Report on Computational Nuclear Physics and AI/ML Workshop

J. Carlson (LANL) in collaboration with A. Lovato (ANL)

- Workshop Outline (Agenda, Participants, etc.)
- Computational Accomplishments during past ~5 years
- Outlook for the next 5-10 years
- Workshop resolutions

Computational Nuclear Physics and AI/ML Workshop

- Organized by:
  - Alessandro Lovato (ANL)
  - Joe Carlson (LANL)
  - Phiala Shanahan (MIT)
  - Bronson Messer (ORNL)
  - Witold Nazarewicz (FRIB/MSU)
  - Amber Boehnlein (JLab)
  - Peter Petreczky (BNL)
  - Robert Edwards (JLab)
  - David Dean (JLab)
- 6-7 September 2022 at SURA in Washington, DC
- 60 registered participants (40 in person, 20 on line), including DOE
- https://indico.jlab.org/event/581/
  - All talks archived
  - Short white paper being prepared for the LRP

Computational Nuclear Physics and AI/ML Workshop

6-7 September, 2022 / SURA headquarters

Organized by:
Alessandro Lovato – Joe Carlson (LANL), Phiala Shanahan (MIT), Bronson Messer (ORNL)
Witold Nazarewicz (FRIB/MSU), Amber Boehnlein (JLab), Peter Petreczky (BNL)
Robert Edwards (JLab), David Dean (JLab)

Admin support: Jae Cho jcho@jlab.org Tea Jojua tjojua@sura.org Sherry Thomas sthomas@jlab.org

Schedule
Registration, schedule, and other information can be found at: https://indico.jlab.org/event/581/

Tuesday, 6 September
1:00 – 1:05 Welcome, David Dean and Sean Hearne
1:05 – 1:20 DOE remarks, Tim Hallman
1:20 – 2:00 QCD, William Detmold (JLab) and Swagato Mukherjee (BNL)
2:00 – 2:40 Quantum many-body problems, Thomas Papenbrock (UT/ORNL)
2:40 – 3:00 BREAK
3:00 – 3:40 Fundamental Symmetries,Emanuele Mereghetti (LANL)
3:40 – 4:20 Astrophysics, George Fuller (UCSD)
4:20 – 5:00 AI/ML, Amber Boehnlein (JLab)
5:00 – 5:40 Preliminary list of recommendations discussion (Peter Petreczky, lead)
5:40 – 7:30 Reception

Wednesday, 7 September
7:45 – 8:30 Continental Breakfast
8:30 – 10:00 Breakout Sessions
1. QCD (Phiala Shanahan, lead)
2. Nuclear Structure and fundamental symmetries (Alessandro Lovato, lead)
3. Astrophysics (Bronson Messer, lead)

10:00 – 10:30 Break
10:30 – 12:00 Breakout reports
12:00 – 1:00 Lunch
1:00 – 2:30 Recommendations discussion and next steps

Jefferson Lab Thomas Jefferson National Accelerator Facility SURA

Major Topical Areas Discussed During Workshop

- Lattice QCD
- Nuclear Structure and Reactions
- Nuclear Astrophysics
- Artificial Intelligence and Machine Learning
  - Some discussion of Quantum Computing

Computational-related items in NP theory effort

- SciDAC-5 projects

    Femto-scale Imaging of Nuclei using Exascale Platforms
    Nuclear Computational Low Energy Initiative (NUCLEI)
    Fundamental nuclear physics at the exascale and beyond (LQCD)

    collaborations with CS and applied math have led to breakthroughs

- JLAB LQCD cluster

- Theory Topical Collaborations (to be decided)

- NSF Centers/Collaborations (N3AS, NP3M, BAND, …)

- Computational Access (NERSC, INCITE,…, local facilities)

Lattice QCD

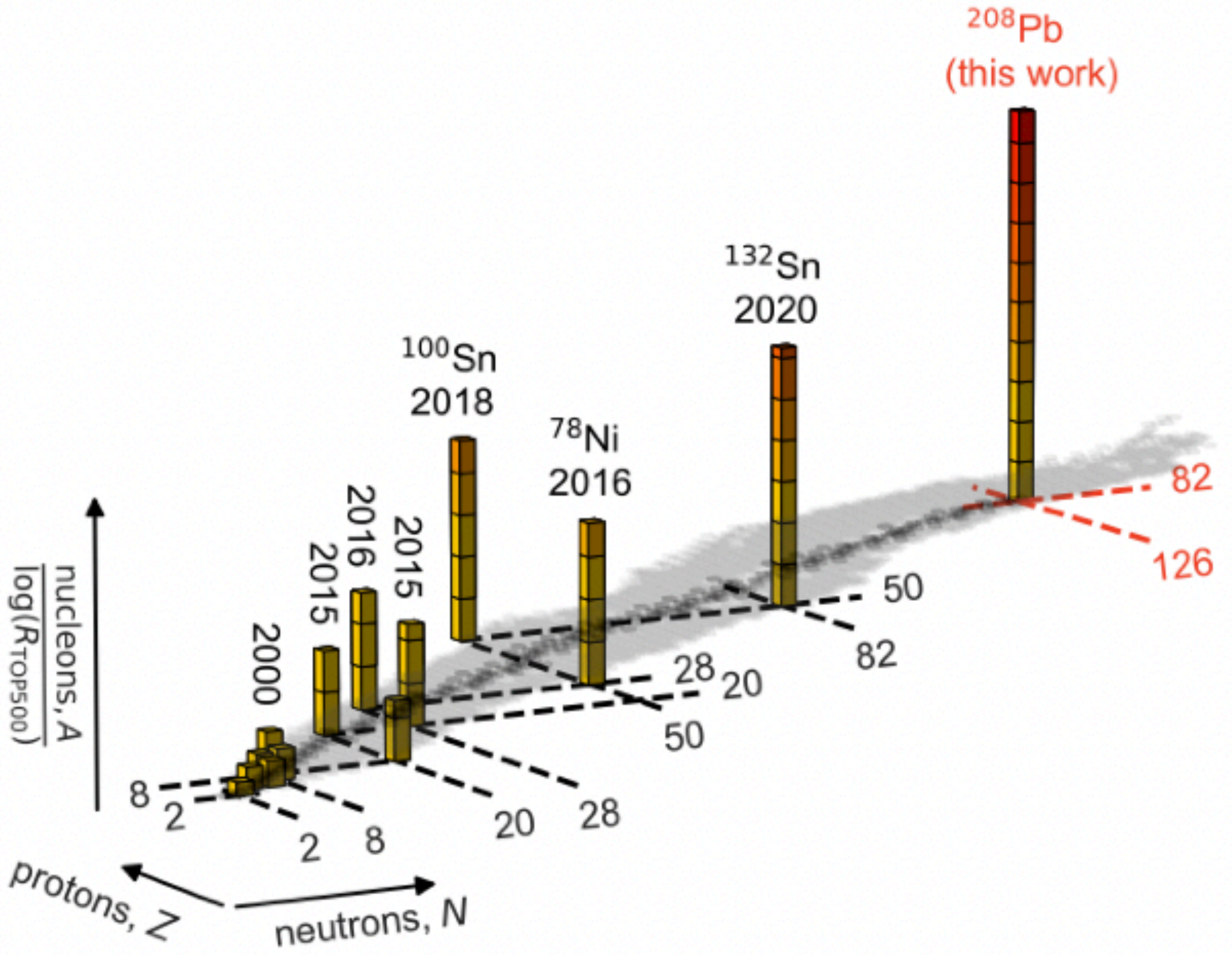
- Great progress since 2015:
  - Hadronic Spectra
  - Parton Distribution Functions from equal-time lattice correlators in the large momentum limit
  - Single-Nucleon Matrix Elements
    - Nucleon axial charge g_A and nucleon EW form factors
  - Two-Nucleon Matrix Elements
    - NN low-energy scattering and HN scattering
  - …

Nuclear Structure and Reactions

- Tremendous progress in last 5-10 years:
  - Larger Nuclei with ab-initio methods (up to Pb)
  - EW transitions at low momentum and energies
  - QE and beyond electron and neutrino scattering from nuclei
  - Stronger, more systematic connections to nuclear astrophysics:
    supernovae and neutron stars (dense matter EOS, neutrinos,…)
  - Stronger, more systematic connections to fundamental symmetries
    Beta decay, double beta decay, nuclear EDM, neutrino-nucleus, …
  - Greatly enhanced efforts on error estimation, AI/ML, …
  - Quantified DFT (fast emulators for UQ)
  - Towards real-time propagation

Nuclear Stucture/Reaction Highlights

Larger Nuclei with Ab-Initio Approaches (CC, IMSRG)



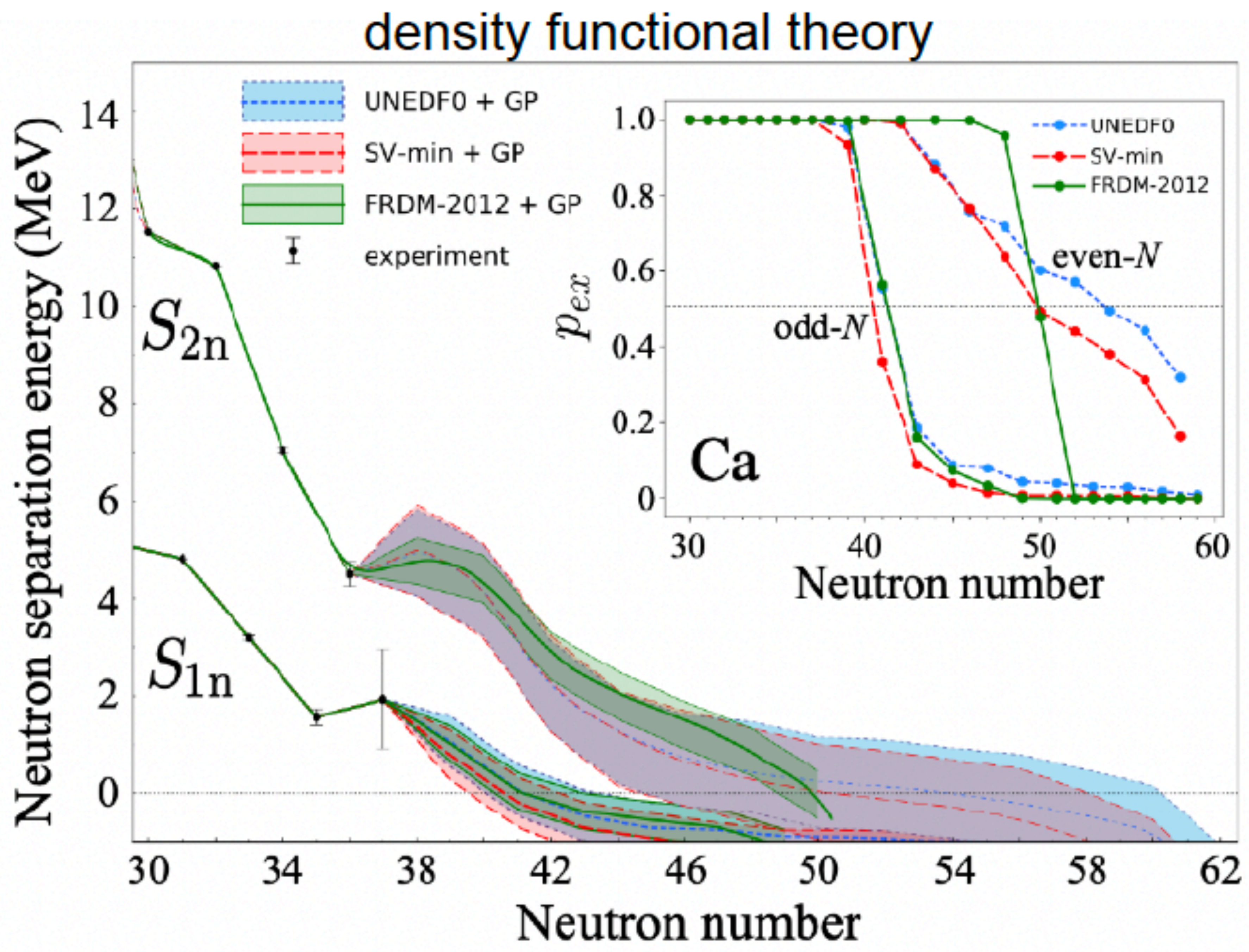
FRIB

Argonne NATIONAL LABORATORY

ATLAS

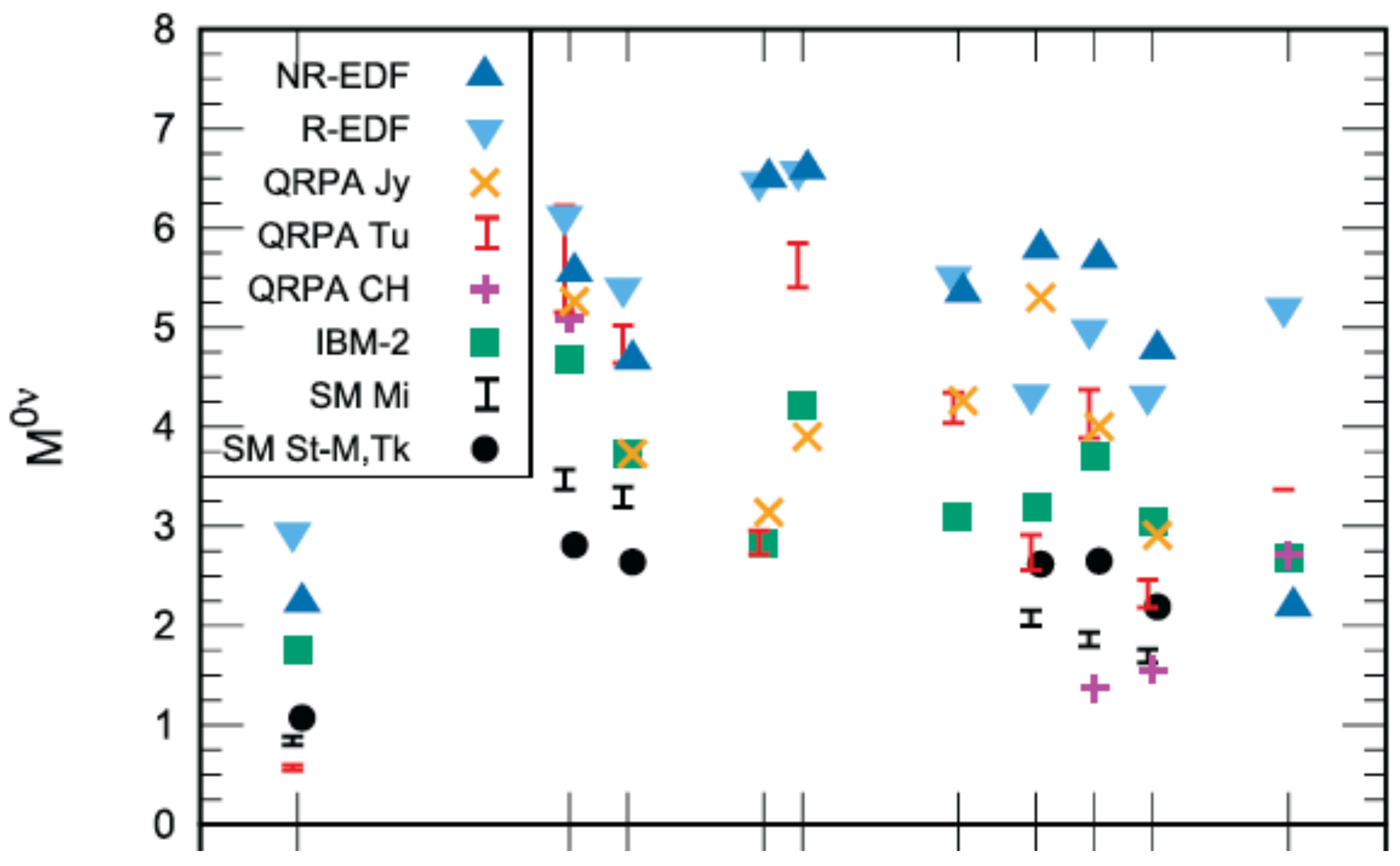
ARUNA

Neutron-rich nuclei



Nuclear Structure and Reactions connections to FS, Astro

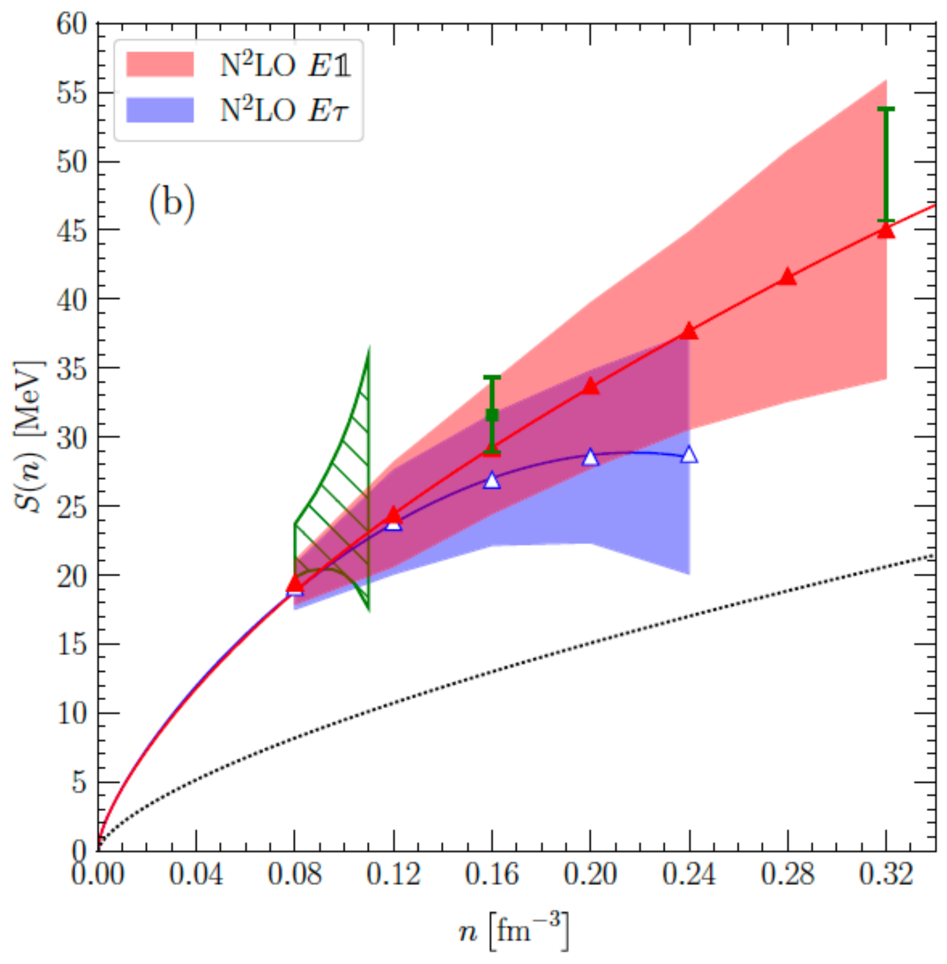
Neutrinoless Double Beta Decay



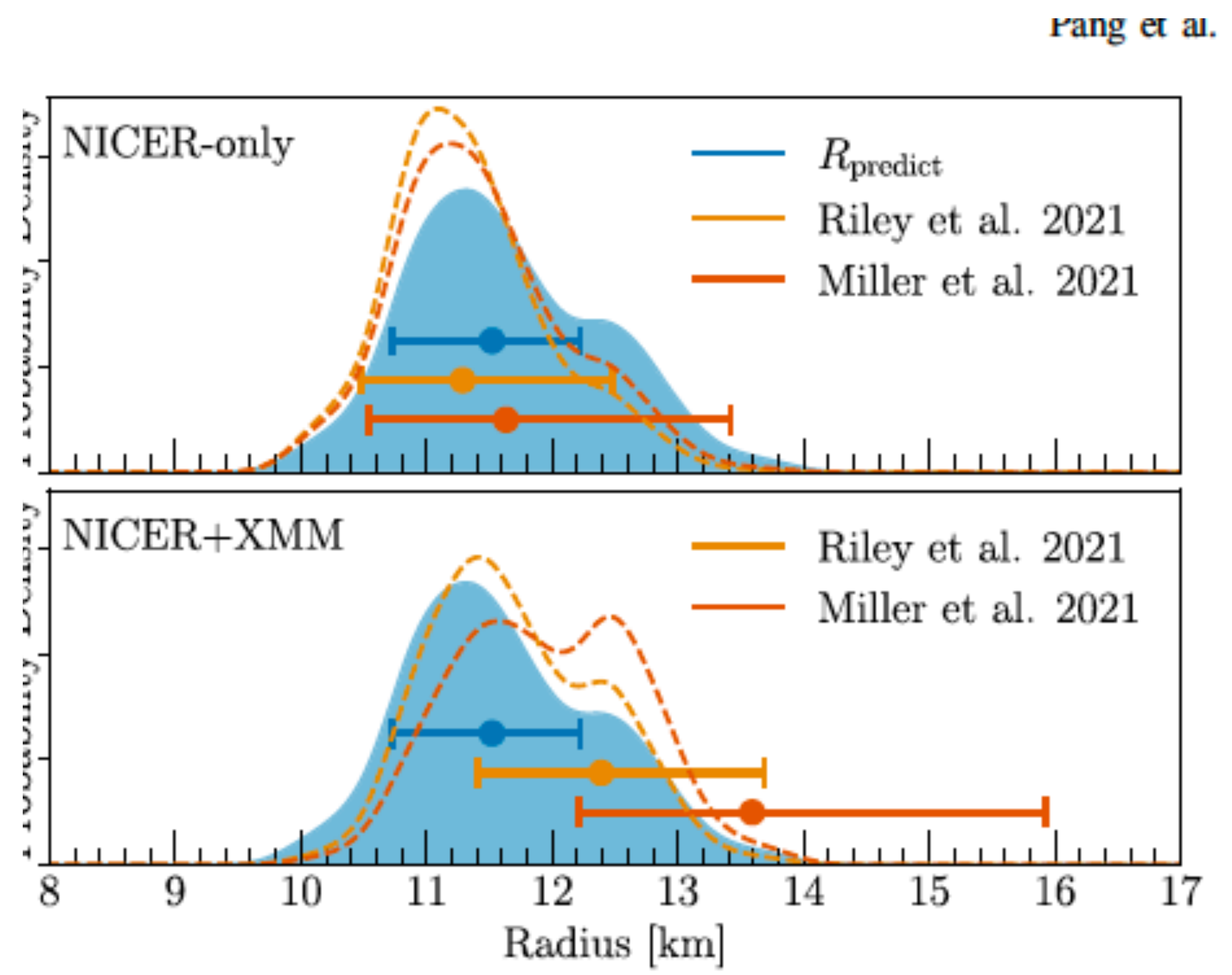
Also beta decay, nuclear EDM, Neutrino-nucleus scattering, …

Neutron Stars

Nuclear Theory + GW (LIGO) + EM (NICER/XMM)

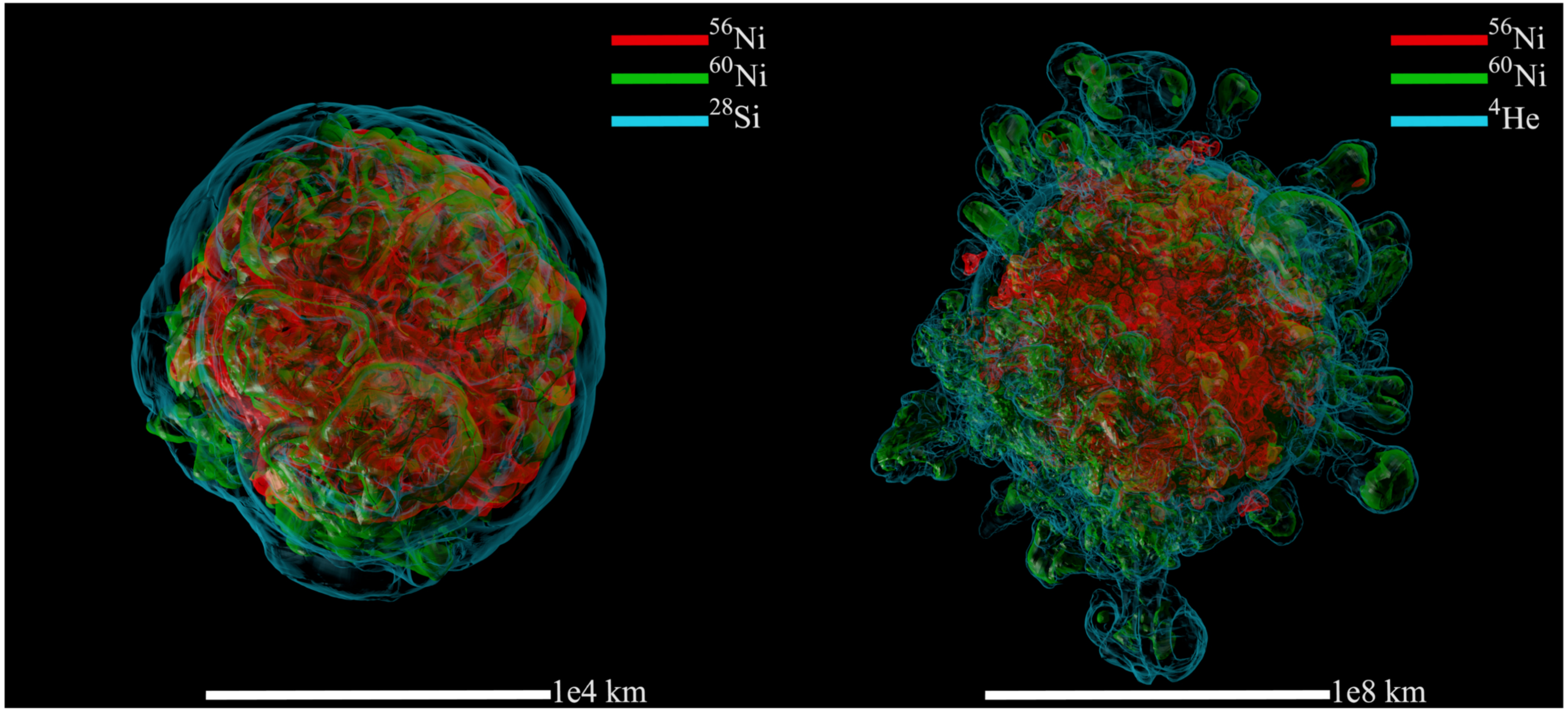


NM EOS



Neutron Star Mass-Radius

Highlights from Nuclear Astrophysics: Nucleosynthesis and SN



SN Nucleosynthesis, courtesy of Bronson Messer

Increased Efforts in Artificial Intelligence and Machine Learning

- New efforts in:
  - UQ and Model Mixing
  - Many-body approaches (tensor networks, etc.)
  - Bayesian methods for emulation

Important challenges for the next 5-10 years

- Large Neutron-Rich Nuclei: masses and decays
  - Confronting FRIB, ATLAS data, …
  - Input to important new experiments
- AI/ML approaches to emulation, UQ, and many-body theory
- Connections to Astro and Fundamental Symmetries
  - Double Beta Decay and beta decay for BSM, nuclear EDM
  - Neutron Skins and Neutron Star Matter
  - Improved EOS (higher densities, finite T, …)
  - Neutrinos in astrophysical environments

- Nuclear Dynamics: Electron and Neutrino Inclusive Scattering
  - Reactions at low energies (resonances, …)
  - Reactions at higher energy - ~quasi-elastic energy regime in ab initio,
    - Coexistence phenomenon and Large amplitude collective motion in fission and fusion

Resolution from the Computational Nuclear Physics meeting

High-performance computing is essential to advance nuclear physics on the experimental and theory frontiers. Increased investments in computational nuclear physics will facilitate discoveries and capitalize on previous progress. Thus, we recommend a targeted program to ensure the utilization of ever-evolving HPC hardware via software and algorithmic development, which includes taking advantage of novel capabilities offered by AI/ML.

The key elements of this program are to:

1) Strengthen and expand programs and partnerships to support immediate needs in HPC and AI/ML, and also to target development of emerging technologies, such as quantum computing, and other opportunities.

2) Take full advantage of exciting possibilities offered by new hardware and software and AI/ML within the nuclear physics community through educational and training activities.

3) Establish programs to support cutting-edge developments of a multi-disciplinary workforce and cross-disciplinary collaborations in high-performance computing and AI/ML.

4) Expand access to computational hardware through dedicated and high-performance computing resources.

Adopted (with modifications) by the QCD Town Hall meeting We ask for a similar adaptation from this Town Hall meeting