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

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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
Physics of Nuclei & Matter

- NN interactions & chiral effect field theory
- Light Nuclear Spectra
- Heavy neutron-rich nuclei (FRIIB)
- 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

Structured Mesh Spatial Discretization
Unstructured Mesh Spatial Discretization
Time Integrators
Solution of Linear Systems
Solution of Eigenvalue Problems
Synergistic activities link the eight areas together
Numerical Optimization
Uncertainty Quantification
Data Analytics

**NUCLEI areas w/ ongoing collaborations**

**Potential future NUCLEI collaborations**
Papers / Talks in 2018

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)

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

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 (\(\uparrow\) or \(\downarrow\)), isospins (n or p) and separation of the nucleons (\(\mathbf{r}_i, \mathbf{r}_k\))

Use chiral formulations of NN and NNN interactions;

*Either Delta-full or Delta-less*

Fit NN using Pounders to NN data,

NNN to light nuclei using DMEM for memory management,

w/o Deltas, AFDMC

No-core Shell Model (NCSM)
Diagonalizes in HO basis

GFMC:
Uses MC for spatial d.o.f.

AFDMC:
Uses MC for space, spin & isospin

With Deltas, GFMC

GFMC calculations

Piarulli, 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 state 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

NuCCOR kernel - Summit: 1 GPU, 7 cores

NuCCOR kernel - Summit: Multiple GPU's

“everything is a tensor contraction”

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)

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%

**FIG. 1.** Comparison of the experimental matrix elements $R(\text{GT})$ with the theoretical calculation based on the “free-nucleon” Gamow-Teller operator. Each transition is indicated by a point in the $x$-$y$ plane, with the theoretical value given by the $x$ coordinate of the point and the experimental value by the $y$ coordinate.

**FIG. 2.** Comparison of the experimental values of the sums $T(\text{GT})$ with the corresponding theoretical value based on the “free-nucleon” Gamow-Teller operator. Each sum is indicated by a point in the $x$-$y$ plane, with the theoretical value given by the $x$ coordinate of the point and the experimental value by the $y$ coordinate.

**TABLE I.** Experimental and theoretical $M(\text{GT})$ matrix elements. The experimental data have been taken from [19].

$\beta^+ + I^\prime$ are the branching ratios. All other quantities explained in the text.
Beta decay in light and medium-mass nuclei

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

NN correlations and currents are critical - also for quasi elastic scattering
Short-range structure of Nuclei: electron and neutrino scattering


The short-range structure of neutron matter: neutron star cooling and gravitational waves.

**Impact**
- We found that the neutron star MXB 1659-29 is the first with a firmly detected thermal component in its x-ray spectrum that needs a fast neutrino-cooling process.
- In particular, we found that it has a core luminosity that substantially exceeds that of a modified Urca reaction and is consistent with the direct Urca reaction operating in a small fraction of the core.
- Future measurements of the temperature variation of the neutron star core during quiescence should place an upper limit on the core specific heat and serve as a check of the fraction of the neutron star core in which nucleons are unpaired.

**Accomplishments**
- Highlighted as Editors’ Suggestion.
- Featured in Physics (phys.aps.org) as Viewpoint: A rapidly cooling neutron star.
- Featured by Science News, Interesting Engineering, and many international news outlets.

**Objectives**
- Observations of the thermal relaxation of the neutron star crust in the transient system MXB 1659—29 following 2.5 years of accretion allow us to measure the energy deposited into the core during accretion.
- This energy is then re-radiated as neutrinos in about 20 years which allows us to infer the neutron star core temperature.
- MXB 1659-29 had previously been in an outburst and went into quiescence. If the outburst-quiescent cycles observed to date represent the long-time average accretion behavior of the source, then the core neutrino luminosity can be obtained.

The posterior distribution of the neutrino cooling prefactor from the MCMC fits to the MXB 1659-29 cooling curve is consistent with the fast neutrino cooling scenario such as the direct Urca reaction.

**Observed cooling from MXB 1659-29**
- Consistent with ‘fast’ cooling: consistent with direct Urca in the core.

**Constraints on radius and tidal deformability of a neutron star**
- Neutron skin thickness of $^{208}$Pb

**Radius of a 1.4 solar mass neutron star**

**Tidal deformability of a neutron star**


**Constraints on radius and tidal deformability of a neutron star**

Quantum Computing in Nuclear Physics

Computing the Deuteron
On actual quantum computers

Methods for computing
Quantum dynamics
(electron and neutrino scattering)


Roggero, et al, arXiv 1804.01505
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!