Neutrino-Nucleus scattering with *ab initio* **No-Core Shell Model**

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Neutrino-nucleus interactions

 \triangleright Nuclear response at different energy transfer regions is crucial to make the predictions.

(Quasi-)elastic v-nucleus CC/NC interactions

Experiment	Nuclear Target	Reaction	$\sigma_{\rm o}$ $[10^{-46}$ cm ²]	ΔE_{nucl} [MeV] (no det. Thres.)
GALLEX/GNO SAGE	71 Ga ₃₃	$v_e + {}^7Ga \rightarrow e^- + {}^{71}Ge$	$8.611 \pm 0.4\%$ (6T)	0.2327
HOMESTAKE	${}^{37}Cl_{17}$	$v_r + {}^{37}Cl \rightarrow e^- + {}^{37}Ar$	1.725 (F)	0.814
SNO	$2H_1$	$v_e + ^2H \rightarrow e^- + p + p$	(GT)	1.442
DUNE. ICARUS, etc.	$40_{Ar_{18}}$	v_{e} + ⁴⁰ Ar $\rightarrow e^{-}$ + ⁴⁰ K [*]	148.58 (F) 44.367 (GT ₂)	$1.505 +$
			41.567 (GT ₆)	

From Kevin McFarland

Important for solar & supernova ➤ neutrino detection

JUNO, Astrophys.J. 965 (2024) 2, 122

Phenomenological models calculations

❖ **Neutrinos-¹²C & ¹³C cross-sections calculations with phenomenological models**

Neutrinos-¹²C cross-sections from different models

Shell Model (SM) Random Phase Approximation (RPA) Quasi-particle RPA (QRPA) Continuum RPA (CRPA)

a: C.Athanassopoulos and the LSND collaboration, Phys. Rev. C (1997),

- b: R.C.Allen et al., Phys. Rev. Lett (1990),
- c: C.Athanassopoulos and the LSND collaboration, Phys. Rev. C (1997),
- d: B.E.Bodmann and the KARMEN collaboration, Phys. Lett. B (1994)

The results from RPA calculations are far away from experimental data, while the SM calculations are much closer to experimental data

Phenomenological models calculations

❖ **Neutrinos-¹²C & ¹³C cross-sections calculations with shell model**

Neutrino-¹²C charge current cross-sections from shell model with SFO interaction had a good agreement with experimental data

B(M1) and B(GT) strengths of ¹³C from shell model with SFO & CK interaction were still a little far away from experimental data

> *T. Suzuki et al., Phys. Rev. C (2012) T. Suzuki et al., Phys. Rev. C (2019)*

What is Ab Initio in nuclear physics?

Few-Body Syst (2023) 64:77 https://doi.org/10.1007/s00601-023-01857-2

R. Machleidt

What is *ab initio*?

Nuclear structure theory at its basic level is not about fitting data to get "good" results. Fundamental nuclear structure theory is about answering the question:

Do the same nuclear forces that explain free-space scattering experiments also explain the properties of finite nuclei and nuclear matter when applied in nuclear many-body theory?

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What is *ab initio* in nucl

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Ab initio has been used as a label in nuclear theory for over two decades. Its meaning has evolved and broadened over the years. We present our interpretation, briefly review its historical use, and discuss its present-day relation to theoretical uncertainty quantification.

Challenges

- ➢ Self bound quantum many-body problem, with 3A degrees of freedom in coordinate (or momentum) space, as well as spin degree of freedom
- ➢ Strong interactions, with both short-range and long-range pieces
- ➢ Not only 2-body interactions, but also intrinsic 3-body interactions and possibly 4- and higher N-body interactions
- ➢ Uncertainty quantification for calculations needed
	- for comparison with experiments
	- for comparison between different methods

Computational Methods for Nuclear Structure

- \triangleright Few-body methods
	- \triangleright Faddeev Equation for A=3 system
		- \triangleright typically in momentum space
	- \triangleright Faddeev-Yakuboski Equations for A=4 system
		- \geq can nowadays be pushed to A=5 and 6 (Lazauskas)
	- ➢ Hyperspherical Harmonics
		- \triangleright Up to A=6

➢ Many-body methods

- \triangleright Variational Monte-Carlo (A \le =12)
- \triangleright Green's Function Monte-Carlo (A \le =12)

➢ Configuration Interaction (CI) methods (NCSM (A<=20), Coupled Cluster $(A \leq 100)$

 \triangleright Nuclear Lattice Simulations (A \leq =32)

➢ All few- and many-body methods need some levels of High-Performance Computing

Nuclear Interactions

$$
\hat{\mathbf{H}}_{\text{rel}} = \hat{\mathbf{T}}_{\text{rel}} + \sum_{i < j} V_{ij} + \sum_{i < j < k} V_{ijk} + \dots
$$

➢ Nuclear interactions not well-determined

- In principle calculable from QCD
- In practice constrained by (fitting to) experimental (*NN* scattering) data

➢Alphabet of realistic interactions

- Argonne potentials
- Bonn potenitals

• …

- Chiral EFT interactions
- Daejeon16 (based on Idaho-N3LO)

➢Most *NN* potentials need 3*N* forces for agreement with experiments

LENPIC chiral EFT *NN* potential up to N⁴LO

Introduction of NCSM

❖ **No-Core Configuration Interaction / No-Core Shell Model calculations**

➢ **Given a Hamiltonian operator**

$$
\widehat{H} = \sum_{i < j} \frac{(\vec{p}_i - \vec{p}_j)}{2mA} + \sum_{i < j}^A V_{ij} + \sum_{i < j < k} V_{ijk} + \cdots
$$

➢ **Solve the eigenvalue problem for wavefunction of A nucleons**

$$
\widehat{H}\Psi_{\alpha_1\cdots\alpha_A} = \mathbf{E}\Psi_{\alpha_1\cdots\alpha_A}
$$

- \triangleright Expand wavefunction in basis states $|\psi\rangle = \sum \widehat{a}_i |\phi_i\rangle$
- **Express Hamiltonian in basis** $\langle \phi_i | \hat{H} | \phi_i \rangle = H_{ii}$
- ➢ **Diagonalize Hamiltonian matrix**
- ➢ **No-Core: All A nucleons are treated equally**
- ➢ **Complete basis ---- exact result**
- ➢ **In practice**
	- **1. truncate basis**
	- **2. study behavior of observables as function of truncation**
- ➢ **Computational challenge**
	- **1. construct large (10¹⁰ 10¹⁰) sparse symmetric matrix**
	- **2. obtain lowest eigenvalues & eigenvectors corresponding to low-**

 lying spectrum and eigenstates

Barrett et al., Progress in Particle and Nuclear Physics (2013) P. Maris, NCSM_NICC_YTT(2021)

Main Chanllenges

Increase of basis space dimension with A and N_{max}

- ightharpoonup b at least $N_{\text{max}}=8$, preferably $N_{\text{max}}=10$ for meaningful extrapolation and numerical error estimates
- \triangleright More relevant measure for computational needs
	- \triangleright Number of nonzero matrix elements
	- \triangleright Current limit 10¹⁴ (Perlmutter)

National Energy Research Scientific Computing Center

MFDn in the SciDAC era

https://nuclei.mps.ohio-state.edu/nuclei_home.php

(not in NUCLEI)

- Collaborative DOE grants for domain scientists (i.e. nuclear physicists), computer scientists, and applied mathematicians to enable scientific progress through high-performance computing
- Support for students and postdocs to do the hard & tedious work
- UNEDF (2007-2012), NUCLEI(2012-2017, 2017-2022)
	- MFDn: collaboration between ISU (James Vary), Ames Lab (Masha Sosonkina), and Berkeley Lab (Esmond Ng, Chao Yang)
	- Ab Initio: Coupled Cluster, VMC & GFMC, lattice EFT, ...
	- Density Functional Theory for heavy nuclei
	- BIGSTICK: complementary/competing NCCI code (Calvin Johnson)
	- Valence Shell Model (NuShellX, BIGSTICK)

Previous calculations from ab initio NCSM

❖ **Neutrino-¹²C cross-sections calculations with NCSM**

AV8': NN potential CD-Bonn: NN potential AV8' + TM'(99): NN potential + 3N NN potential

The B(M1) calculated values from AV8', CD-Bonn, AV8' + TM'(99) were still a little far away from experimental data

Experimental and calculated B(M1;0⁺0 \rightarrow 1⁺1) values for ¹²C

		CD -Bonn		$AV8' + TM'(99)$	
Interaction	$2\hbar\Omega$	$4\hbar\Omega$	$6\hbar\Omega$	$4\hbar\Omega$	Experiment
(ν_e, e^-)	2.27	3.2	3.69	6.8	$8.9 \pm 0.3 \pm 0.9$ [a]
(ν_{μ}, μ^{-})	0.168	0.275	0.312	0.537	$0.56 \pm 0.08 \pm 0.1$ [b]
μ -capture	1.46	2.07	2.38	4.43	6.0 ± 0.4 [c]

Predicted weak interaction rates of ¹²C. The units are 10⁻⁴² cm² for the (v_e, e^-) **DAR cross section, 10-42 cm² for the** (ν^µ , µ [−]) **DIF cross section, and 10³ sec-1 for** muon capture

a:LSND Collaboration, L. B. Auerbach et al., Phys. Rev. C 64, 065501 (2001).

- b:LSND Collaboration, L. B. Auerbach et al., Phys. Rev. C 66, 015501 (2002).
- c: G. H. Miller et al., Phys. Lett. B 41, 50 (1972);

A. C. Hayes, P. Navrátil, and J. P. Vary, Phys. Rev. Lett. 91, 012502 (2003)

Barrett et al., , Progress in Particle and Nuclear Physics (2013)

Improvements of our calculations

From the previous NCSM calculations of neutrino-¹²C scattering, we can infer that the precision of neutrino-¹²C cross-sections with Ab initio NCSM/NCCI, could be improved by applying new interaction(with the contributions from 3N force), increasing the basis space, including more reaction channels and excited states.

❖ **Highlights in our calculations**

 1. New interaction – Daejeon16

Dimensions of many body matrix in Nmax6: 3.26x10⁷ ; Nmax10: 7.83x109

- **2. Larger basis space for calculations(up to Nmax=10)**
- **3. Higher excitation energy (at least 20 MeV~ 30 states)**
- **4. More channels(neutral current, charged current, nucleon knock-out)**
- **5. Theoretical uncertainty**
- **6. Extrapolation tools (Traditional and machine learning ANN)**
- **7. Calculations of cross sections at reactor neutrino energies**

Current progress

❖ Ground state energy from Daejeon16

NCSM+Daejeon16 has good performance on the calculations of binding energies

We use a simple 3-point exponential extrapolation from the reference paper

$$
E^{\hbar\omega}(N_{\text{max}}) = E^{\hbar\omega}_{\infty} + a e^{(-b N_{\text{max}})}
$$

P. Maris et al., Phys. Rev. C (2021)

❖ **Energy spectra from Daejeon16**

0+ The low lying spectra of ¹²C & ¹³C from Daejeon16 have good agreement with experimental data

❖ **Point Proton Radii of ground state from Daejeon16**

We get the estimations and uncertainties of point proton radii from the "crossing points" The point proton radii values from Deajeon16 quite close to experimental data

❖ **Comparisons on ground state energies and point proton radii between Daejeon16 and other Chiral EFT interactions**

Ground state energies and point proton radii of Carbon-11, 12, 13 from Deajeon16 in good agreement with experiment, even better than NN + NNN interaction.

> *P. Maris et al., Phys. Rev. C (2021) P. Navrátil et al., Phys. Rev. Lett (2007)*

❖ **Comparisons on ground state energies and point proton radii between Daejeon16 and other Chiral EFT interactions**

Ground state energies and point proton radii of Boron 11, 12, 13 & Nitrogen 12, 13 from Deajeon16 in good agreement with experiment, even better than chiral N3LO interaction.

❖ **Comparisons on M1 and E2 transitions between**

NCCI-Daejeon16 and other calculations

The CK-POT, CK, SFO interactions were performed in shell model calculations

Hw = 15 MeV in Daejeon16 and chiral interactions

Electromagnetic transitions of Carbon12 & 13 from Deajeon16 are not so close to experiment, but reasonable.

P. Navrátil et al., Phys. Rev. Lett (2007) T. Suzuki et al., Phys. Rev. C (2012) H. Sagawa et al., EPJ Web of Conferences (2018)

Next plan

1. Cross section

$$
\left(\frac{d\sigma}{d\Omega}\right)_{\substack{v_e\\v_e}} = \frac{2}{\pi} G_F^2 \cos^2\theta_c F(Z,\epsilon) \frac{\epsilon^2}{2J_i+1} \cos^2\frac{\theta}{2} \left\{ \sum_{J=0}^{\infty} |\langle J_f || \hat{\mathcal{M}}_J + \frac{\omega}{q} \hat{\mathcal{L}}_J || J_i \rangle|^2 \right. \\ \left. + \left[-\frac{q_\mu^2}{2q^2} + \tan^2\frac{\theta}{2} \right] \sum_{J=1}^{\infty} [|\langle J_f || \hat{T}_J^{\text{el}} || J_i \rangle|^2 + |\langle J_f || \hat{T}_J^{\text{mag}} || J_i \rangle|^2 \right] \\ \left. + 2 \tan\frac{\theta}{2} \left[-\frac{q_\mu^2}{q^2} + \tan^2\frac{\theta}{2} \right]^{1/2} \sum_{J=1}^{\infty} \text{Re}\left(\langle J_f || \hat{T}_J^{\text{mag}} || J_i \rangle \langle J_f || \hat{T}_J^{\text{el}} || J_i \rangle^* \right) \right\},
$$

3. The multipole operators in the equation of charged-current cross section can be expressed in terms of the 7 basic operators

$$
\begin{split} &M_{JM_J}^{\pm}(q{\bf x})=F_1^{(1)}\big(q_\mu^2\big)M_J^{M_J}(q{\bf x})\tau_{\pm},\\ &T_{JM_J}^{\rm el\,\pm}(q{\bf x})=\frac{q}{M_N}\bigg(F_1^{(1)}(q_\mu^2)\Delta_J^{/M_J}(q{\bf x})+\frac{1}{2}\mu^{(1)}(q_\mu^2)\varSigma_J^{M_J}(q{\bf x})\bigg)\tau_{\pm},\\ &T_{JM_J}^{\rm mag\,\pm}(q{\bf x})=-\frac{iq}{M_N}\bigg(F_1^{(1)}(q_\mu^2)\Delta_J^{M_J}(q{\bf x})-\frac{1}{2}\mu^{(1)}(q_\mu^2)\varSigma_J^{/M_J}(q{\bf x})\bigg)\tau_{\pm},\\ &M_{JM_J}^5\pm(q{\bf x})=\frac{iq}{M_N}\bigg(F_A^{(1)}(q_\mu^2)\varOmega_J^{\prime M_J}(q{\bf x})+\frac{1}{2}\omega F_P^{(1)}(q_\mu^2)\varSigma_J^{\prime M_J}(q{\bf x})\bigg)\tau_{\pm},\\ &L_{JM_J}^5(q{\bf x})=i\bigg(F_A^{(1)}(q_\mu^2)-\frac{q^2}{2M_N}F_P^{(1)}(q_\mu^2)\bigg)\varSigma_J^{\prime M_J}(q{\bf x})\tau_{\pm},\\ &T_{JM_J}^{\rm el5\,\pm}(q{\bf x})=iF_A^{(1)}(q_\mu^2)\varSigma_J^{\prime M_J}(q{\bf x})\tau_{\pm},\\ &T_{JM_J}^{\rm mag5\,\pm}(q{\bf x})=F_A^{(1)}(q_\mu^2)\varSigma_J^{M_J}(q{\bf x})\tau_{\pm},\\ \end{split}
$$

2. The multipole operators in the equation of charged-current cross section are defined by

$$
\hat{\mathcal{M}}_{JM_J;TM_T} \equiv \int d\mathbf{x} \mathbf{M}_J^{M_J}(q\mathbf{x}) \hat{\mathcal{J}}_0(\mathbf{x})_{TM_T} = \hat{M}_{JM_J;TM_T} + \hat{M}_{JM_J;TM_T}^5,
$$
\n
$$
\hat{\mathcal{L}}_{JM_J;TM_T} \equiv \frac{i}{q} \int d\mathbf{x} \left[\vec{\nabla} M_J^{M_J}(q\mathbf{x}) \right] \cdot \hat{\mathcal{J}}(\mathbf{x})_{TM_T} = \hat{\mathcal{L}}_{JM_J;TM_T} + \hat{\mathcal{L}}_{JM_J;TM_T}^5,
$$
\n
$$
\hat{T}_{JM_J;TM_T}^{\text{el}} \equiv \frac{1}{q} \int d\mathbf{x} \left[\vec{\nabla} \times \mathbf{M}_{JJ}^{M_J}(q\mathbf{x}) \right] \cdot \hat{\mathcal{J}}(\mathbf{x})_{TM_T} = \hat{T}_{JM_J;TM_T}^{\text{el}} + \hat{T}_{JM_J;TM_T}^{\text{el5}},
$$
\n
$$
\hat{T}_{JM_J;TM_T}^{\text{mag}} \equiv \int d\mathbf{x} \mathbf{M}_{JJ}^{M_J}(q\mathbf{x}) \cdot \hat{\mathcal{J}}(\mathbf{x})_{TM_T} = \hat{T}_{JM_J;TM_T}^{\text{mag}} + \hat{T}_{JM_J;TM_T}^{\text{mag5}},
$$

4. 7 basic operators)

$$
M_J^{M_J}(q\mathbf{x}),
$$

\n
$$
\Delta_J^{M_J}(q\mathbf{x}) \equiv \mathbf{M}_{JJ}^{M_J}(q\mathbf{x}) \cdot \frac{1}{q} \vec{\nabla},
$$

\n
$$
\Delta_J^{M_J}(q\mathbf{x}) \equiv -i \left[\frac{1}{q} \vec{\nabla} \times \mathbf{M}_{JJ}^{M_J}(q\mathbf{x}) \right] \cdot \frac{1}{q} \vec{\nabla} = [J]^{-1} \left[-J^{1/2} \mathbf{M}_{JJ+1}^{M_J}(q\mathbf{x}) + (J+1)^{1/2} \mathbf{M}_{JJ-1}^{M_J}(q\mathbf{x}) \right] \cdot \frac{1}{q} \vec{\nabla}
$$

\n
$$
\Sigma_J^{M_J}(q\mathbf{x}) \equiv \mathbf{M}_{JJ}^{M_J}(q\mathbf{x}) \cdot \vec{\sigma},
$$

\n
$$
\Sigma_J^{M_J}(q\mathbf{x}) \equiv -i \left[\frac{1}{q} \vec{\nabla} \times \mathbf{M}_{JJ}^{M_J}(q\mathbf{x}) \right] \cdot \vec{\sigma} = [J]^{-1} \left[-J^{1/2} \mathbf{M}_{JJ+1}^{M_J}(q\mathbf{x}) + (J+1)^{1/2} \mathbf{M}_{JJ-1}^{M_J}(q\mathbf{x}) \right] \cdot \vec{\sigma},
$$

\n
$$
\Sigma_J^{mJ_J}(q\mathbf{x}) \equiv \left[\frac{1}{q} \vec{\nabla} M_J^{M_J}(q\mathbf{x}) \right] \cdot \vec{\sigma} = [J]^{-1} \left[(J+1)^{1/2} \mathbf{M}_{JJ+1}^{M_J}(q\mathbf{x}) + J^{1/2} \mathbf{M}_{JJ-1}^{M_J}(q\mathbf{x}) \right] \cdot \vec{\sigma},
$$

\n
$$
\Omega_J^{M_J}(q\mathbf{x}) \equiv M_J^{M_J}(q\mathbf{x}) \vec{\sigma} \cdot \frac{1}{q} \vec{\nabla},
$$

Haxton et al., Comput. Phys. Commun(2008)

Computer Resources

- 1. Perlmutter (3072 CPU nodes, 1536 GPU nodes)
- 2. Nova (ISU, ~250 CPU nodes)
- 3. ¥7.5 million (HAUST, 70-80 CPU nodes)

Conclusions

- ➢ **Ground state energies and spectra of stable p-shell nuclei from Daejeon16 in good agreement with experiment; electromagnetic transitions are reasonable**
- ➢ **Improve the accuracy of calculations: increasing the basis space**
- ➢ **Demanding computer resources**
- ➢ **Theoretical uncertainty**
- ➢ **Comparison with future experimental data**