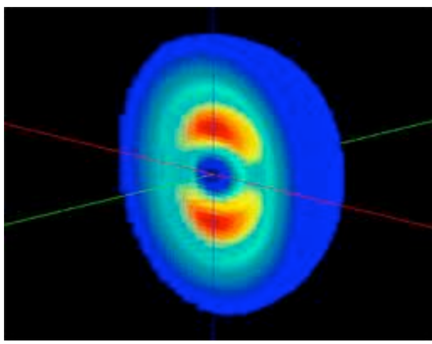
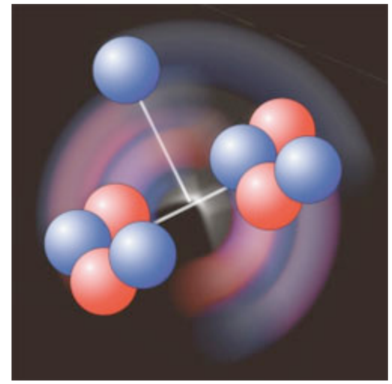
Computational Nuclear Physics

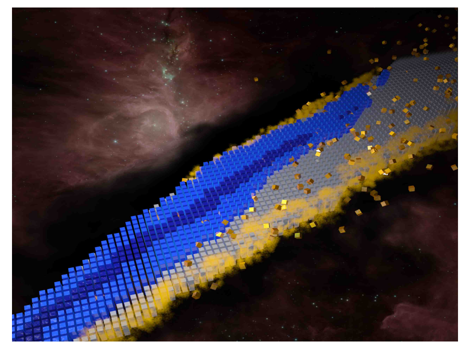
Joe Carlson

Nuclear, Particle, Astrophysics and Cosmology Group

Theoretical Division, LANL

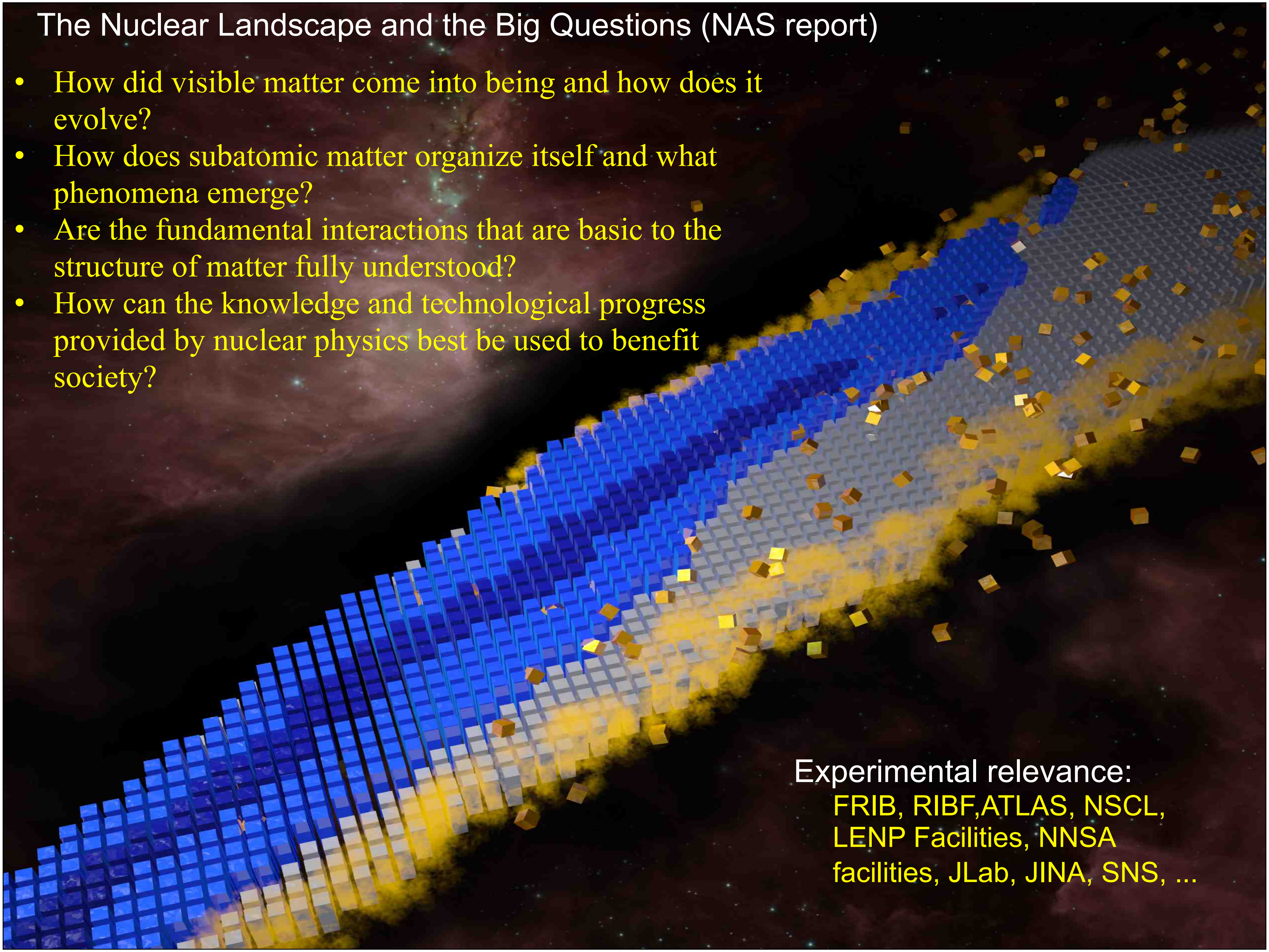






Building Complex Structures and phenomenon from simple interactions

QUCS 2012, NARA



The Nuclear Landscape and the Big Questions (NAS report)

- 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?

Experimental relevance:

FRIB, RIBF,ATLAS, NSCL, LENP Facilities, NNSA facilities, JLab, JINA, SNS, ...

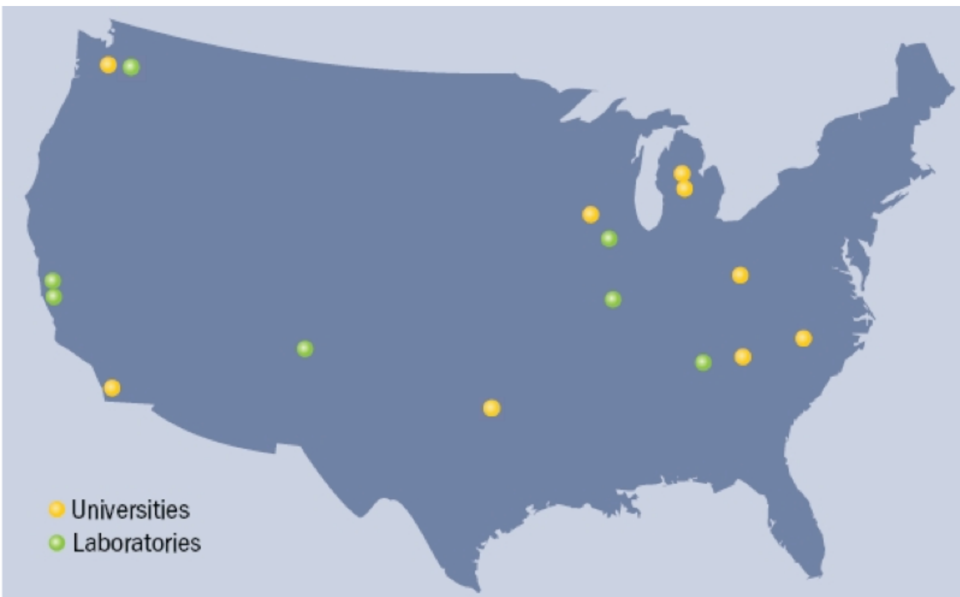
Nuclear Physics SciDAC projects

SCIDAC projects : UNEDF ➪ NUCLEI

National (and international) effort

Physicists, Computer Scientists and Applied Mathematicians

15 institutions, 2011 19 postdocs + 11 students



Both People and
Computational Resources are critical

~120M core-hours in 2012

For a popular description of UNEDF, see:
SciDAC Review Winter 2007
http://www.scidacreview.org/0704/pdf/unedf.pdf
Nucl. Phys. News 21, No. 2, 24 (2011)
Office of Science "Highlight Series":
http://science.energy.gov/news/in-focus/2011/03-28-11-s/

Junior Scientists in SciDAC

POST-DOCTORAL ASSOCIATES (2010)

Christopher Calderon, LBNL (staff, Numerica co.)
Joaquin Drut (Professor, UNC)
Stefano Gandolfi, LANL (staff, LANL)
Kai Hebeler, OSU (TRIUMF)
Heiko Hergert, MSU (OSU)
Jason Holt, UTK/ORNL
Eric Jurgenson, LLNL (staff, LLNL)
Markus Kortelainen, UTK (U. Jyväskylä)
Plamen Krastev, UCSD (research, Harvard)
Pieter Maris, ISU (Research Prof. ISU)
Eric McDonald, MSU (staff scientist, MSU)
Gustavo Nobre, LLNL (BNL, NNDC)
Junchen Pei, UTK (Prof., Pekin U.)
Nicolas Schunck UTK (staff, LLNL)
Roman Senkov, CMU
Ionel Stetcu, UW (staff, LANL)
Jun Terasaki, UNC (staff, U. Tsukuba)
Stefan Wild, ANL (staff, ANL)

Relevant instruction (workshops, courses) is crucial for the future of the field

Effect of UNEDF on workforce

Year-1: 9 students, 17 postdocs;
Year-2: 12 and 12;
Year-3: 10 and 18;
Year-4: 11 and 19

2010: Early Career Award

2010: Math/CS Staff ANL

2011: Faculty UNC/Chapel Hill

2010:Staff LLNL

2012: Faculty Guelph

2012: Harvard Research Computing

Why is Nuclear Physics Important?

Many-body physics:

Strong coupling of spin to space (tensor, spin-orbit)

Strong Pairing (Δ / E_F from 0.03~0.3)

Competition between single-particle evolution and pairing

Clustering (^{8}Be, ^{12}C Hoyle state, ...)

Nuclear physics:

Neutron-rich nuclei and limits of stability

Nucleosynthesis: light (BBN fusion) & heavy elements (SN, neutron star)

Correlations and nuclear response

Ties to other fields:

fundamental symmetries and BSM (ββ decay, superallowed β decay,...)

astrophysics (reactions, neutrinos, gravity waves, ...)

cold atom physics (superfluidity, universality, Efimov, ...)

Illustrate progress and challenges

Starting point:

Two- plus three-nucleon interactions (phenomenological, EFT)

$$H = \sum_i T_i + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk}$$

V_{ij} fit to many NN experimental data

V_{ijk} has O(5) parameters, typically fit to few-nucleon systems

One- plus two-body charges and current operators:

$$\rho = \sum_i \rho_i + \sum_{i<j} \rho_{ij}$$

$$\mathbf{j} = \sum_i \mathbf{j}_i + \sum_{i<j} \mathbf{j}_{ij}$$

+ similarly for weak interaction; few parameters fit to data

Computational Methods

Light Nuclei: Quantum Monte Carlo

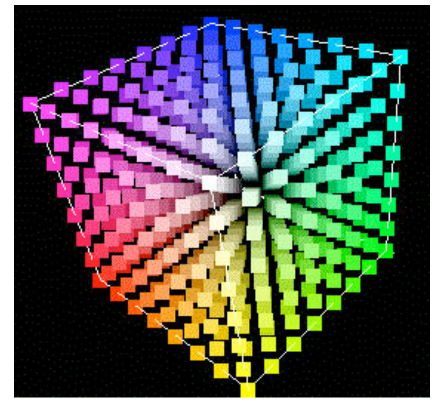
Configuration Interaction

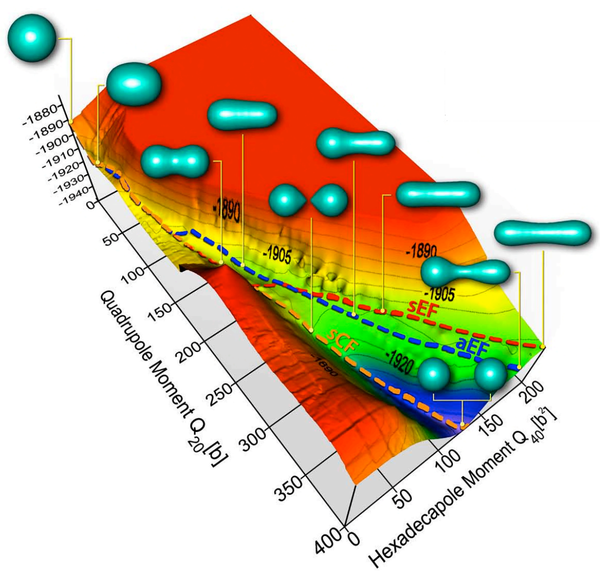
Medium Mass Nuclei: Coupled Cluster

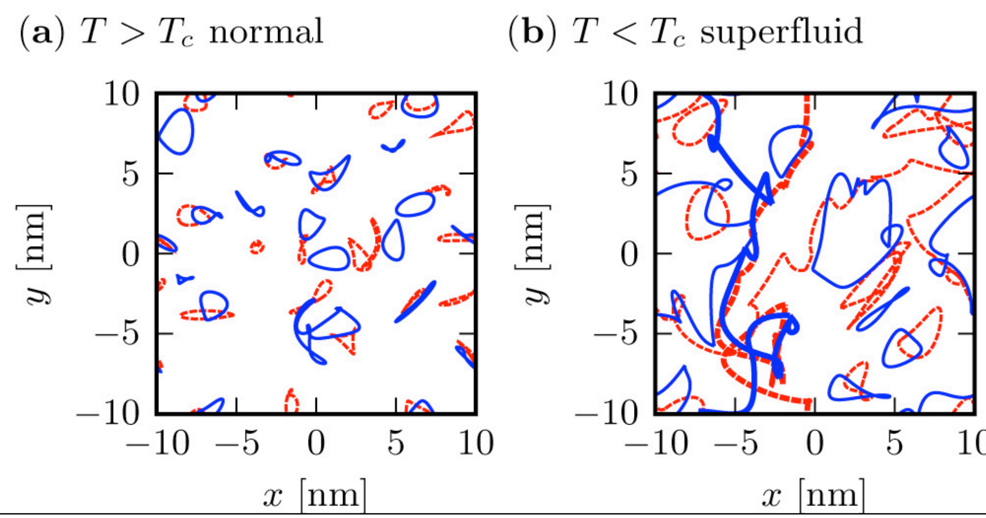
Heavy Nuclei: Density Functional Theory

Nucleonic Matter: Quantum Monte Carlo

Density Functional Theory

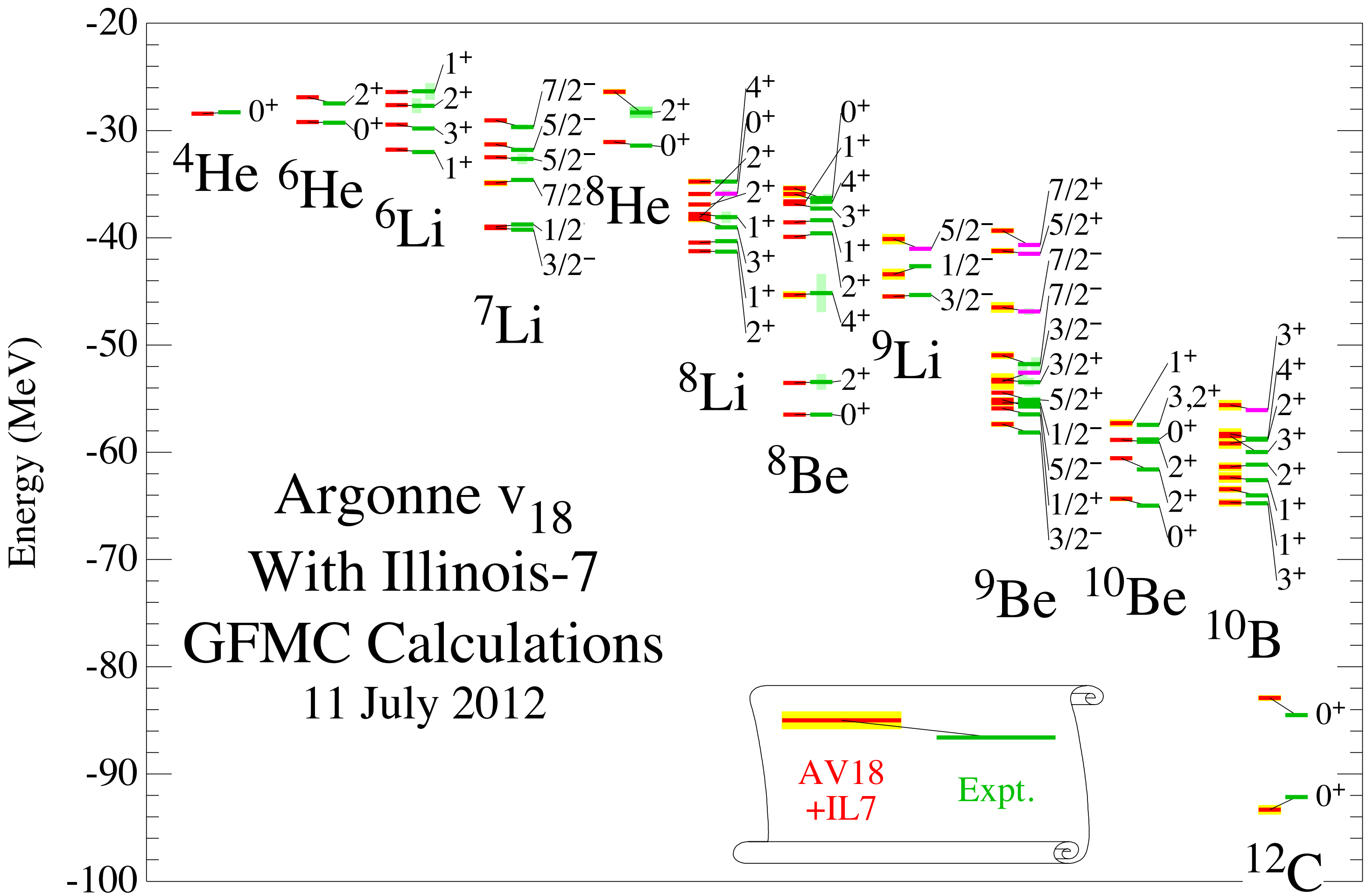






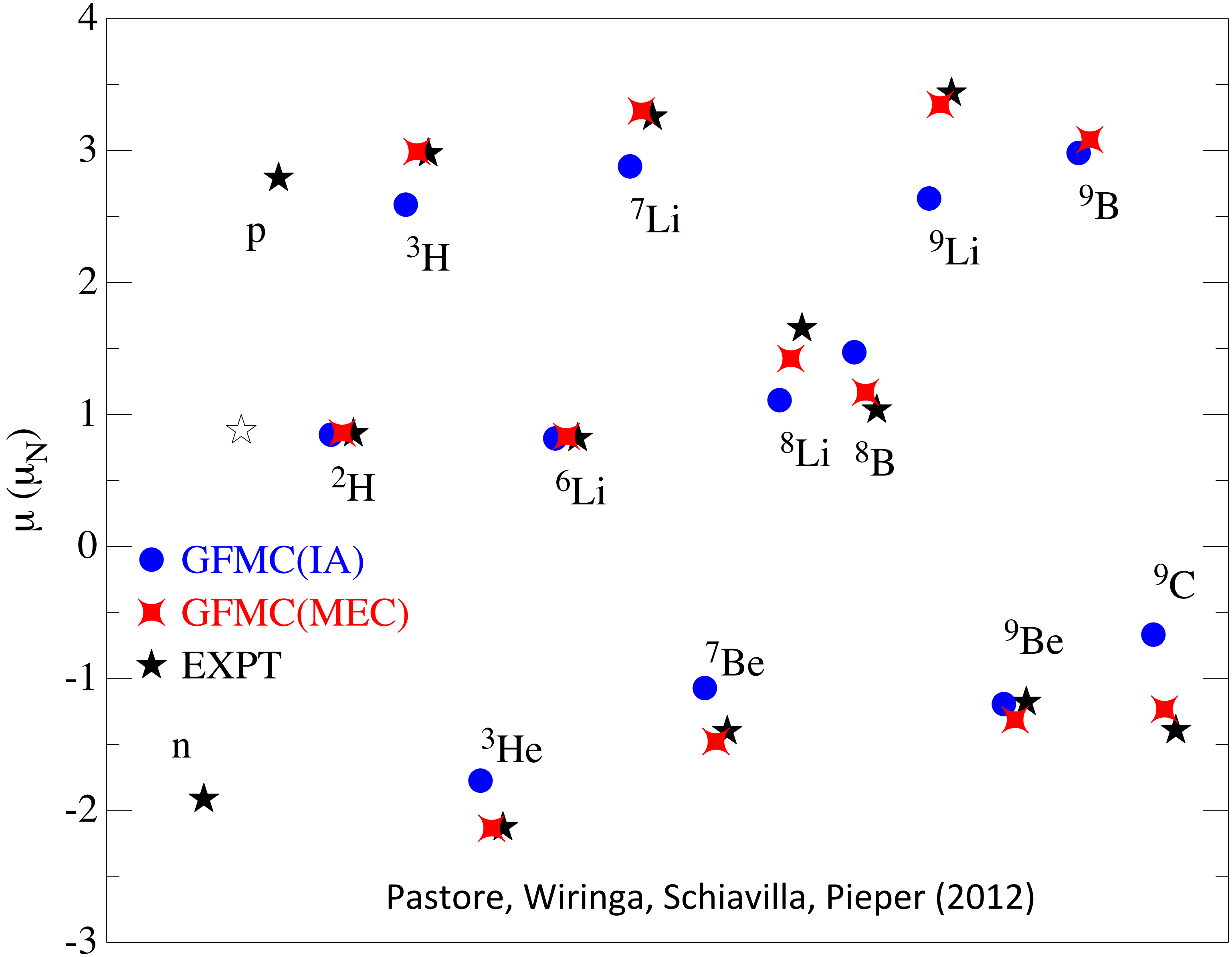
Light Nuclei

Spectra reproduced with `realistic' NN + NNN interactions

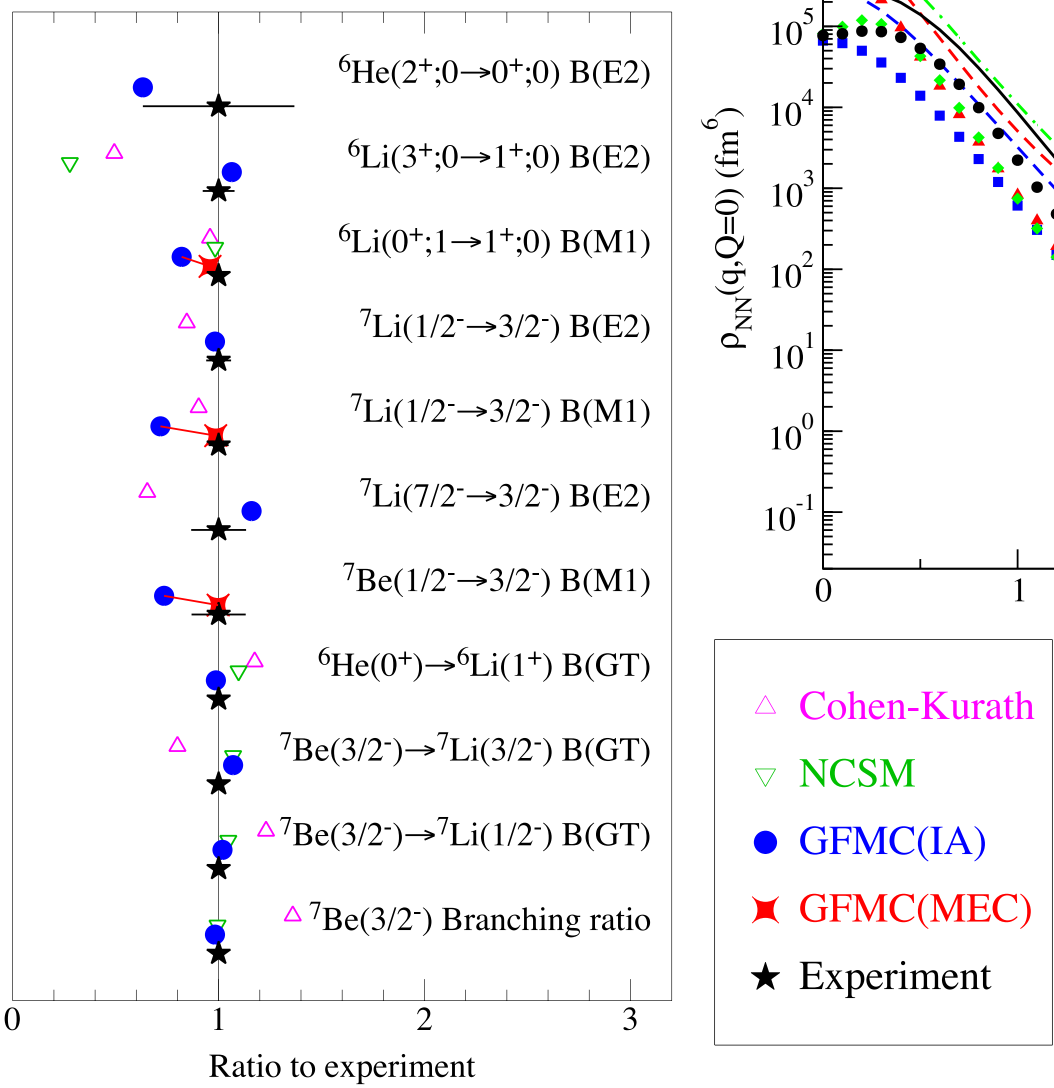


Pieper, Wiringa, et al.

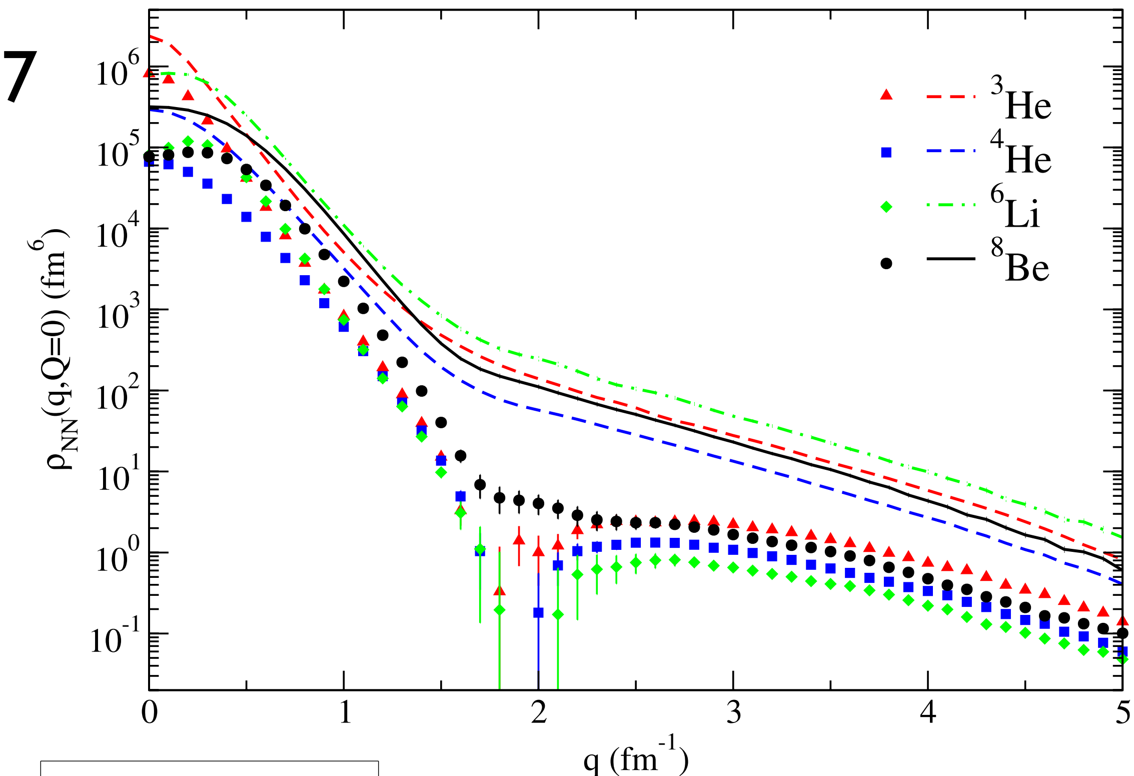
Magnetic moments of light Nuclei



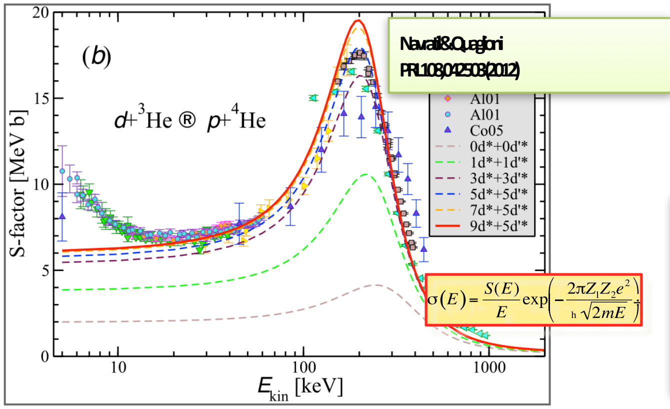
EM Transitions A=6,7



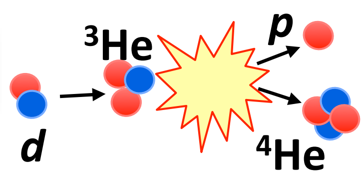
Back to Back momenta np vs. pp



Light Nuclear Reactions



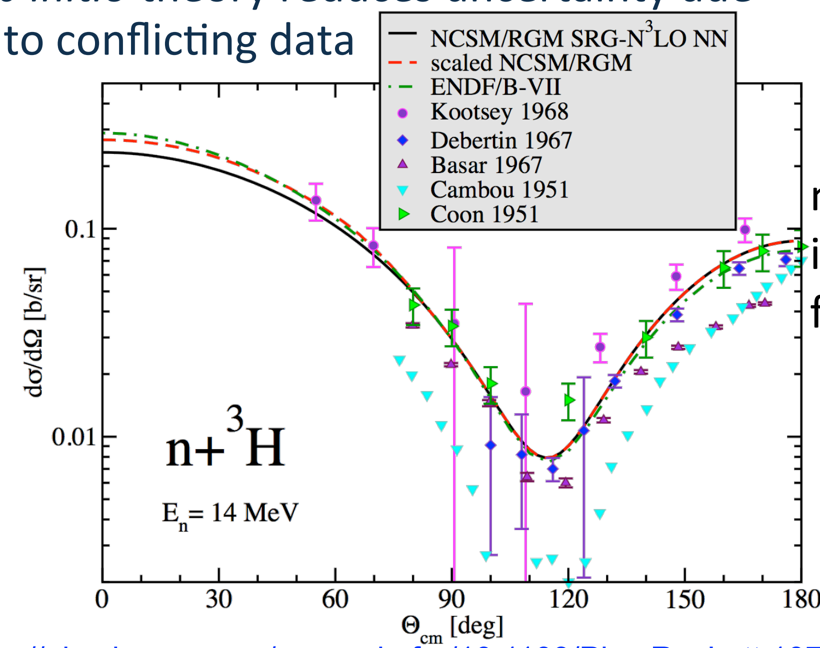
Data deviate from NCSM/RGM results at low energy due to lab. electron-screening



NCSM/RGM is pioneering *ab initio* calculations of light-nuclei fusion reaction with NN interaction. Here, ^{3}He(d,p) ^{4}He S-factor.

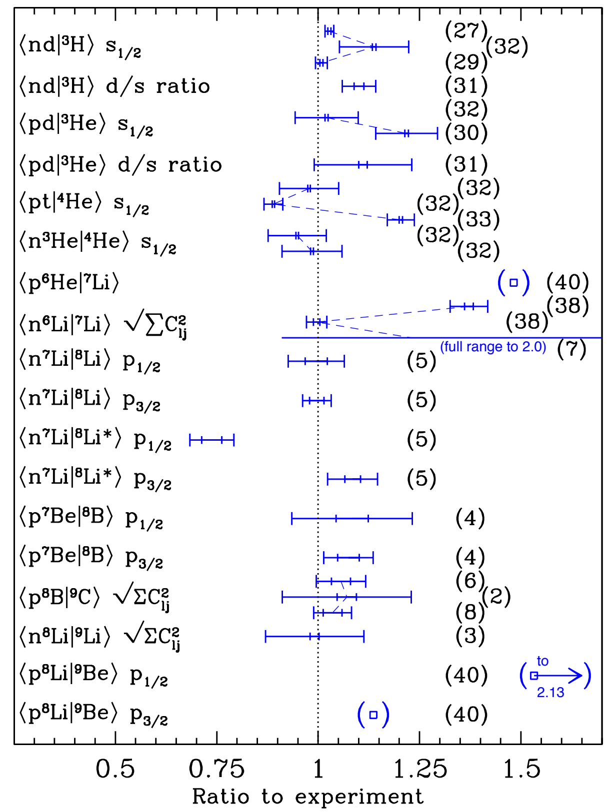
Navratil, Quaglioni,...

Ab initio theory reduces uncertainty due to conflicting data



n+3H important for NIF

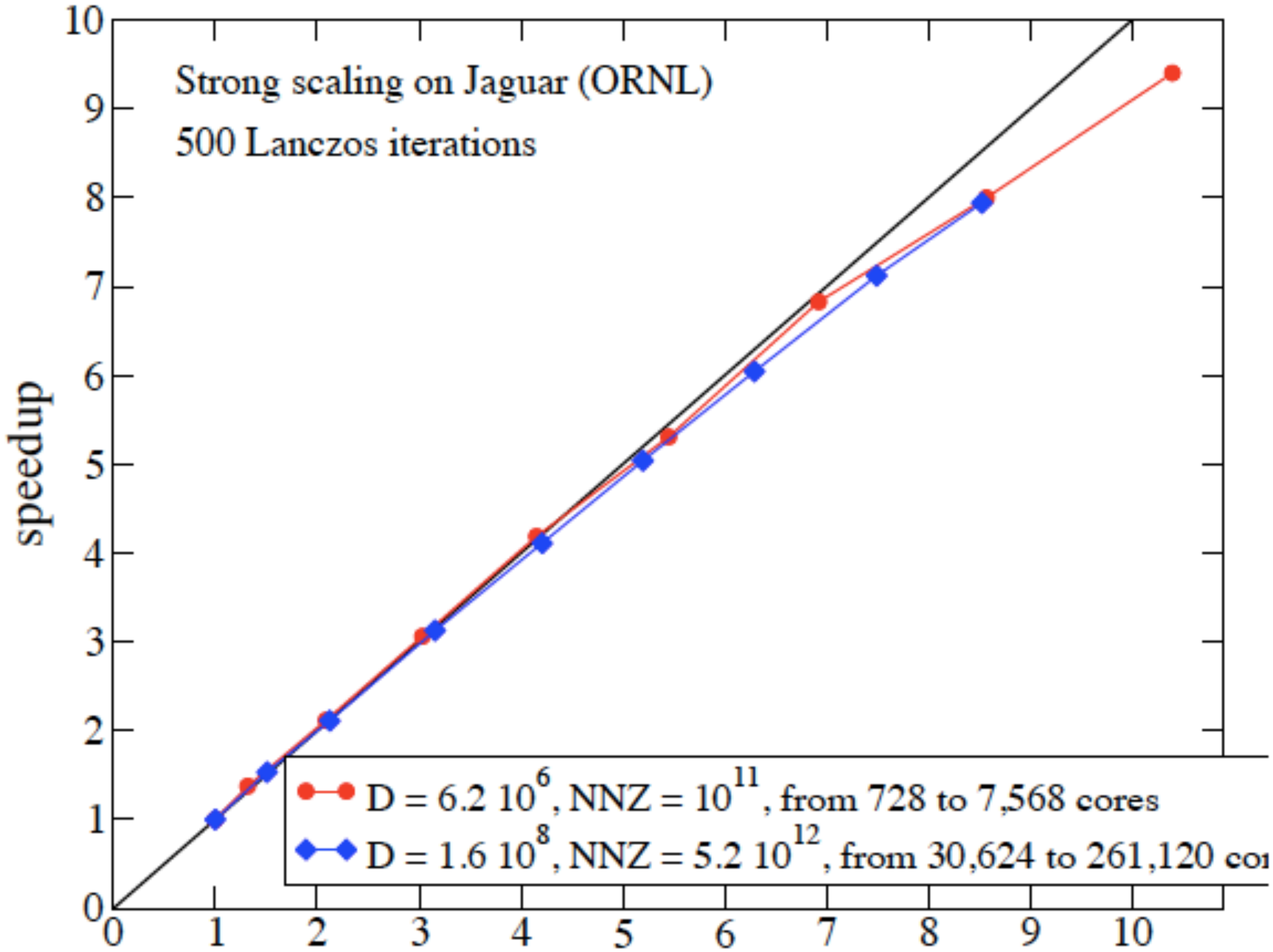
http://physics.aps.org/synopsis-for/10.1103/PhysRevLett.107.122502



ANCs from light nuclei
Nollett and Wiringa (2012)

Also recently width calculations : Nollett

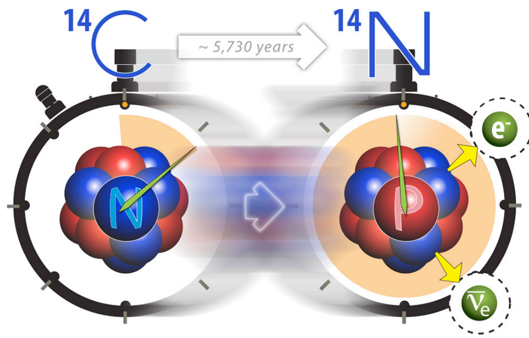
Scaling of Large Scale Configuration Interaction Calculations



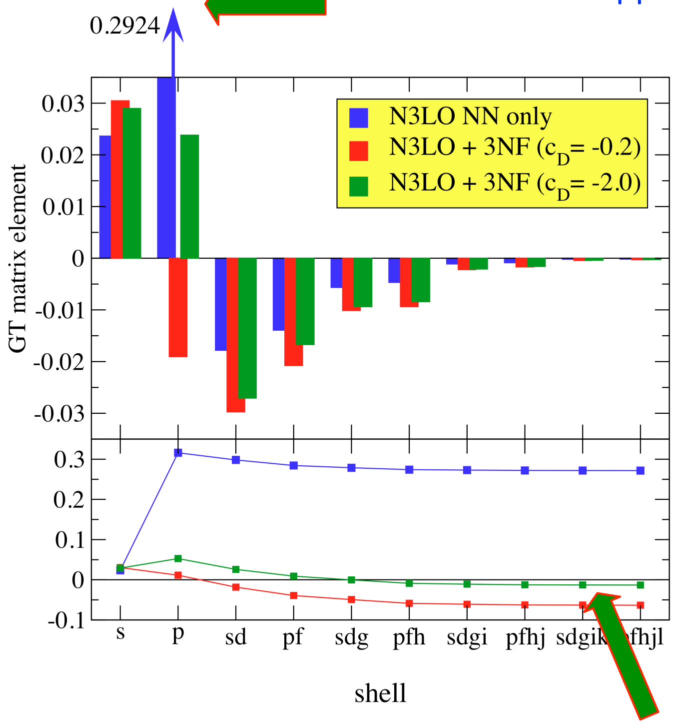
Vary, Ng, Maris,...
Iowa State, LBNL, ...

Anomalously Long Lifetime of Carbon-14 and the importance of 3-nucleon forces

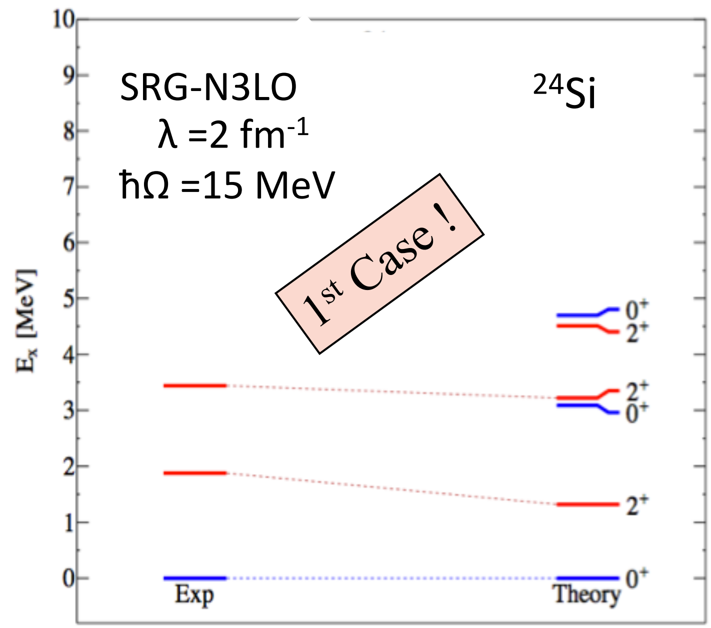
Maris, et al,
Phys. Rev. Lett. 106, 202502 (2011)



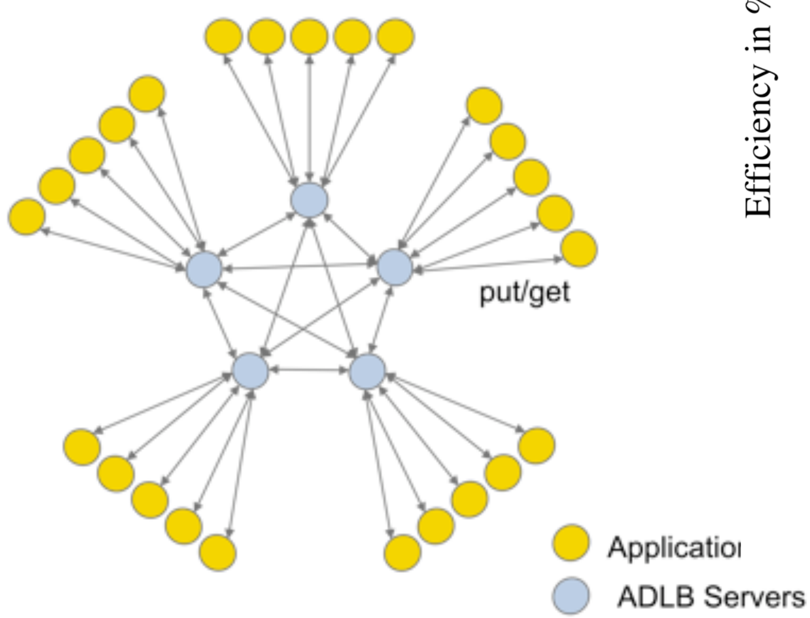
3-nucleon forces suppress critical component

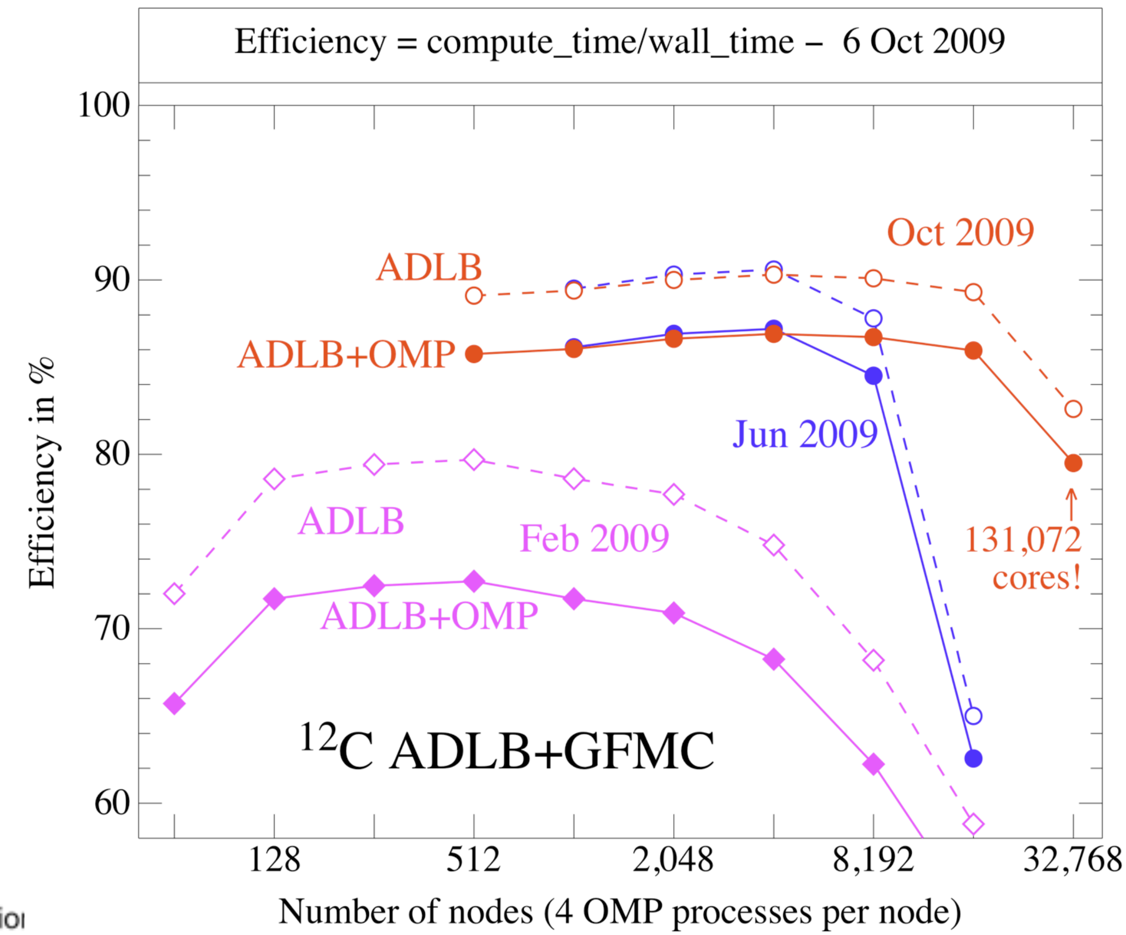


net decay rate
Is very small



Asynchronous Dynamic Load Balancing (ADLB) Library

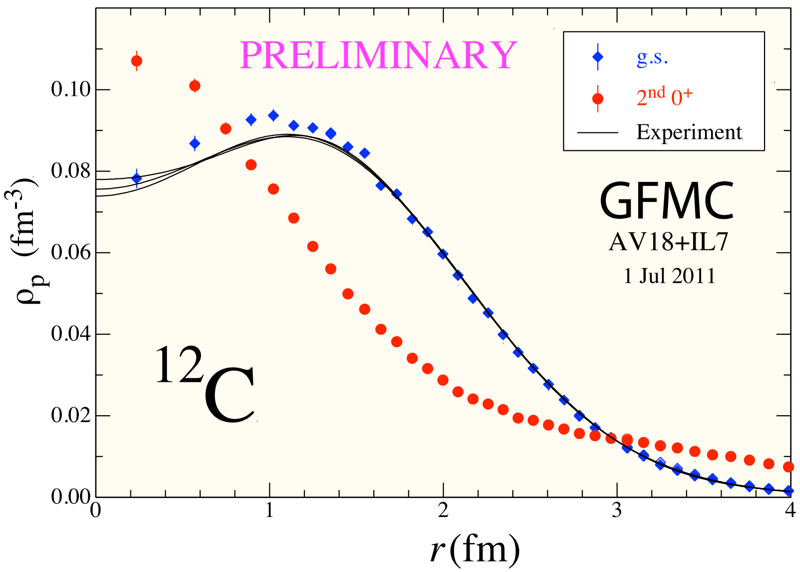


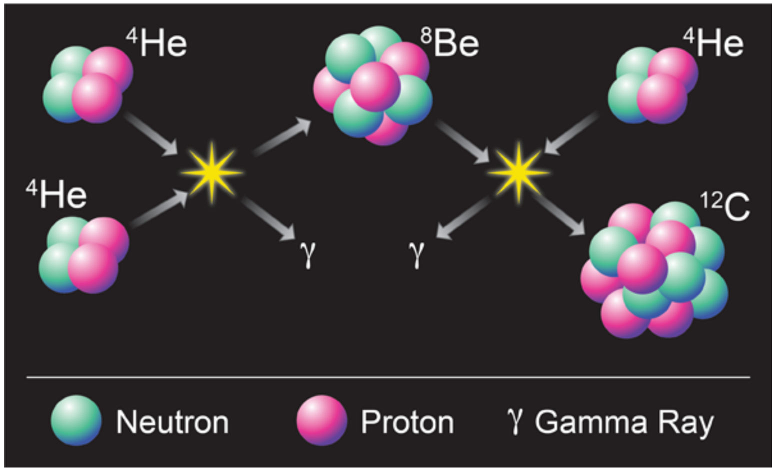


Lusk, Pieper, Butler
SciDAC Review 2010

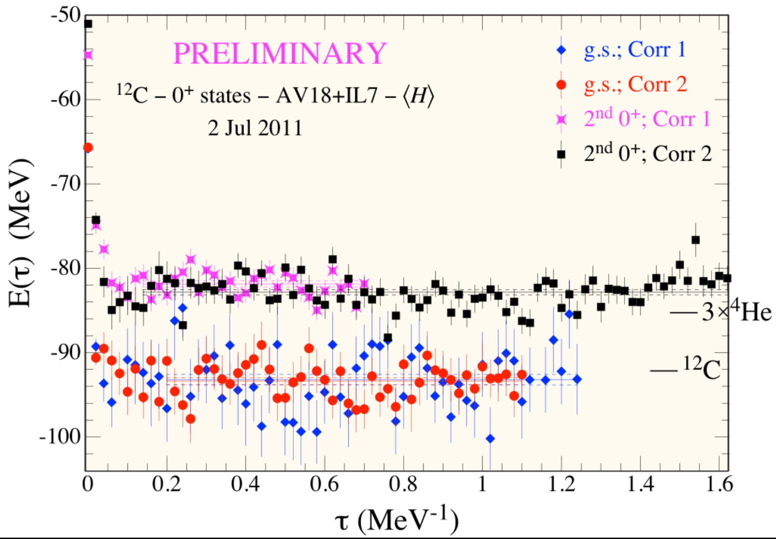
Ab initio description of ^{12}C

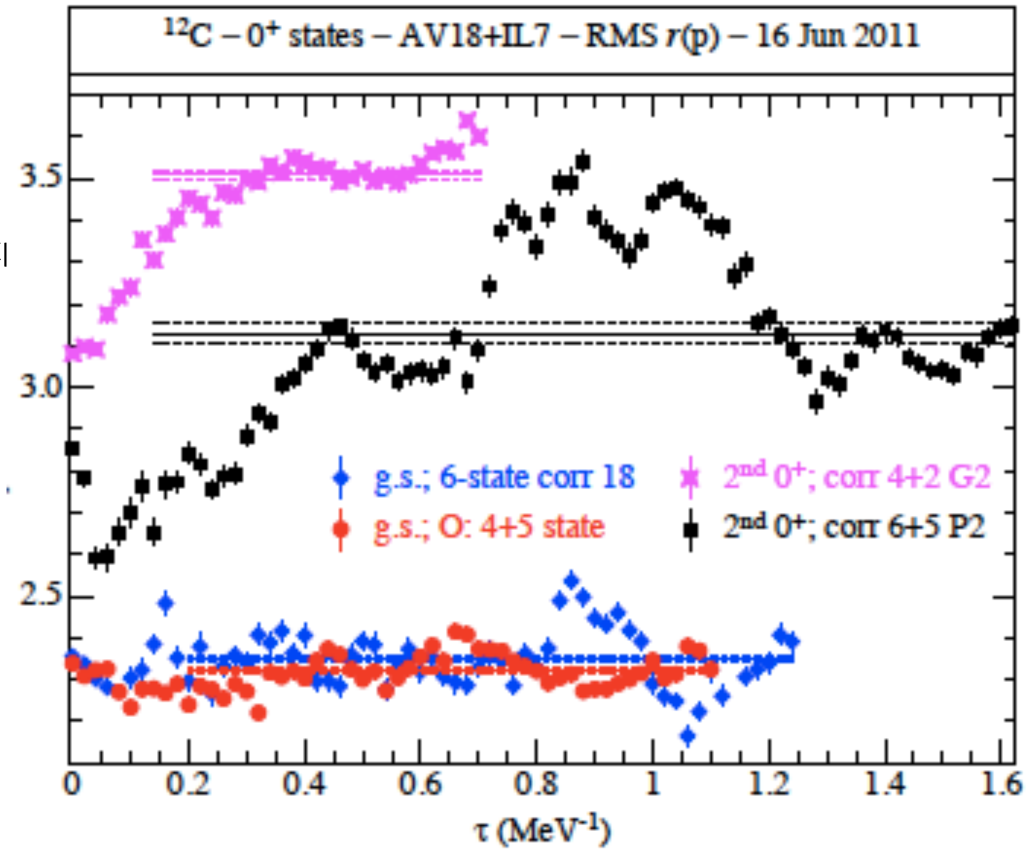
GFMC (Pieper et al.)



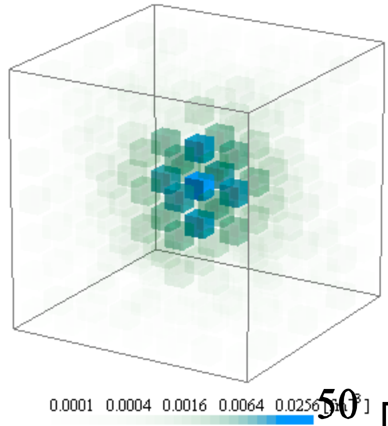


The ADLB (Asynchronous Dynamic Load-Balancing) library & GFMC. GFMC energy 93.5(6) MeV; ex[illegible] 92.16 MeV. GFMC pp radius 2.35 fm; expt. 2.33 fm.

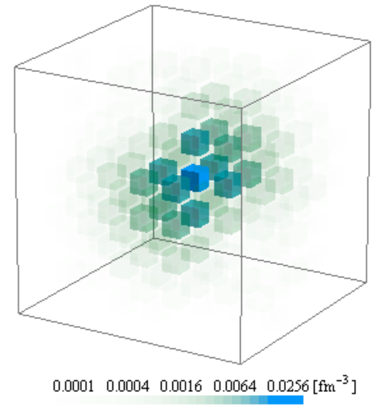




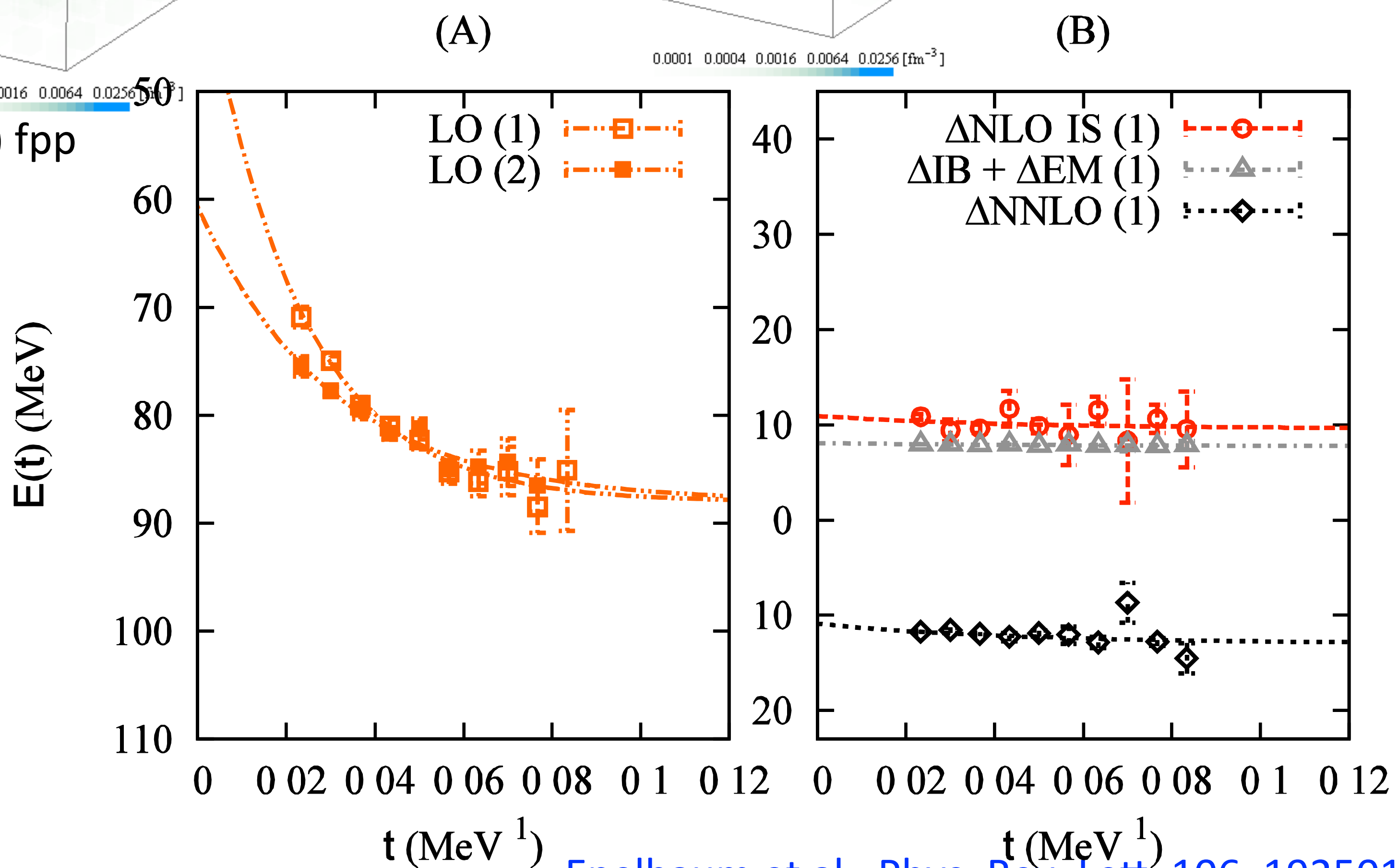
Lattice EFT (Lee, Epelbaum, Meissner,…)



0+(1) fpp



0+(2) fpp

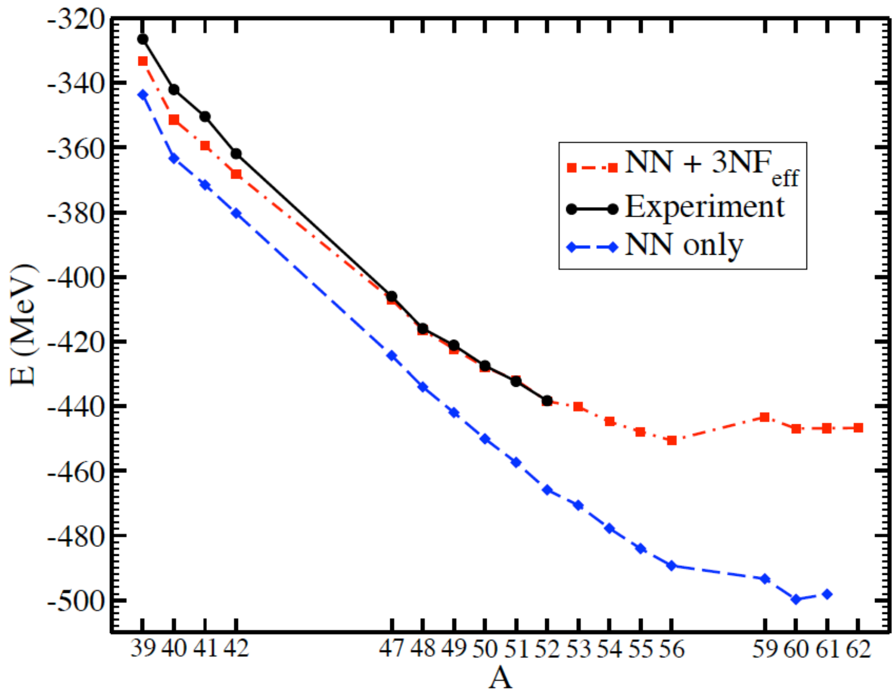


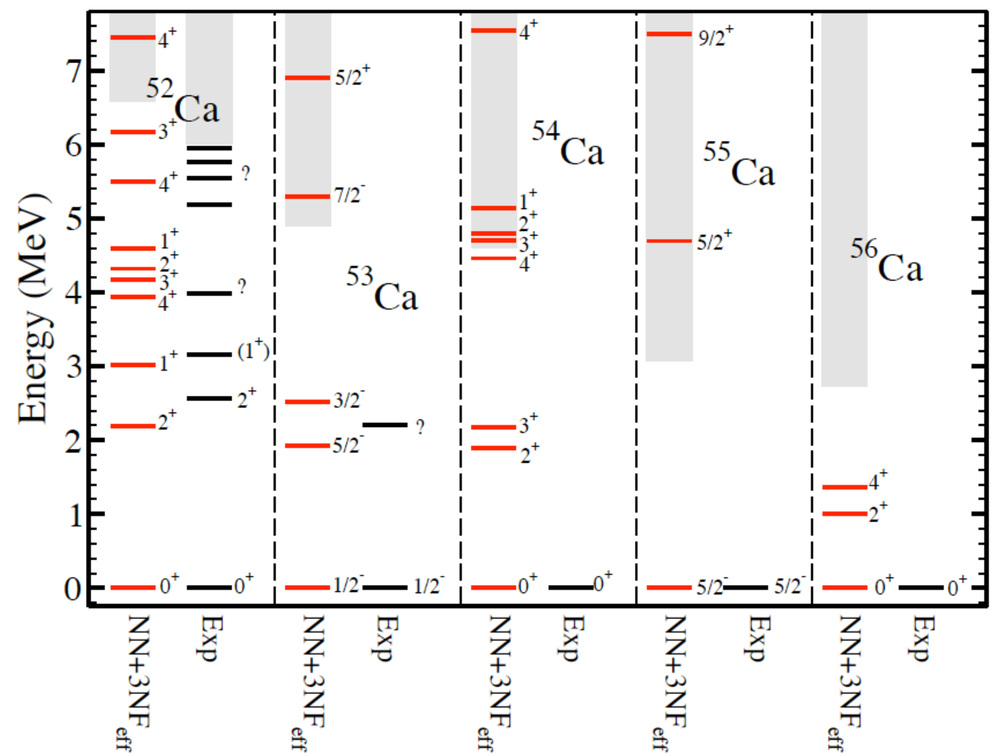
Epelbaum et al., Phys. Rev. Lett. 106, 192501 (2011)

Medium-Mass Nuclei: Coupled-cluster method

Description of medium-mass open nuclear systems

G. Hagen et al., Phys. Rev. Lett. 109, 032502 (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

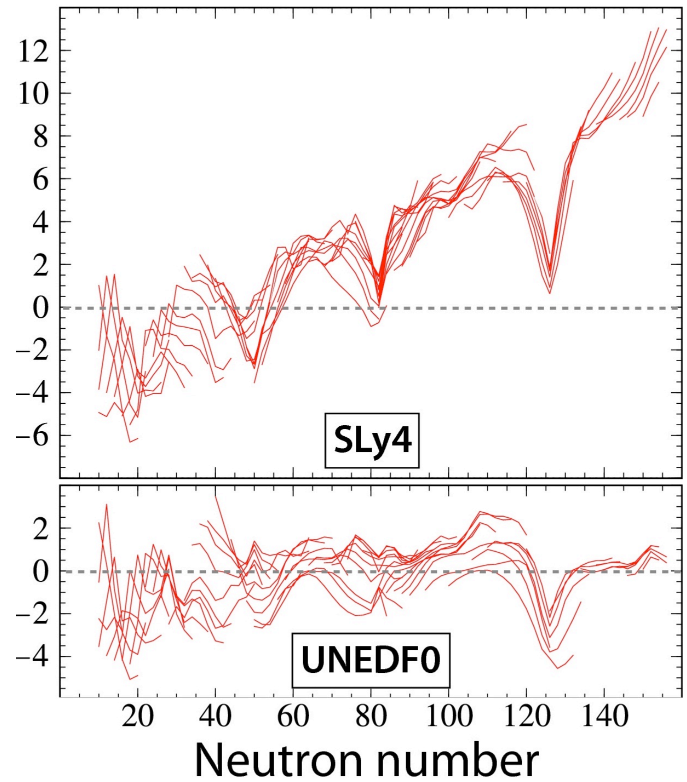
$\frac{1}{2}^+$ virtual state

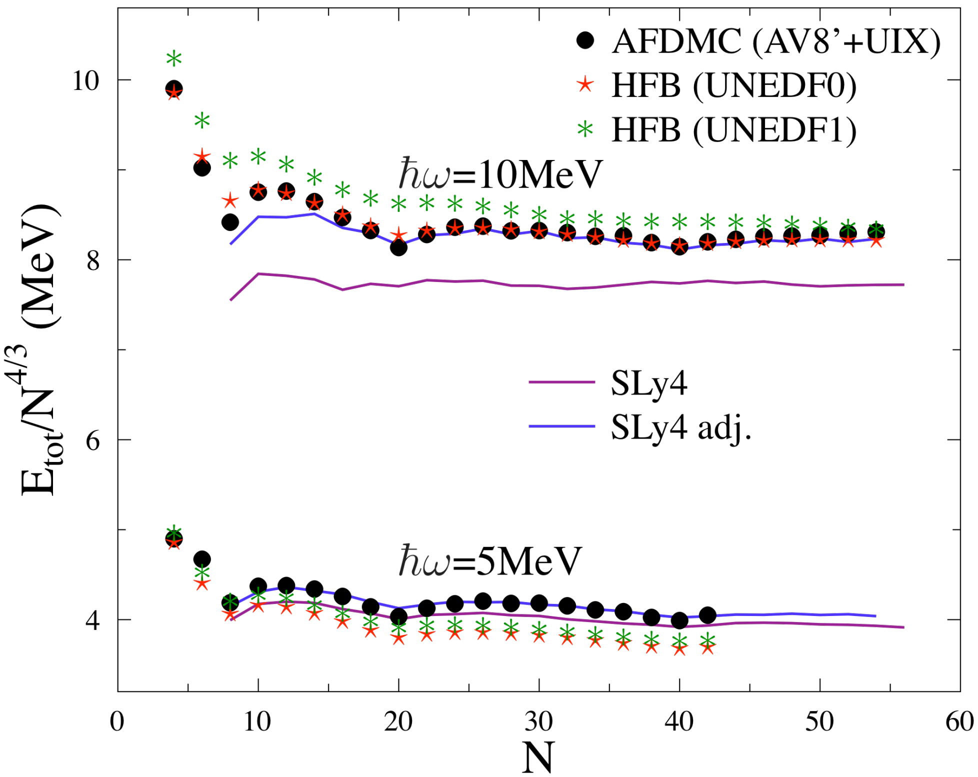
- Strong coupling to continuum for neutron rich calcium isotopes
- Level ordering of states in the *gds* shell is contrary to naïve shell model picture

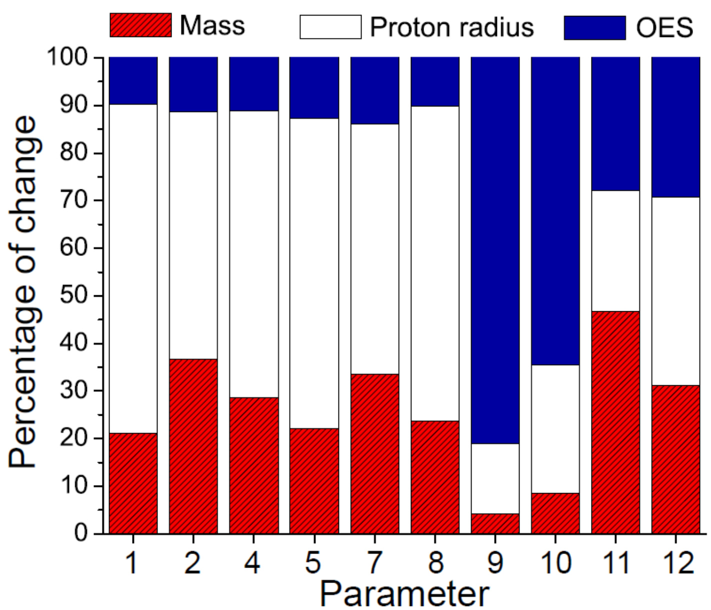
Improved Density Functionals

Neutron Drops, Masses, Fission,…

Derivative-free optimization, uncertainty quantification







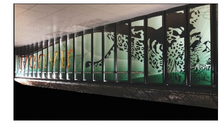
http://www.deixismagazine.org/2011/03/cranking-up-the-speed-of-dft/

http://www.deixismagazine.org/2011/03/pounding-out-atomic-nuclei/

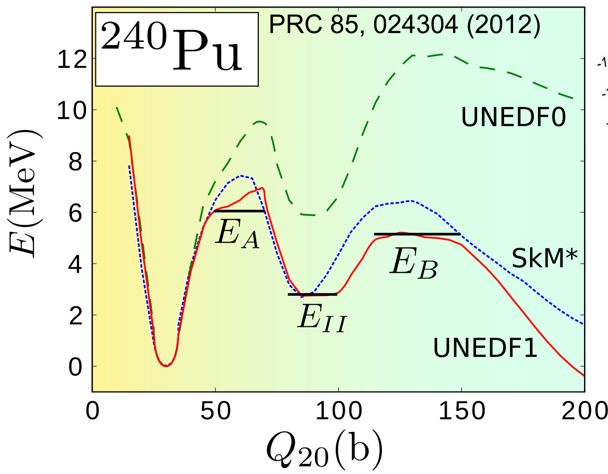
http://www.mcs.anl.gov/news/detail.php?id=720

LACM, Fission: the ultimate challenge

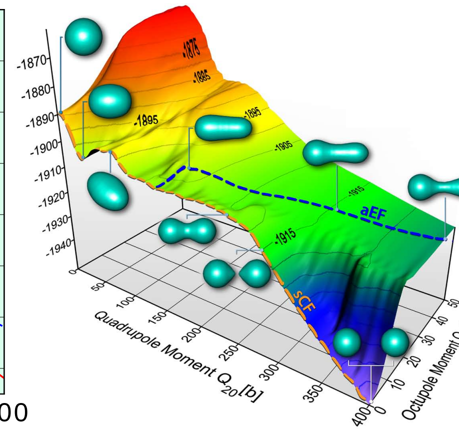
Stability of the heaviest nuclei, r-process, advanced fuel cycle, stockpile stewardship…



Optimized Functionals

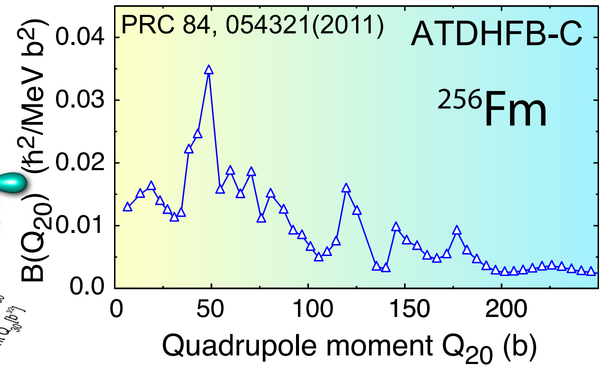


Large-scale DFT

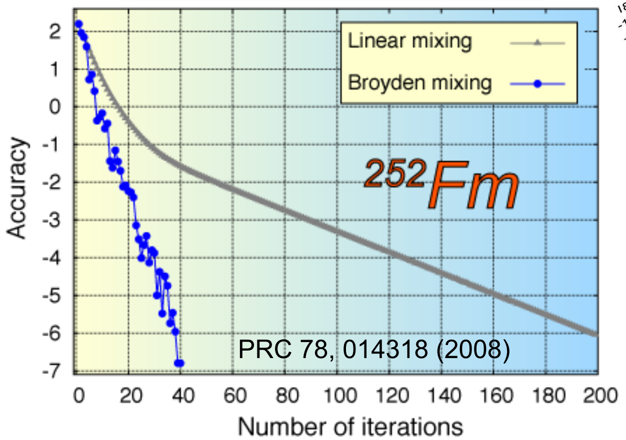


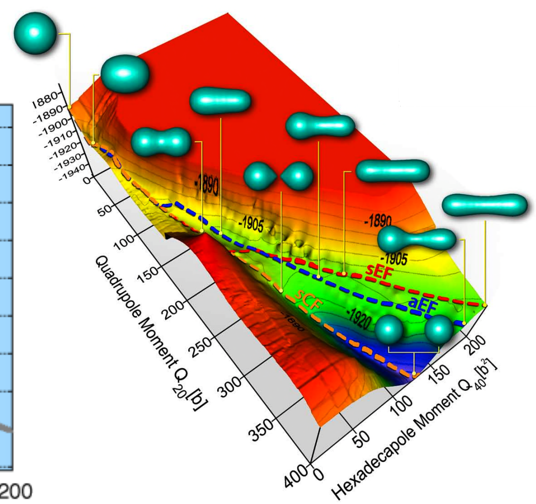
PRC 80, 014309 (2009)

Collective dynamics



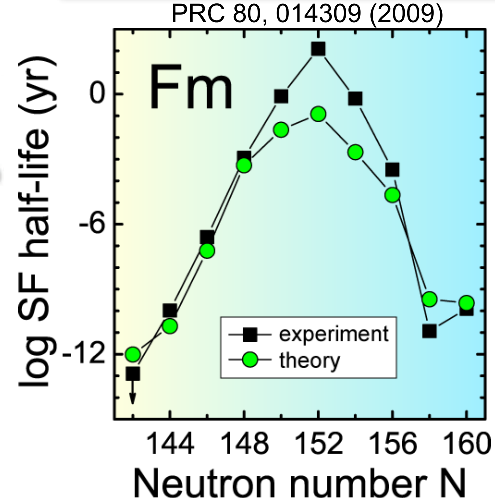
Numerical Techniques





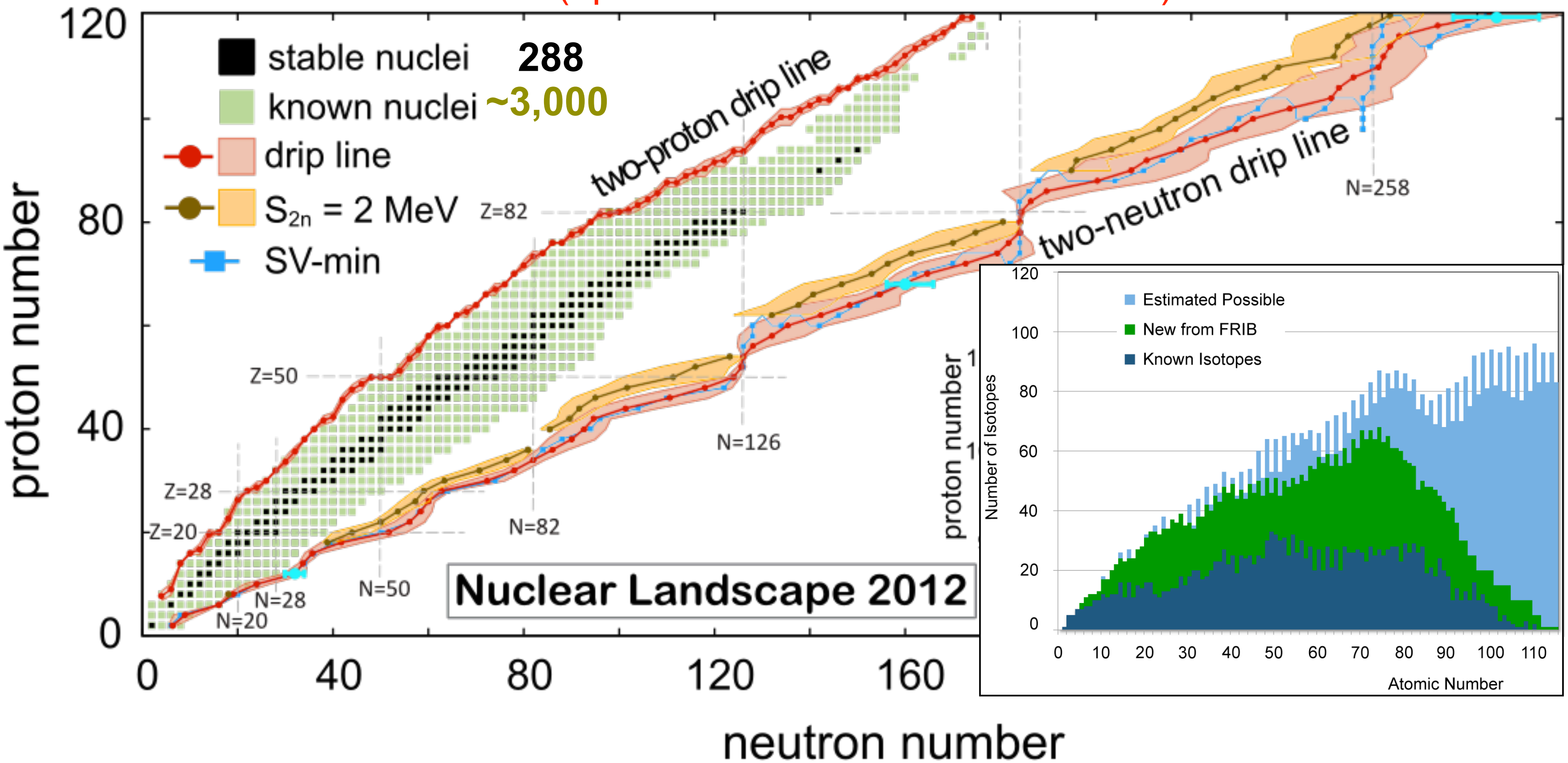
Confrontation with experiment; predictions

PRC 80, 014309 (2009)



The limits: Skyrme-DFT Benchmark 2012

- Systematic errors (due to incorrect assumptions/poor modeling)
- Statistical errors (optimization and numerical errors)



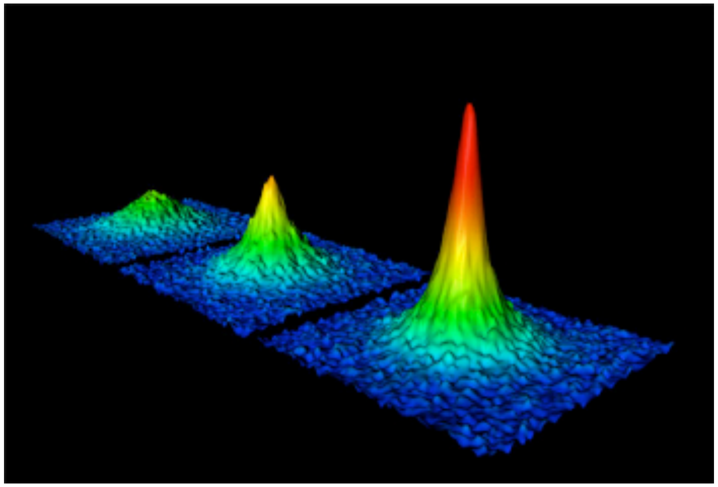
How many protons and neutrons can be bound in a nucleus?

Skyrme-DFT: 6,900±500$_{syst}$

Erler et al.,
Nature 486, 509 (2012)

http://www.livescience.com/21214-atomic-nuclei-variations-estimate.html
http://www.sciencedaily.com/releases/2012/06/120627142518.htm

Neutron Matter: from very low to high density



Low-Density (dilute) near free Fermions to near Unitarity

range of the interaction < interparticle spacing

Stringent tests of many-body calculations with strong correlations

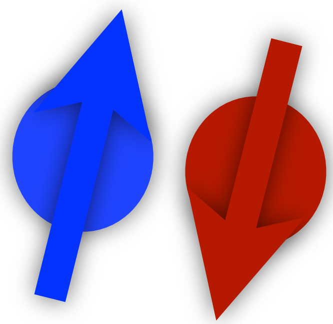
Analytically known at extremely low density

E / E_{FG} rapidly decreases to ~ 1/2 with increasing k_F a

Pairing Gap very large, up to ~ 0.5 Ef in cold atoms

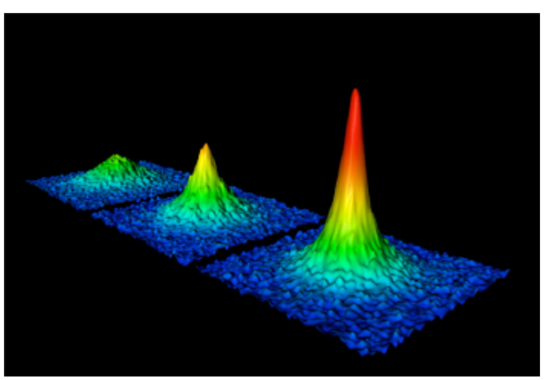
Unitary Regime and Low-Density Neutron Matter

Experimental Results in Cold Atoms



$$H = \sum_i T_i + \sum_{i<j} V_0 \, \delta(r_{ij})$$

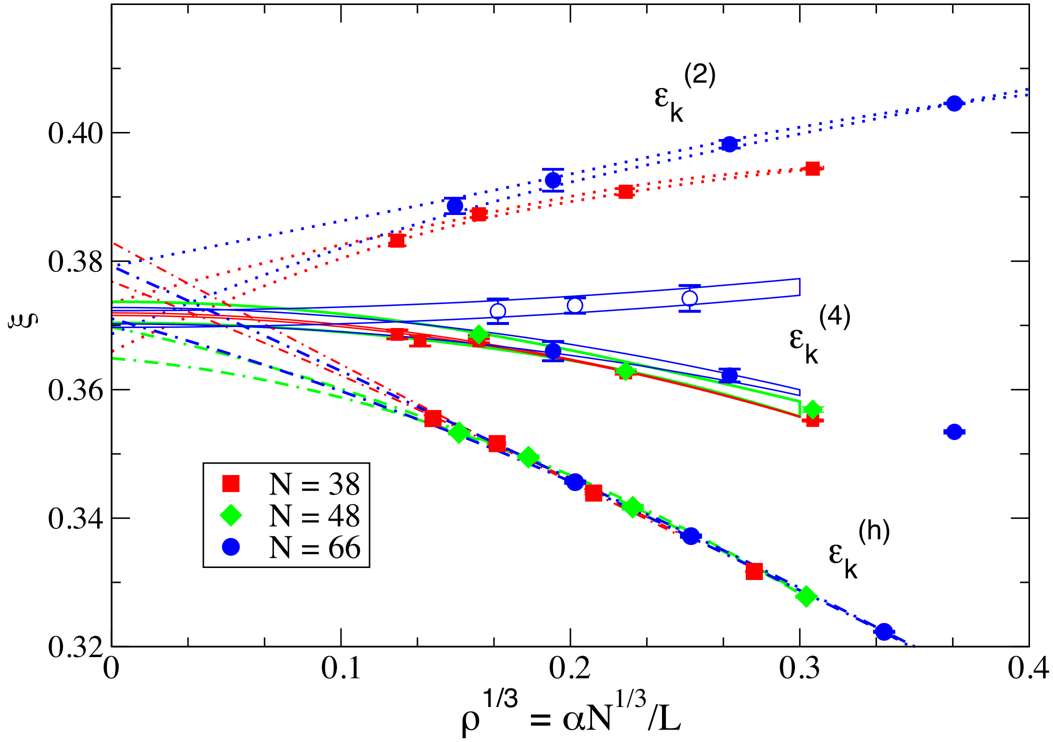
Fermi Condensates 2004



- (nearly) Free Fermions
- (nearly) Free Bosons
- ‘Universality’ and the BCS-BEC transition
- Polarons
- Efimov States
- Superfluid Fermions (s-, p-, d-wave,... pairing)
- Exotic Polarized Superfluids(FFLO,...)
- PseudoGap States
- Itinerant Ferromagnetism
- \`Perfect’ Fluids
- Reduced Dimensionality
- More than pairing (3-,4-body condensates, ...)
- Bose, Fermi Hubbard Models,

Towards largest Nuclei: neutron-rich matter

Equation of state: cold atoms and low-density neutron matter



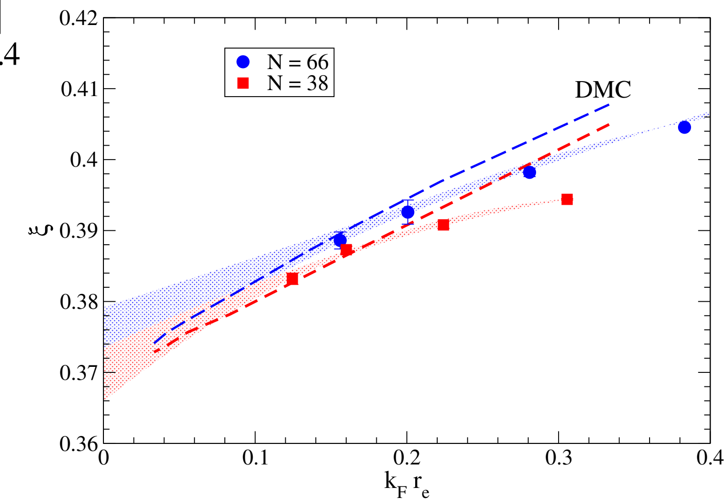
Effective Range Dependence

$$E / E_{FG} = \xi + S\, k_F\, r_e + \ldots.$$

ξ = 0.372(5) QMC

0.375(5) Expt (MIT)

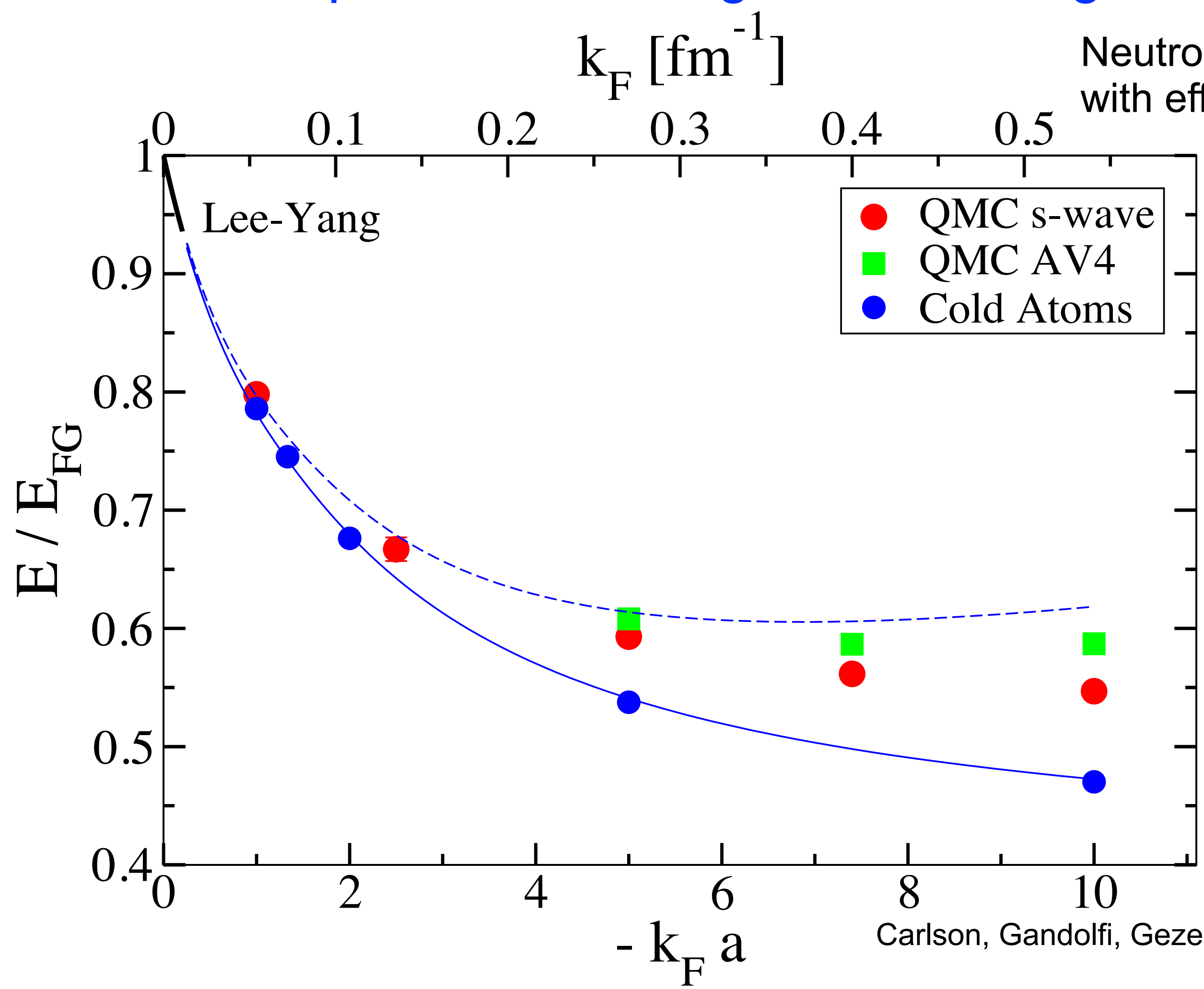
S = 0.12(3) QMC



Towards largest Nuclei: neutron-rich matter

Equation of State: Cold atoms and Neutron Matter comparison including effective range terms

Neutron Matter and cold atoms with effective range term

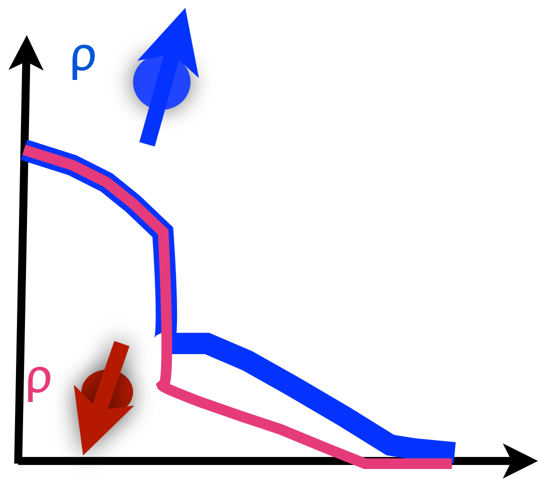


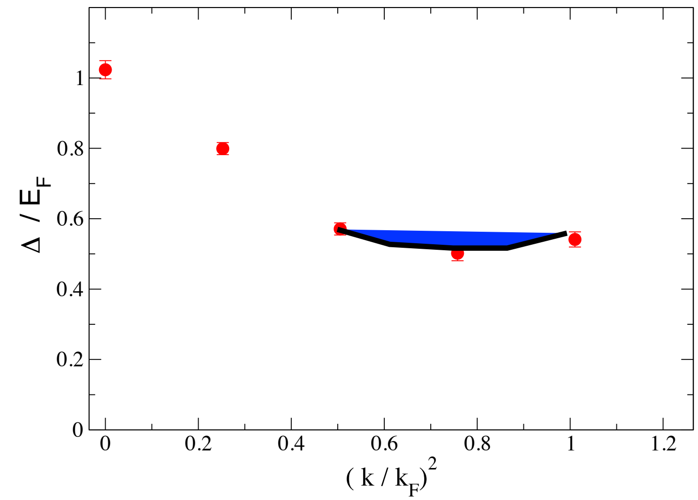
Carlson, Gandolfi, Gezerlis, PTEP (2012) in press

Laboratory tests of strongly-paired many-body problem

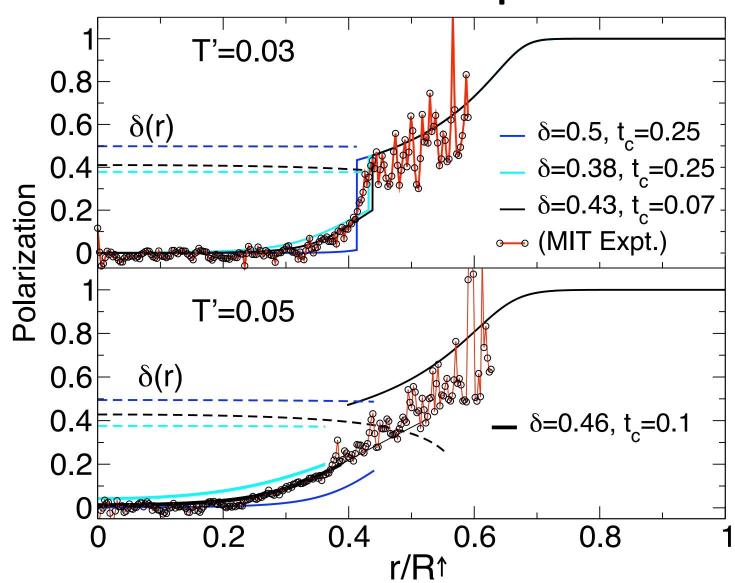
Superfluid pairing gap in cold atoms

Spin up, down densities





Measurements of polarization in a trap



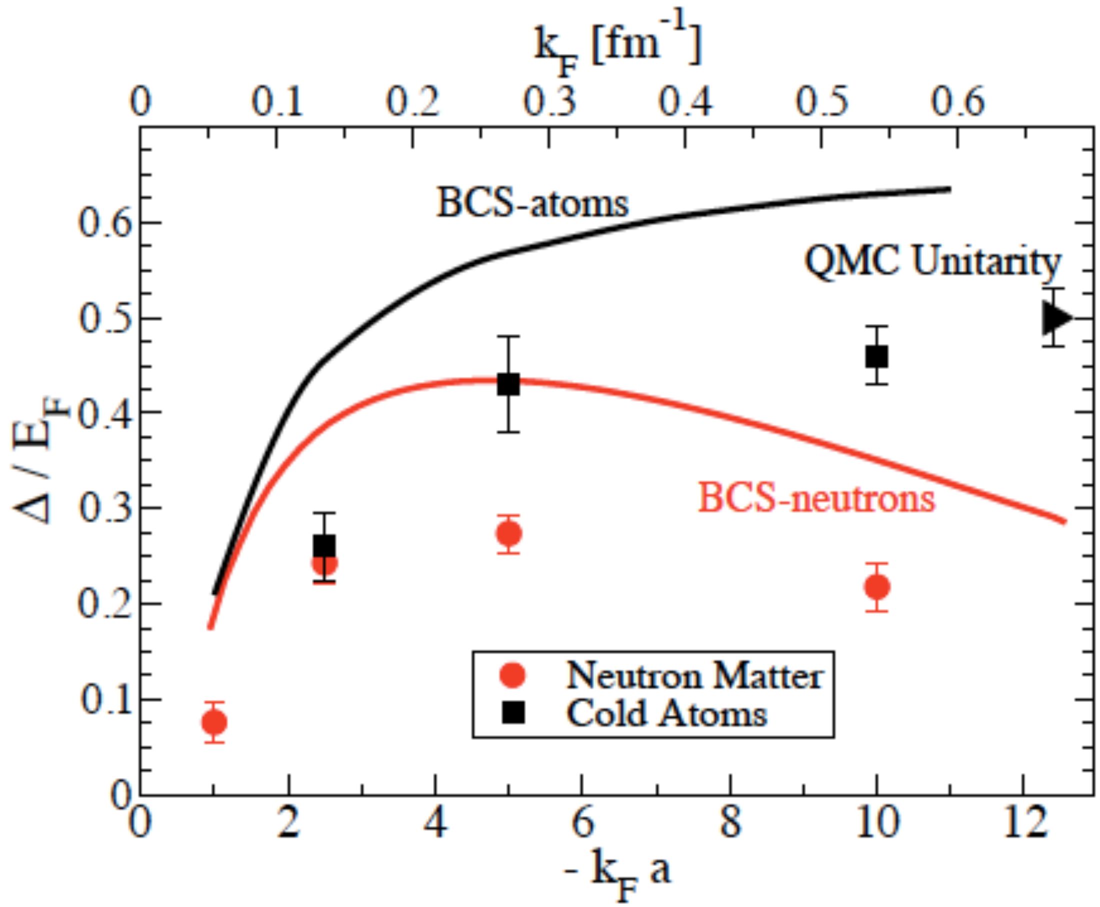
Largest Δ/E_f

$$\Delta = \delta \frac{\hbar^2 k_F^2}{2m}$$

$$\delta = 0.45(05)$$

JC and Reddy, PRL 2007
analyzing MIT data

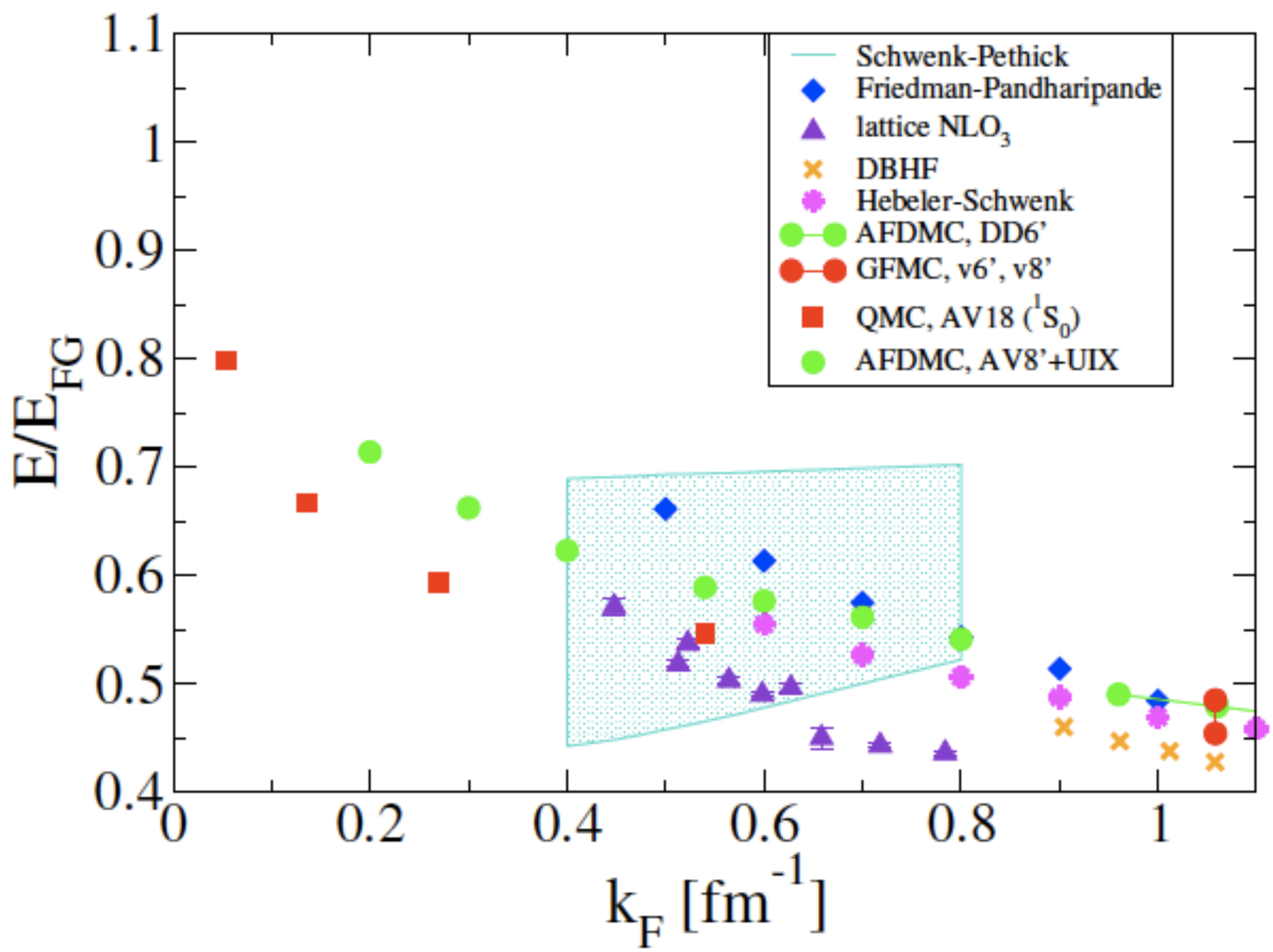
Neutron Matter
Pairing Gap at low density



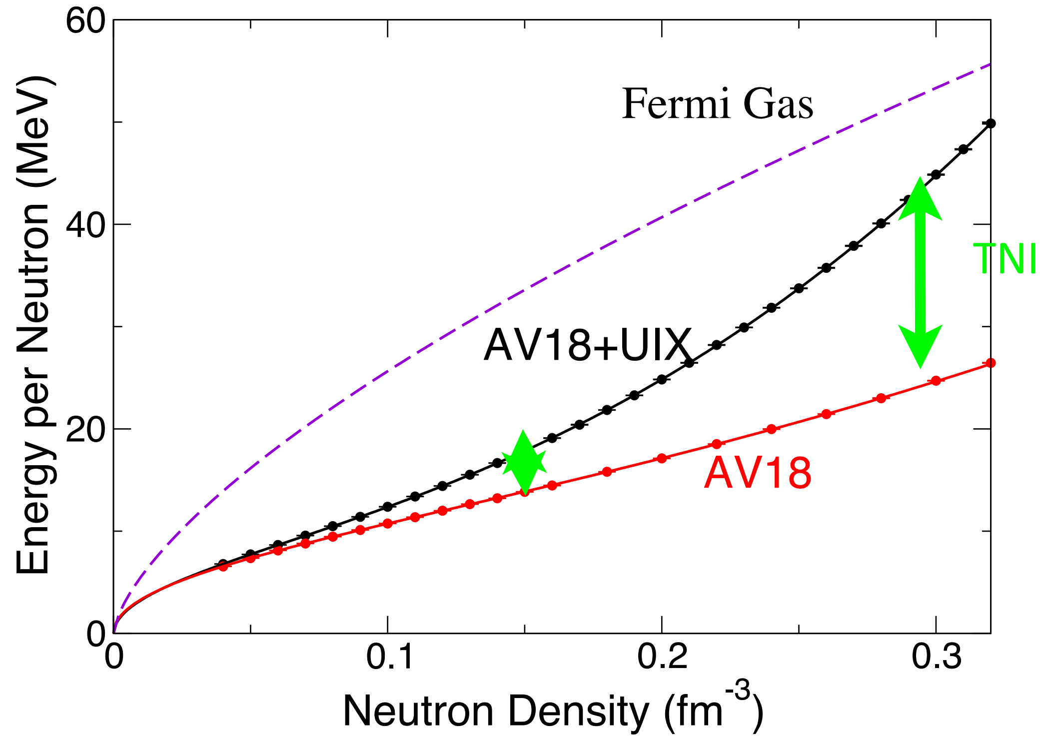
Transition from weak pairing (Gorkov correction) to near unitarity

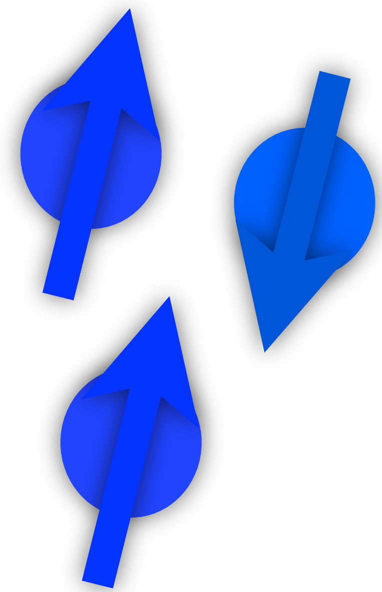
Low-moderate density EOS

All methods based on NN interactions give similar results



Neutron Star (Mass/Radius) requires neutron matter at higher (<2-3 ρ_0) densities



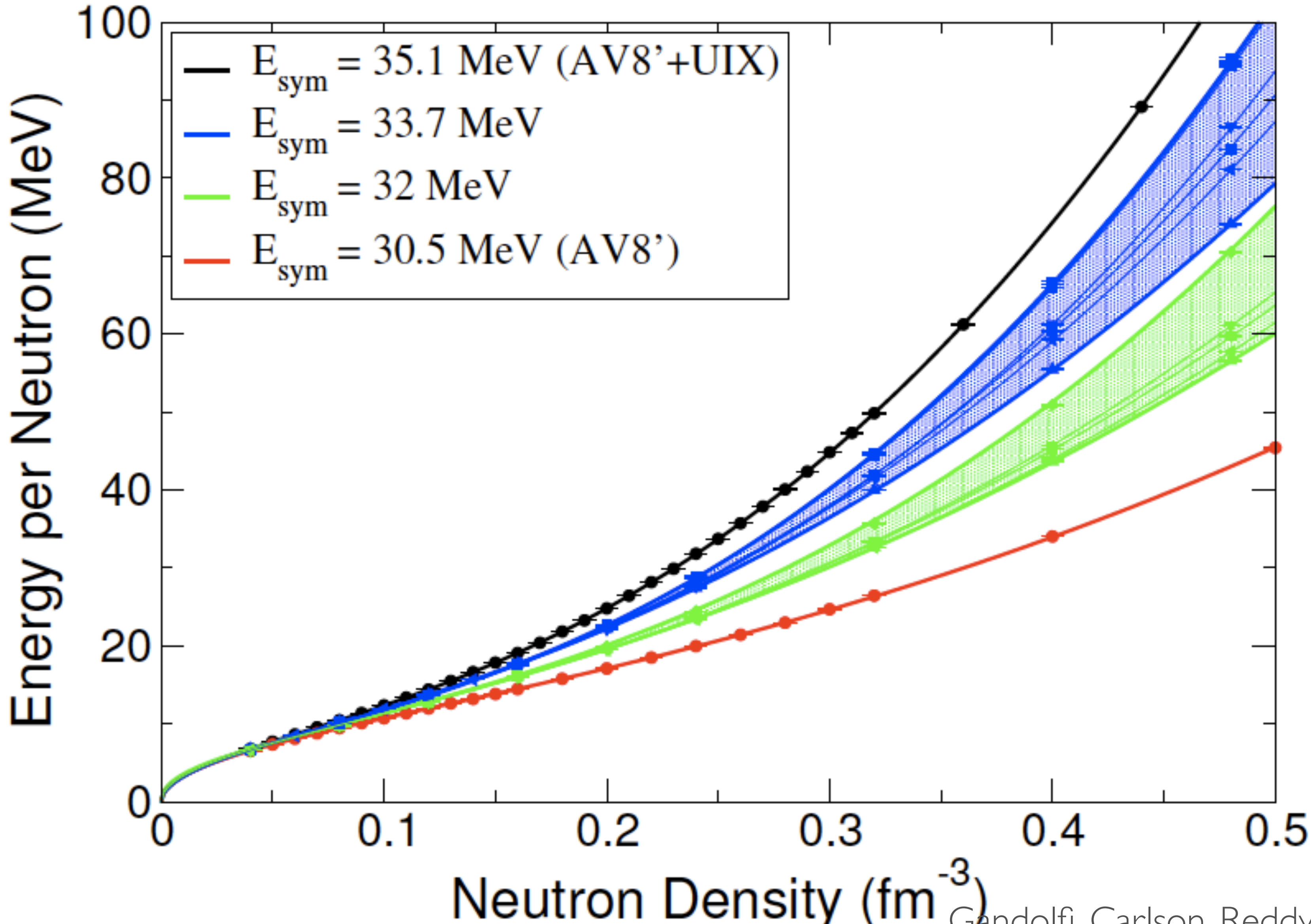


TNI quite small (~ 4 MeV) at saturation density

moderate at 2x saturation density (< 1/2 E_{FG})

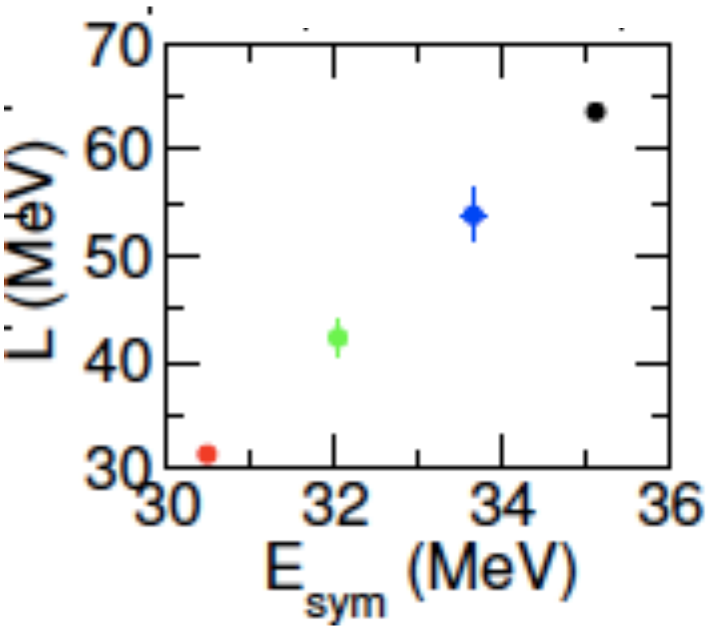
Very small contribution from 2π TNI

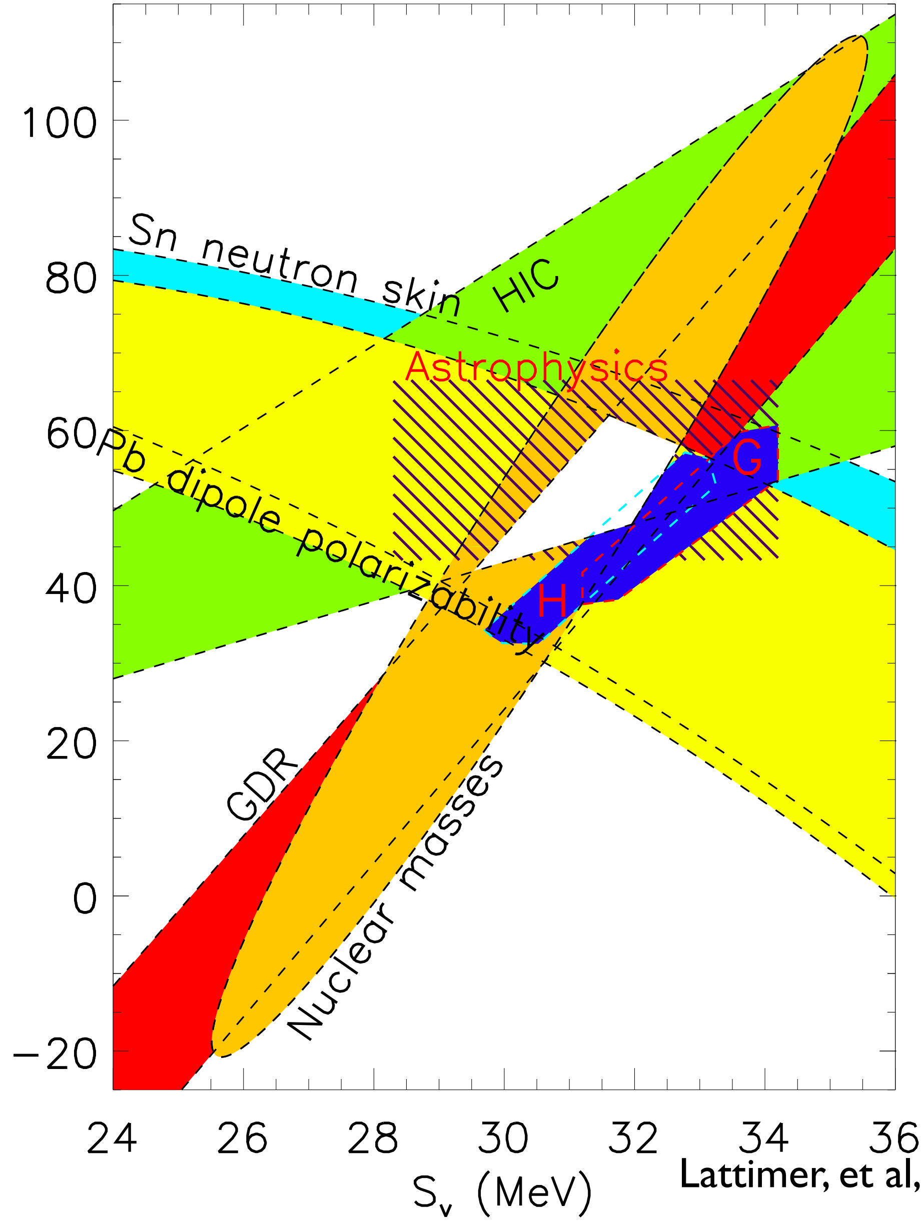
Neutron Matter EOS and 3-nucleon interactions



Gandolfi, Carlson, Reddy 2011

Very Strong Correlation between Symmetry Energy and its Density Dependence

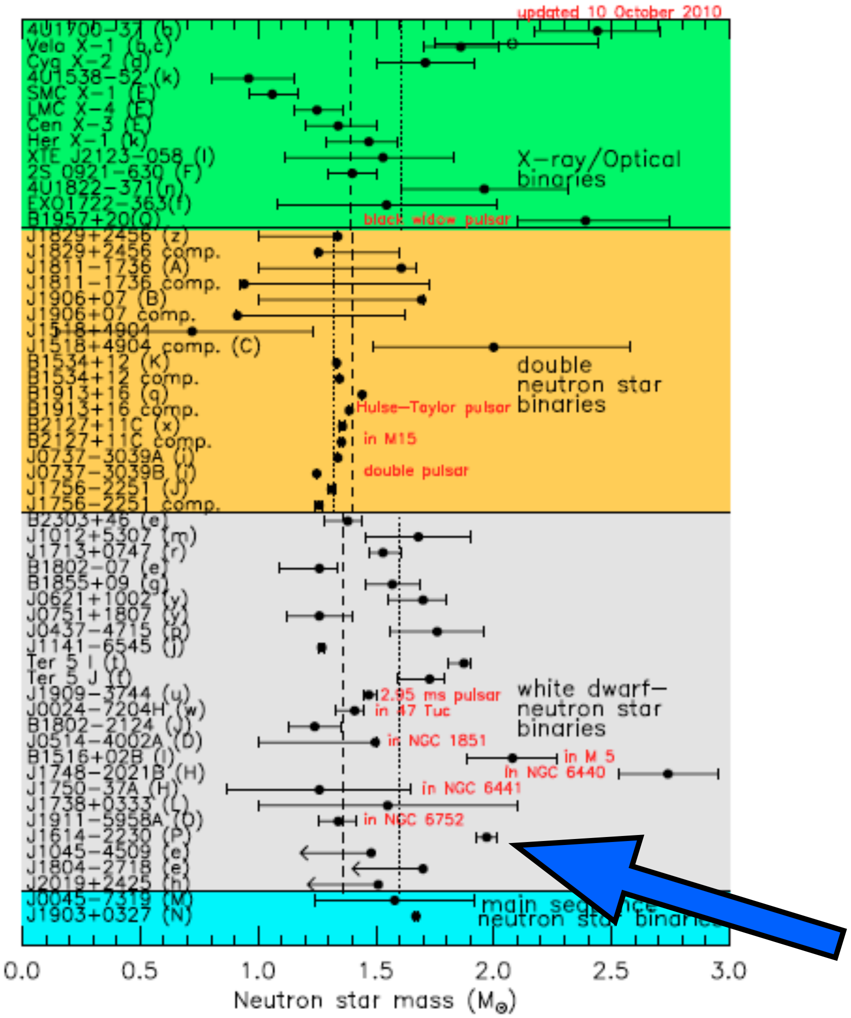




Lattimer, et al, 2012

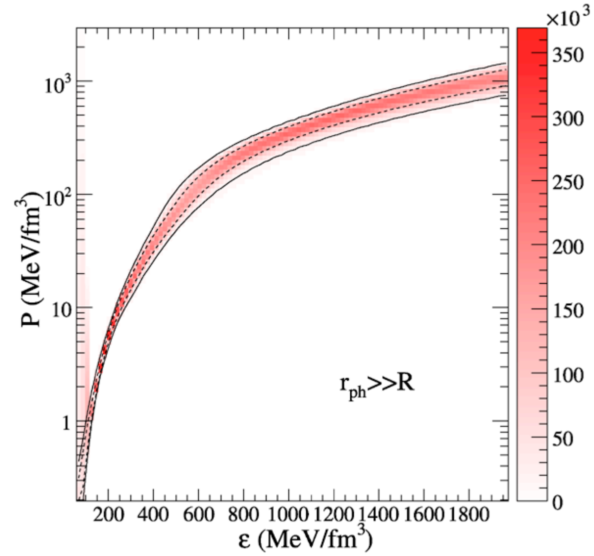
Astrophysical Constraints

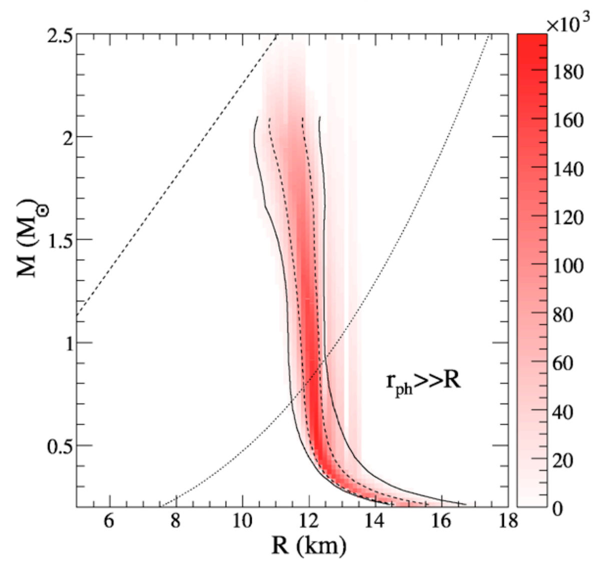
Neutron Star masses



Demorest, et al, Nature, 2010

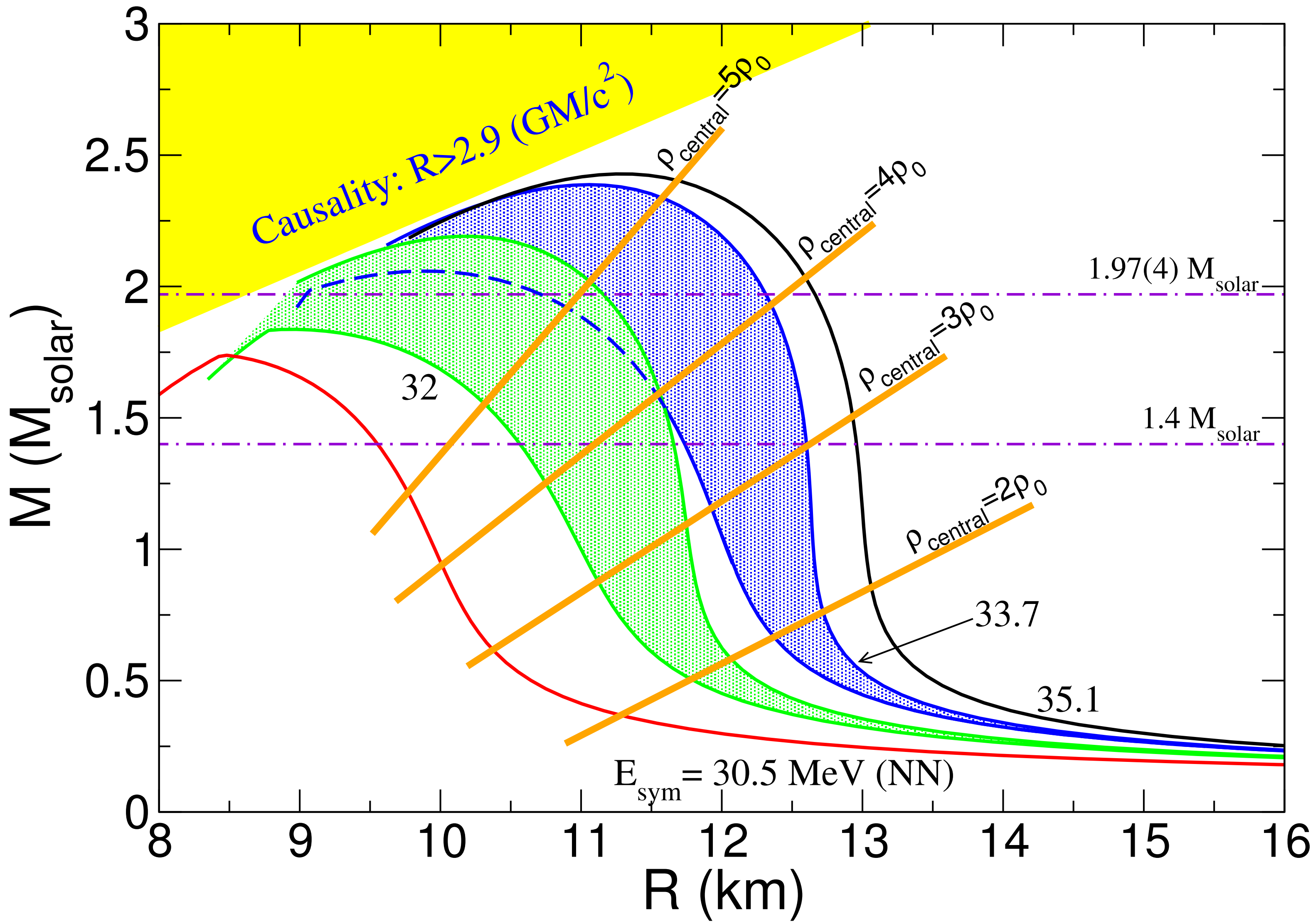
Photospheric radius expansion bursts, Thermal Emission



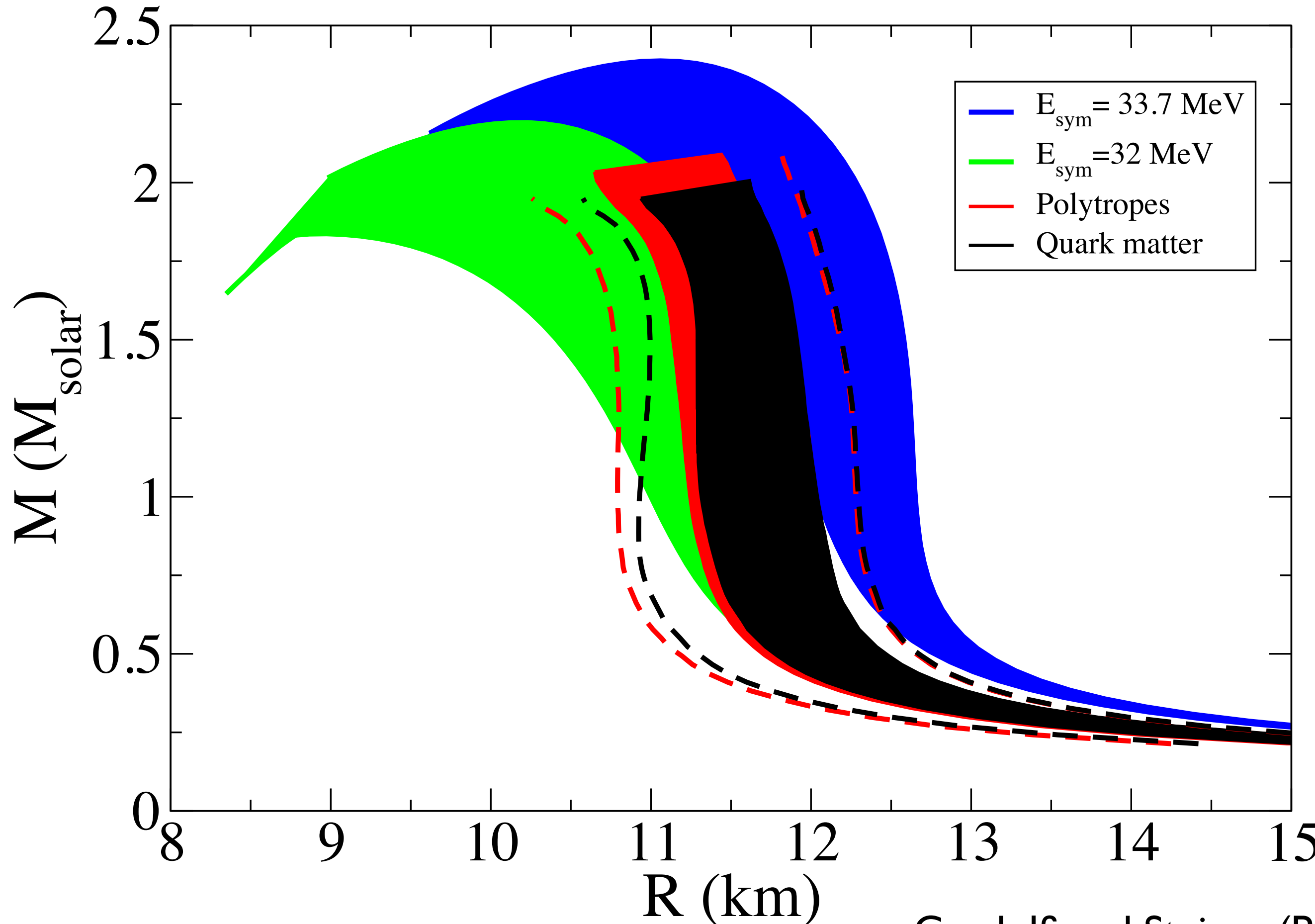


Steiner, Lattimer, Brown: Astrophys. J. 722, 33 (2010); Lattimer, Astrophysical Space Science (2011).

Mass/Radius Bands for Different Symmetry Energies



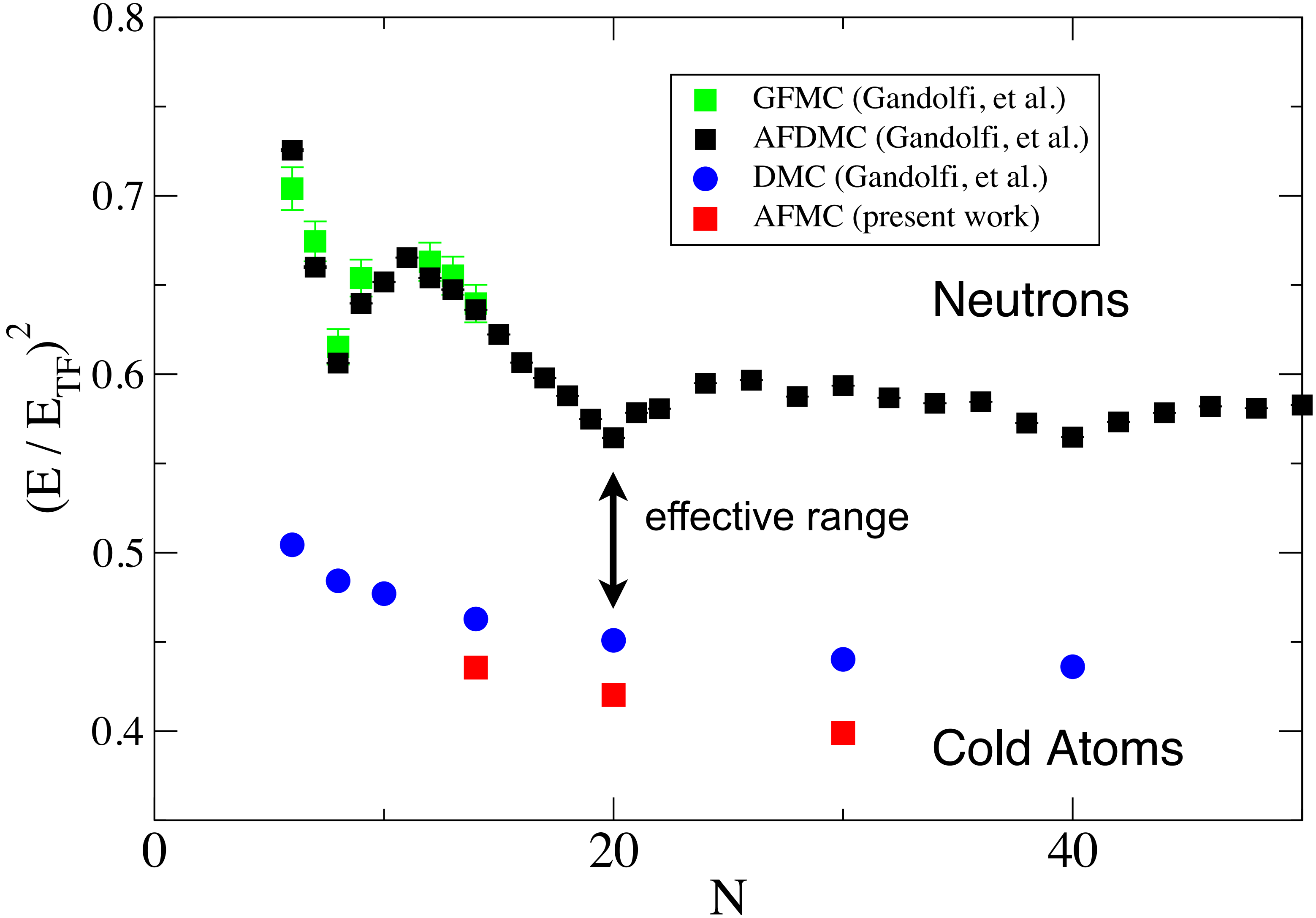
Combined constraints on EOS and Mass/Radius from Nuclear Physics and Astrophysical Observations



Gandolfi and Steiner (PRL 2012)

EOS critical in gravity waves, supernovae, ...

Inhomogeneous Matter:
Neutron Star Crusts / Optical Lattices

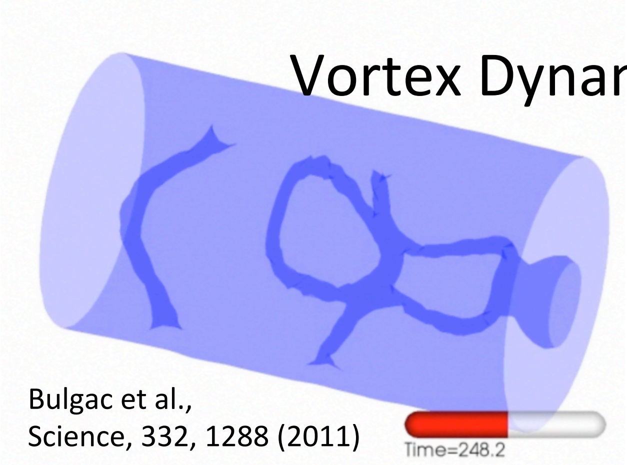


Cold atoms versus neutron drops

Can be used to optimize density functionals

Further Directions in Cold Atoms

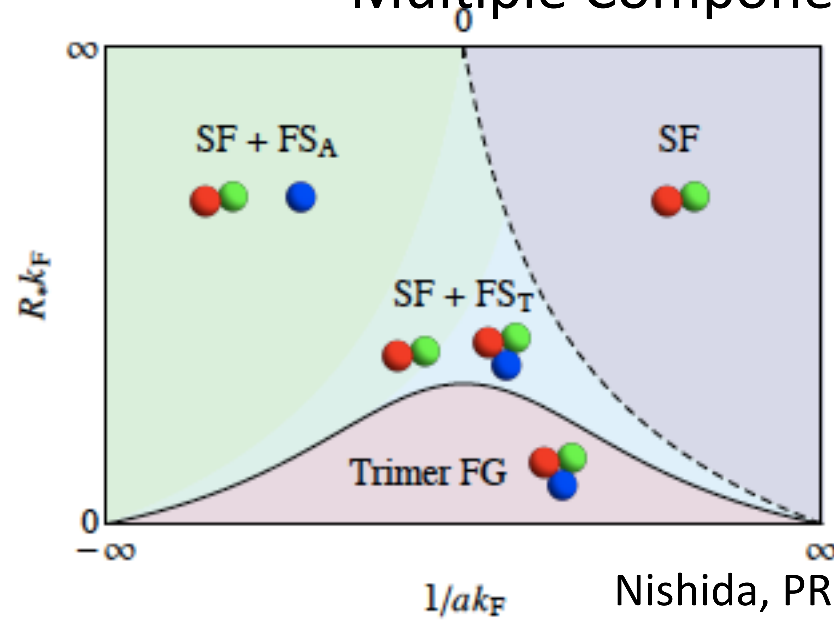
Vortex Dynamics



Bulgac et al.,
Science, 332, 1288 (2011)

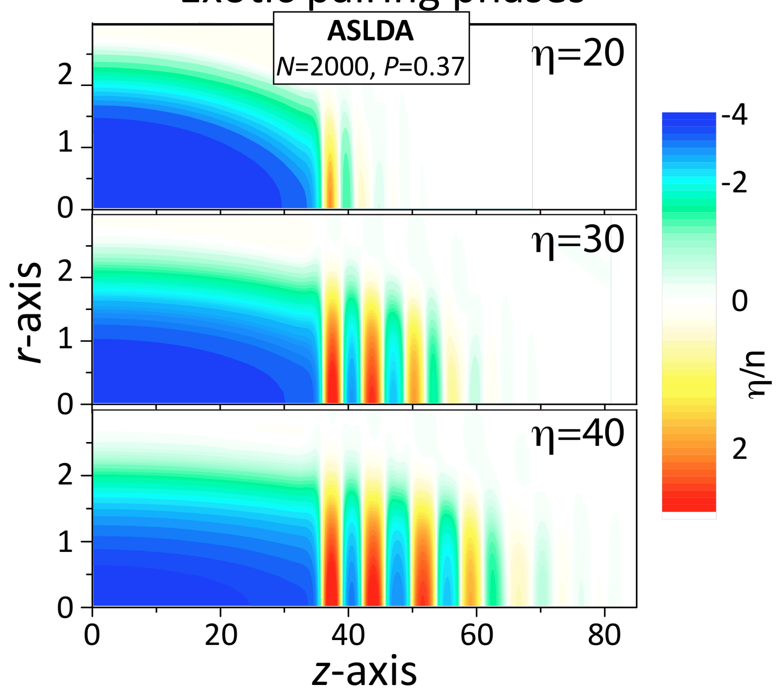
http://www.physicstoday.org/resource/1/phtoad/v64/i8/p19_s1

Multiple Components



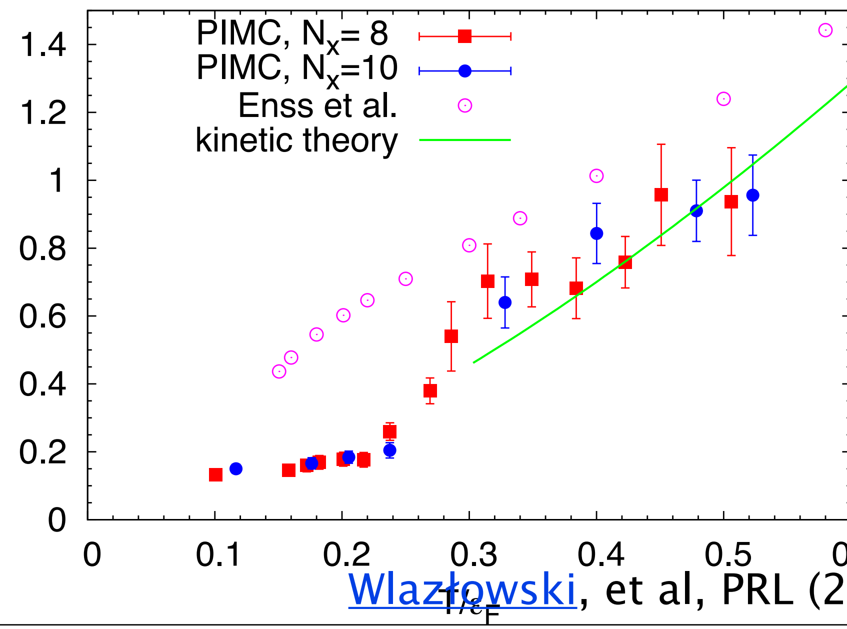
Nishida, PRL (2012)

Exotic pairing phases



J. Pei et al., Phys. Rev. A 82, 021603(R) (2010)

Viscosity over Entropy



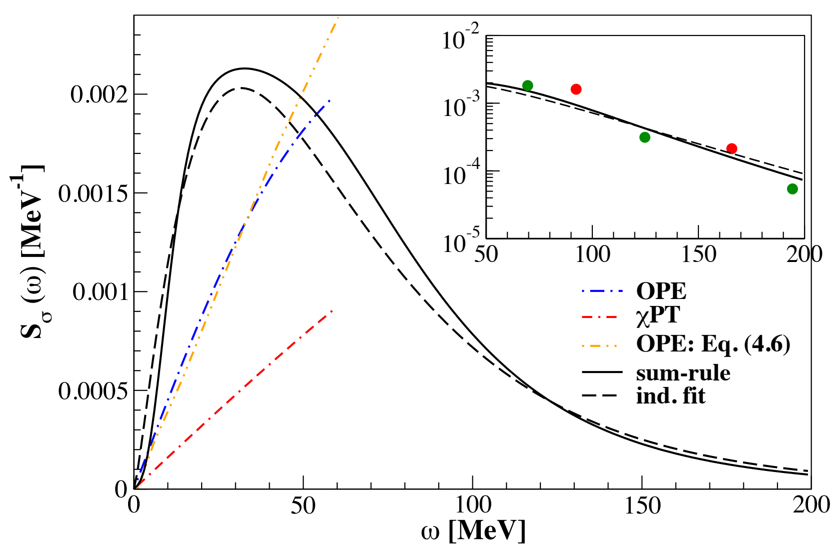
Wlazłowski, et al, PRL (2012)

Further Directions in Nuclear Physics: Neutrino Physics

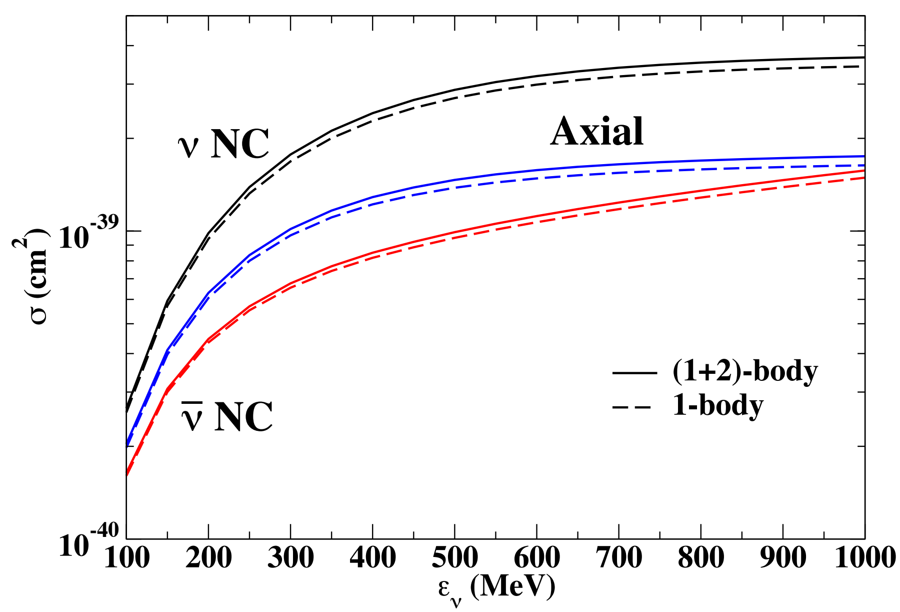
Nuclear structure is critical:
Double-beta decay
neutrino-nucleus scattering

Low to High energy
Small to Large A

Spin (weak) Response of Neutron Matter



Neutrino-Deuteron Scattering



q~0 A=∞

q very large, A=2

Conclusions:

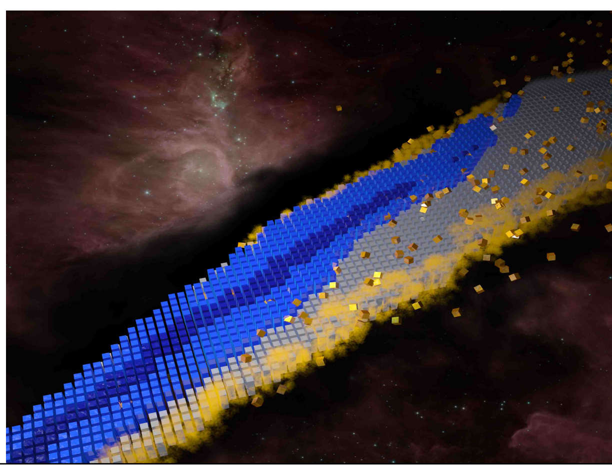
Important progress in computational nuclear physics and our understanding of nuclear reactions.

Nuclear Structure is a fascinating subject with deep connections to:

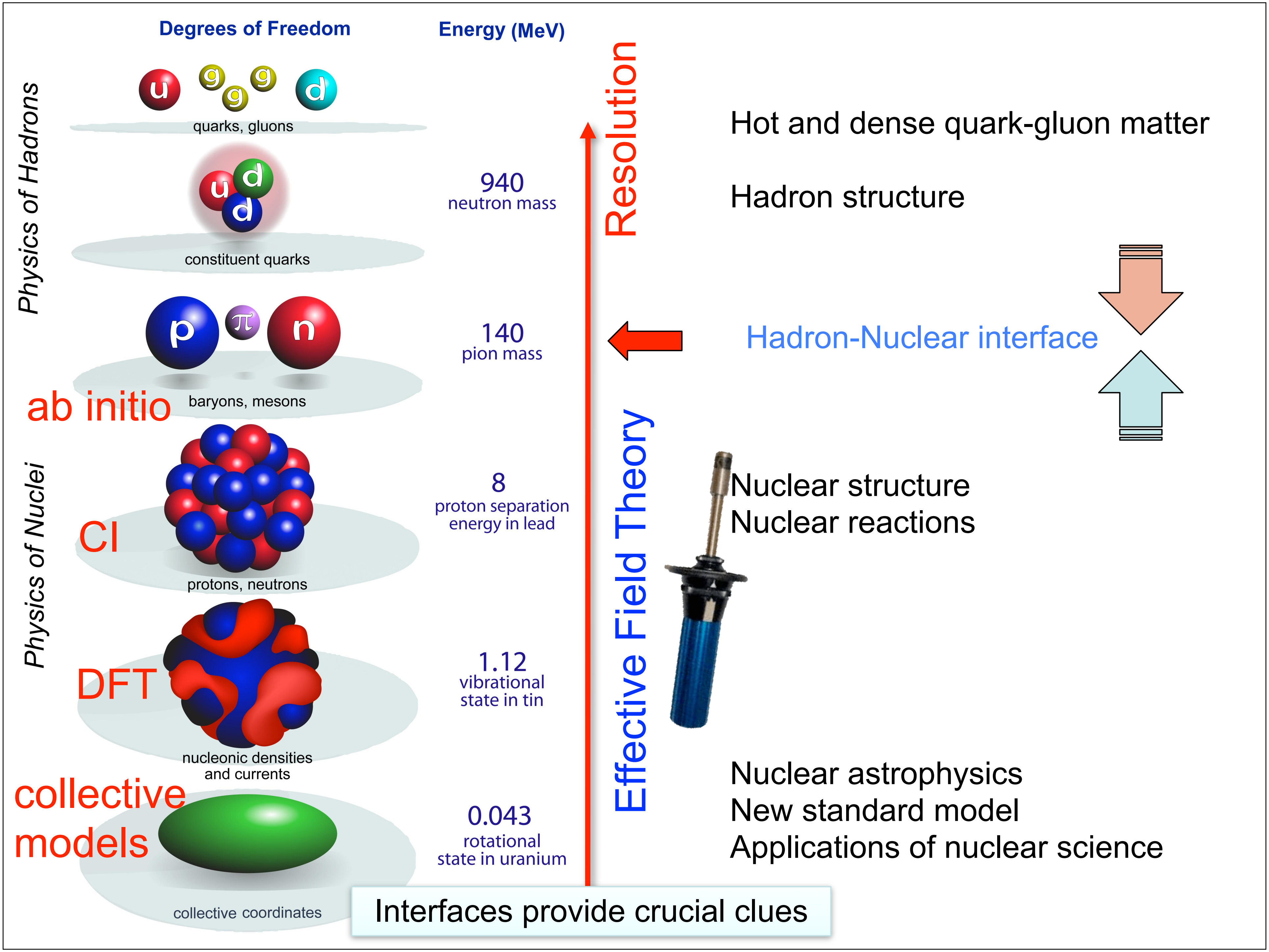
Many-Body Theory: Condensed Matter/ Cold Atoms

Astrophysics: r-process, neutron stars, supernovae

Neutrino physics and fundamental symmetries:
double-beta decay, neutrino oscillations, ...

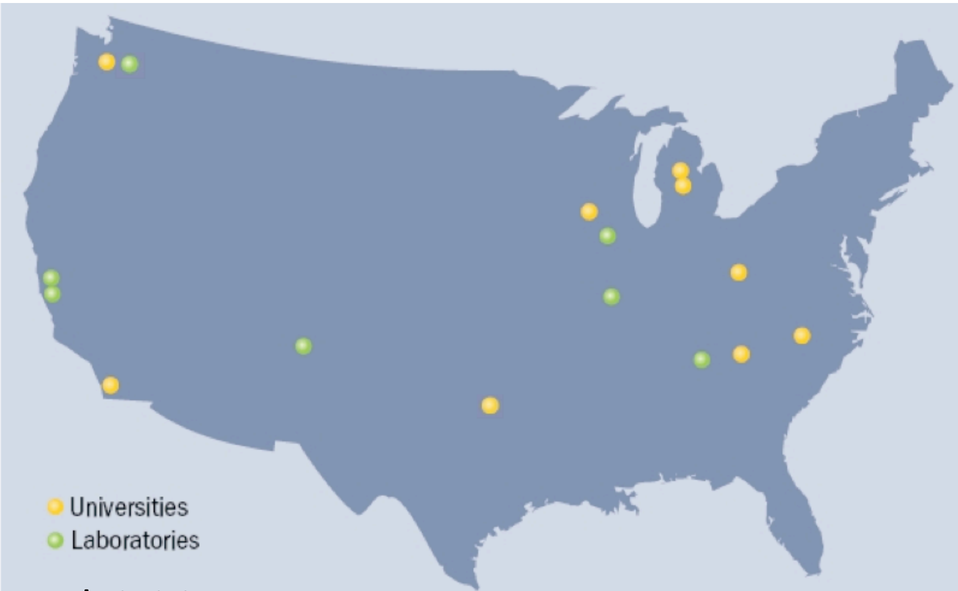


Backup


Degrees of Freedom
Energy (MeV)
Physics of Hadrons
quarks, gluons
constituent quarks
baryons, mesons
Physics of Nuclei
ab initio
CI
DFT
collective models
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 dense quark-gluon matter
Hadron structure
Hadron-Nuclear interface
Nuclear structure
Nuclear reactions
Nuclear astrophysics
New standard model
Applications of nuclear science
Interfaces provide crucial clues

EXAMPLE: *Universal Nuclear Energy Density Functional*

(other, smaller, collaborations exist: NuN, TORUS, PetaApps,…)



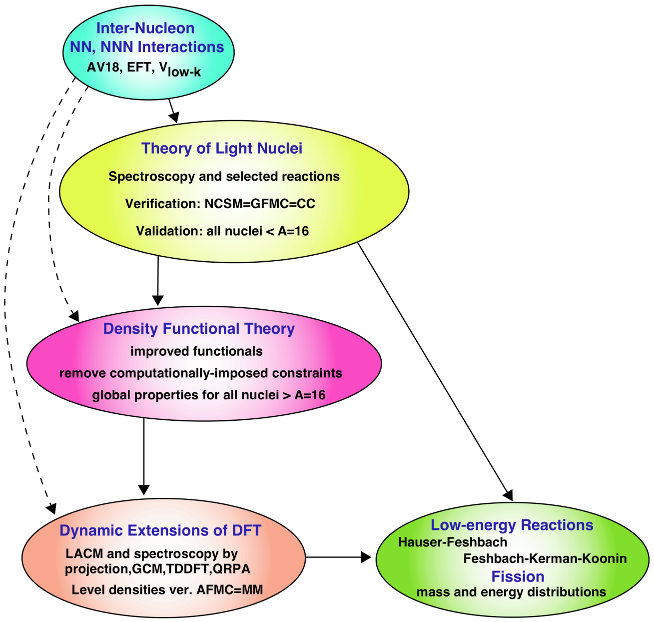
- Ab initio structure
- Ab initio functionals
- DFT applications
- DFT extensions
- Reactions

Focus on:
- Predictive power
- Robust extrapolations
- Validation
- Guidance

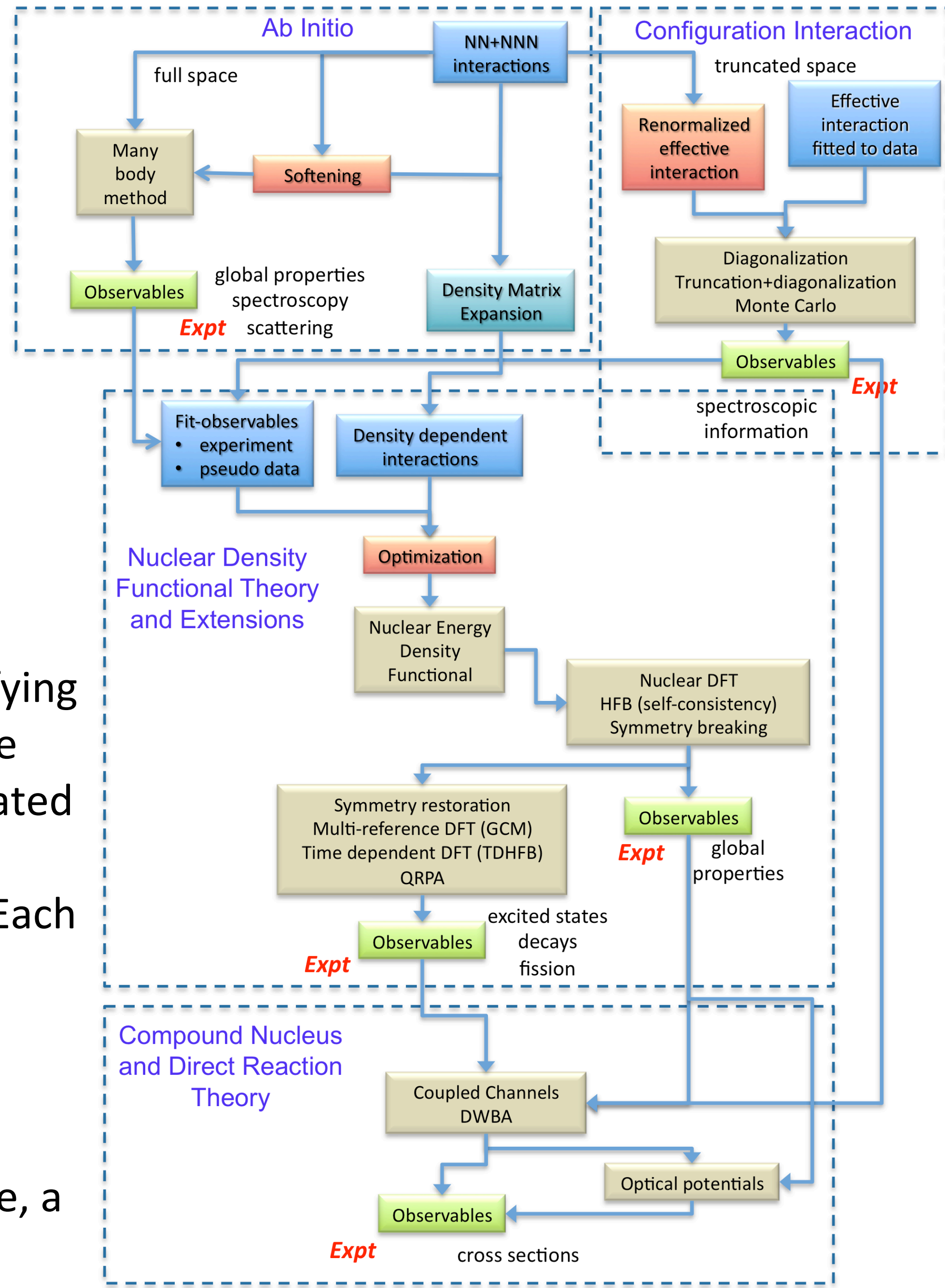
- Funded for 5 years by DOE (NP/SC, NNSA, ASCR)
- 9 universities and 7 national labs
- Junior scientists: 11 students, 19 postdocs/year
- ~50 researchers in
  - physics
  - computer science
  - applied mathematics
- International partners

For a popular description of UNEDF, see:
- SciDAC Review Winter 2007 http://www.scidacreview.org/0704/pdf/unedf.pdf
- Nucl. Phys. News 21, No. 2, 24 (2011)
- Office of Science "Highlight Series": http://science.energy.gov/news/in-focus/2011/03-28-11-s/

UNEDF in 2007



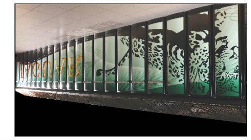
UNEDF in 2011



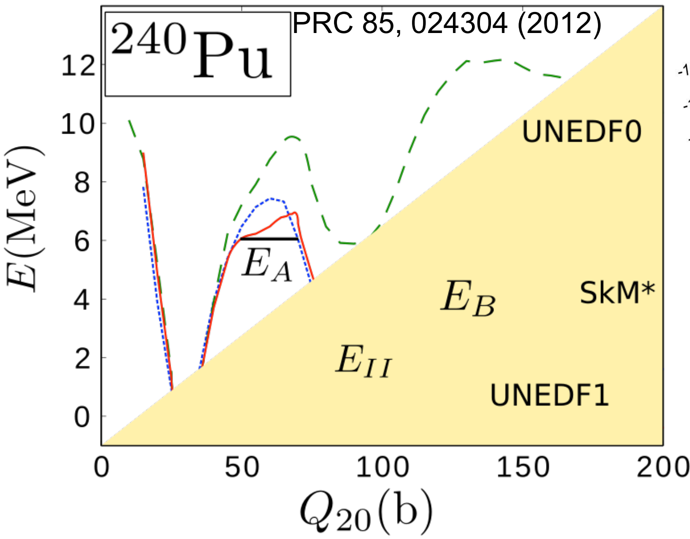
- As UNEDF has matured, it has been satisfying to see the increased coherence within the effort; the project has created and facilitated an increasing interplay among the major sections *where none existed previously*. Each of the main physics areas now includes collaborations that cross over into other sectors.
- A fair number of applications are now running on the biggest machines available, a vast change from when UNEDF started.

LACM, Fission: the ultimate challenge

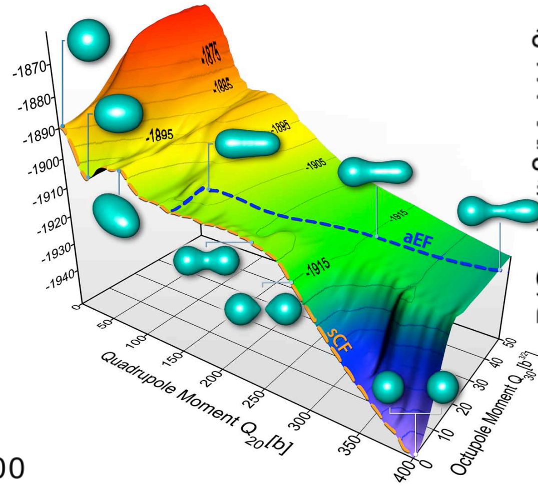
Stability of the heaviest nuclei, r-process, advanced fuel cycle, stockpile stewardship…



Optimized Functionals

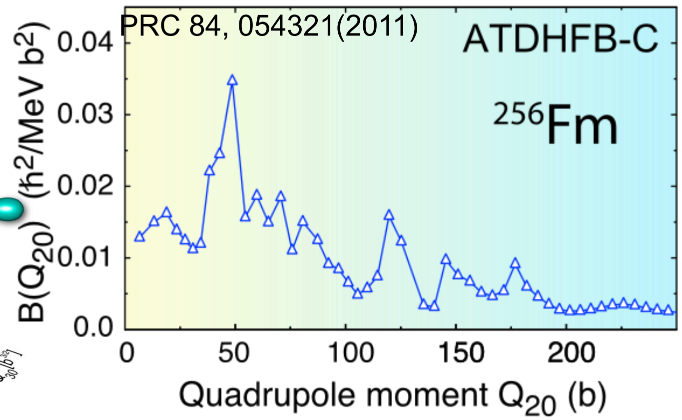


Large-scale DFT

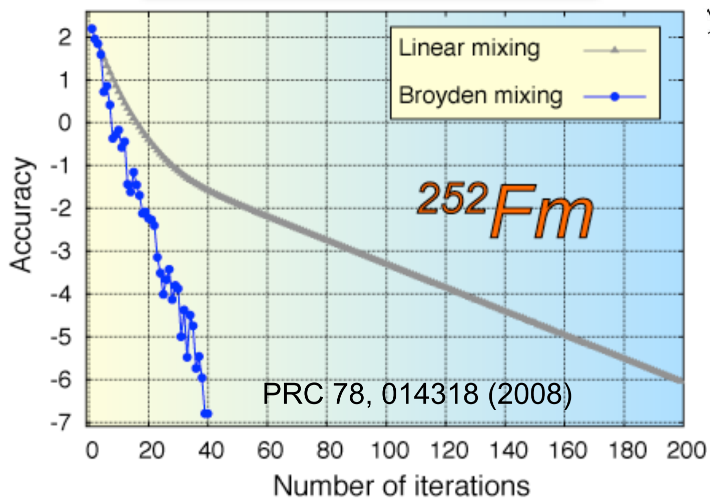


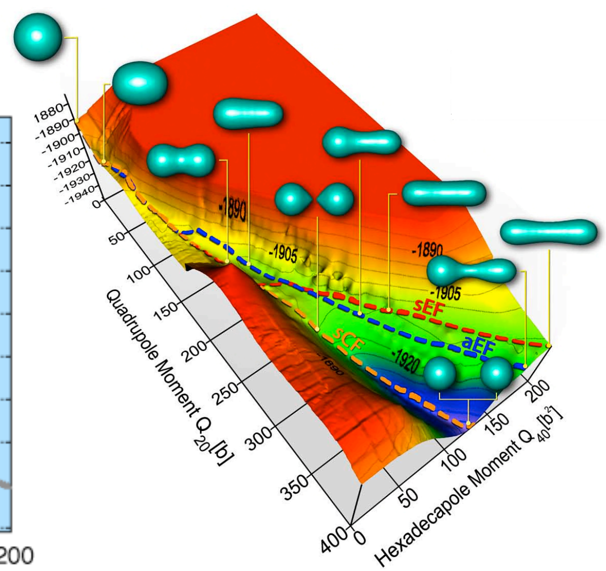
PRC 80, 014309 (2009)

Collective dynamics



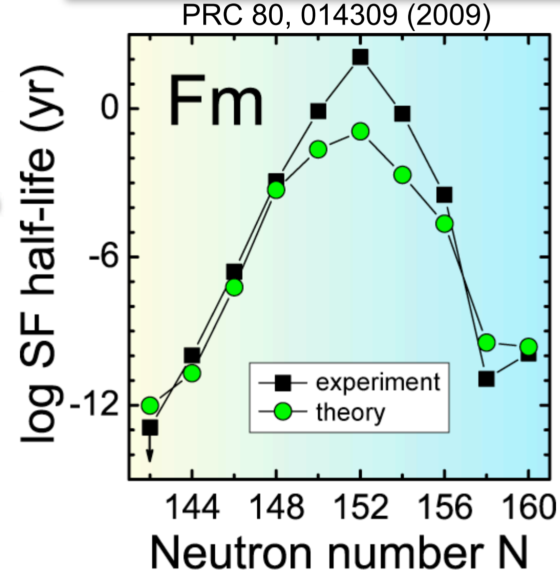
Numerical Techniques

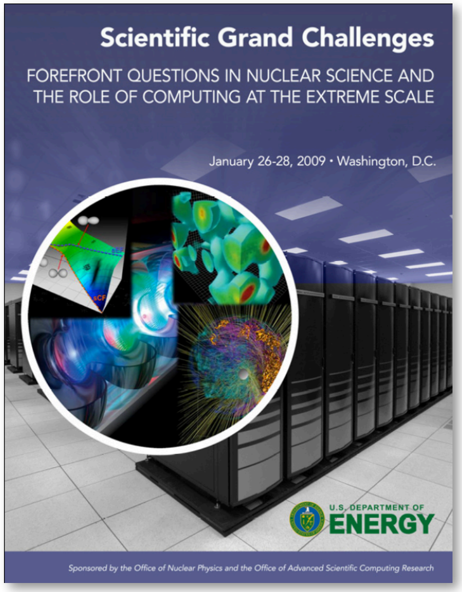




Confrontation with experiment; predictions

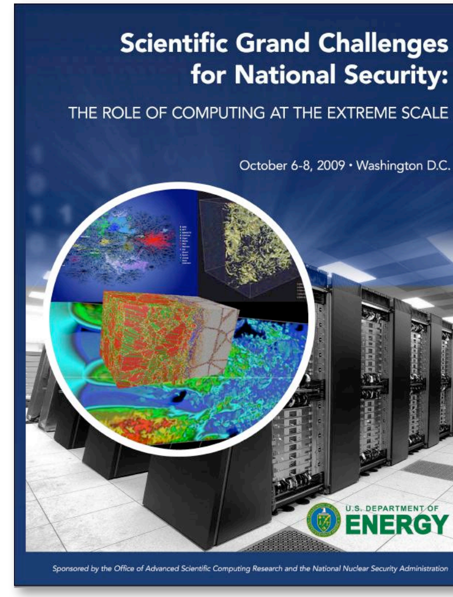
PRC 80, 014309 (2009)





Two DOE-sponsored workshops on exascale computing for nuclear physics, one common conclusion:

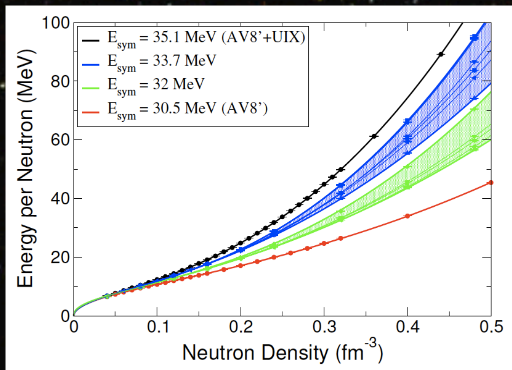
The microscopic descriptions of nuclear fusion and fission are our Priority Research Directions.



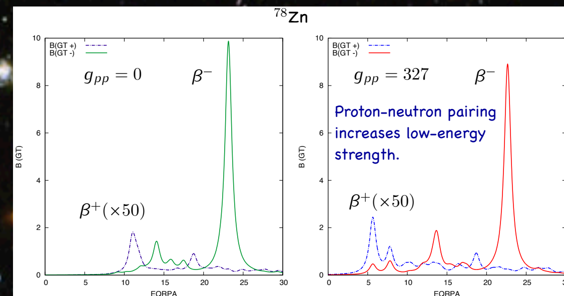
“The ultimate outcome of the nuclear fission project is a treatment of many-body dynamics that will have wide impacts in nuclear physics and beyond. The computational framework developed in the context of fission will be applied to the variety of phenomena associated with the large amplitude collective motion in nuclei and nuclear matter, molecules, nanostructures and solids”

“Fusion reactions in light nuclei are critical for both basic science and NNSA applications. These reactions aid in understanding the early universe and provide the energy that powers the stars. These reactions are also essential elements of NNSA science..”

Quest for understanding the neutron-rich matter on Earth and in the Cosmos



Phys. Rev. C 85, 032801(R) (2012)



RNB Facilities/ NuN topical collaboration

Nuclear matter equation of state

Nuclear observables

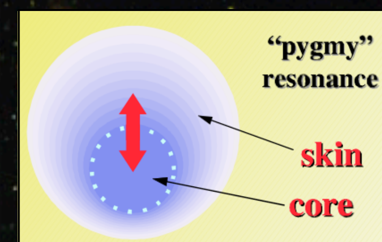
Nuclear interactions

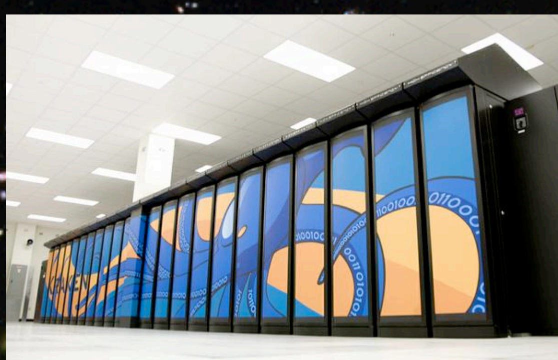
Many body theory

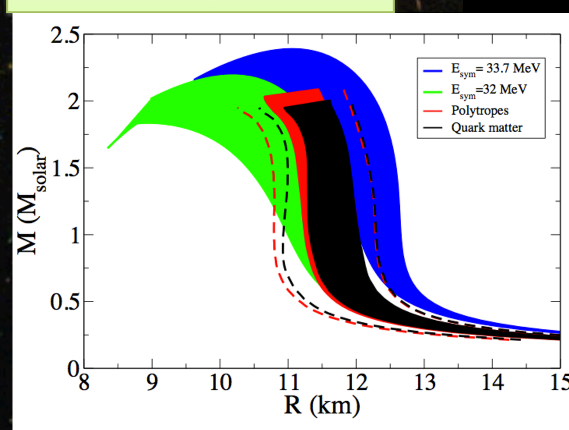
Neutron star crust

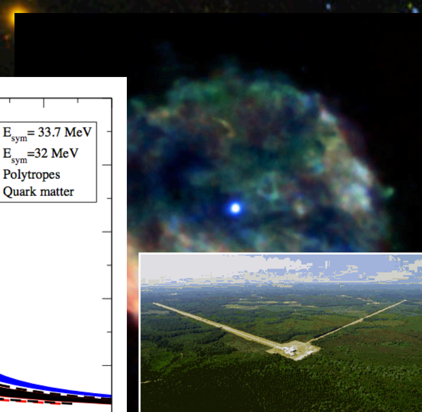
Astronomical observables

Microphysics (transport,…)









Phys. Rev. Lett. 108, 081102 (2012)

Science on NBCNEWS.com

How many neutrons, protons can get along? Maybe 7,000

New study comes closer than ever to finding answer by estimating number of variations that can exist in an atom

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LiveScience
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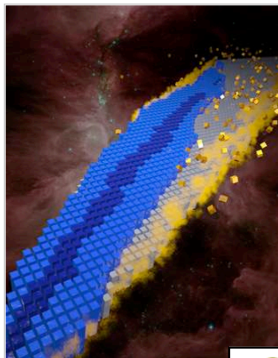

Andy Sproles / Oak Ridge National...

Scientists have long wondered whether there is a limit to the number of protons and neutrons that can be clustered together to form the nucleus of an atom. A new study comes closer than ever to finding the answer by estimating the total number of nucleus variations that can exist.

The periodic table of elements includes 118 known species of atoms, and each of these exists (either naturally or synthetically) in several versions with differing numbers of neutrons, giving rise to a total of about 3,000 different atomic nuclei. As technology has

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Pounding out atomic nuclei

Mike May | March 7th, 2011 | Updated: March 16th, 2011 — Email This Post | Print | Share This

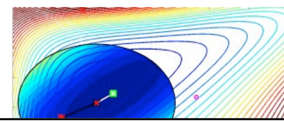
FILED UNDER Argonne,

Thousands of tiny systems called atomic nuclei – specific combinations of protons and neutrons – prove extremely difficult to study but have big implications for nuclear stockpile stewardship. To describe all of the nuclei and the reactions between them, a nationwide collaboration is devising powerful algorithms that run on high-performance computers.

Nuclear reactions, from fission in reactors to fusion in stars, depend on interactions between protons and neutrons that are building blocks of atomic nuclei.

Describing all of the nuclei and the reactions between them, however, demands powerful algorithms running on high-performance computers.

The Universal Nuclear Energy Density Functional (UNEDF) collaboration, which was created by the Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) program, focuses on developing such descriptions.



The UNEDF collaboration includes researchers from seven national laboratories – Ames, Argonne, Lawrence Berkeley, Lawrence Livermore, Los Alamos, Oak Ridge, and Pacific Northwest – and nine universities: Central Michigan, Iowa State, Michigan State, Ohio State, San Diego State, North Carolina at Chapel Hill, Tennessee-Knoxville, Texas A&M in Commerce and University of Washington. Recently, researchers in this collaboration made a significant advance through the use of density functional theory (DFT).

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Science News

Physicists Pin Down Proton-Halo State

ScienceDaily (May 27, 2010) — A halo may be difficult to acquire in terms of virtue, but it can also be tough to calculate in terms of physics. Thomas Papenbrock, associate professor of physics and astronomy at the University of Tennessee, Knoxville, and his colleagues Gaute Hagen from Oak Ridge National Laboratory and Morten Hjorth-Jensen from the University of Oslo have managed to do just that, however, and report their findings in *Physical Review Letters*

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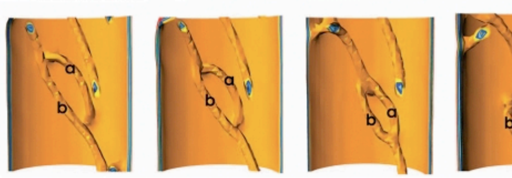
« Fluorescing diamonds inside living cells | Physics Update

Stirring superfluids

By Physics Today on June 13, 2011 10:52 AM | No TrackBacks

If you chill fermions enough, they can pair up to form bosons and settle into a single c... ground state, a Bose–Einstein condensate. In the case of helium-3 atoms, the resultin... superfluid that flows without dissipation—provided the flow is not so energetic that it b... apart or destroys the ground state's coherence. Until now, theorists could characterize... in fermionic superfluids, but not the vigorous turbulence that results from shaking or st... Bulgac of the University of Washington in Seattle and his colleagues have adapted de... functional theory—a computational approach originally devised to calculate molecula... —and applied its time-dependent extension to model turbulent fermionic superfluids. ... underlying quantum mechanical equations are straightforward, solving them required ... of the world's most powerful supercomputers, Jaguar at Oak Ridge National Laborato... Tennessee. In their simulations, Bulgac and his colleagues agitated a fermionic super... shooting spherical projectiles through it or by stirring it with a laser beam. Turbulent su... known to harbor tubes of quantized vorticity. As the figure below shows, the simulatio... how two vortex tubes (marked a and b) joined to form a ring, which then opens in a ma... reminiscent of the unzipping of a DNA molecule during transcription. Bulgac's model c... astronomers understand another agitated superfluid: the interior of a rapidly spinning ... (A. Bulgac et al., *Science* 332, 1288, 2011.)—Charles Day



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03.28.11

Universities and DOE National Laboratories Join Forces to Understand the Nucleus of an Atom

Find out about this collaboration's efforts and accomplishments toward completing a portrait of the nuclear landscape.

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Nuclear physics is the study of the tiny, massive core of an atom, a complex micro-world of particles and forces. Nearly all the mass in the visible universe is locked away in atomic nuclei, as is nearly all the energy. The physics of the nucleus lies at the heart of element formation in exploding stars, as well as sources of energy for public use and national defense. Scientists strive for a comprehensive, unified description of all nuclei, a portrait of the nuclear landscape which incorporates all nuclear properties and forces in one framework. Such a model would allow for more accurate predictions of the nuclear reactions involved in all sorts of processes, from the creation of new elements to the improvement of nuclear reactors.

Around 50 researchers — theoretical physicists, computer scientists, and applied mathematicians — from nine U.S. universities, seven national laboratories, and research institutes across Europe and Japan, have come together in an effort to develop a more complete description of the atomic nucleus and its interactions. Their computational nuclear physics project, known as Universal Energy Density Functional (UNEDF), is led by Ewing Lusk (Argonne National Laboratory) and Witold Nazarewicz (University of Tennessee/Oak Ridge National Laboratory). The project is part of the U.S. Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) program, funded by the Office of Science.

A nucleus is one of the most complicated environments in nature because all fundamental forces come into play. The four fundamental forces are called the strong force, the weak force, electromagnetic force, and gravity. The constituents of a nucleus are protons and neutrons (collectively referred to as nucleons), which are themselves made of fundamental particles known as quarks and gluons. Each

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Quantum quirk makes carbon dating possible

› 15 July 2011 by David Shiga
› Magazine issue 2821. Subscribe and save

RADIOCARBON dating relies on carbon-14 to decode an object's age, but the isotope has steadfastly refused to divulge the key to its own unusual longevity. The answer, it seems, lies in the bizarre rules of quantum physics.

Carbon-14 decays with a half-life of 5730 years, so it is often used to date objects up to about 50,000 years old (anything older would have negligible amounts of the stuff).

But most other atoms that decay in the same way - by converting one of their neutrons into a proton - disappear in less than a day. So what's different about carbon-14?

The nucleus of the carbon-14 isotope has six protons and eight neutrons. When it decays, one of the neutrons turns into a proton, and also releases an electron and a neutrino. The result is a nitrogen-14 nucleus with seven protons and seven neutrons.

International Impact of UNEDF

- JUSTIPEN (Japan)
- FUSTIPEN (France)
- FIDIPRO (Finland)
- individuals worldwide

- Annual collaboration meetings of UNEDF with JUSTIPEN and FIDIPRO
- Helping our Japanese colleagues to sharpen the case for nuclear theory supercomputing (K-machine)
- Significant impact on low-energy nuclear theory effort worldwide (example: INPC 2010)
- Unique worldwide (no other program has such a broad scope and such close PHY/CS/AM partnerships)

What makes this possible?

- Computational Resources
- Physicists (particularly early career are critical)
- Math/CS research and people (Lusk)

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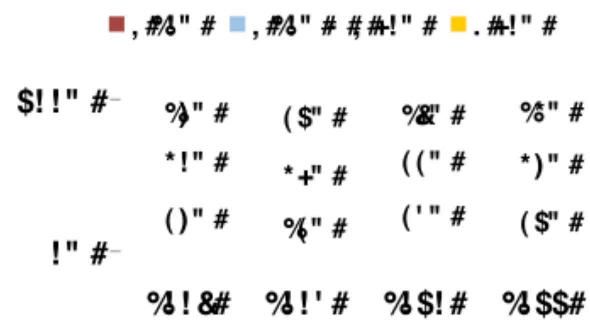
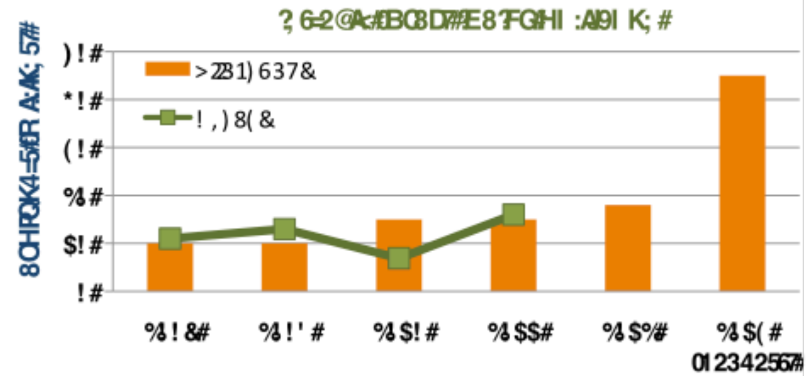
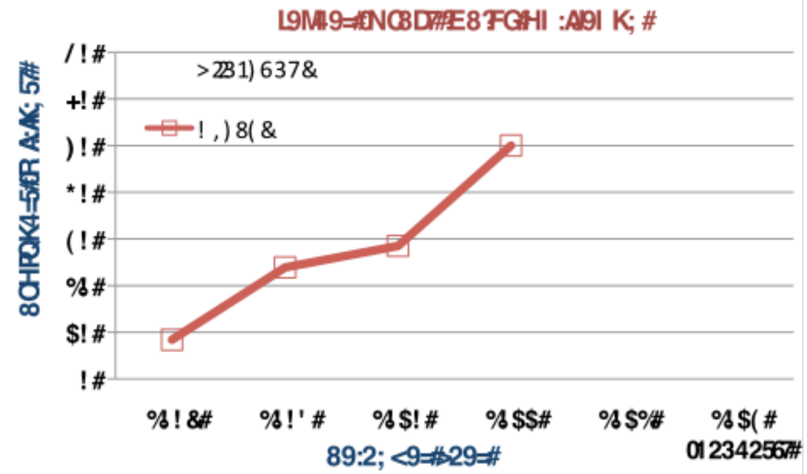




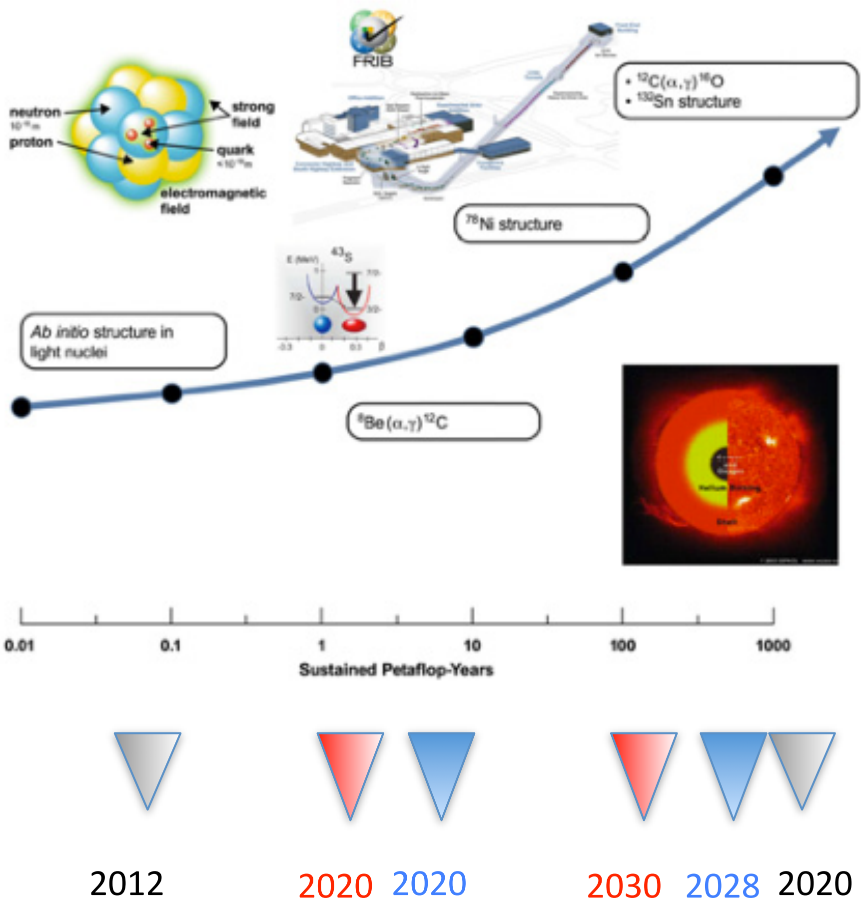


Total Resource Usage / Request / Needs

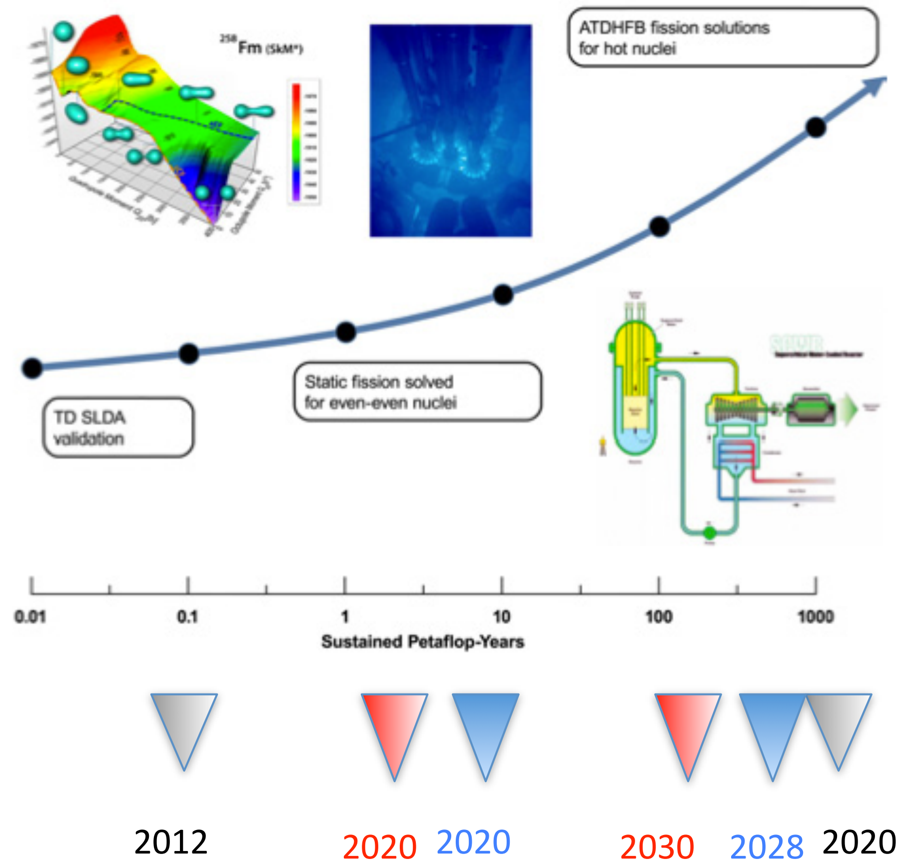
	2009	2010	2011	2012	2013
INCITE					
Intrepid	12	9	14	19	45
Jaguar	22	28	50	35	65
NERSC	2	3	3	4	10
Jaguar	20	25	35	50	150
LLNL, LANL,	20	25	25	30	40
TOTAL	70	90	120	140	300

In million core-hours (approximate)

Nuclear Reactions



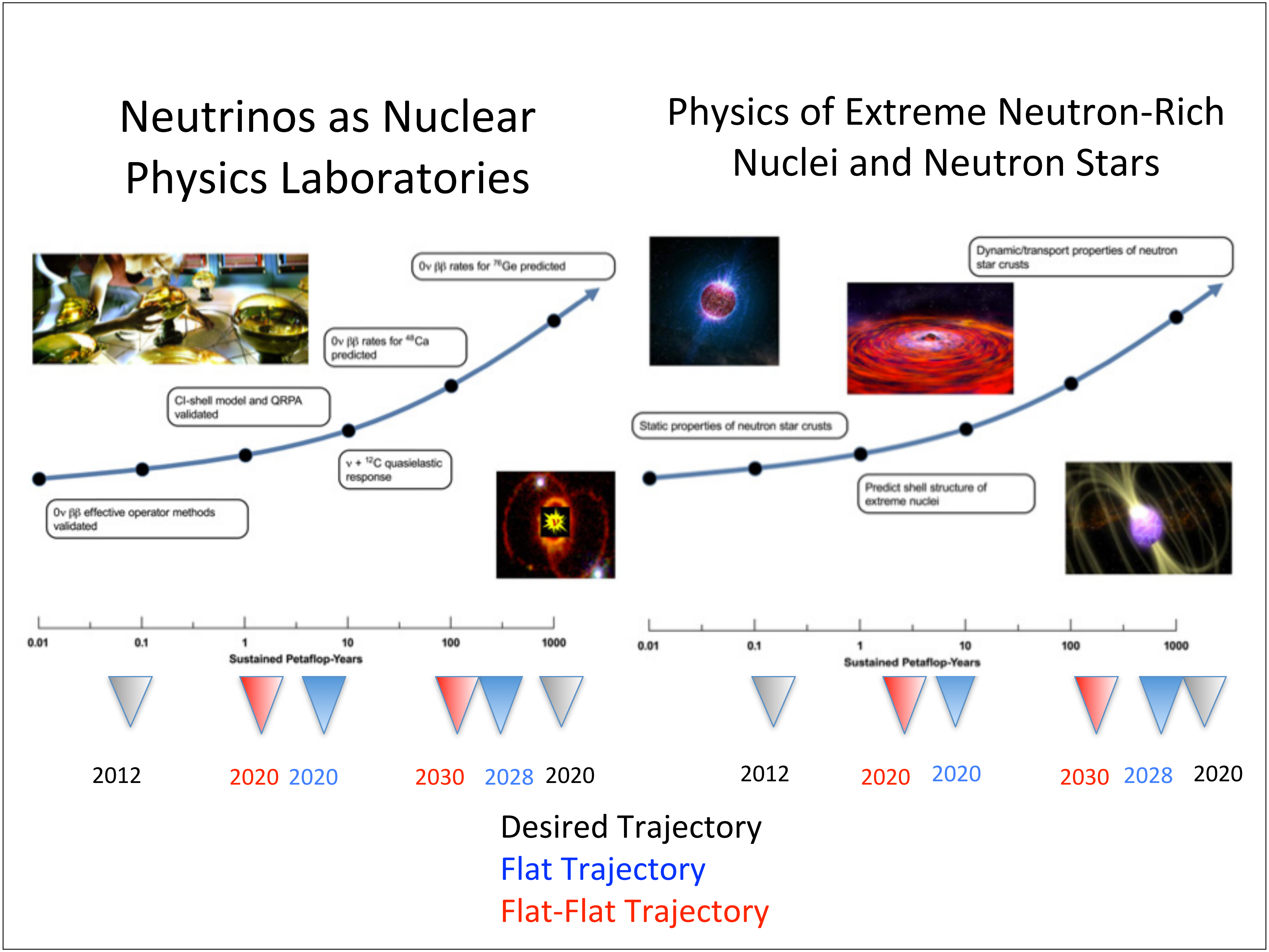
Microscopic Theory of Fission



Desired Trajectory

Flat Trajectory

Flat-Flat Trajectory



Neutrinos as Nuclear Physics Laboratories
Physics of Extreme Neutron-Rich Nuclei and Neutron Stars
0ν ββ rates for 76Ge predicted
0ν ββ rates for 48Ca predicted
CI-shell model and QRPA validated
ν + 12C quasielastic response
0ν ββ effective operator methods validated
0.01
0.1
1
10
100
1000
Sustained Petaflop-Years
2012
2020 2020
2030 2028 2020
Dynamic/transport properties of neutron star crusts
Static properties of neutron star crusts
Predict shell structure of extreme nuclei
0.01
0.1
1
10
100
1000
Sustained Petaflop-Years
2012
2020 2020
2030 2028 2020
Desired Trajectory
Flat Trajectory
Flat-Flat Trajectory

Junior Scientists in UNEDF

POST-DOCTORAL ASSOCIATES (2010)

Christopher Calderon, LBNL (staff, Numerica co.)
Joaquin Drut (Professor, UNC)
Stefano Gandolfi, LANL (staff, LANL)
Kai Hebeler, OSU (TRIUMF)
Heiko Hergert, MSU (OSU)
Jason Holt, UTK/ORNL
Eric Jurgenson, LLNL (staff, LLNL)
Markus Kortelainen, UTK (U. Jyväskylä)
Plamen Krastev, UCSD (research, Harvard)
Pieter Maris, ISU (Research Prof. ISU)
Eric McDonald, MSU (staff scientist, MSU)
Gustavo Nobre, LLNL (BNL, NNDC)
Junchen Pei, UTK (Prof., Pekin U.)
Nicolas Schunck UTK (staff, LLNL)
Roman Senkov, CMU
Ionel Stetcu, UW (staff, LANL)
Jun Terasaki, UNC (staff, U. Tsukuba)
Stefan Wild, ANL (staff, ANL)

Relevant instruction (workshops, courses) is crucial for the future of the field

Effect of UNEDF on workforce

Year-1: 9 students, 17 postdocs;
Year-2: 12 and 12;
Year-3: 10 and 18;
Year-4: 11 and 19

2010: Early Career Award

2010: Math/CS Staff ANL

2011: Faculty UNC/Chapel Hill

2010:Staff LLNL

2012: Faculty Guelph

2012: Harvard Research Computing

Mathematics and Computer Science in Two Nuclear Physics SciDAC Projects

UNEDF: 2007-2011

NUCLEI: 2012-2016 (hopefully)

Outline

- The UNEDF project just ending
  - goals
  - structure
  - Math/CS areas
- Some Specific accomplishments
- The NUCLEI project just starting (no logo yet)
- Lessons learned

Universal Low-Energy Density Functional (UNEDF)

- Sponsors: NP, ASCR, and NNSA
- Math/CS goals of this SciDAC-2 project:
  - Improve algorithms and software in support of moving codes (existing, for the most part) to petascale computing facilities, thus enabling new scientific results
  - Achieve results in mathematics and computer science applicable outside the project
- Structure:
  - Not a Math/CS team and a physics team
  - Rather, a collection of specific projects requiring math/CS and physics both, tied together by an overarching physics objective

Math/CS Areas

- Optimization
- Load Balancing
- Eigenvalues
- Frameworks
- Programming Models

- Each one part of a specific physics subproject of UNEDF

Computer Science in UNEDF

- Several partnerships; model collaborations
- Collaborations established before proposal was submitted

Green's Function Monte Carlo

Physics challenge: ab-initio description of 12C, 14C, 16O

Computational challenges: 800,000 core hours each on Argonne's IBM BlueGene/P for 12C. 14C is 60 times harder, and 16O is more than 1,000 times harder.

Exploiting BG/Q will require a redesign of the ADLB Load Balancing Library.

Coupled-cluster Code Suite

Physics challenge: ab-initio description of structure and reaction properties of medium-mass and heavy nuclei.

Computational challenges: iteratively solve coupled, non-linear equations scaling roughly as O(N4). Current calculations include N~1,000 (oxygen and calcium isotopes) with calculations planned to N~7,000 (nickel and tin isotopes). To address scaling issues and facilitate feature additions, a generalized tensor contraction engine (TCE) and global arrays will be implemented. Improved I/O, checkpoint and fault tolerance tools will be required, as well as adaptive mesh technologies for collision modeling.

No-Core Shell Model

Physics challenge: ab-initio description of light nuclei

Computational challenges: typically solve for the lowest 10-20 eigenvalues and eigenvectors of a large sparse symmetric matrix with dimensions up to 1010. A single case can run for about 5 hours of wallclock time using the full Jaguar PF machine (~240,000 cores) including post processing. Future applications will involve significantly increased matrix dimensions.

Nuclear Density Functional Theory

Physics challenge: global description of nuclear properties and decays (including fission) throughout the nuclear landscape with the focus on medium-mass and heavy nuclei.

Computational challenges: huge systems (over 107) of integro-differential equations per configuration solved iteratively. This is usually done by projection into a pre-determined basis with subsequent computations employing mostly dense matrices. Various boundary conditions assumed leading to discrete, resonance, and scattering problems. A realistic description of fission requires up to 109 configurations. Requirements: scalable IO; fault tolerance; on-the-fly simulation steering; high-dimensional array manipulations via tensor contractions; novel use of visualization tools for analysis. The use of adaptive multi-resolution techniques such as MADNESS framework will be required to solve extreme problems. MADNESS parallel runtime ensures efficient execution on leadership computers.

Nuclear Density Functional Optimizations

Physics challenge: Simulation-based, derivative-free optimization involving 10-20 parameters; sensitivity analysis for uncertainty and correlation estimations.

Computational challenges: Efficient parameter estimation and multilevel optimization algorithms for large scale (many core) DFT calculations. Estimating derivatives of noisy simulations.

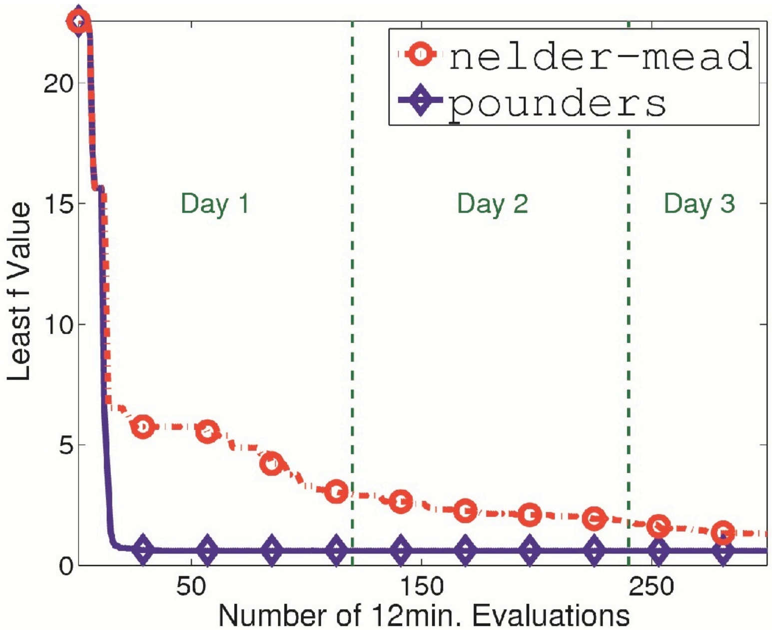
Time-dependent Density Functional Theory

Physics challenge: Dissipative nuclear processes - nuclear fission and fusion, nuclear reactions, and time-dependent phenomena in nuclei and related systems (cold gases, neutron stars)

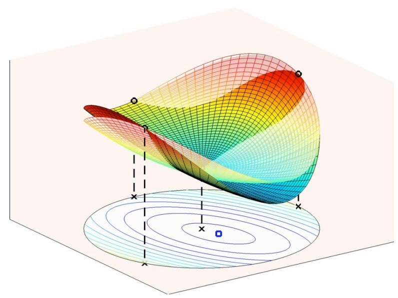
Computational challenges: Determination of nuclear ground states requires full diagonalization of large matrices (O (106) and higher) - one diagonalization requires the whole JaguarPF for several hours today; efficient I/O for large data volumes for check point and restart; in situ analysis for reduction of large data and novel use of visualization tools for analysis. A real time stochastic formulation of the current approach will require new communication algorithms for reductions and overlaps, fault tolerance, in situ data reductions, likely higher precision numerics, and improved I/O.

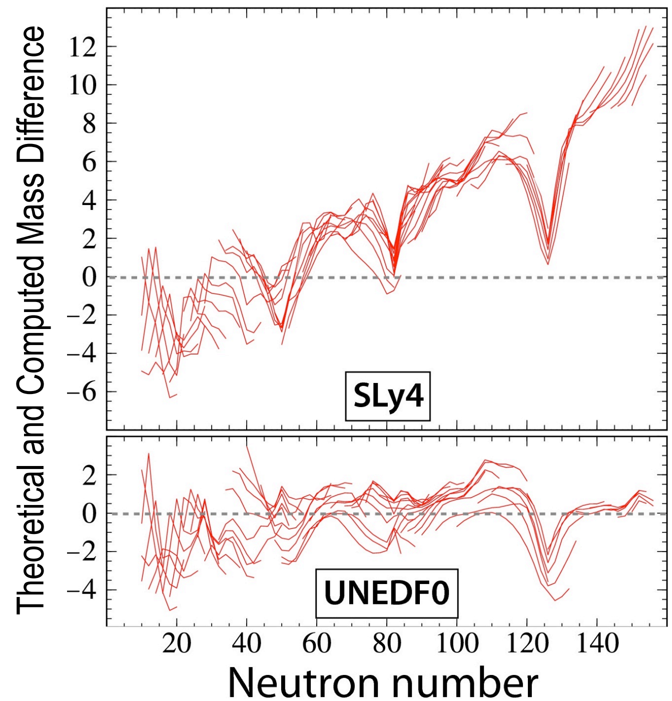
Derivative-free Optimization for Energy Density Functional Calibration

New algorithm for tuning large-scale nuclear structure simulations turns days into hours



- Energy density functional (EDF) predictions rely on large-scale computer simulations that must be calibrated to experimental data
- TAO 2.0's **POUNDERS** developed for UNEDF to exploit the mathematical structure of this calibration problem
- Substantial computational savings over alternative algorithms enables fitting of complex EDFs



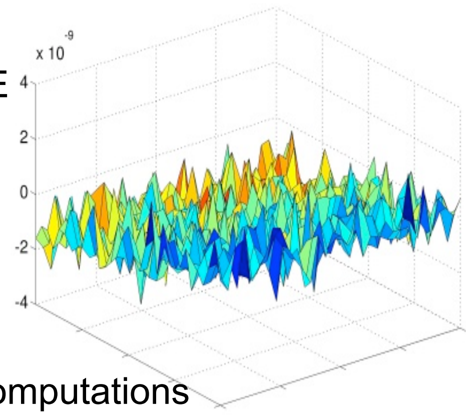


- Previous optimizations required too many evaluations to obtain desirable features exhibited by *UNEDF0, UNEDF1, …*
- Derivative-free sensitivity analysis procedure developed for UNEDF exposes correlations and constraining data in 1 minute using 20k cores
  - *"Nuclear Energy Density Optimization" Kortelainen et al., PhysRevC '10.*
  - *"N.E.D.O.: Large Deformations" Kortelainen et al., PhysRevC '12.*
  - *"Occupation Number-based Energy Functional for Nuclear Masses" Bertolli et al., PhysRevC '12.*

Optimal Derivatives of Noisy Numerical Simulations

Computational Noise

In all computations of DOE interest containing
- adaptivity,
- discretizations
- iterative methods
- petaflops,
- roundoff errors

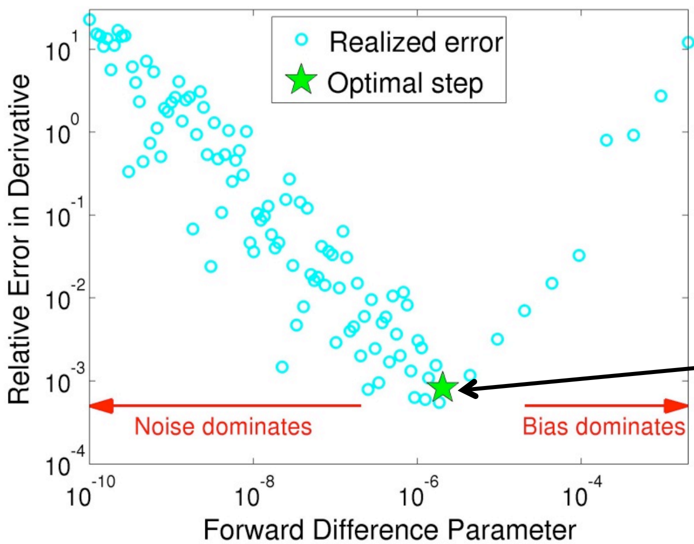


❖Includes *deterministic* computations

Noise Impacts in UNEDF & Beyond

- Uncertainty in computed outputs
- Unstable derivative estimates for sensitivity analysis
- Can be unrelated to/overwhelm truncation error
- Blurs relationship between tolerance values and stability

Our optimal forward difference parameter



Tools & Techniques

- *ECNoise* provides reliable estimates of stochastic and deterministic noise in few simulations
- Nonintrusive **stability bounds for extreme scale simulations**, can instruct precision levels/tolerances for subroutines
- Optimal difference parameters calculated without computationally expensive parameter sweeps

Optimal step was obtained with only two simulation evaluations. *Classical approach (circles): result of a sweep across 100 difference parameters, each point requiring a new simulation.*

"Estimating Computational Noise," Moré & Wild, SIAM Sci. Comp., '11

"Estimating Derivatives of Noisy Simulations," Moré & Wild, ACM TOMS'12

Making a simple programming model scalable: The Asynchronous Dynamic Load Balancing Library

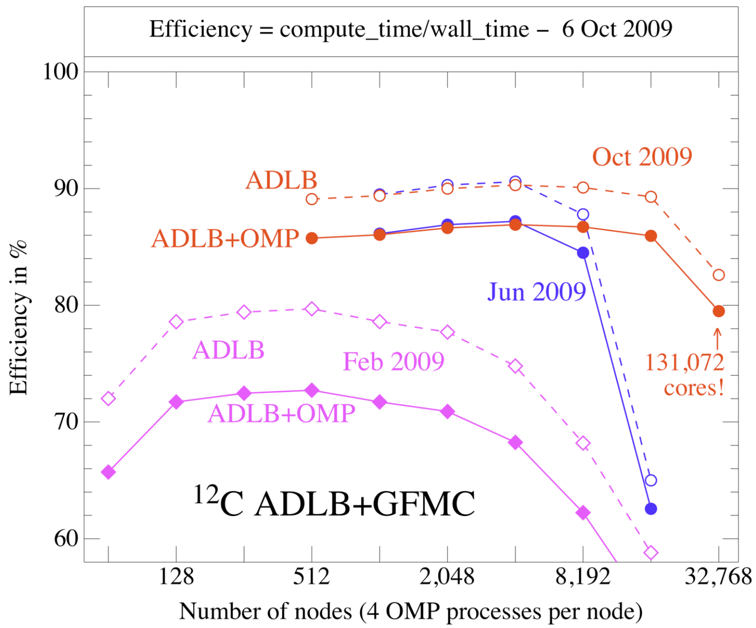
Objectives

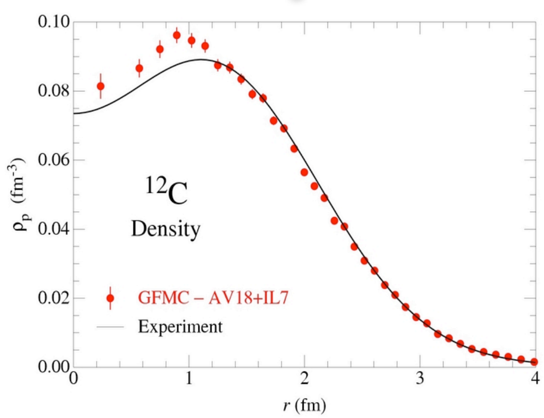
- Enable Green's Function Monte Carlo calculations for ^{12}C on full BG/P as part of UNEDF project
- Simplify programming model
- Scale to leadership class machines

Impact

- Demonstrate capabilities of simple programming models at petascale and beyond
- Show path forward with hybrid programming models in library implementation

Improved Efficiency (compute time/wall time) with more nodes





Progress

- Initial load balancing was of CPU cycles
- Next it became necessary to balance memory utilization as well
- Finally ADLB acquired the capability to balance message flow
- "More Scalability, Less Pain" by E. Lusk, S.C. Pieper and R. Butler published in SciDAC Review 17, 30 (2010)

MFDn: Total-J Progress

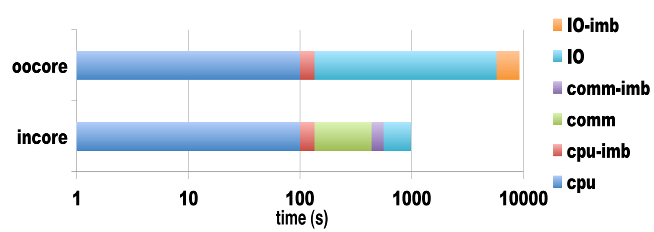
- **M-scheme approach:** works directly on the Hamiltonian, extracts all low energy states
- **J-scheme approach:** alternative to find a large number of low energy states for a prescribed total angular momentum (J) value
- **Targeted applications:** investigation of nuclear level densities, evaluation of scattering amplitudes
- **Total-J code:** implementation of the J-scheme approach in Fortran, MPI
- **CS Challenges in Total-J:** Three distinct phases, each with very different computing and storage characteristics

Phase 1: Construction of the J-basis

Implemented a multi-level greedy load balancing algorithm

Phase 2: Invariant Subspace Projection

In-core implementation to reduce I/O overheads in the out-of-core version



^{6}Li, N_{max}=14, J=3

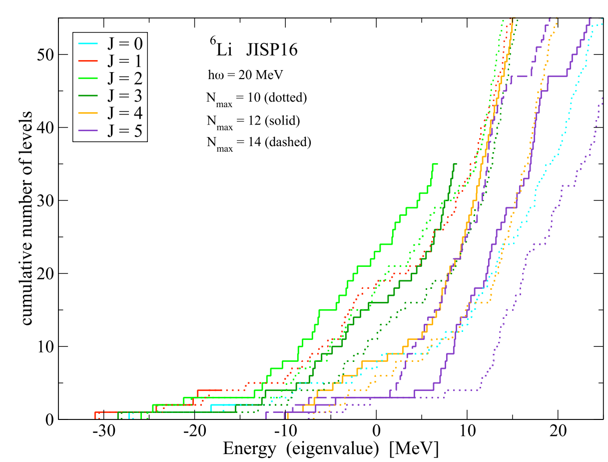
dimension of H ~ 1.7x10^8

10x speed-up, default striping

4x speed-up, optimal striping

Application:

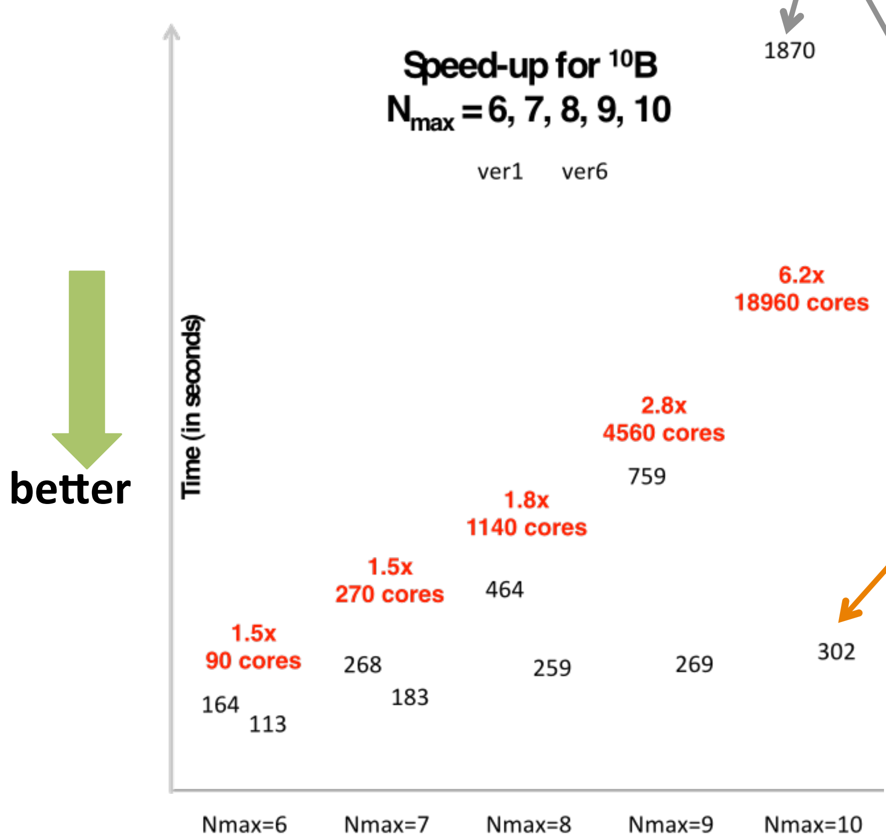
Predicting the Nuclear Level Density of ^{6}Li (PRELIMINARY)



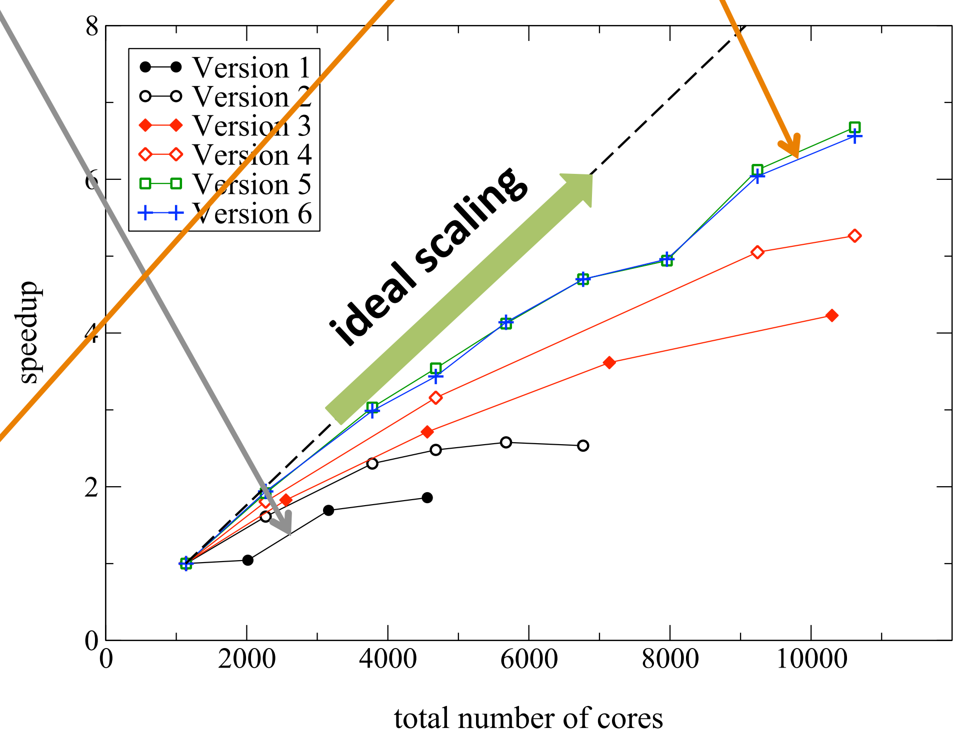
M-scheme: Performance Improvements

ver1: SC'08 paper
(beginning of SciDAC2)

ver6: current release
(end of SciDAC2)



Weak Scaling



Strong Scaling for ^{10}B, N_{max} = 8

One Demonstration of NP – ASCR Coupling: Over 20 joint publications resulting from UNEDF

- "Real-Time Dynamics of Quantized Vortices in a Unitary Fermi Superfluid," A. Bulgac, Y.-L. Luo, P. Magierski, K.J. Roche, and Y. Yu, Science 332, 1288 (2011).
- "Origin of the anomalous long lifetime of ^{14}C," P. Maris, J. P. Vary, P. Navratil, W. E. Ormand, H. Nam, and D. J. Dean, Phys. Rev. Lett. 106, 202502 (2011).
- "More Scalability, Less Pain," E. Lusk, S.C. Pieper and R. Butler, SciDAC Review 17, 30 (2010).
- "Nuclear Energy Density Optimization," M. Kortelainen, T. Lesinski, J. More, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, and S. Wild, Phys. Rev. C 82, 024313 (2010).
- "One-quasiparticle States in the Nuclear Energy Density Functional Theory," N. Schunck, J. Dobaczewski, J. McDonnell, J. More,, W. Nazarewicz, J. Sarich, and M.V. Stoitsov, Phys. Rev. C 81, 024316 (2010).
- "Scaling of ab-initio nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, International Conference on Computer Science, ICCS 2010, Procedia Computer Science 1, 97 (2010).
- "Hamiltonian light-front field theory in a basis function approach," J. P. Vary, H. Honkanen, Jun Li, P. Maris, S. J. Brodsky, A. Harindranath, G. F. de Teramond, P. Sternberg, E. G. Ng, C. Yang, Phys. Rev. C 81, 035205 (2010).
- "Ab initio nuclear structure: The Large sparse matrix eigenvalue problem," J.P. Vary, P. Maris, E. Ng, C. Yang, and M. Sosonkina, J. Phys. Conf. Ser. 180, 012083 (2009).
- "Fast Multiresolution Methods for Density Functional Theory in Nuclear Physics," G. I. Fann, J. Pei, R. J. Harrison, J. Jia, J. Hill, M. Ou, W. Nazarewicz, W. A. Shelton, and N. Schunck, Journal of Physics: Conference Series 180, 012080 (2009).
- "Solution of the Skyrme-Hartree-Fock-Bogolyubov equations in the Cartesian deformed harmonic-oscillator basis. (VI) HFODD (v2.38j): a new version of the program," J. Dobaczewski, W. Satula, B.G. Carlsson, J. Engel, P. Olbratowski, P. Powalowski, M. Sadziak, J. Sarich, N. Schunck, A. Staszczak, M. Stoitsov, M. Zalewski, H. Zdunczuk, Comp. Phys. Comm. 180, 2361 (2009).
- "Towards The Universal Nuclear Energy Density Functional," M. Stoitsov, J. More, W. Nazarewicz, J. C. Pei, J. Sarich, N. Schunck, A. Staszczak, and S. Wild, Journal of Physics: Conference Series 180, 012082 (2009).
- "Deformed Coordinate-Space Hartree-Fock-Bogoliubov Approach to Weakly Bound Nuclei and Large Deformations," J.C. Pei, M.V. Stoitsov, G.I. Fann, W. Nazarewicz, N. Schunck and F.R. Xu, Phys. Rev. C 78, 064306 (2008).
- "Time-Dependent Density Functional Theory Applied to Superfluid Nuclei," A. Bulgac and K.J. Roche, J. Phys.: Conf. Ser. 125, 012064 (2008).
- ...

A SciDAC-3 Project: Nuclear Computational Low Energy Initiative (NUCLEI)

- Mostly same cast as UNEDF
- Targeting next generation architectures on path to exascale
- Examples of specific plans in Math/CS…

Optimization Plans in NUCLEI

New Optimization Capabilities

- State-of-the art mathematical/numerical optimizations of next-generation EDFs *(with LLNL, ORNL, Tennessee)*
- Optimization of basis states and non-perturbative coupling constants arising in chiral Hamiltonians *(with ISU)*
- Enable nucleus lifetime computations with collective action minimizations *(with LLNL, others)*

- Exploit additional parallelism at the simulation-optimization interface
- Extend POUNDERS to address missing states and available sensitivity information
- Incorporate uncertainties and QUEST technologies

Coupling NUCLEI Subgroups

- Incorporate new observables from various NUCLEI subgroups
  - giant resonance data,
  - binding energy of neutron droplets in a trap,
  - …

Deploy code optimization tools

- Introduce performance, energy, and resilience tools developed by the SUPER SciDAC Institute for use in NUCLEI codes
- Deliver representative NUCLEI computational kernels to SUPER

Future Plans for the Asynchronous Dynamic Load Balancing Library

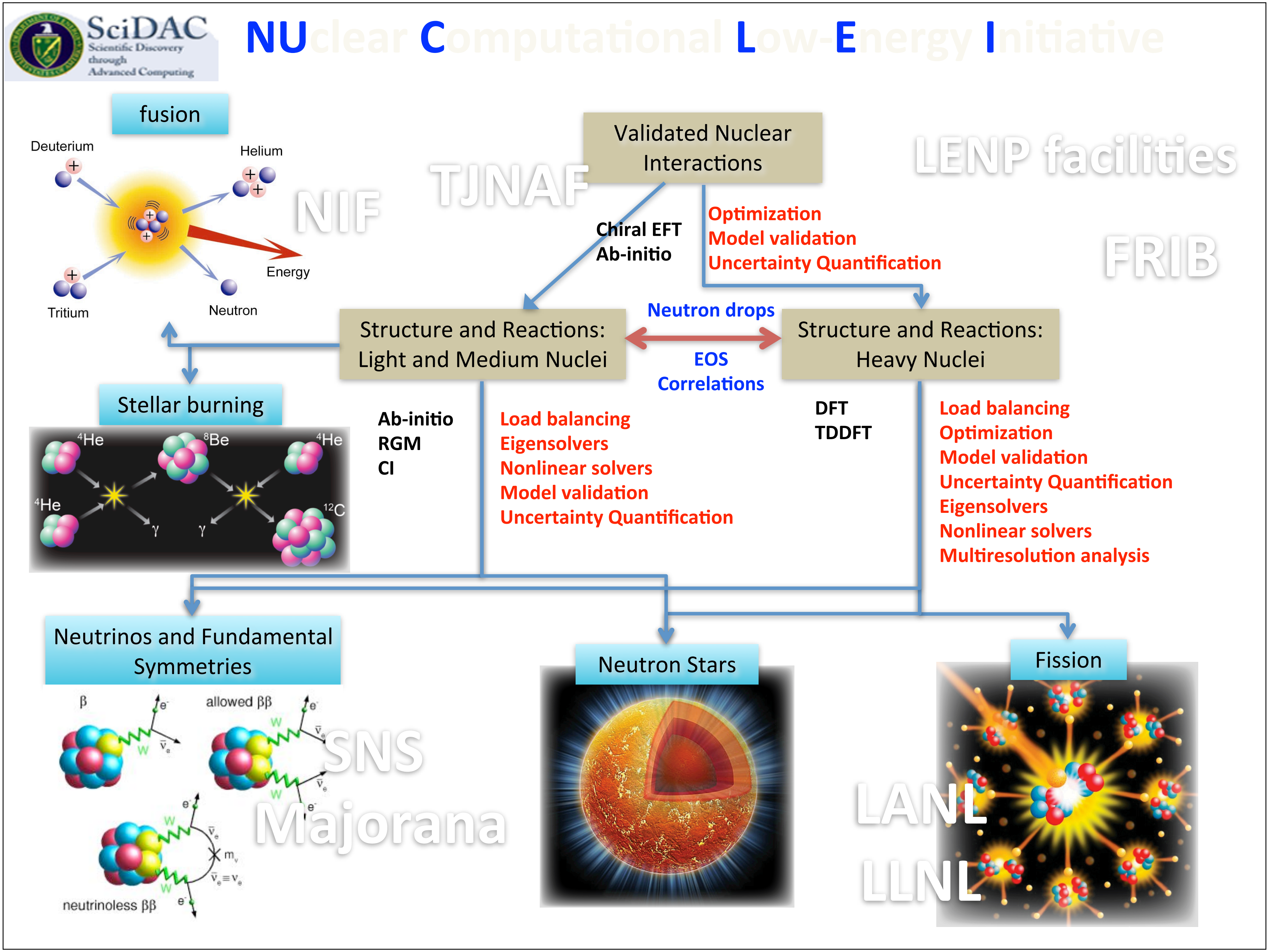
- The Exascale target for GFMC (Green's Function Monte Carlo) code is ^{16}O.
- The overall structure of GFMC can remain the same if
  - Effective use of many-core nodes can be made
    - may need to go beyond current OpenMP approach
  - ADLB can support multi-node parallelism on single work units
- This will require major changes to ADLB that take advantage of new features in MPI-3.

MFDn: Future Work

- Version 14 (under development)
  - Efficient construction of the Hamiltonian, faster SpMV
  - 3-body interaction support is underway
- MFDn on different architectures
  - Investigating the use of GPU (Titan) and BG/Q (Mira) platforms
  - Out-of-core implementation on SSD-equipped clusters
- Compression of the Hamiltonian to enable the study of heavier nuclei

Summary (for Math/CS)

- The structure of the UNEDF project was the key to its success
  - Math/CS//Physics partnerships formed locally at proposal-writing stage, and developed over the 5-year timeframe of the project
- Significant science resulted
- Future looks bright
  - Many hard steps now behind us
    - Collaborations quite deep at this point
    - Codes have been significantly improved for scalability
  - Many interesting steps ahead of us
    - Exascale provides new set of challenges


SciDAC
Scientific Discovery through Advanced Computing
NUclear Computational Low-Energy Initiative
fusion
Deuterium
Helium
Energy
Tritium
Neutron
NIF
TJNAF
Validated Nuclear Interactions
LENP facilities
Chiral EFT
Ab-initio
Optimization
Model validation
Uncertainty Quantification
FRIB
Neutron drops
Structure and Reactions: Light and Medium Nuclei
EOS
Correlations
Structure and Reactions: Heavy Nuclei
Stellar burning
4He
8Be
4He
4He
12C
γ
γ
Ab-initio
RGM
CI
Load balancing
Eigensolvers
Nonlinear solvers
Model validation
Uncertainty Quantification
DFT
TDDFT
Load balancing
Optimization
Model validation
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Nonlinear solvers
Multiresolution analysis
Neutrinos and Fundamental Symmetries
β
allowed ββ
neutrinoless ββ
SNS
Majorana
Neutron Stars
Fission
LANL
LLNL