Nuclear Structure (and Dynamics) Thrust

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NTNP Goals and Objectives

- **BETA-3**
  - Y1: Develop software and file formats to deploy EFT transition operators in ab initio calculations. [MSU, ND, ORNL/UTK, UNC, …] ⟷ **[BETA-2]**
  - Y1: Convergence analysis for (superallowed) beta decays using VS-IMSRG and IM-GCM. [MSU, ND, UNC, …]
  - Y1: R&D to compute δ_C, δ_{NS} corrections in HOBET. [UCB] ⟷ **[BETA-2]**
  - **Y2: Compute δ_C in superallowed beta decays in VS-IMSRG and IM-GCM. [MSU, ND, …]**
  - **Y3: Calculation of δ_C, δ_{NS} in light nuclei with various methods & benchmarking [ANL, LANL, MSU, ND, ORNL/UTK, UNC, WUSTL, …]**
  - Y4: R&D for using QMC with STA for calculation of δ_{NS}. [ANL, LANL, ODU, WUSTL, …] ⟷ [MSU, ND ORNL/UTK] ?
  - **Y4 & Y5: Ab initio calculations of δ_C, δ_{NS} in light and medium-mass nuclei.**
- **BETA-4**
  - **Y5: Study impact of ab initio calculation of δ_C, δ_{NS} on CKM unitarity [LANL, UMass, UW] ⟷[BETA-3]**

NTNP Goals and Objectives

- **EDM-3 [MSU, ND, UNC, …]**
  - Y1: Develop software and file formats to deploy EFT transition operators in ab initio calculations
  - Y1: Preliminary VS-IMSRG result for the Schiff moment of ^{199}Hg
  - **Y3: VS-IMSRG results with uncertainties for Schiff moments of ^{199}Hg and ^{129}Xe**
  - Y4: Preliminary IM-GCM Schiff moment in ^{225}Ra
  - **Y5: IM-GCM Schiff moment for ^{225}Ra with uncertainty analysis**

NTNP Goals and Objectives

- **XSEC-4 [ANL, LANL, ODU, WUSTL …]**
  - Y4: Calculations of inclusive electroweak cross sections in A = 4,12,16 nuclei with QMC methods supplemented by factorization schemes (Short-Time-Approximation and Spectral Function formalism).
  - Y4: R&D for ^{40}Ca
  - **Y5: Electroweak cross sections in ^{40}Ca**

- **XSEC-5 [ANL, LANL, ODU, WUSTL …]**
  - Y3: Relativistic effects in the STA and tests on $_{4}$He. R&D to extend STA to include exclusive channel.
  - Y4: Relativistic effects in STA and tests on $_{12}$C. Preliminary results in STA of π-production induced by electrons for A = 3. Exclusive results for neutrino- and electron-$_{12}$C cross sections in SF formalism.
  - **Y5: Determination of theoretical uncertainties in calculations of inclusive and exclusive cross sections induced by lepton scattering.**

Nuclear Structure Teams

- MSU: S. Bogner, H. Hergert
- Notre Dame: R. Stroberg
- UNC-Chapel Hill: J. Engel
- ODU: A. Gnech, R. Schiavilla,
- ORNL / UTK: G. Hagen, T. Papenbrock
- ANL: A. Lovato, N. Rocco, R. Wiringa
- WUSTL: L. Andreoli, G. King, J. Bub, S. Pastore, M. Piarulli, A. McCoy

Challenges: Many-Body Methods

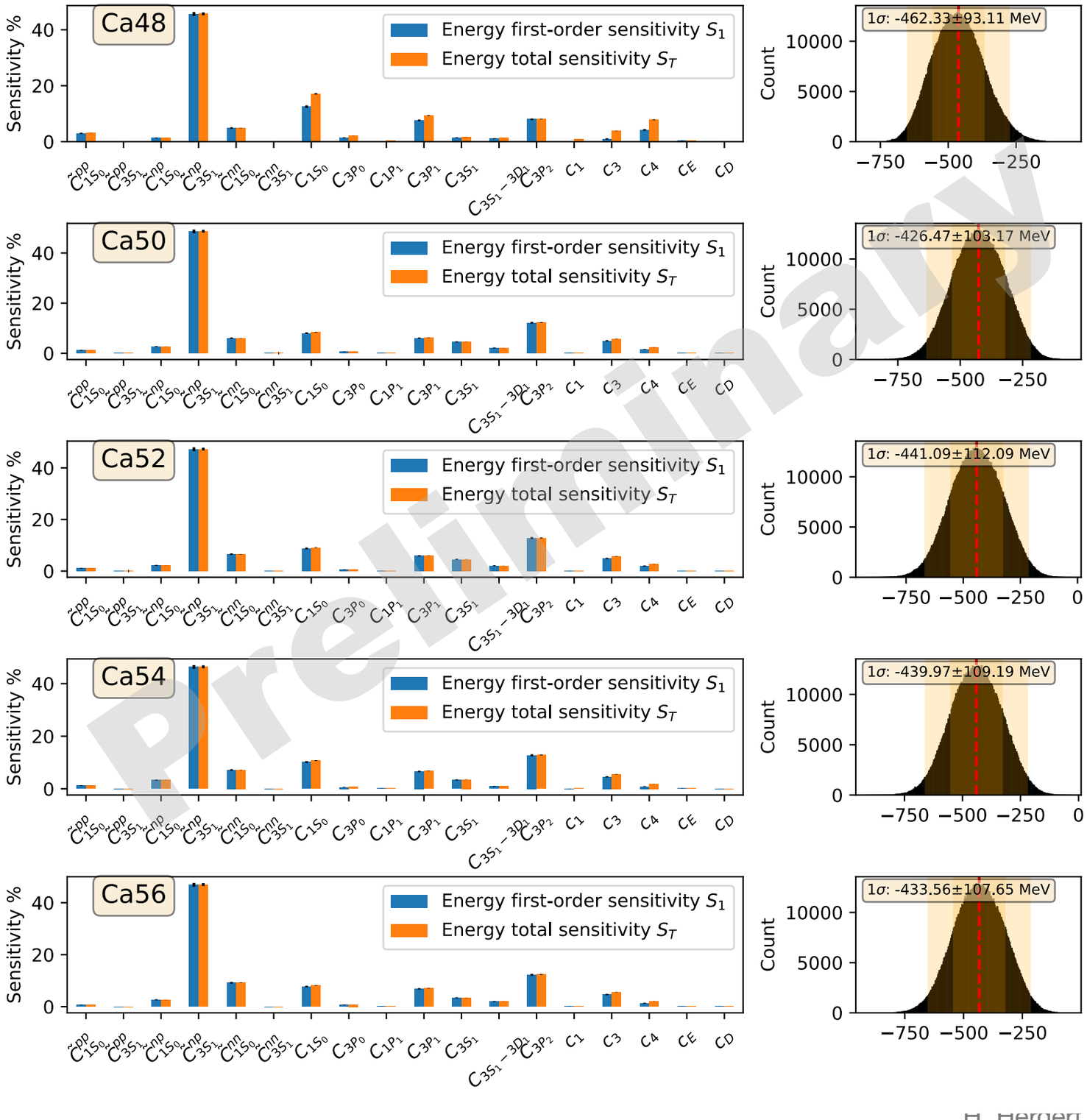
- continuous **efficiency improvements** **(proactive sharing)**
  - leverage potential synergies with other efforts (e.g., NUCLEI SciDAC)
- improvements to **many-body truncations**
  - necessary ingredient for **uncertainty quantification**
- necessary extensions of many-body methods
  - IM-GCM: odd nuclei
  - CC: symmetry projection, triaxial deformation (maybe?)
  - **summation over intermediate states** (e.g. for computation of δ_{NS}) - or **alternative ideas**?

Uncertainty Quantification

- major advances through the systematic use of **Bayesian techniques** (e.g. history matching…) and **emulators**
- **reduced-basis methods (e.g., eigenvector continuation)** for wave-function methods: NCSM, SA-NCSM, Coupled Cluster
- **new:** parametric emulator for IMSRG flows based on Dynamic Mode Decomposition
- **new:** Gaussian process emulators for VS-IMSRG transition matrix elements

Parametric DMD

***J. Davison, J. Crawford**, S. Bogner, HH, in preparation*



- $NNLO_{sat}$, NN+3N
- $e_{max} = 12,$ $E_{3max} = 14$
- 1M+ samples
- **5+ order of magnitude reduction in computational effort**

Uncertainty Quantification

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- **reduced-basis methods (e.g., eigenvector continuation)** for wave-function methods: NCSM, SA-NCSM, Coupled Cluster
- **new:** parametric emulator for IMSRG flows based on Dynamic Mode Decomposition
- **new:** Gaussian process emulators for VS-IMSRG transition matrix elements
- Emulators/model reduction for **free-space SRG**?
- Emulation for **QMC** methods?

Implementation and Deployment

Y1: Develop software and file formats to deploy EFT transition operators in ab initio calculations

- **consistent transition operators** from EFT (and LQCD?)
  thrusts ⟷ **[BETA-2] (EDMs?)**
  - routines for momentum- and coordinate-space expressions (Jacobi variables) - maybe Jacobi HO?
  - contributions separated by LEC, to facilitate interfacing with emulators
- may require adaptations to existing workflows because of symmetry breaking

Discussion

- Collaboration repository for codes and matrix elements?
- Echoing previous talk(s) - Slack (or alternative) workspace?
- Announce and proactively share new tools
- Maintain list of expertise a la FRIB Theory Alliance?

List of Potential Nuclear Theory Collaborators - In order to support the experimental program at FRIB right from the start, the FRIB TA Executive Board (TA-EB) has compiled a list of theorists who are willing to provide their expertise to experimental groups. Theorists can contribute to successful proposals and experiments by providing background information, suggesting experts who can address specific questions, and by collaborating directly. In turn, experimentalists can support theorists by incorporating and acknowledging the input, as well as by including them in proposals and collaborative work beyond. All users of the list are expected to use the information therein solely for the purpose of scientific discussion and collaboration. Any concerns should be reported to the Theory Alliance Executive Board. Updated 12 06 22

Name	Email address	Website	Areas of current interest	Resources (formal, computational, theory networks/collaboration) available	Other areas of expertise	Wish list for experimental data
Alex Brown	brown@nscl.msu.edu	https://people.nscl.msu.edu/~brown/	Structure of sd shell nuclei (Structure includes beta and gamma decay, moments, One and two nucleon spectroscopic factors) Structure in the region of 42Si Structure of pf shell nuclei Structure for Z=29-50 up to N=56 Structure in the regions of 132Sn and 208Pb Rms radii and neutron skins connected to the neutron equation of state Rapid-proton capture rates Level densities from the shell model Structure aspects of double Di-proton decay	Shell-model codes Oxbash and NuShellX		Structure data for the regions of 42Si, 60Ca, and 78Ni Rms charge radii of proton-rich nuclei
Witek Nazarewicz	witek@frib.msu.edu	https://people.nscl.msu.edu/~witek/www/Nazarewicz.htm	Nuclear structure; global properties of nuclei; nuclear collective motion Decay spectroscopy; physics of open systems Large amplitude collective motion; nuclear fission Nuclear input for nuclear astrophysics Uncertainty quantification for nuclear models; Bayesian inference Hyperfine interactions	NUCLEI SCIDAC (http://nuclei.mps.ohio-state.edu) BAND collaboration (https://www.ohio.edu/news/2020/05/ohio-leads-new-3-7-million-projectadvance-nuclear-physics-experiments) Several international collaborations	High performance computing Theory of open quantum systems	Masses, radii, and moments of radioactive nuclei Spin-isospin excitations Multi-particle decays; inter-nucleon correlations Data on superheavy nuclei Data on mirror nuclei Data on neutron-rich nuclei, including beta-decay information
Jutta Escher	escher1@llnl.gov	https://people.llnl.gov/escher1	Improving nuclear structure inputs for nuclear reactions: level densities, gamma-ray strength functions, optical-model potentials Integrating nuclear structure and reaction theory: inelastic scattering and transfer reactions Indirect methods for determining nuclear reaction cross sections for astrophysics and other applications Interplay of statistical and direct reactions, formation, and decay of compound nuclei		Symmetry-based approaches in nuclear structure and reactions	Elastic and inelastic scattering cross sections Decay properties of compound nuclei
Daniel Phillips	phillid1@ohio.edu	https://www.ohio.edu/cas/phillid1	Halo nuclei and quantum universality Bayesian inference Astrophysical reactions for light nuclei; R-matrix theory Neutron-neutron interactions	BAND collaboration (https://bandframework.github.io/) BUQEYE collaboration (https://buqeye.github.io/) Collaboration with several physicists at TU Darmstadt	Electron & photon scattering from light nuclei Effective Field Theory Three-body dynamics Parity violation	Neutron-neutron correlations in the final state Energies, radii, B(E1) strengths of weakly bound s-wave & p-wave states near the driplines
Jorge Piekarewicz	jpiekarewicz@fsu.edu	http://web2.physics.fsu.edu/~piekarewicz/	Neutron-rich matter on heaven and earth; Neutron stars, neutron skins, giant resonances; Covariant density functional theory; Bayesian statistics	Calibration and implementation of unified covariant density functional codes to describe ground-state properties of finite nuclei, their linear (RPA) response, and properties of neutron stars.		Masses of exotic neutron-rich nuclei of relevance to the neutron star crust; Neutron densities and neutron skins of very neutron-rich nuclei to constrain EOS; Electric dipole polarizability along isotopic chains; Charge radii of mirror and exotic nuclei; constraints on the EOS at twice saturation density from heavy-ion collisions of highly asymmetric nuclei
Kevin Fossez	fossez@nscl.msu.edu	https://kevinfossez.github.io/	Nuclear structure including the continuum (ab initio, shell model); Halo structures, two-neutron/proton decay, many-body resonances. Collective motion.	NUCLEI collaboration; (Ab initio) Gamow shell model (GSM), density matrix renormalization group (DMRG) method, In-medium similarity renormalization group (IMSRG), particle-plus-rotor model.	High-performance computing. Shell model interactions. Radiative capture reactions, alpha clustering.	Energies and spin-parity at the drip lines in the sdfp region. Decay widths and decay channels. Beta-decay spectroscopy of proton-rich nuclei.
Filomena Nunes	nunes@frib.msu.edu	https://fimmnunes.wixsite.com/mysite	direct nuclear reactions, few-body methods for reactions, optical potential, uncertainty quantification in reactions		Halo nuclei and few-body models for halos	systematic study of elastic on several isotopic chains. simultaneous measurement of breakup and elastic. transfer measurements on neutron rich heavy nuclei
Dean Lee	leed@frib.msu.edu	https://leedeanj.wixsite.com/leegroup	nuclear clustering, forces, structure, thermodynamics, liquid-gas transition, equation of state, superfluid pairing, microscopic calculations	NUCLEI collaboration Nuclear Lattice EFT Collaborstion	Quantum computing Machine learning	Cluster states, nuclear correlations, multifragmentation distributions
Jon Engel	engelj@physics.unc.edu https://physics.unc.edu/engelj/	http://www.physics.unc.edu/~engelj/	Fundamental symmetries in nuclei: double-beta decay, atomic electric dipole moments. Nuclear astrophysics: weak interactions in nucleosynthesis, r process. Nuclear structure: density-functional theory, in-medium generator-coordinate method.	DBD Topical Theory Collaboration NUCLEI collaboration	Group theoory in nuclear physics	Beta-decay spectroscopy Strength distributions for forbidden/retarded operators