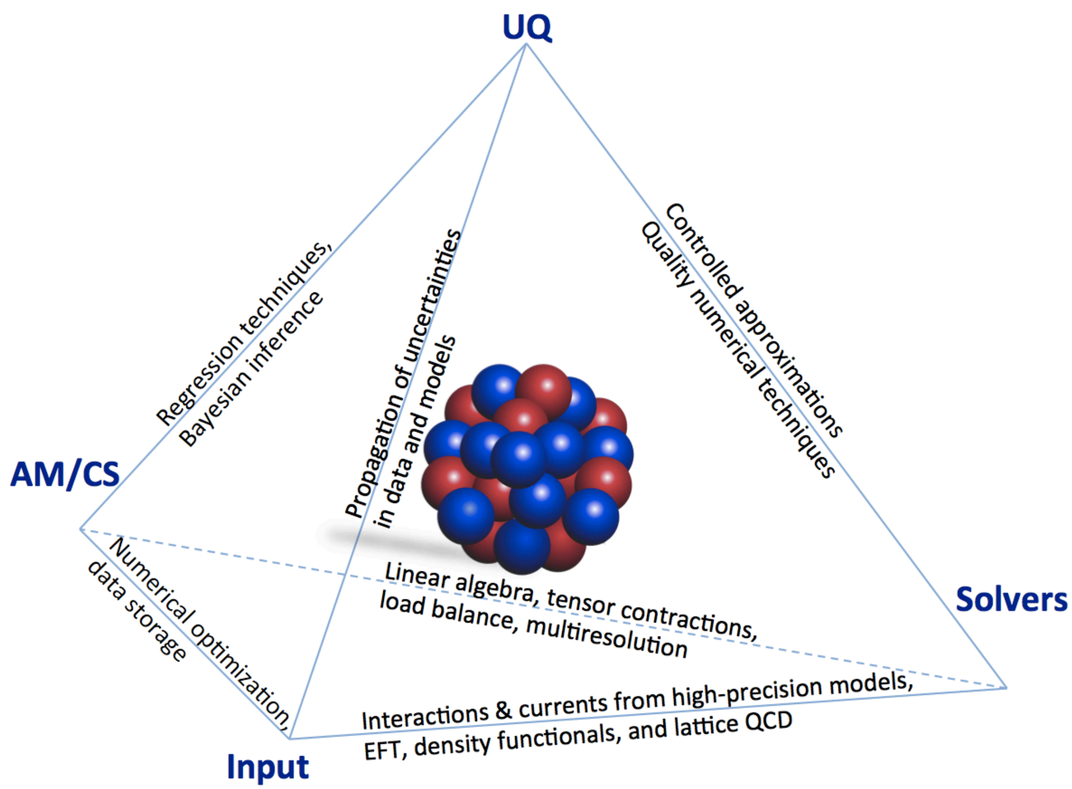
NUCLEI

Nuclear Computational Low-Energy Initiative

A SciDAC-4 Project



Solving the nuclear quantum few- and many-body problem

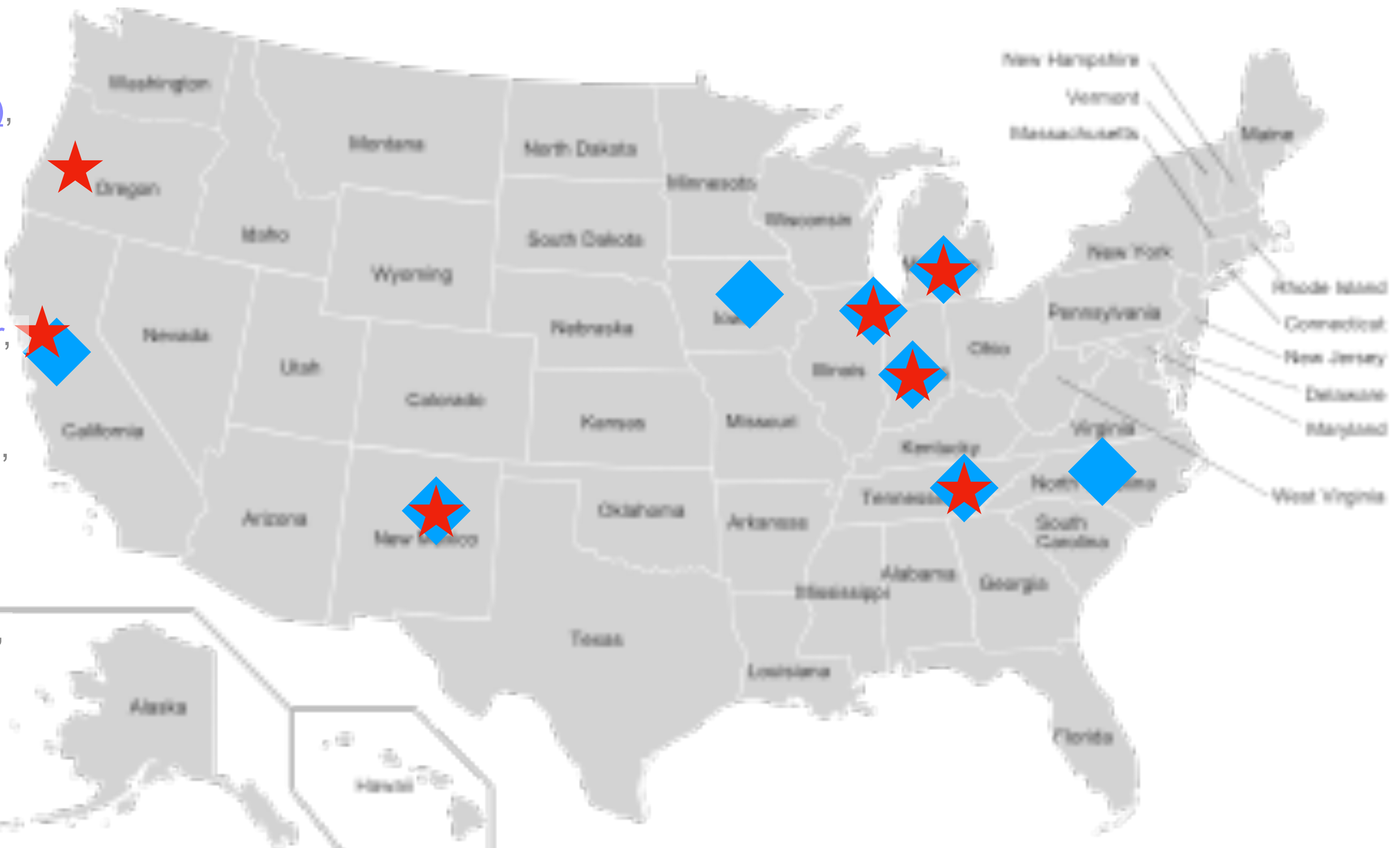
Direct connections to LQCD and TEAMS

computingnuclei.org

Funded by DOE/SC (NP and ASCR) and NNSA

People & Institutions

Argonne National Laboratory
R. Butler, A. Lovato, E. (Rusty) Lusk, S. Narayanan, J. ONeal, M. Piarulli (p), S. Pieper, S. Wild, R. Wiringa
Indiana University
D. Berry, F. Fattoyev (p), C. Horowitz, Zidu Lin (g)
Iowa State University
R. Basili (g), M. Lockner (g), P. Maris, J. Vary
Lawrence Berkeley National Laboratory
E. Ng, C. Yang
Lawrence Livermore National Laboratory
M. Kruse (p), E. Ormand, G. Papadimitriou (p),
S. Quaglioni, N. Schunck
Los Alamos National Laboratory
J. Carlson, S. Gandolfi, E. Lawrence,
H. Nam, A. Roggero (p)
Michigan State University
Md. Afibuzzaman (g), H.M. Aktulga, S. Bogner,
M. Chen (g), K. Fossez (p), S. Guiliani (p),
H. Hergert, D. Lee, T. Li (g), J. Lietz (g),
D. Lonardoni (p), W. Nazarewicz, E. Olsen (p),
S. Wang (p), J. Yao (p)
Oak Ridge National Laboratory
G. Fann, G. Hagen, G. Jansen
Ohio State University
R. Caulfield (g), R. Furnstahl, J. Melendez (g),
A. Tropiano (g), Y. Zhang (p)
University of North Carolina at Chapel Hill
J. Engel, E. Ney (g)
University of Oregon
B. Norris, S. Pollard (g)
University of Tennessee
W Jiang (p), T. Morris (p), S. Novario (p), T. Papenbrock, Z. Sun (p)



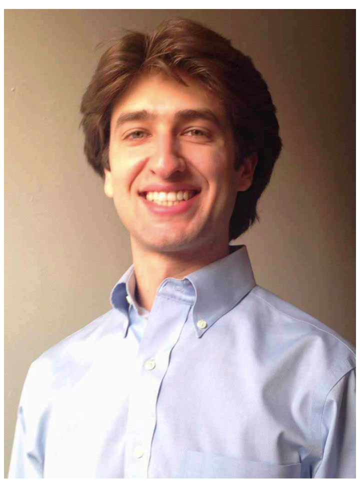
Good News: People



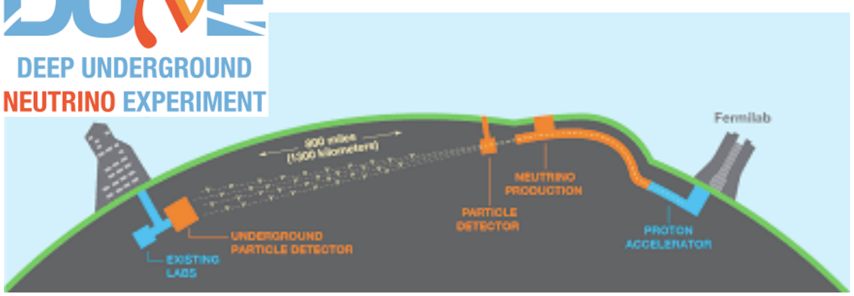
Maria Piarulli (ANL → **Washington University**)
Saori Pastore (LANL→ **Washington University**)
Rodrigo Navarro Perez (LLNL, Ohio→ **San Diego State U**)
All named to new faculty positions in 2018

NUCLEI researcher Pieter Maris (ISU)
elected to NUGEX

Matt Caplan (Indiana)
2018 APS dissertation
award in Nuclear Physics



Stefano Gandolfi (LANL)
Received DOE
Early Career Award in
Nuclear Physics (2018).



Physics of Nuclei & Matter

- *NN interactions & chiral effect field theory*
- *Light Nuclear Spectra*
- *Heavy neutron-rich nuclei (FRIB)*
- *Beta Decay*
- *Nuclear Structure and dynamics*

  at short-ranges (NN separation)
- *Electron Scattering (JLAB)*
- *Neutrino Scattering (DUNE)*
- *Neutron Stars (LIGO)*
- *New support from NNSA:*

  light ion reactions and fission

  strong connections to lattice QCD

  and nuclear astrophysics

ASCR-supported work in NUCLEI

SciDAC Institutes in Blue

- Algorithmic/Automatic Differentiation: S.H. Krishna Narayanan
- Eigenvalue Solvers/Linear Algebra: Esmond Ng, Chao Yang (FASTMath)
- High-Performance Computing: Hai Ah Nam
- Load Balancing/Memory Management: Ralph Butler, Rusty Lusk
- Multiresolution/Nonlinear Approximation: George Fann
- Numerical Optimization: Jared O'Neal, Stefan Wild (FASTMath)
- Performance Optimization: H. Metin Aktulga, Gustav Jansen
- Performance Optimization: Boyana Norris (RAPIDS), Sam Pollard
- Uncertainty Quantification: Earl Lawrence

RAPIDS Focus Areas

Application Engagement & Community Outreach

Tiger Teams, Liaisons, and Outreach

Data Understanding

- ★ Scalable methods
- Robust infrastructure
- ◆ Machine learning

Platform Readiness

- Roofline modeling
- ★ Hybrid programming
- Deep mem. hierarchy
- ★ Autotuning
- Correctness

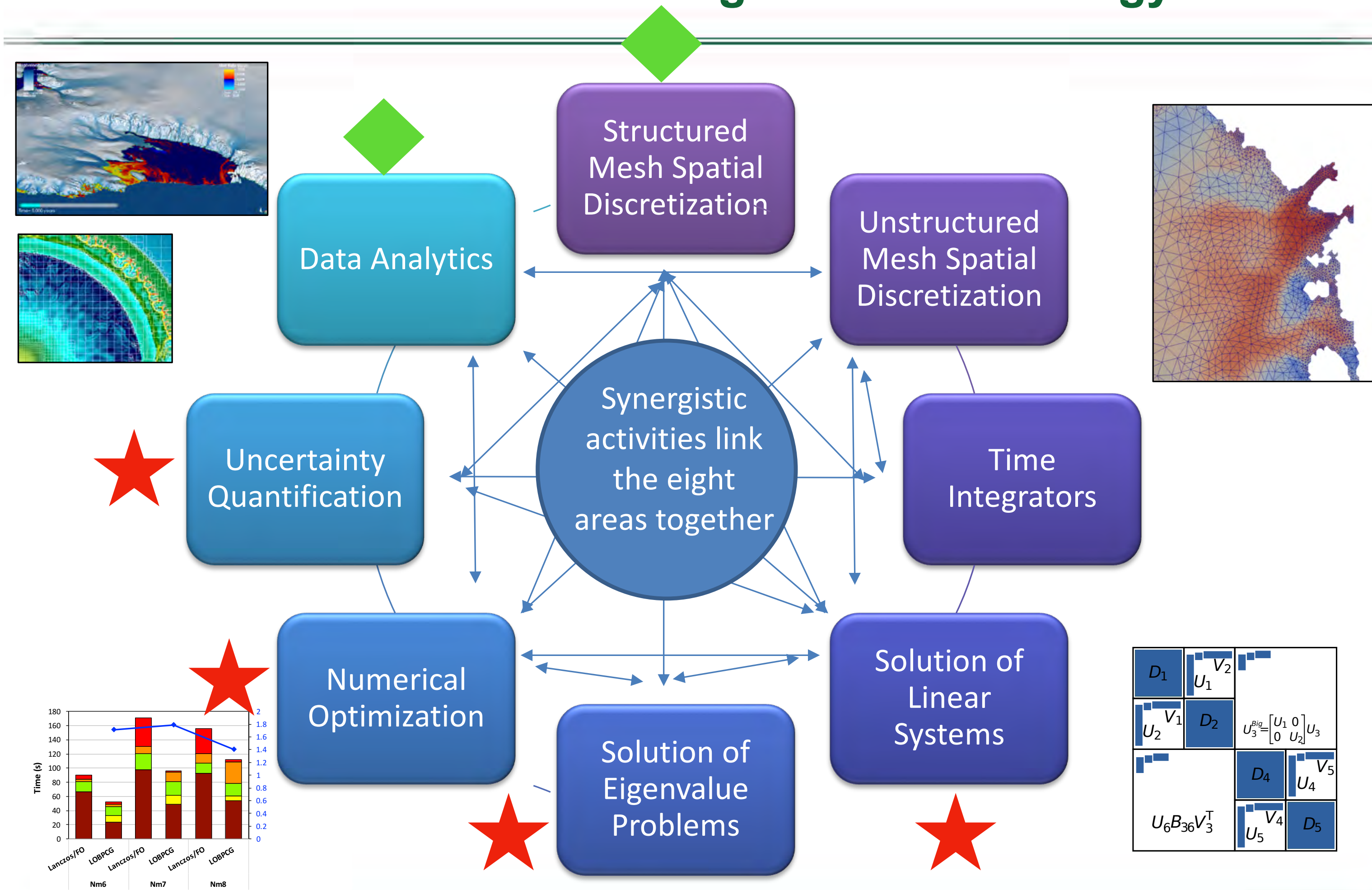
Scientific Data Management

- I/O libraries
- Coupling
- ◆ Knowledge management

★ **NUCLEI areas w/ ongoing collaborations**

◆ **Potential future NUCLEI collaborations**

FASTMath is focused on eight core technology areas



U.S. DEPARTMENT OF ENERGY | Office of Science

FASTMATH

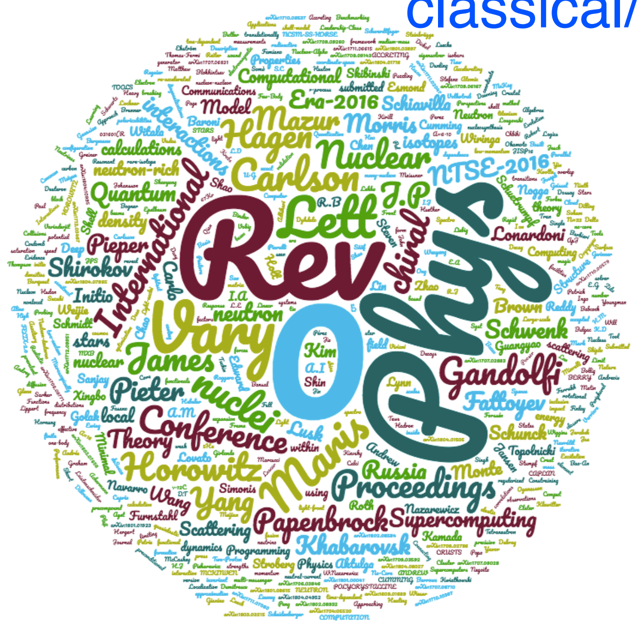
★ **NUCLEI areas w/ ongoing collaborations**

◆ **Potential future NUCLEI collaborations**

Papers / Talks in 2018

No-Core Shell Model
Coupled Cluster
AFMC
DFT
Leadership-class supercomputers
Deep Learning
Quantum Computing
Tin isotopes
Neutron Stars
Tetra-neutron
Localization
Chiral Dynamics
Weak Transitions
Electron and Neutrino Scattering

Papers/Talks: 2018
41 Papers and 35 talks
including 10 Physical Review Letters,
1 Nature Physics
6 joint physics and Math/CS
6 methods papers (including
classical/quantum computing



Annual Meeting: UTK May 29-June 31
~50 participants

Chiral Interactions and Light Nuclear Spectra

$$H = \sum_i \frac{-\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk}$$

Interactions depend upon spins (↑ or ↓), isospins (n or p)

and separation of the nucleons ($\mathbf{r}_{ij}$, $\mathbf{r}_{ik}$)

Use chiral formulations of NN and NNN interactions;

Either Delta-full or Delta-less

Fit NN u*sing Pounders to NN data,*

NNN to light nuclei

u*sing DMEM for memory management,*

No-core Shell Model (NCSM)

Diagonalizes in HO basis

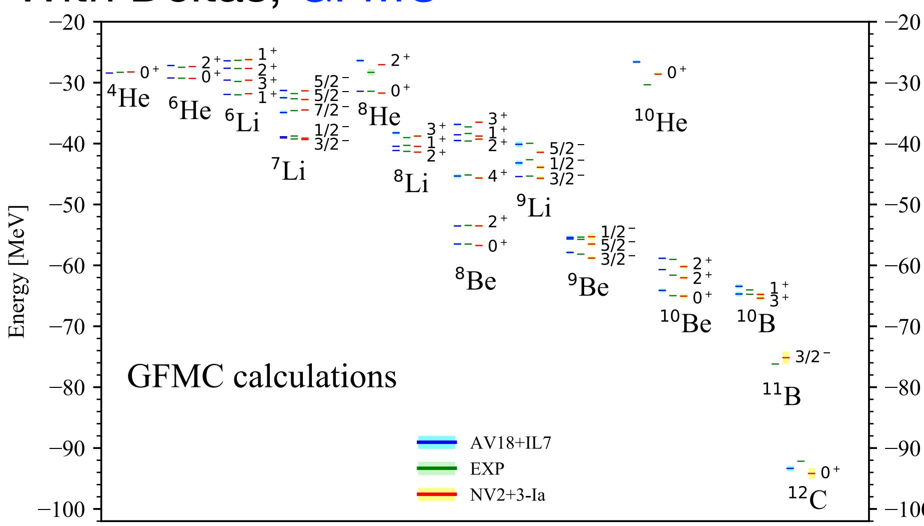
GFMC:

Uses MC for spatial d.o.f.

AFDMC:

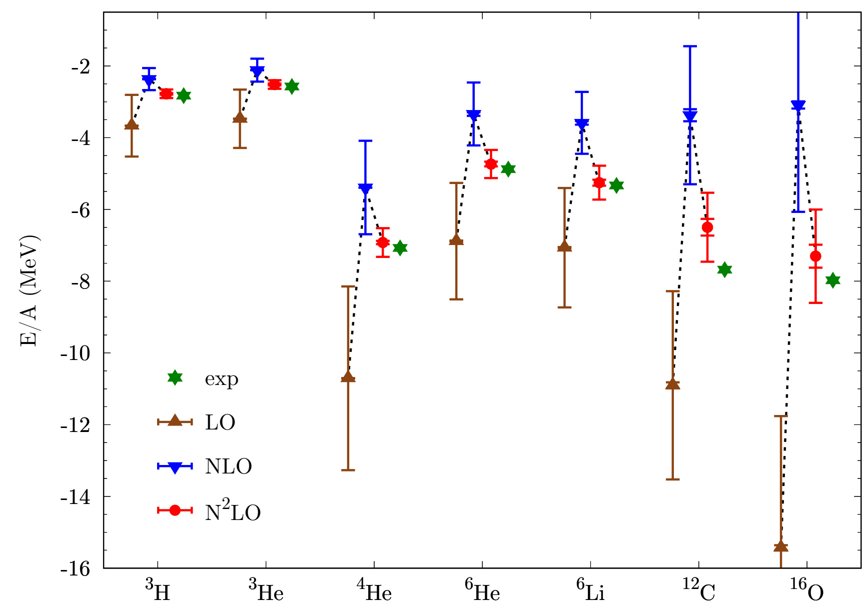
Uses MC for space, spin & isos

With Deltas, GFMC



Piarulli, et al, PRL 2018

w/o Deltas, AFDMC

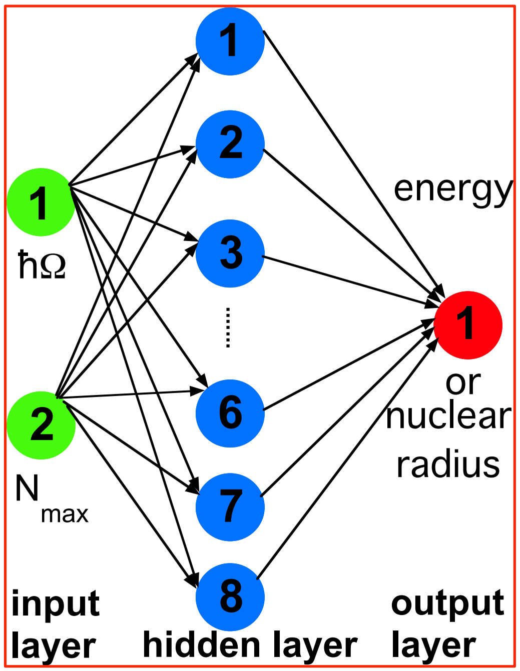


Lonardoni, et al., PRL 2018

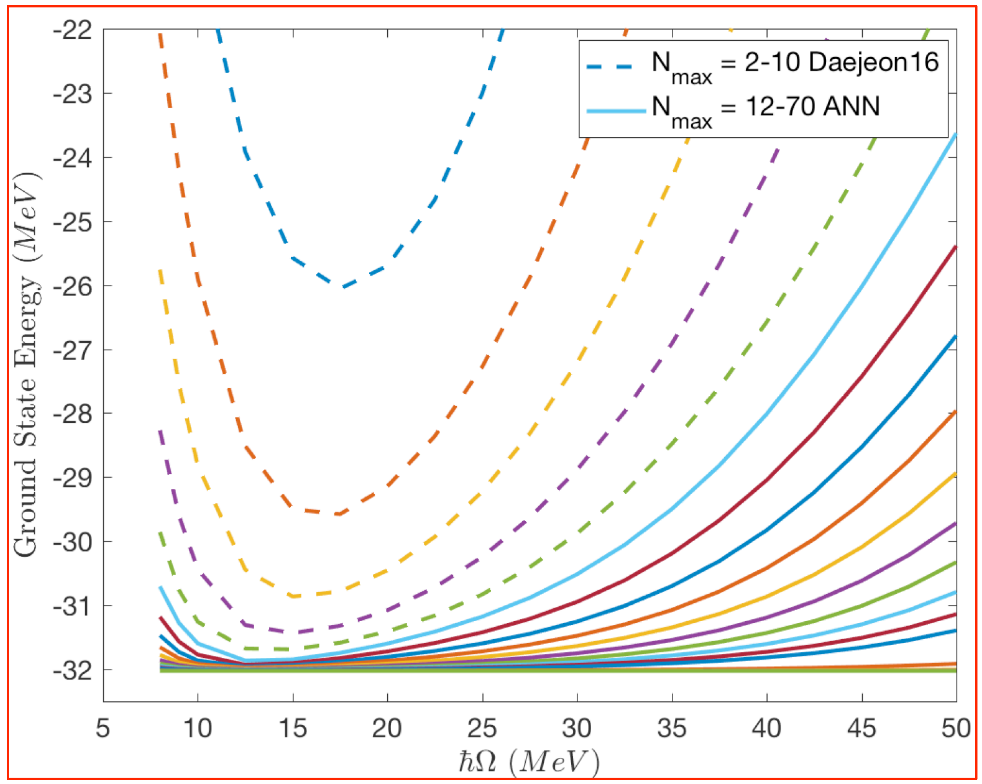
See Piarulli & Wild poster

Deep Learning for Nuclear Binding Energy and Radius

Developed an artificial neural network for NCSM
Demonstrated predictive power



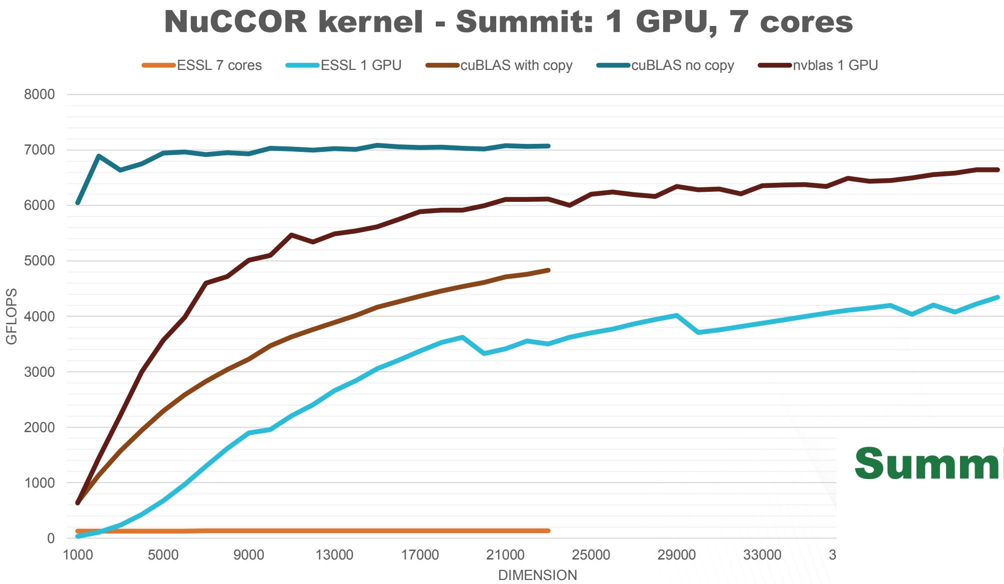
Architecture of neural network **(above)** used successfully to extrapolate the ^{6}**Li** ground stat energy from modest basis spaces (dashed line sequence) to extreme basis spaces (solid line sequence) achieving independence of basis parameters (flat line in **left figure**).



Best Paper Award: COMPUTATION TOOLS 2018, Barcelona
G.A. Negoita, et al. (w/ Esmond Ng and James Vary)

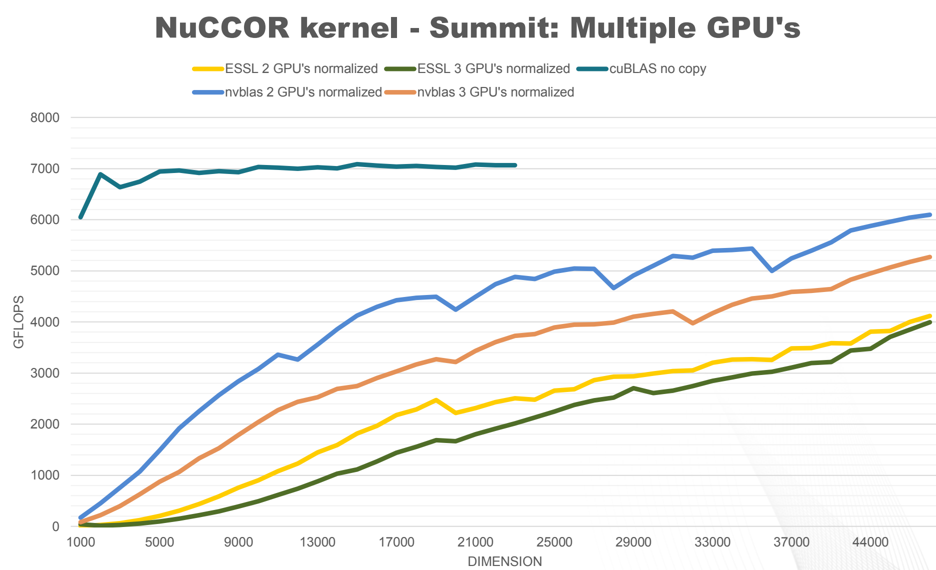
Coupled Cluster for heavier nuclei

Summit performance



"everything is a tensor contraction"

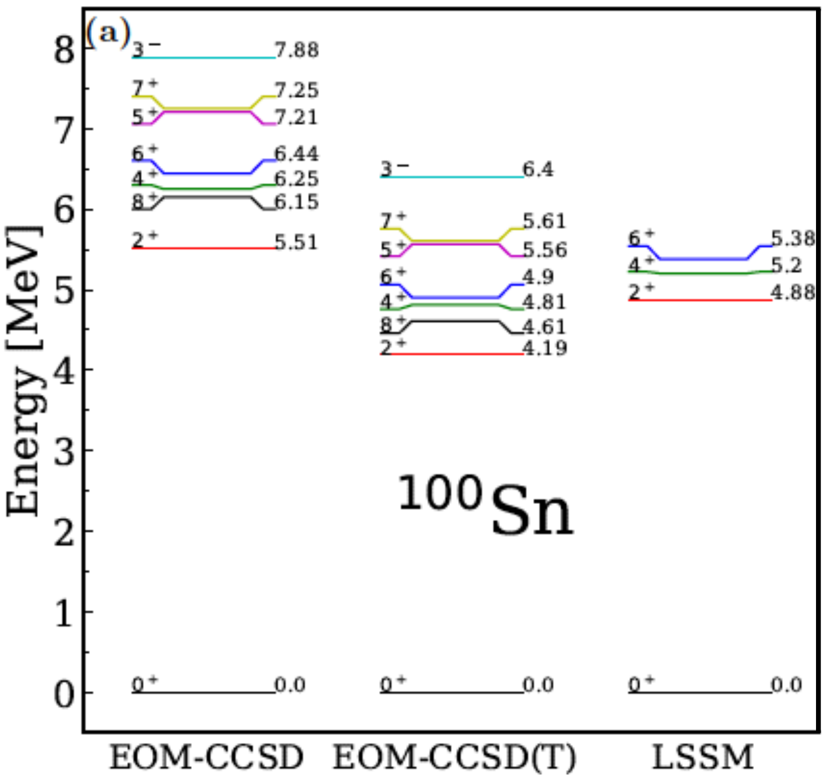
Summit performance



See Jansen and Hergert poster

Coupled Cluster and In-medium SRG for heavier nuclei

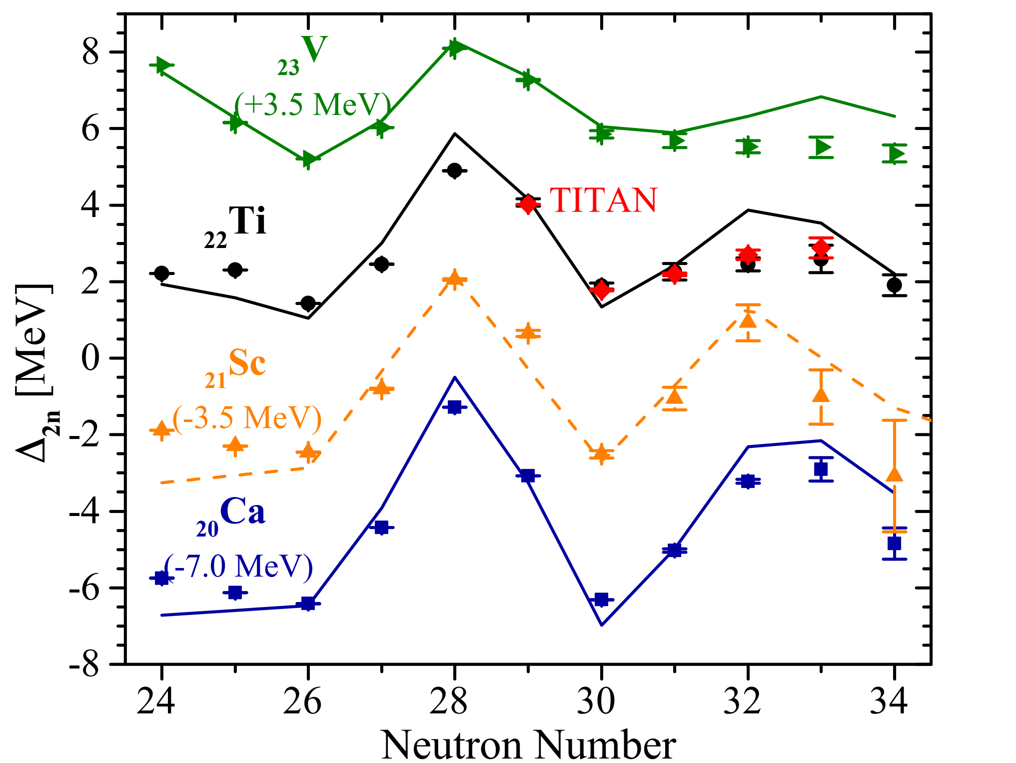
Low-lying states in Tin 100
(50 neutrons and 50 protons)



T. Morris et al, PRL 2018

Large gap to 2+ state indicates doubly magic
Lays the groundwork for more neutron-rich isotopes
Relevant to nucleosynthesis

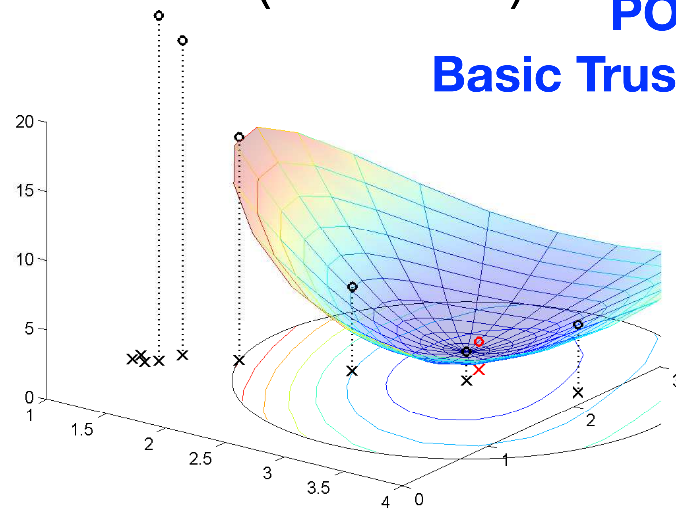
Shell closure for N=32 for
Different isotopes expos vs. theory (IMSRG)



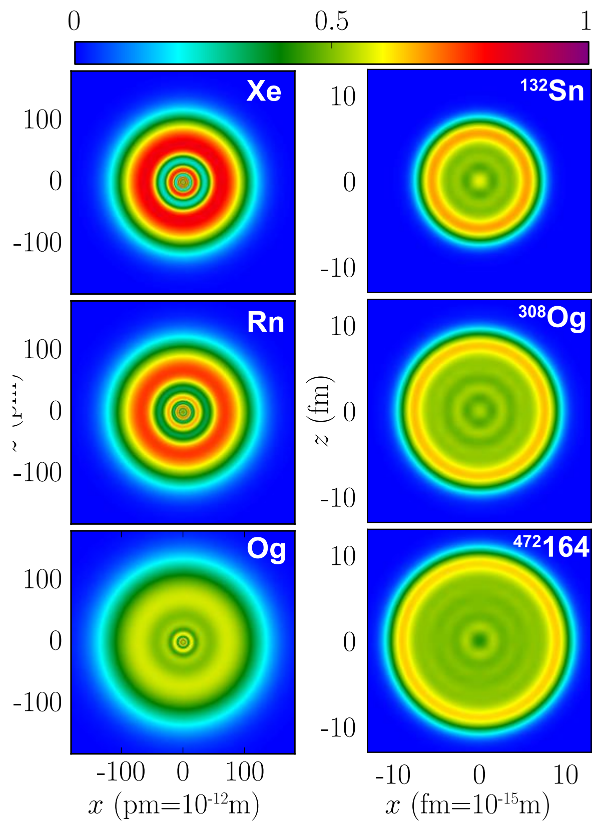
E. Leistenschneider, et al. PRL (2018)
Accurate treatment for open shell nuclei

See Jansen and Hergert poster

Density function theory for very heavy nuclei: Oganesson (Z=118)



Left: electronic localization for noble gases
Right: neutron localization in heavy nuclei



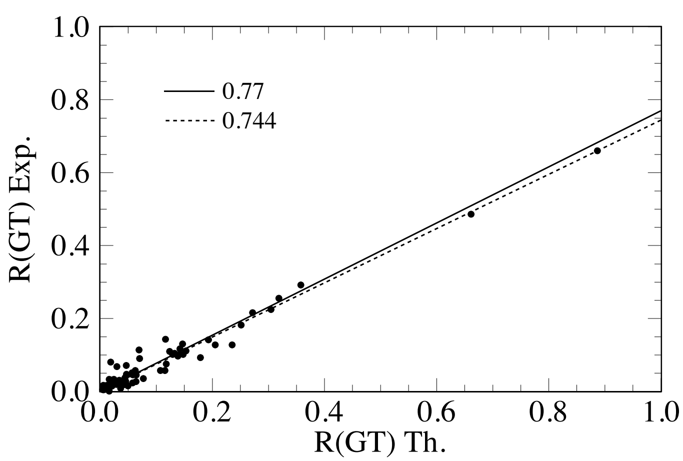
Using density functional theory
and advanced computational techniques,
We study the transition from
strong shell structure (localization)
to uniform matter.
Shell structure transitions to uniform
matter in large nuclei

P. Jerabek, et al,
PRL 2018

Weak Interactions in Nuclei
From beta decay to quasi elastic scattering

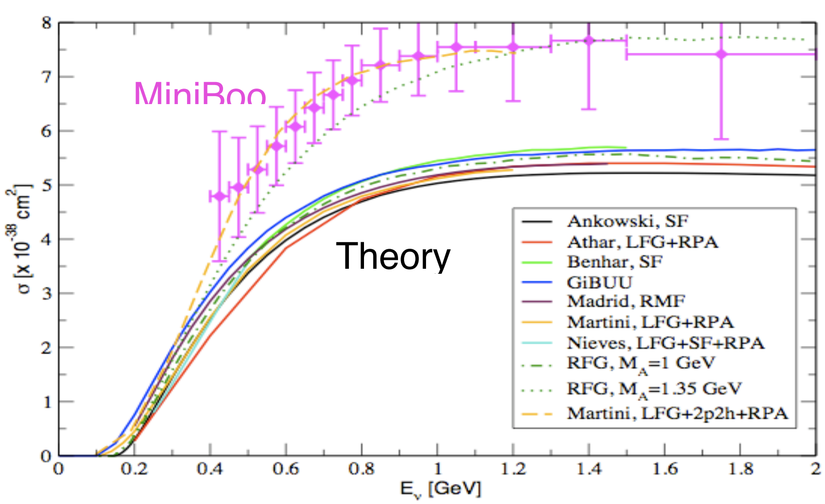
Historically significant issues:
Over predicting beta decay
Under predicting quasi elastic scattering

Beta Decay



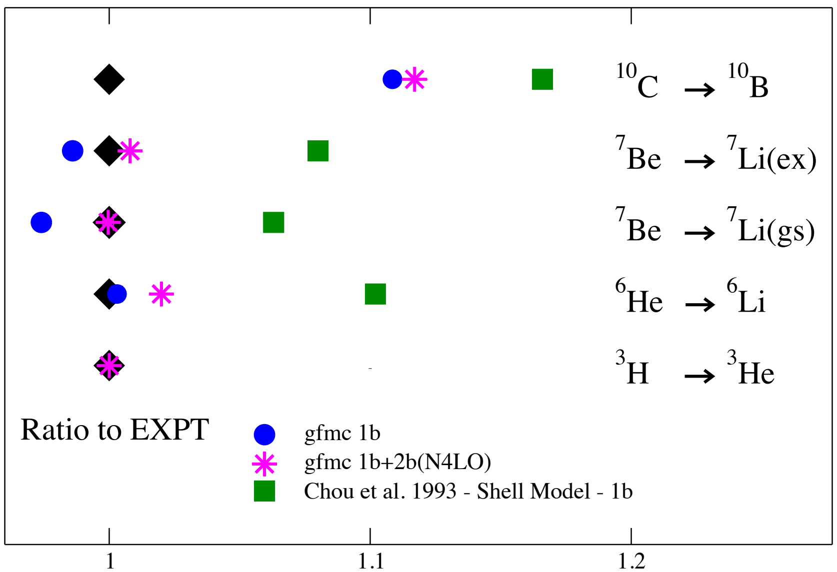
Empirically need to decrease rate (matrix element squared) by ~50%

Quasielastic Scattering



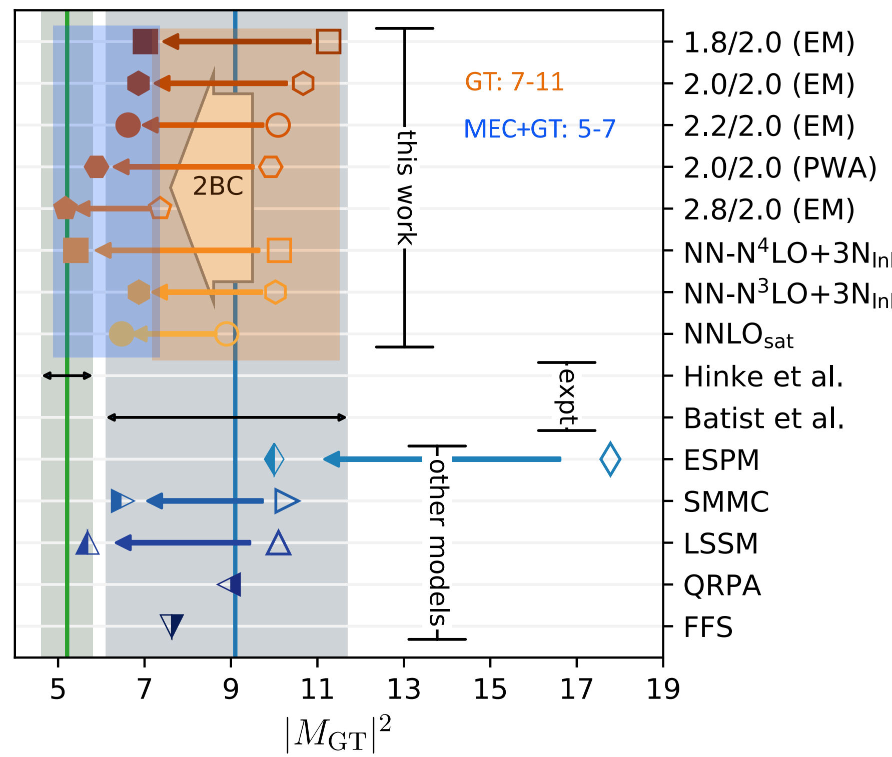
Empirically need to increase rate (matrix element squared) by ~30-40%

Beta decay in light and medium-mass nuclei



Pastore, et al PRC (2018)

Super allowed Gamow-Teller decay of $^{10(}$

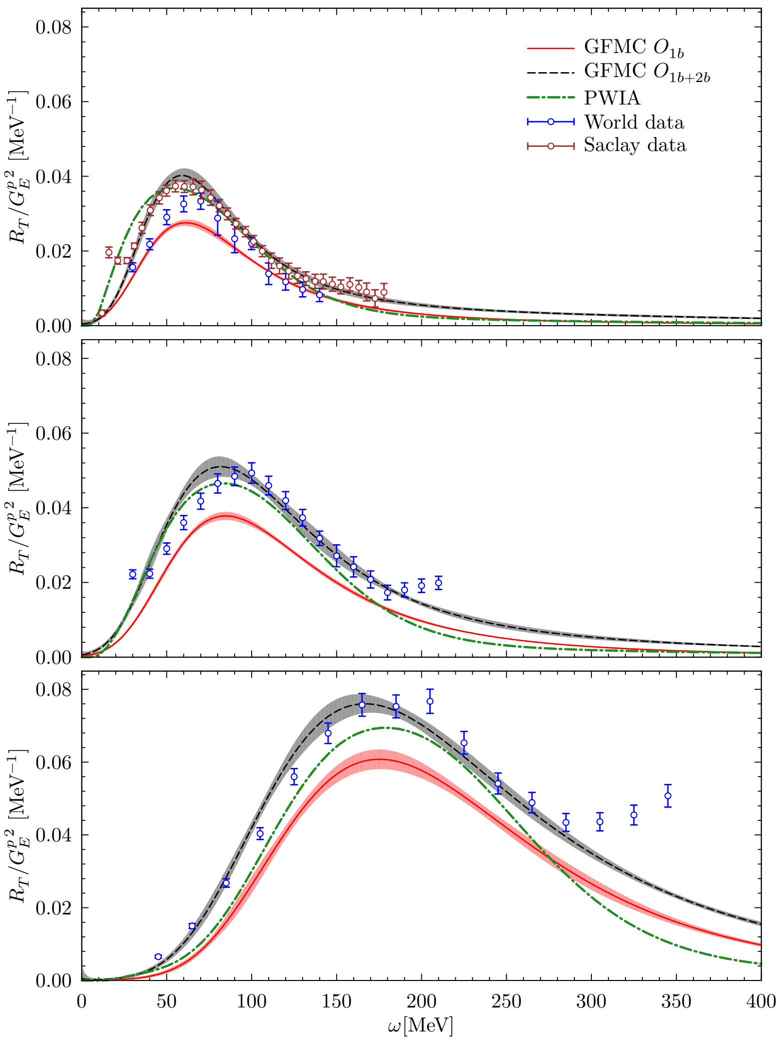


Hagen, et al, CC

NN correlations and currents are critical - also for quasi elastic scattering

Short-range structure of Nuclei: electron and neutrino scattering

e^- scattering

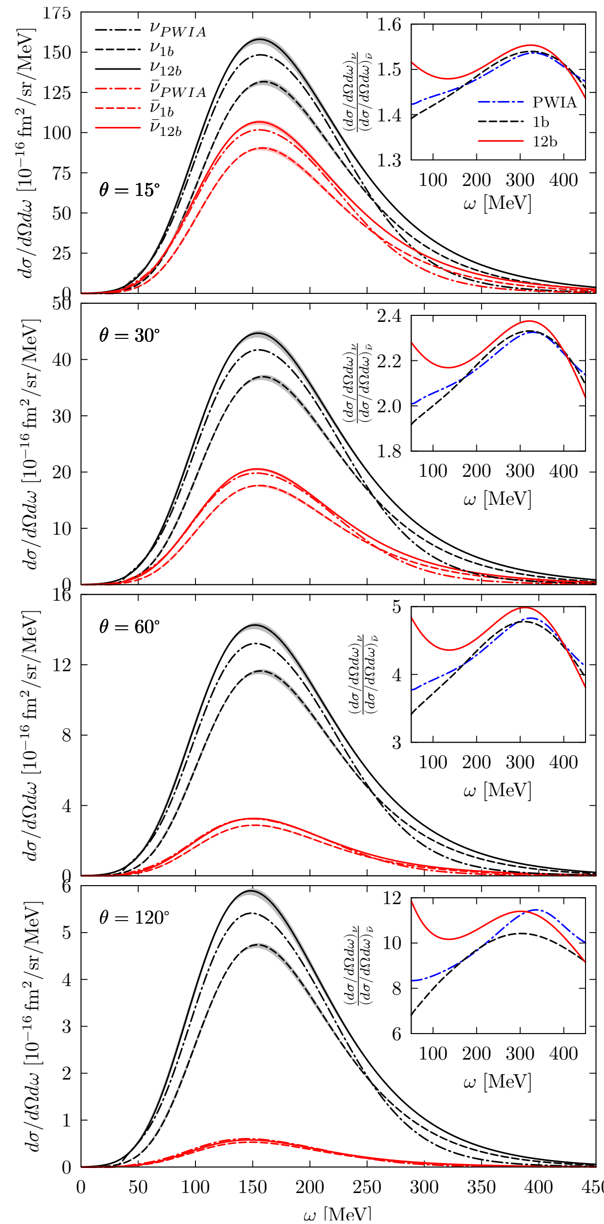


Lovato, et al, PRL (2016)

ν scattering

anti-ν

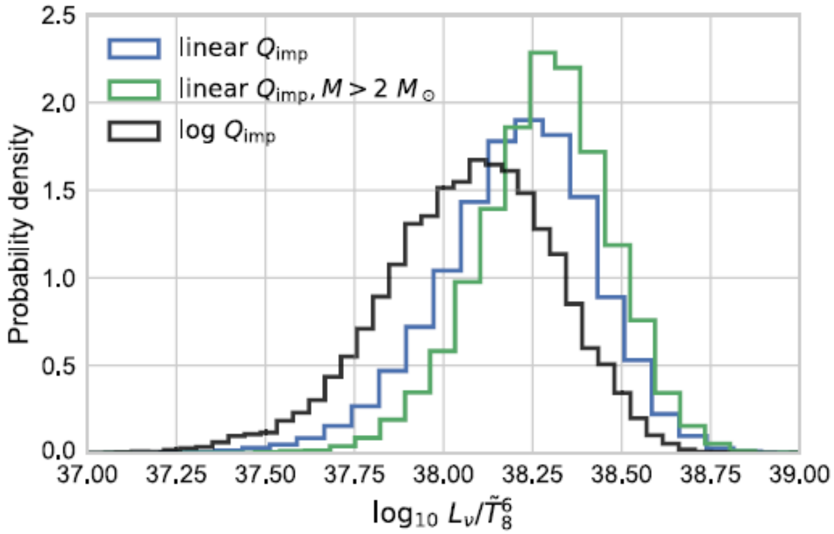
ν



Lovato, et al, PRC (2018)

Short-range structure of Neutron Matter: Neutron star cooling and gravitational Waves

Observed cooling from MXB 1659-29 consistent with 'fast' cooling: consistent with direct Urca in the core

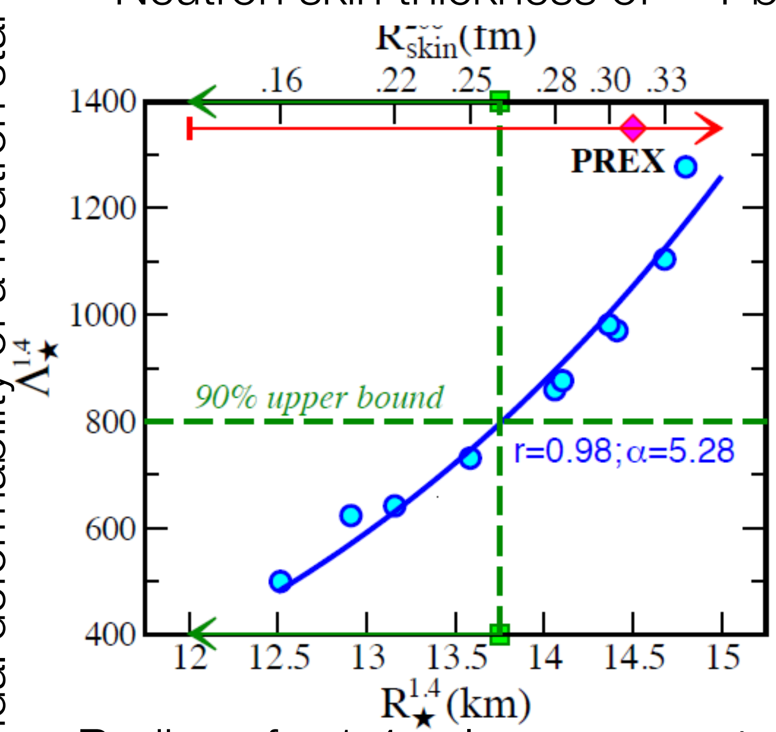


Edward F. Brown, C. J. Horowitz, et al., Phys. Rev. Lett. 120, 172701 (2018).

Constraints on radius and tidal deformability of a neutron star

Neutron skin thickness of ^{208}Pb

Tidal deformability of a neutron star



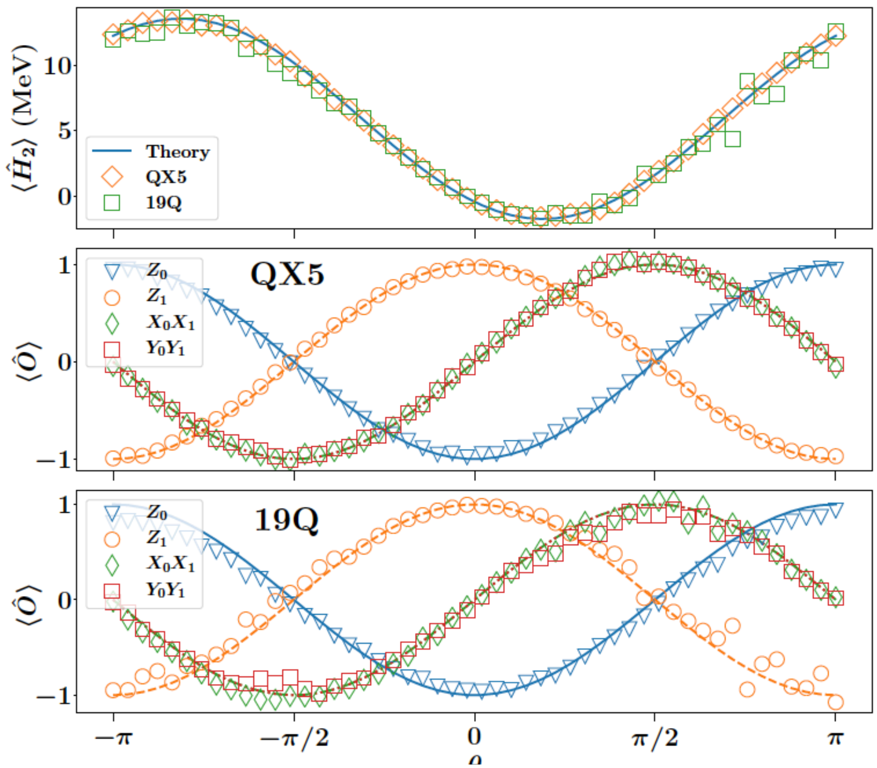
Radius of a 1.4 solar mass neutron star

F. J Fattoyev, J. Piekarewicz,

and C. J. Horowitz, Phys. Rev. Lett. 120, 172702 (2018).

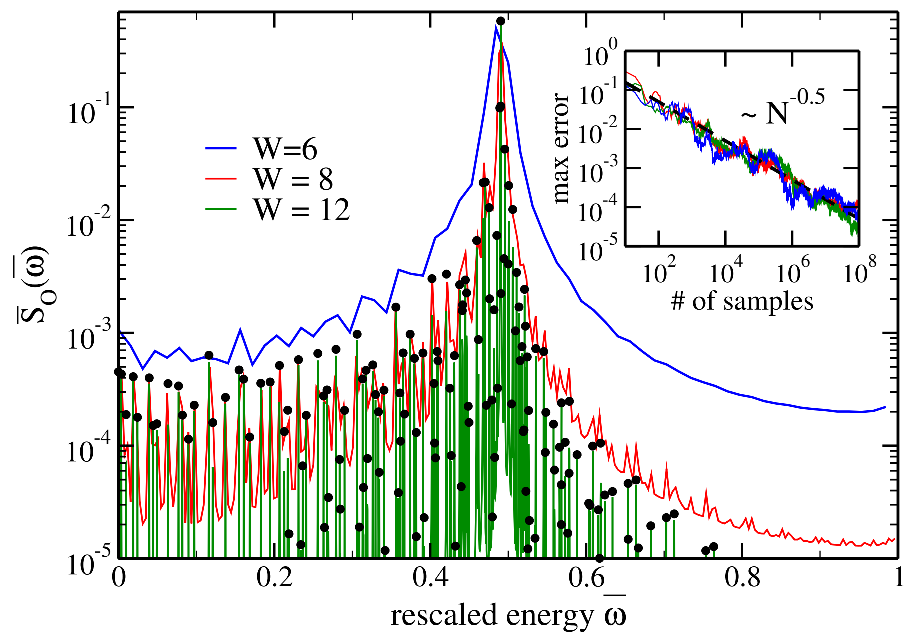
Quantum Computing in Nuclear Physics

Computing the Deuteron
On actual quantum computers



E. F. Dumitrescu et al., Phys. Rev. Lett.
Phys. Rev. Lett. 120, 210501 (2018).

Methods for computing
Quantum dynamics
(electron and neutrino scattering)



Roggero, et al, arXiv 1804.01505

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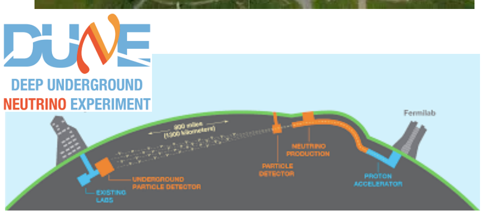

Conclusions

Exciting Era for Nuclear Physics:

Many New Capabilities for Computing Nuclear Structure and Dynamics:

Many new experiments and observations

- ***Ab-initio calculations of nuclear structure and decay***
- ***Neutron-rich nuclei and r-process nucleosynthesis***
- ***Weak interactions at low-energy (beta decay) and***
- ***high-energy (electron and neutrino scattering)***
- ***Neutrinos in astrophysics***
- ***Gravitational waves and neutron star structure***

Outstanding early career scientists
to take advantage
of these opportunities

Funded by DOE/SC (NP and ASCR) and NNSA: Thank you!