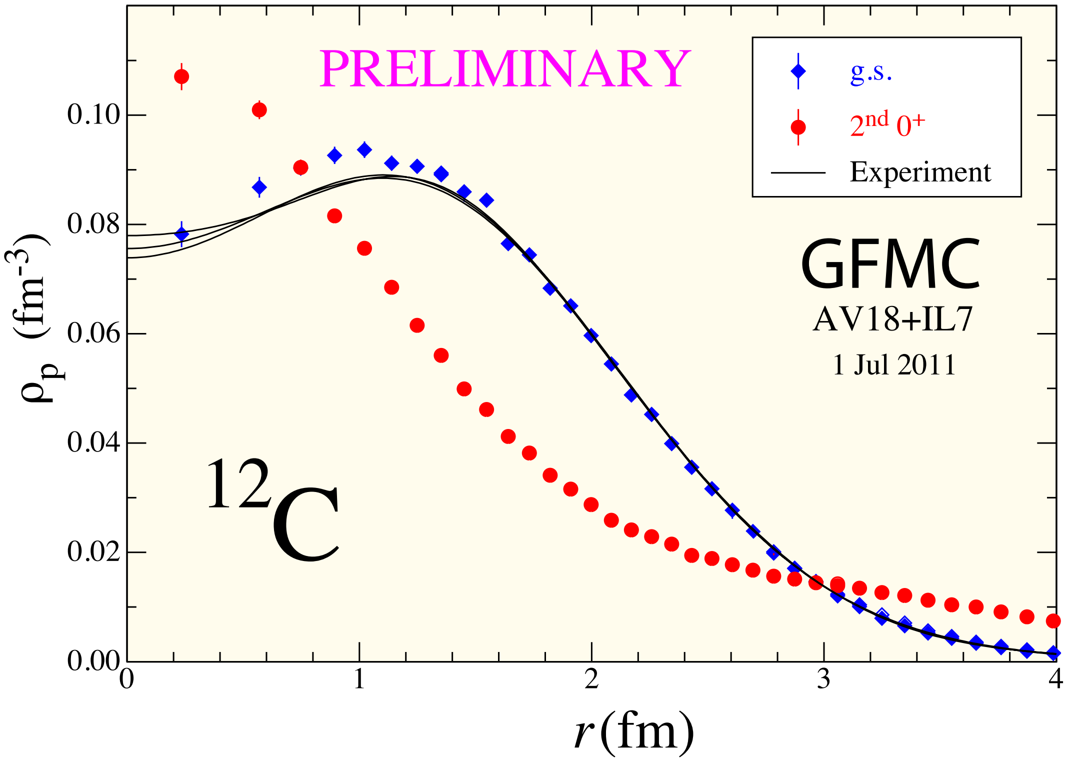
Nuclear structure
Nuclear reactions

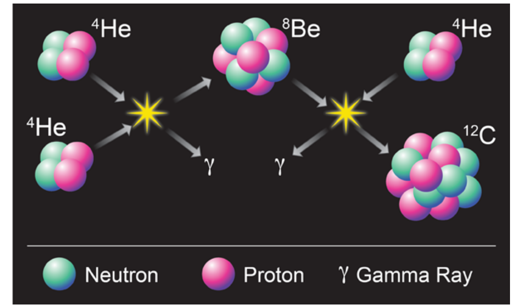
Third Law of Progress in Theoretical Physics by Weinberg:

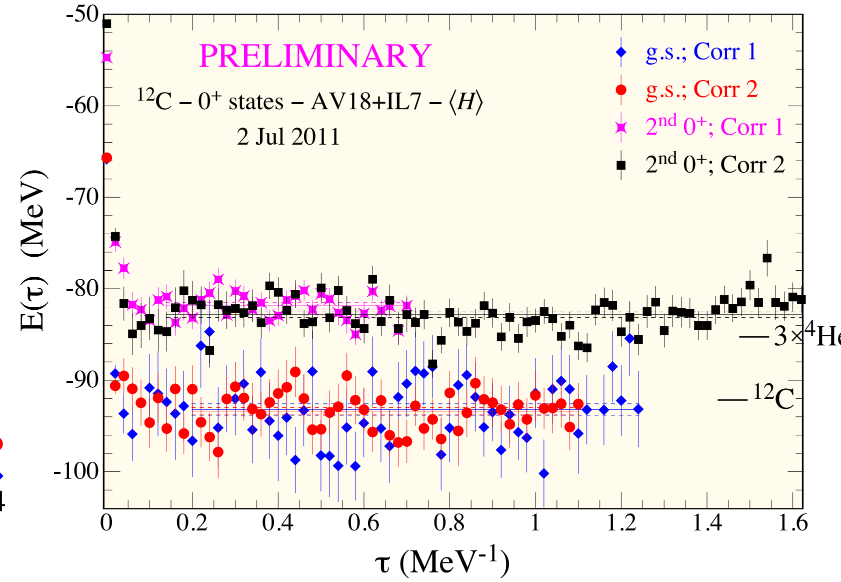
"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

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

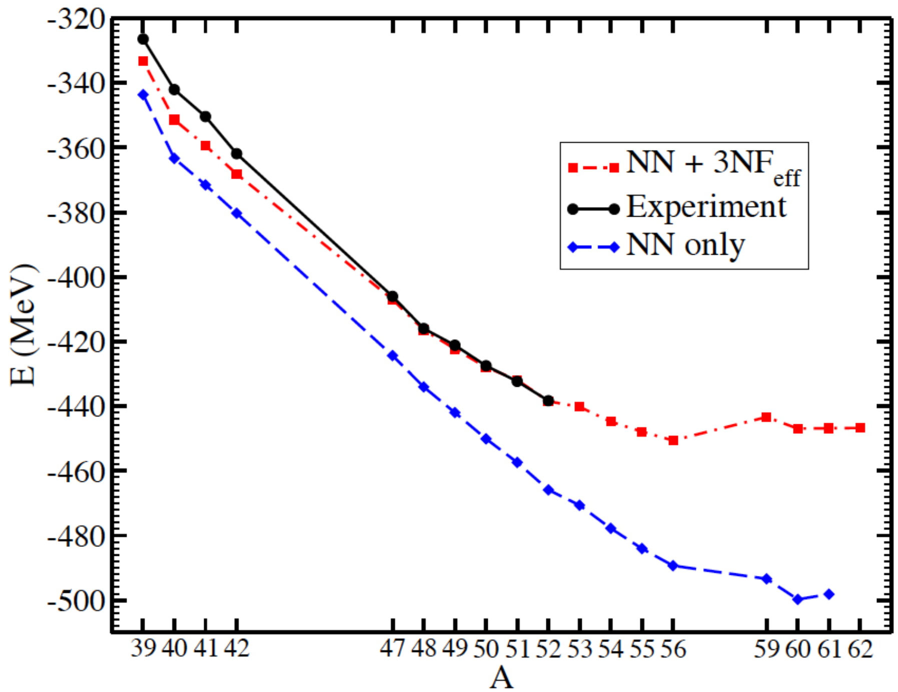
Epelbaum et al., Phys. Rev. Lett. 106, 192501 (2011)

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.

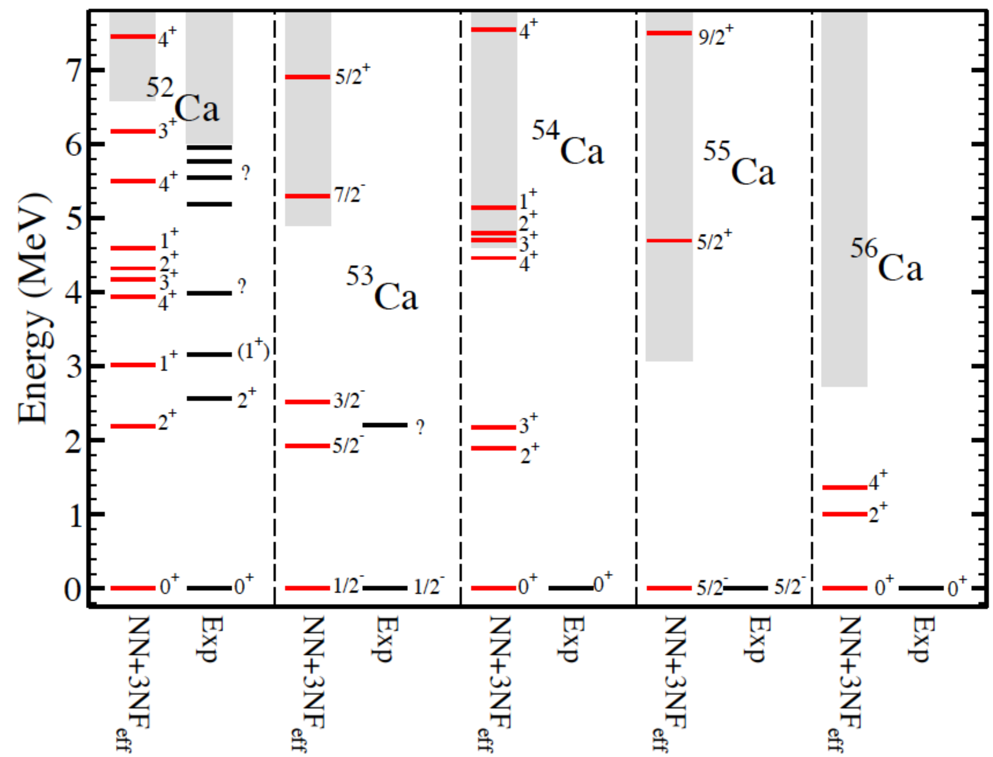
	0_2^+	$2_1^+, J_z = 0$	$2_1^+, J_z = 2$
LO $[O(Q^0)]$	−94(2)	−92(2)	−89(2)
NLO $[O(Q^2)]$	−82(3)	−87(3)	−85(3)
IB + EM $[O(Q^2)]$	−74(3)	−80(3)	−78(3)
NNLO $[O(Q^3)]$	−85(3)	−88(3)	−90(4)
Experiment	−84.51	−87.72	

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

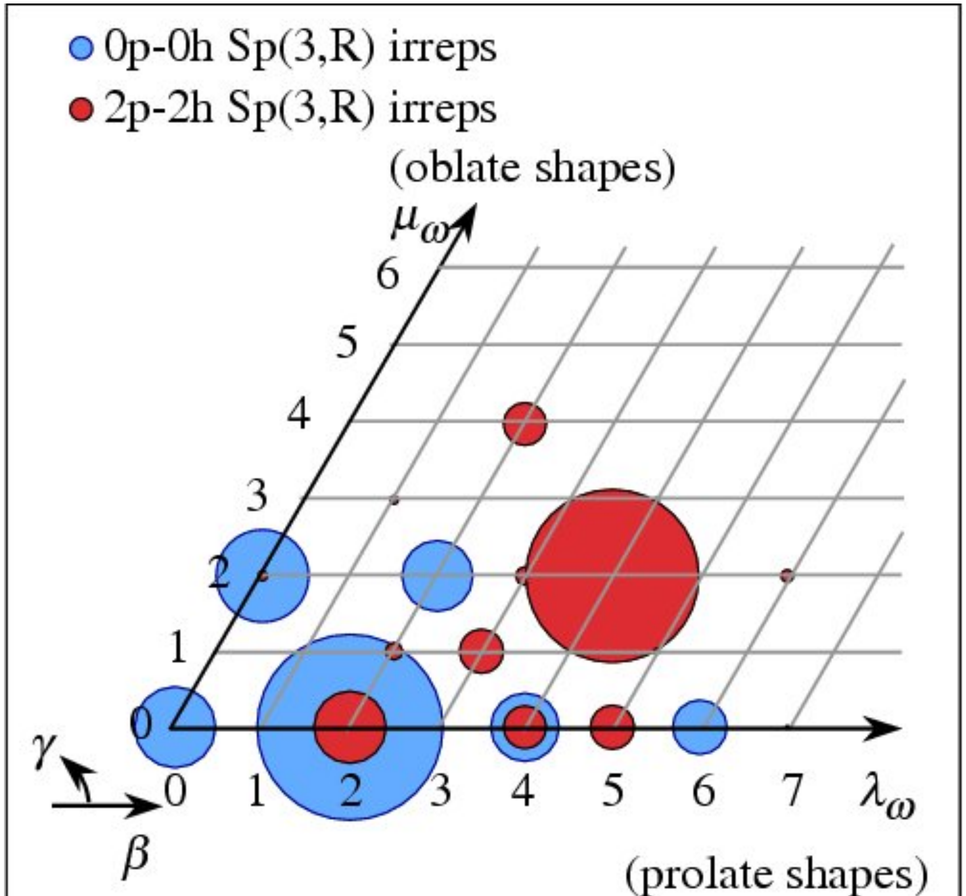
- Strong coupling to continuum for neutron rich calcium isotopes
- Level ordering of states in the *gds* shell is contrary to naïve shell model picture

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)

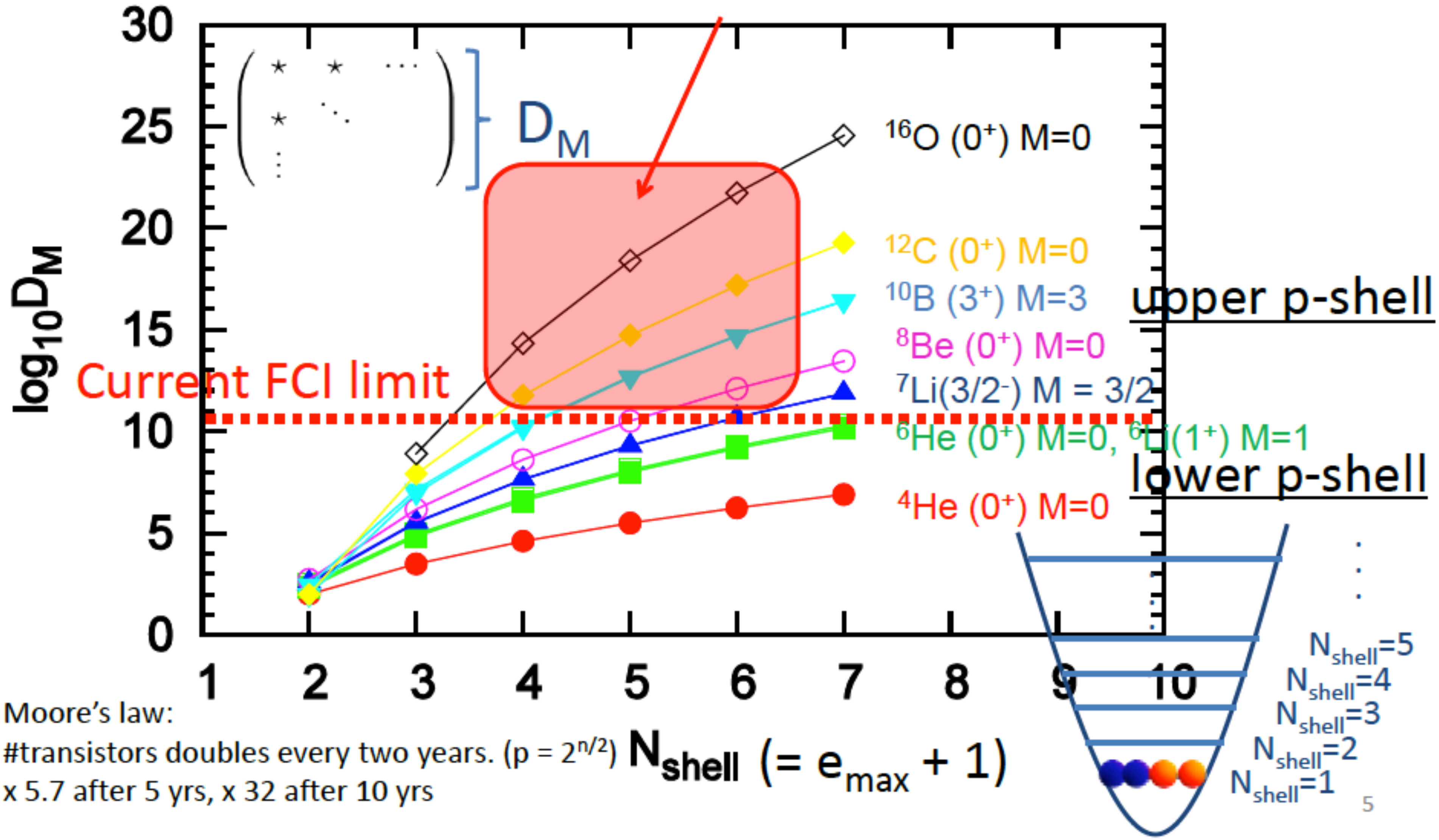


first 0+ excited state of 16O

- Effective truncation scheme
- Very promising approach to cluster states

No Core Monte Carlo Shell Model

Dimension of M-scheme basis for p-shell nuclei



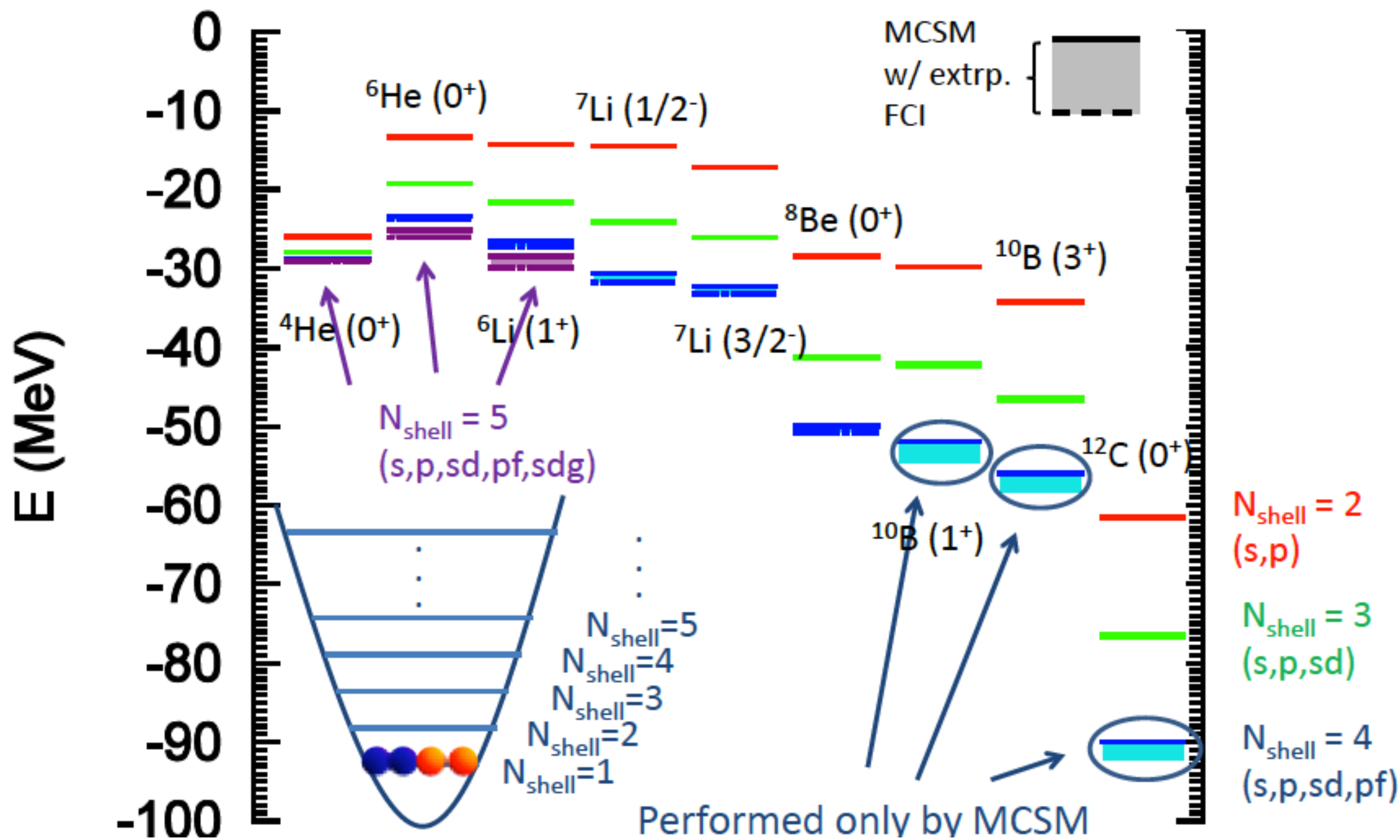
Moore's law:

#transistors doubles every two years. ($p = 2^{n/2}$)

x 5.7 after 5 yrs, x 32 after 10 yrs

T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary

Energies of the Light Nuclei



Collaborations with Pacific National University developed the NN interaction used to make these predictions

“Proton-Dripping Fluorine-14”

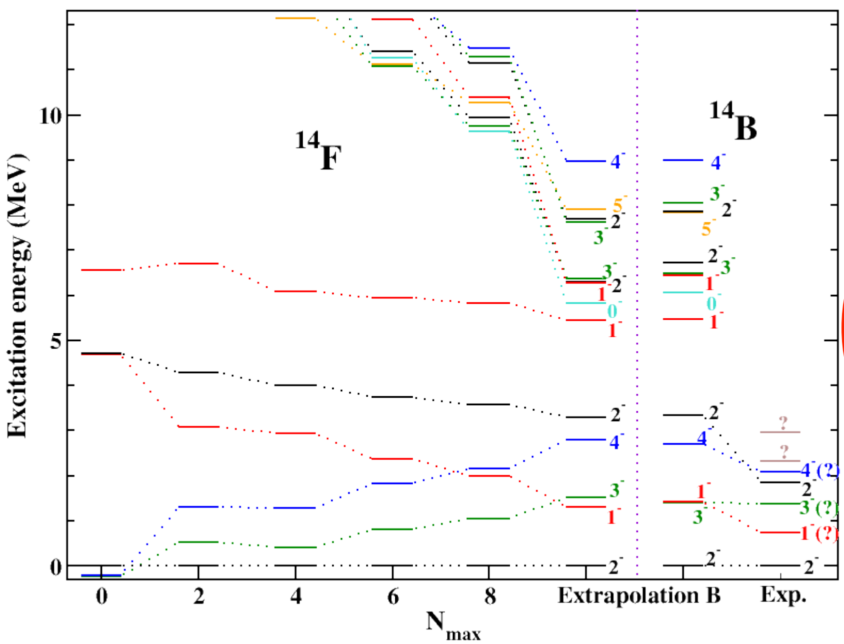
Objectives

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

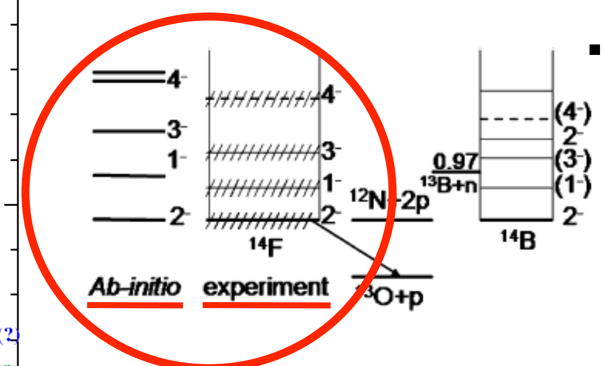
Impact

- 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. Shirokov and J.P. Vary, Phys. Rev. C 81 (2010) 021301(R)



Experiment confirms our published predictions!



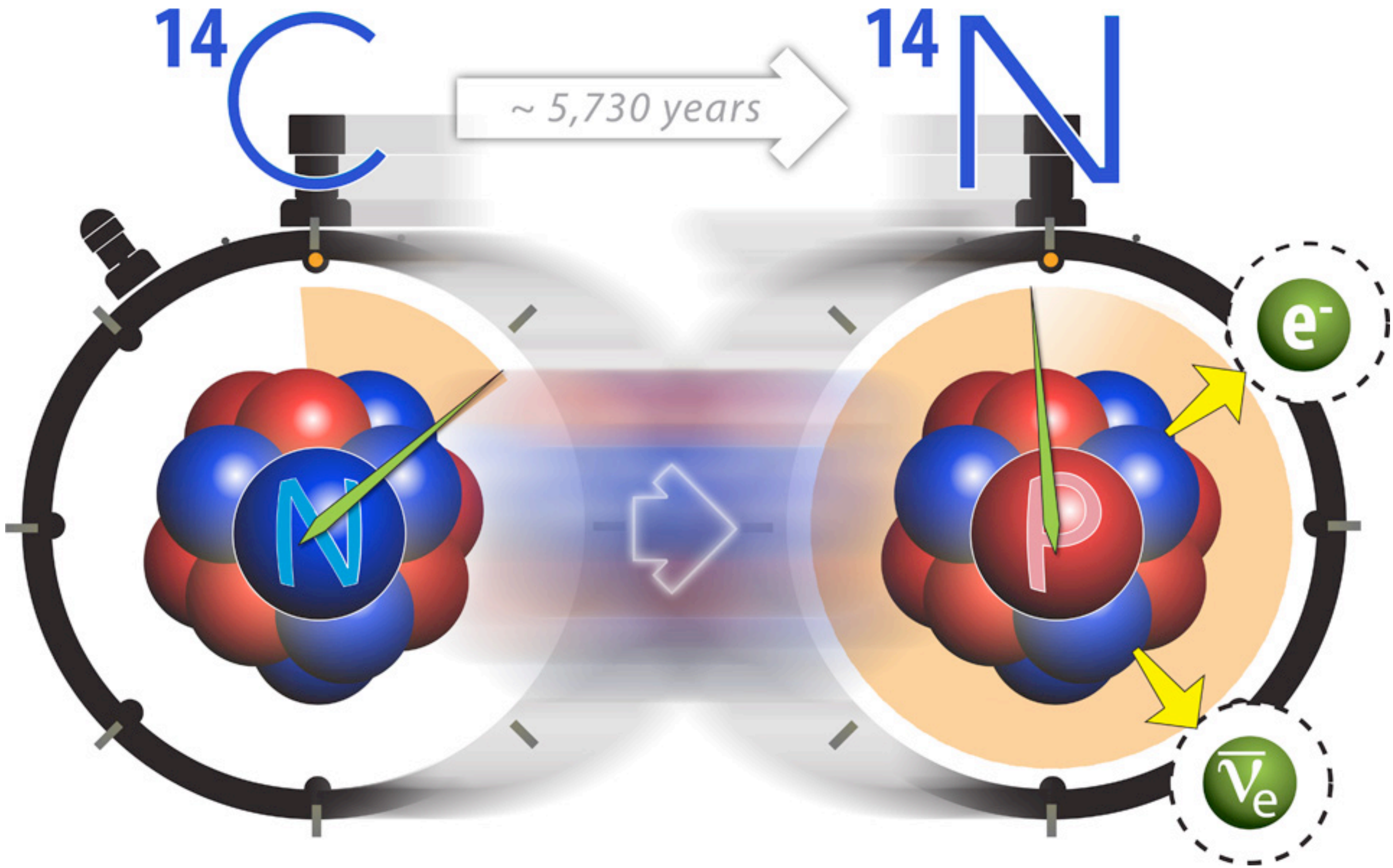
V.Z. Goldberg et al., Phys. Lett. B 692, 307 (2010)

- Dimension of matrix solved for 14 lowest states ~ 2x10^{9}
- Solution takes ~ 2.5 hours on 30,000 cores (Cray XT4 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)

U.S. DEPARTMENT OF ENERGY | Office of Science

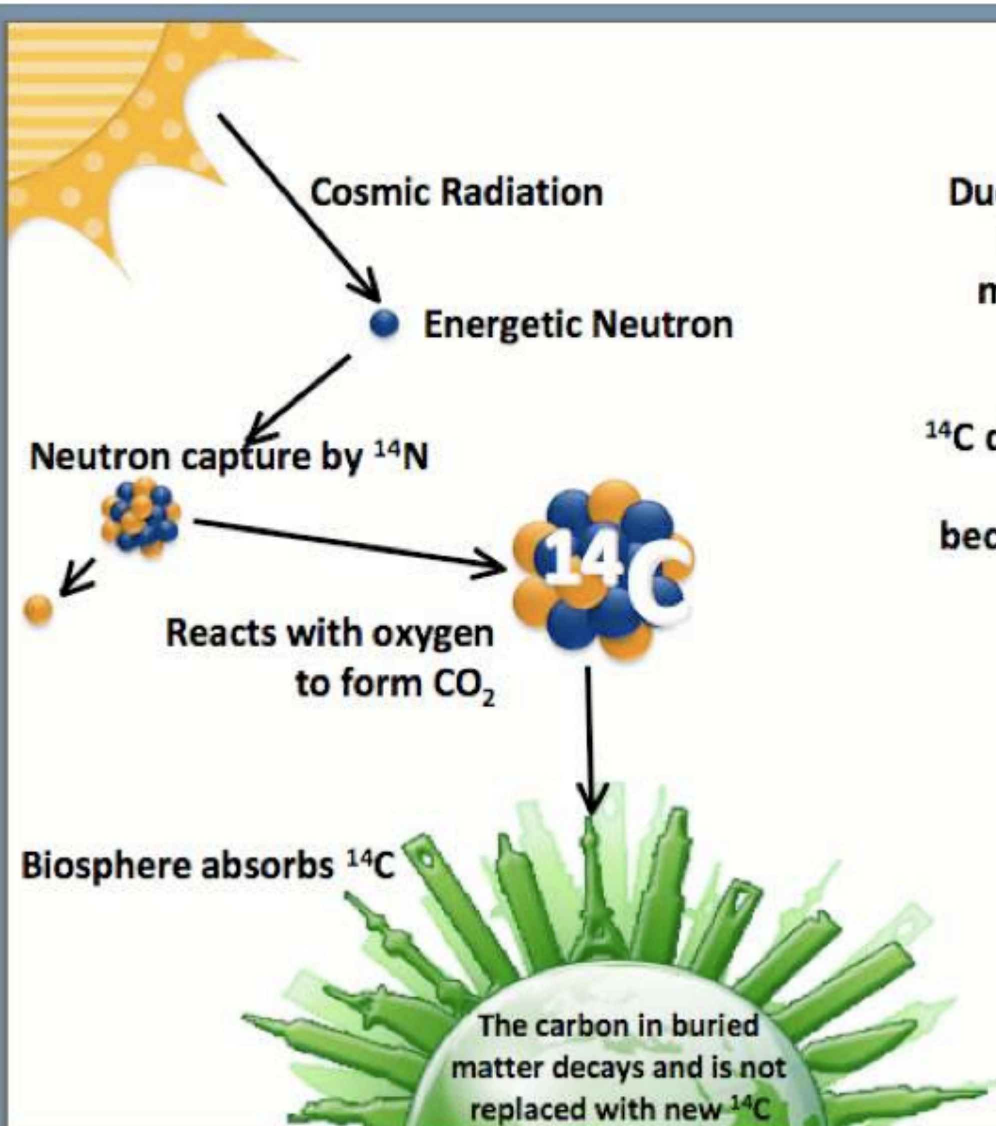
INCITE — Advancing America's Science and Industrial Competitiveness

UNEDF SciDAC Collaboration — Universal Nuclear Energy Density Functional



14C
~ 5,730 years
14N
N
p
e-
νe

Petascale Early Science – Ab-initio structure of Carbon-14



Due to its long half-life, ^{14}C has been used in dating organic materials, up to 60,000 years old, since the 1950's.

^{14}C decays into ^{14}N through beta decay, where a neutron becomes a proton, an electron, and an antineutrino.

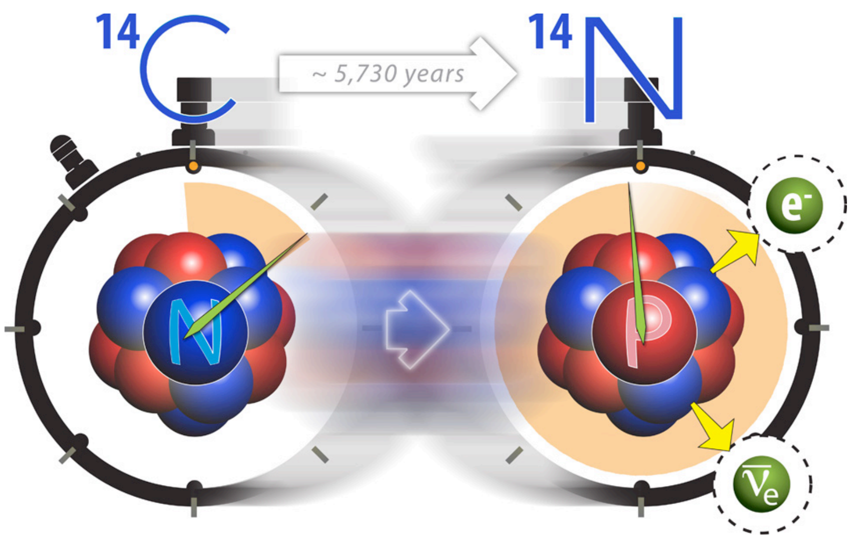
"Anomalous Long Lifetime of Carbon-14"

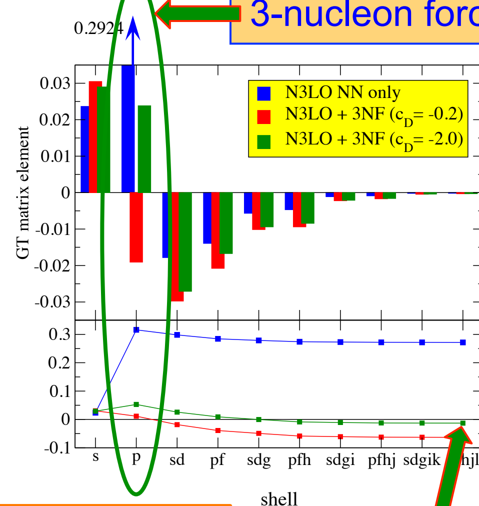
Objectives

- 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 ~ 1×10^9
- 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]

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IOWA STATE UNIVERSITY

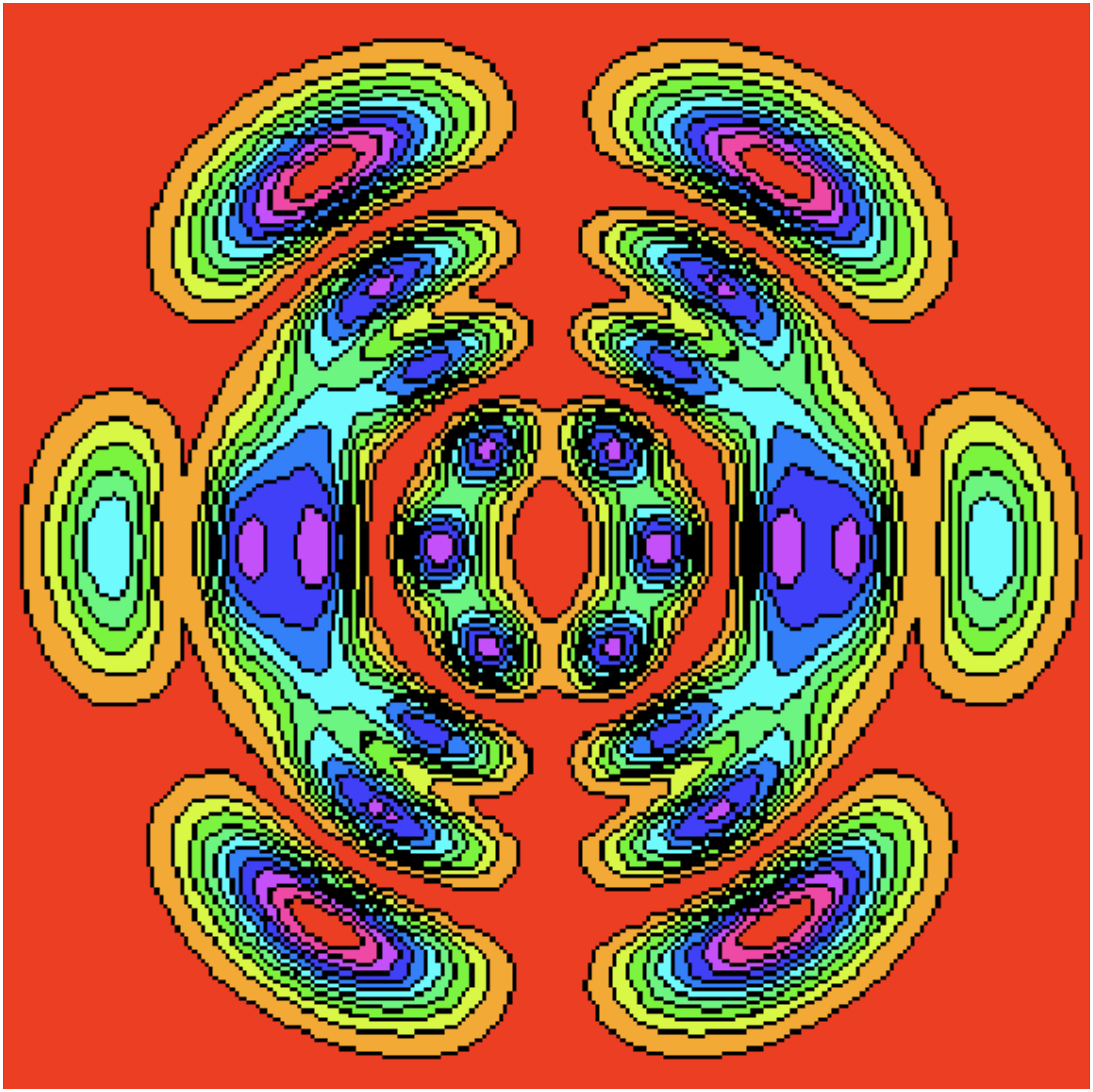
TRIUMF

UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

NNSA

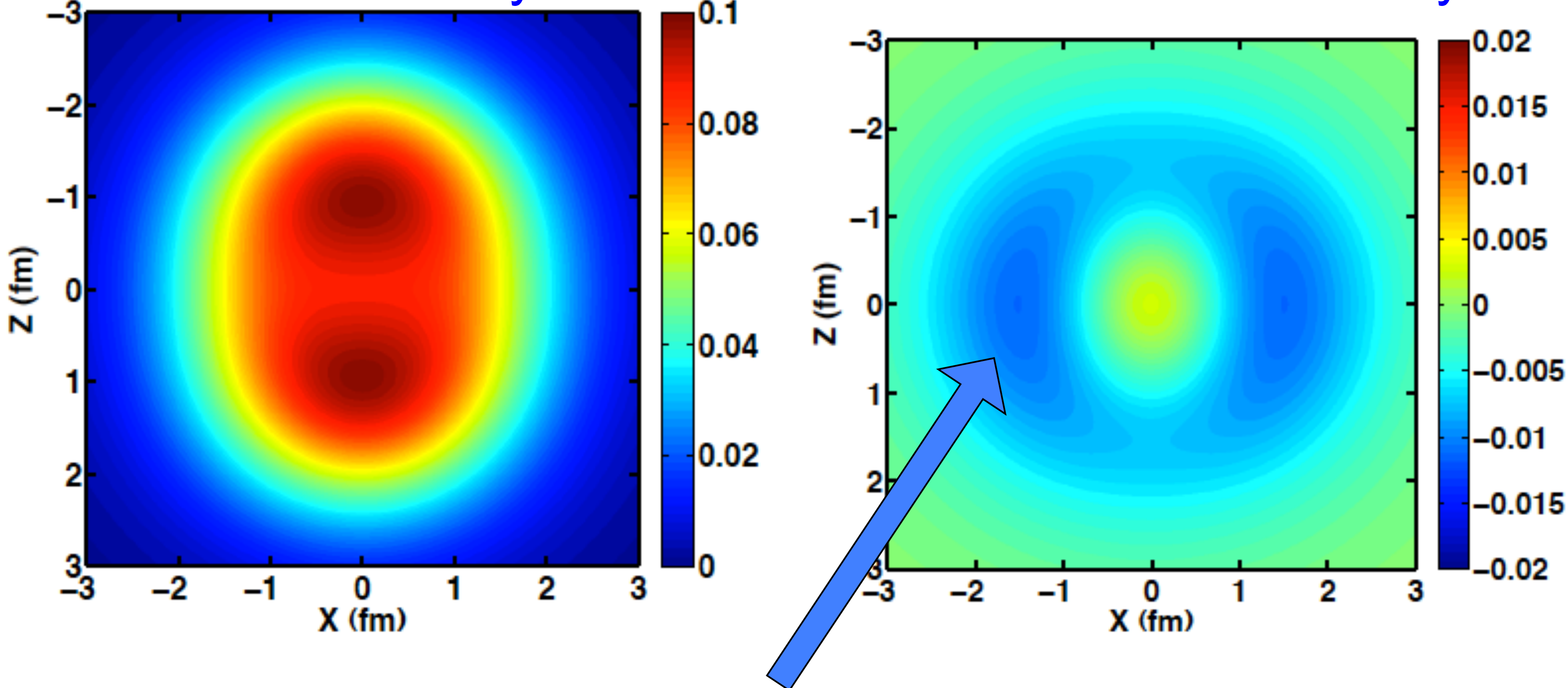
LAWRENCE LIVERMORE NATIONAL SECURITY

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



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

Total density / Neutron – Proton density



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

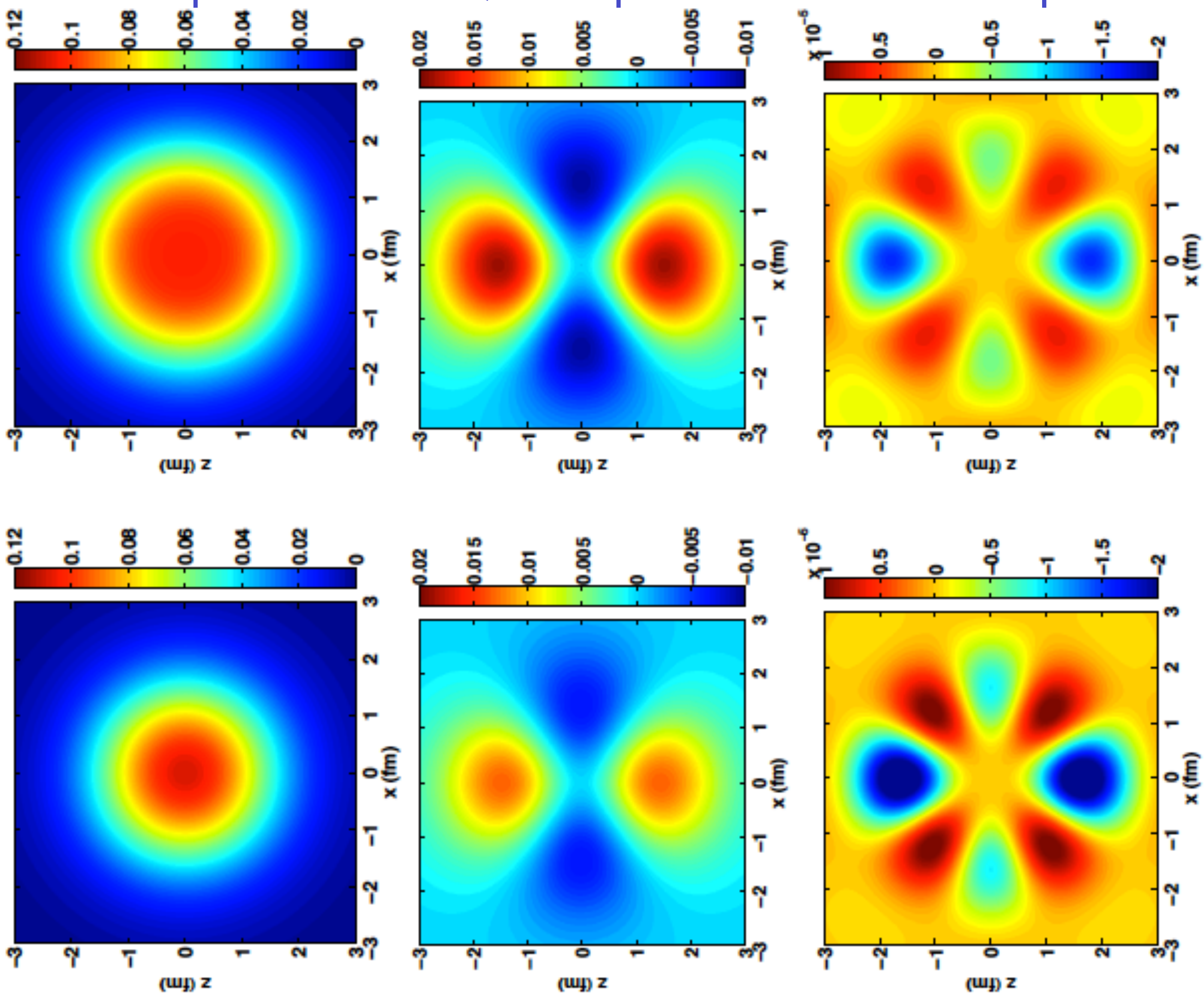
C. Cockrell, J.P. Vary, P. Maris, ArXiv 1201.0724; C. Cockrell, PhD, Iowa State University

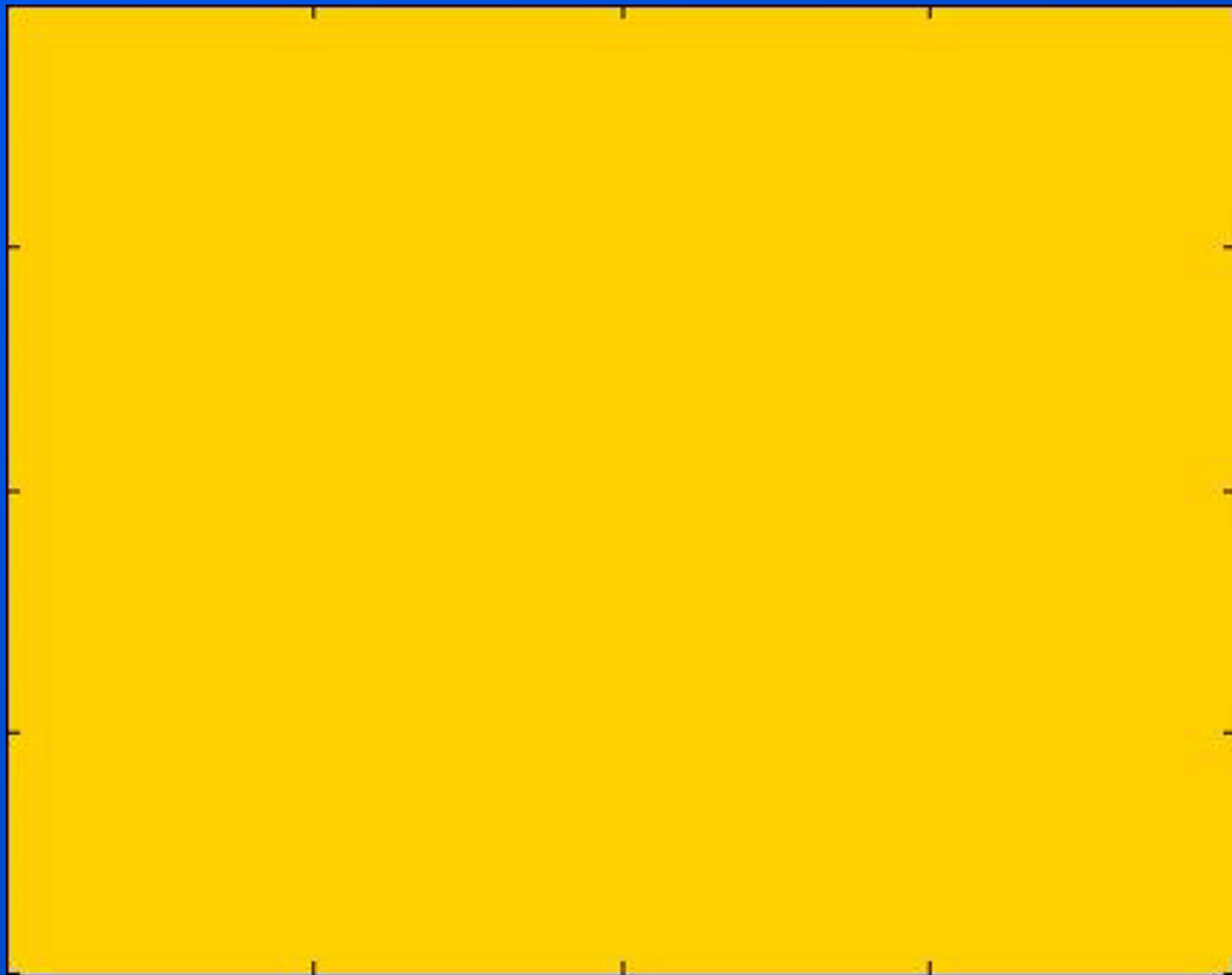
^{8}Li gs
J=2

Monopole Quadrupole Hexadecapole

Neutrons

Protons





J = 2 ground state of ^{8}Li viewed through a hexadecapole filter (Chase Cockrell, PhD)

Ab initio nuclear reactions

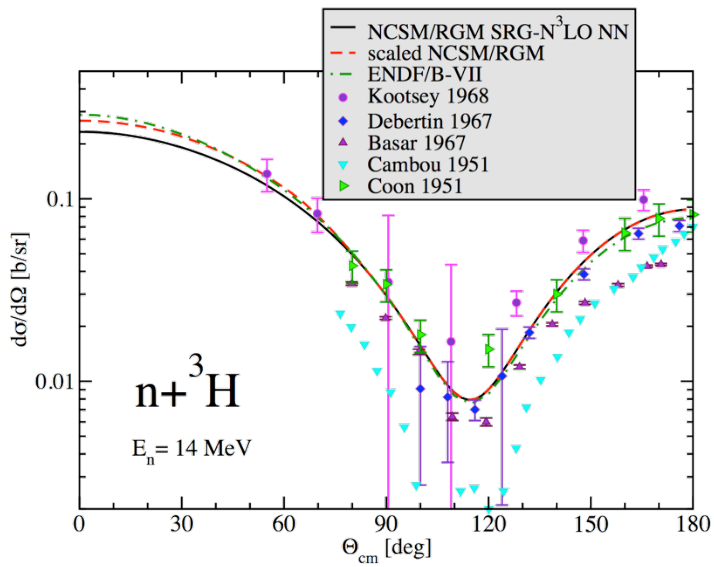
Objectives

- 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

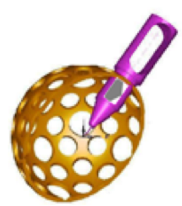
- Computational tools for addressing fusion reactions that power stars and Earth-based fusion facilities such as the National Ignition Facility (NIF)
- Provide research community with accurate evaluations and uncertainties for nuclear astrophysics and fusion diagnostic

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

Simulations on high performance computers provide answers to questions that neither experiment nor analytic theory can answer

It becomes a third leg, in addition to Experiment and Theory, supporting the field of nuclear physics

||

Experiment + Theory + Simulations

Atanasoff-Berry Computer (ABC)

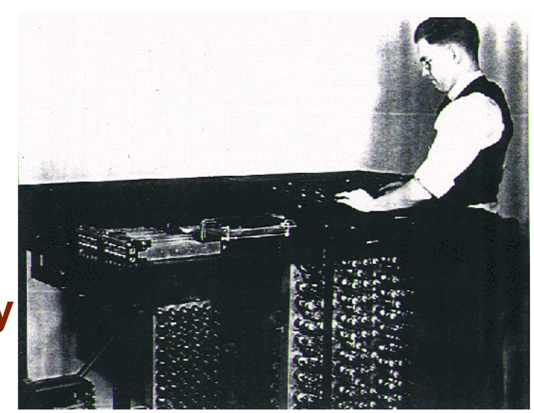

John Vincent Atanasoff
1983 photo


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

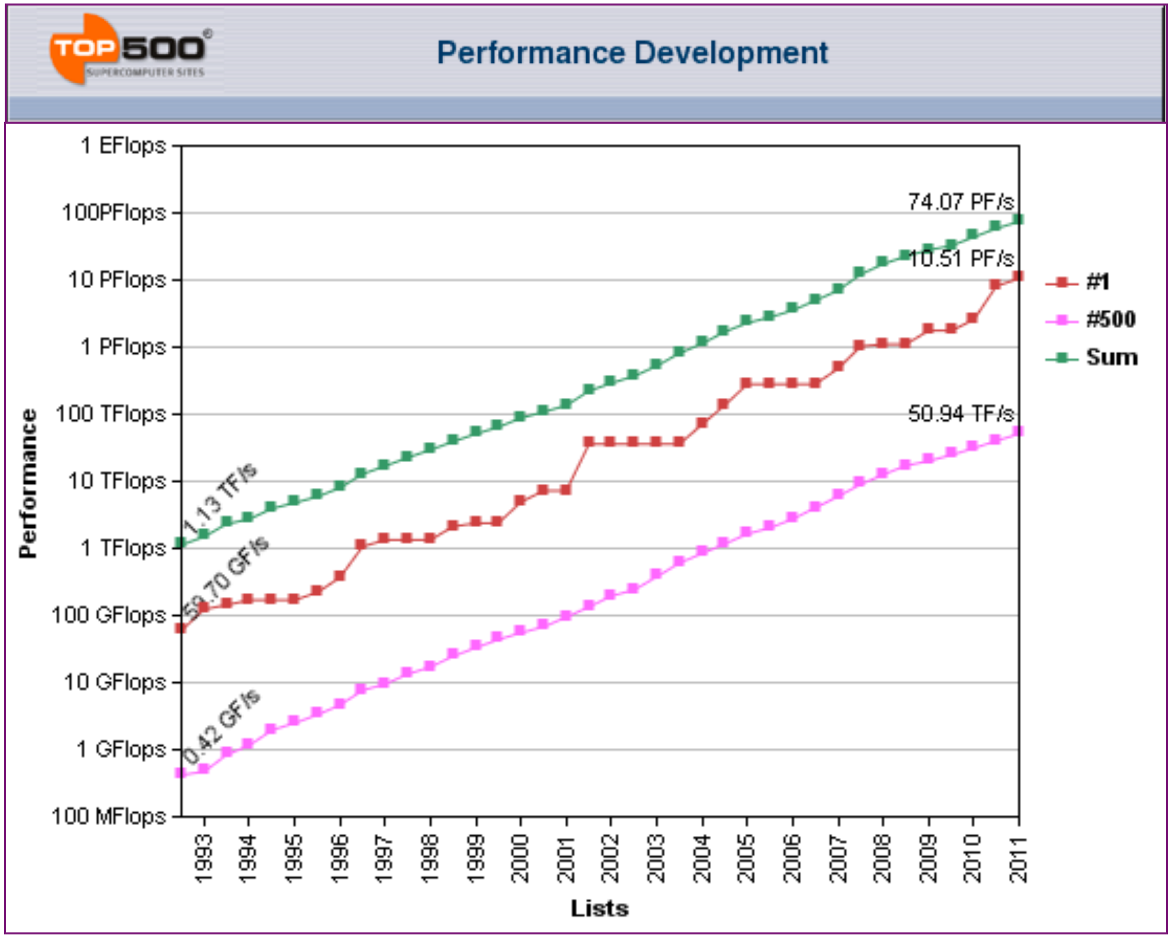
1942 photo of Clifford Berry and the ABC

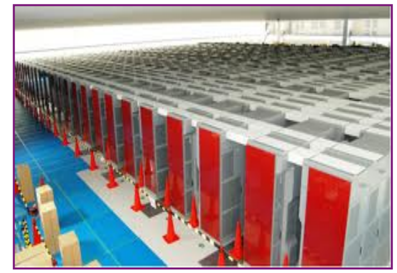


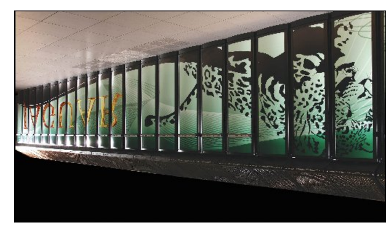
Theoretical Tools and Connections to Computational Science

1Teraflop=10^{12} flops
1peta=10^{15} flops (today)
1exa=10^{18} flops (next 10 years)

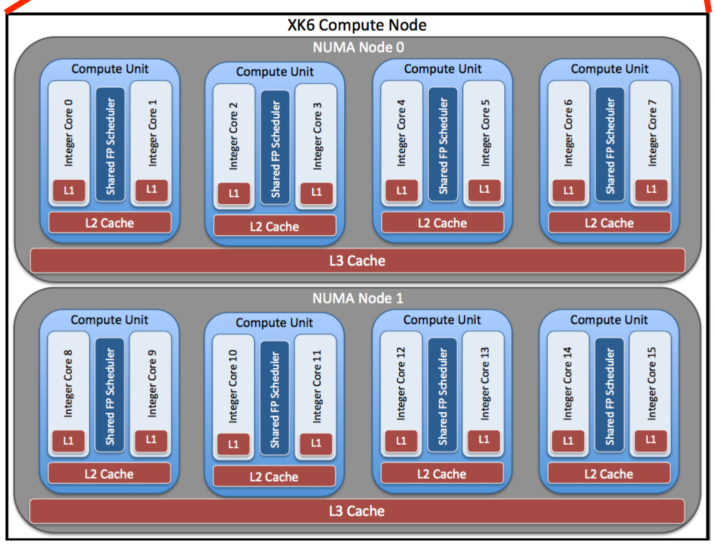
Tremendous opportunities for nuclear theory!







“Leadership Class” Computational Resources



16 “cores” on one compute “node”
Total: 300,000 cores at present
Titan will have 1GPU/node

& INCITE Award 55M cpu-hrs/yr

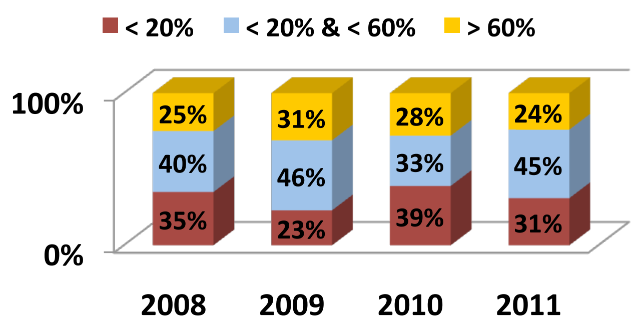
UNEDF Leadership-class computing

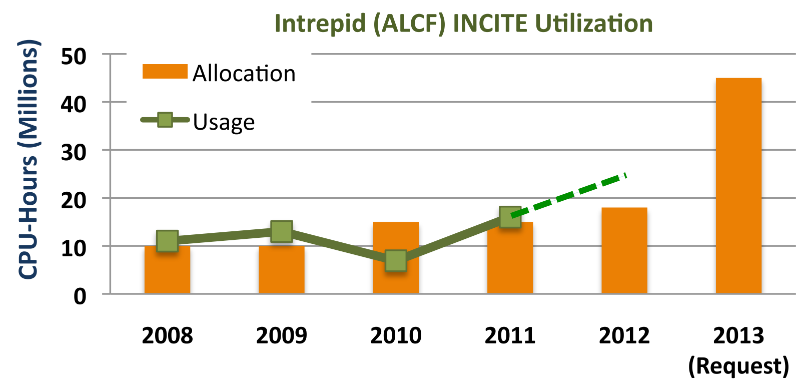
◆ SciDAC collaboration between applied mathematicians, computer scientists, and nuclear physicists leads to efficient utilization of leadership-class computing resources for nuclear physics problems

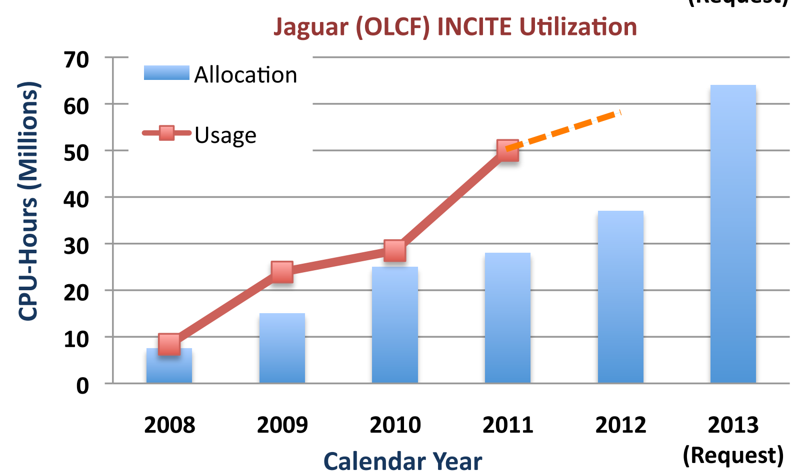
◆ Significant accomplishments, achieved through leadership-class computing

- ➢Ab-initio calculations of C-12
- ➢Understanding long lifetime of C-14
- ➢Microscopic calculations of select medium-mass nuclei
- ➢Improved energy-density functional UNEDF1

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







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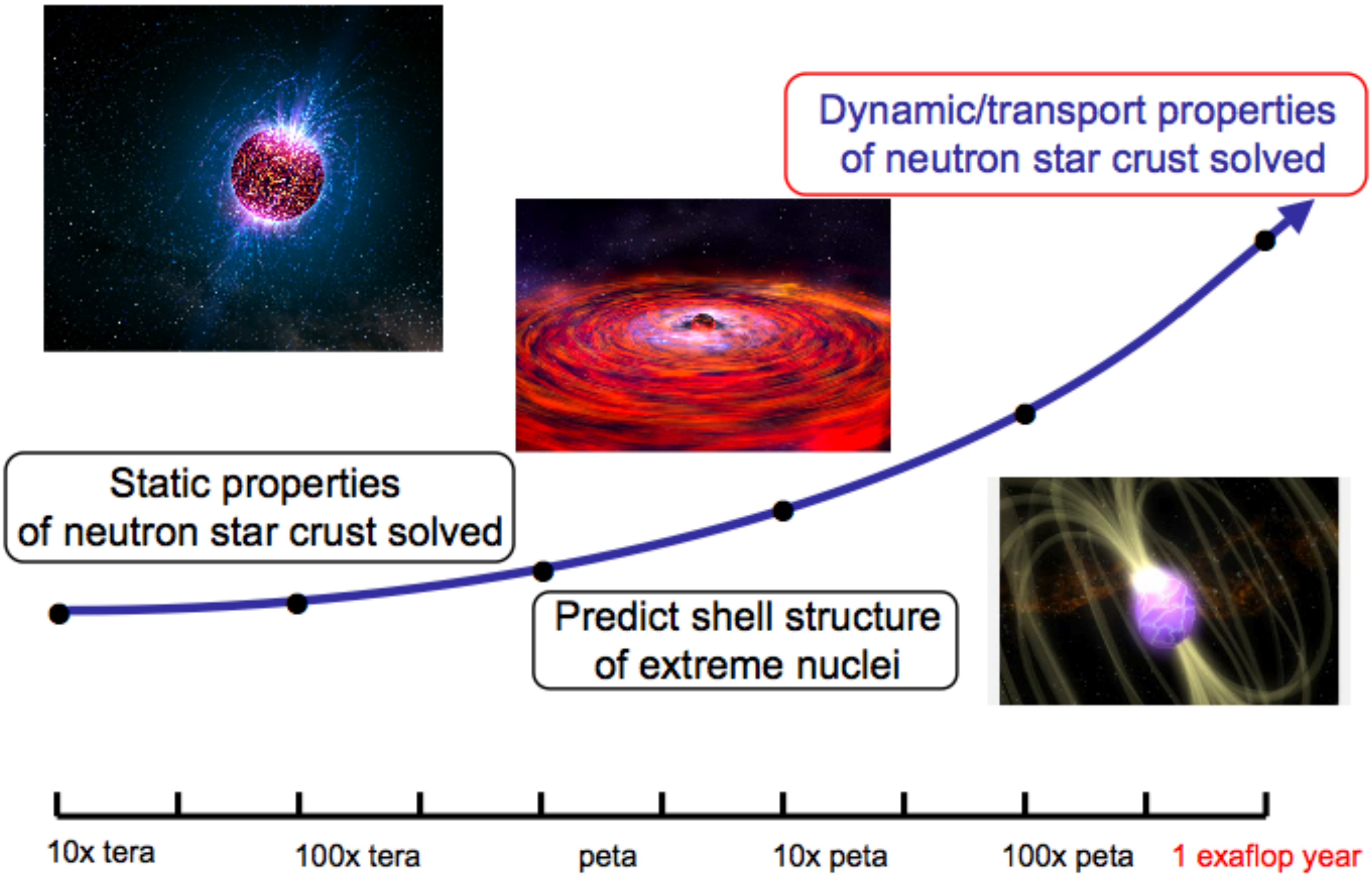
Universal Nuclear Energy Density Functional

Суперкомпьютер «Ломоносов»

Selected science and technology "drivers" for high-performance computing


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

Corporations use HPC to speed product development cycles

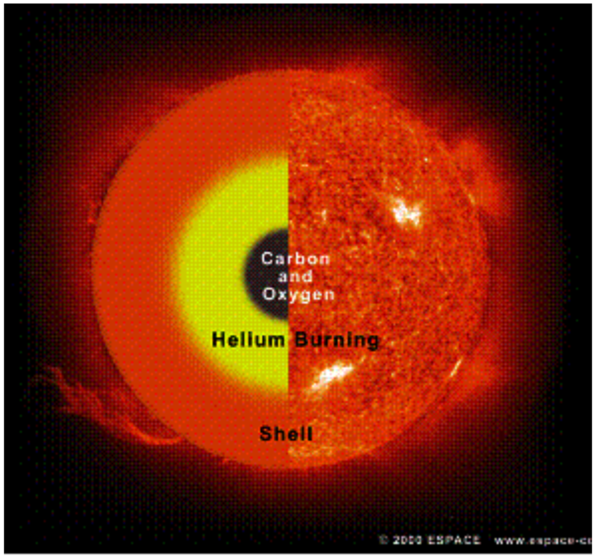
US Council on Competitiveness case studies (15)
http://www.compete.org

Example 1:
"Bringing the power of HPC to Drug Discovery and the Delivery of 'Smarter' Health Care," studies how HPC and computer-aided engineering is helping GNS Healthcare drive the identification of the right cost-effective intervention for the right patient at the right time.
http://www.compete.org/publications/detail/1742/

Example 2:
"HPC Enables Innovation and Productivity at Ford Motor Company."
From Safety Performance to EcoBoost Technology
http://www.compete.org/publications/detail/1664/

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
+ Many More!



^{12}C - At the heart of matter

The first excited 0+ state of ^{12}C, the "Hoyle state", is the key state of ^{12}C formation in the triple-alpha fusion process that occurs in stars.

Due to its role in astrophysics and the fact that carbon is central to life, some refer to this as one of the "holy grails" of nuclear theory.

Many important unsolved problems of the Hoyle state:

Ab initio origins of the triple-alpha structure are unsolved

Breathing mode puzzle - experiments disagree on sum rule fraction

Laboratory experiments to measure the formation rate are very difficult - resulting uncertainties are too large for predicting the ^{12}C formation rate through this state that dictates the size of the iron core in pre-supernova stars

Conclusion: Need *ab initio* solutions of the Hoyle state with no-core method that accurately predicts the ground state binding energy

==> parameter free predictions for the Hoyle state achievable with petascale within 1-2 years

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

Unsolved Mysteries

Driven by new puzzles in our understanding of the physical world, particle physicists are following paths to new wonders and startling discoveries. Experiments may even find extra dimensions of space, mini-black holes, and/or evidence of string theory.

Universe Accelerating?

The expansion of the universe appears to be accelerating. Is this due to Einstein's Cosmological Constant? If not, will experiments reveal a new force of nature or even extra (hidden) dimensions of space?

Why No Antimatter?

Matter and antimatter were created in the Big Bang. Why do we now see only matter except for the tiny amounts of antimatter that we make in the lab and observe in cosmic rays?

Dark Matter?

Invisible forms of matter make up much of the mass observed in galaxies and clusters of galaxies. Does this dark matter consist of new types of particles that interact very weakly with ordinary matter?

Origin of Mass?

In the Standard Model, for fundamental particles to have masses, there must exist a particle called the Higgs boson. Will it be discovered soon? Is supersymmetry theory correct in predicting more than one type of Higgs?

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

Supersymmetry

Extra dimensions (string theory)

Multiple universes

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

- A. Lomonosov

<u>Status report from this workshop</u>

We have successful “models” and we are developing successful predictive theory with wide applicability and the supercomputer simulations to prove that theory

Thank you Pacific National University
and Khabarovsk for hosting this scientific meeting

I welcome your questions!