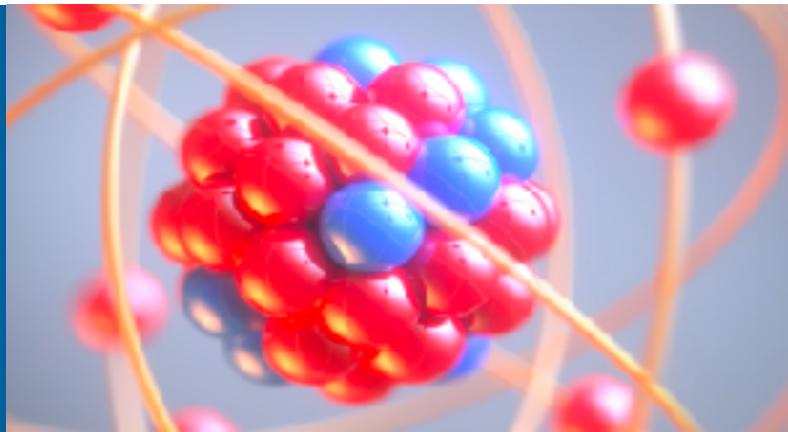


NEUTRINO-NUCLEUS SCATTERING, A QUANTUM MONTE CARLO PERSPECTIVE



ALESSANDRO LOVATO

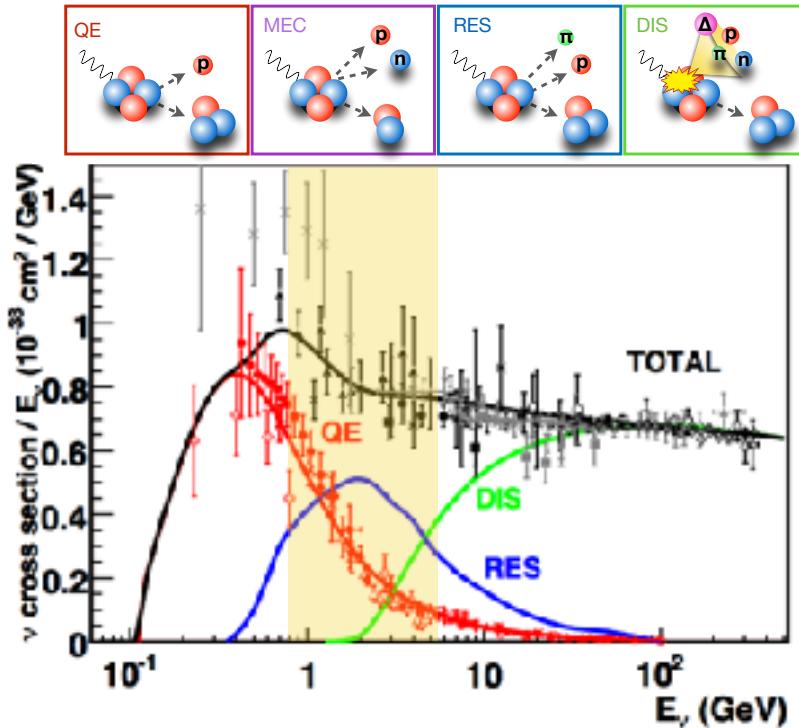
Argonne National Laboratory

22 June 2022
Neutrino Theory Network Workshop

INTRODUCTION

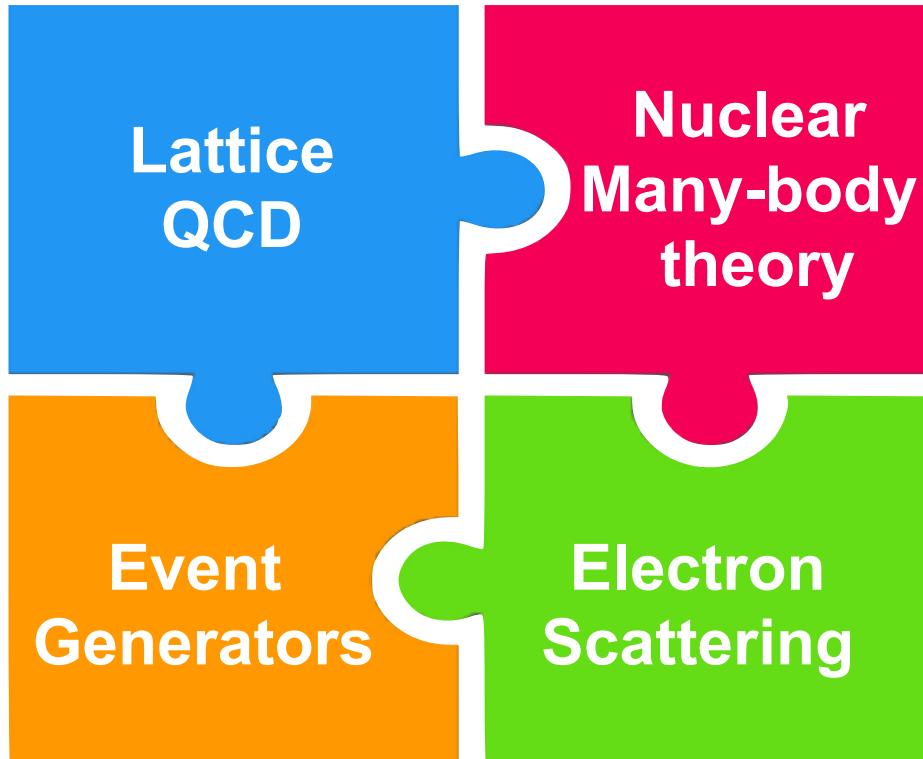
Achieving a robust description of the reaction mechanisms at play in the DUNE energy regime is a **formidable nuclear-theory and high-energy physics challenge**

- Realistic description of nuclear correlations
- Relativistic effects in the current operators and kinematics
- Description of resonance-production and DIS region



INTRODUCTION

A quantitative understanding of neutrino-nucleus scattering requires a synergistic effort



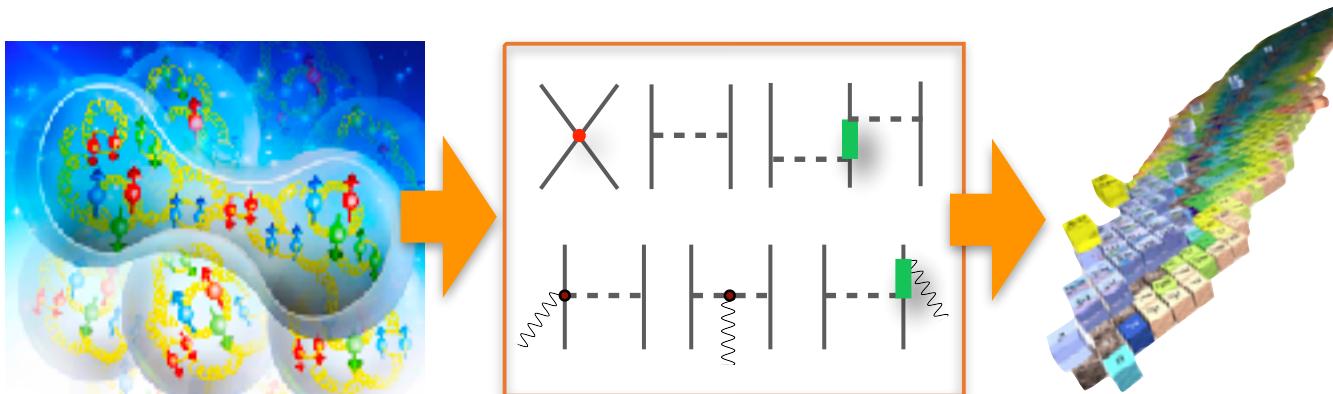
- **Lattice-QCD:** Few-nucleon amplitudes, including elastic and inelastic transitions;
- **Nuclear many-body theory:** Systematically improvable predictions for cross sections with quantified uncertainties;
- **Event generators:** Connect theory with experiments, simulate events using state-of-the art theory models;
- **Electron scattering:** Validate the framework with the exception of the axial contribution.

NUCLEAR MANY-BODY THEORY

- Nuclear effective field theories allow to systematically derive Hamiltonians and consistent electroweak currents

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i < j} v_{ij} + \sum_{i < j < k} V_{ijk} + \dots \quad J = \sum_i j_i + \sum_{i < j} j_{ij} + \dots$$

- They connect the underlying theory of strong interactions, QCD, with nuclear observables

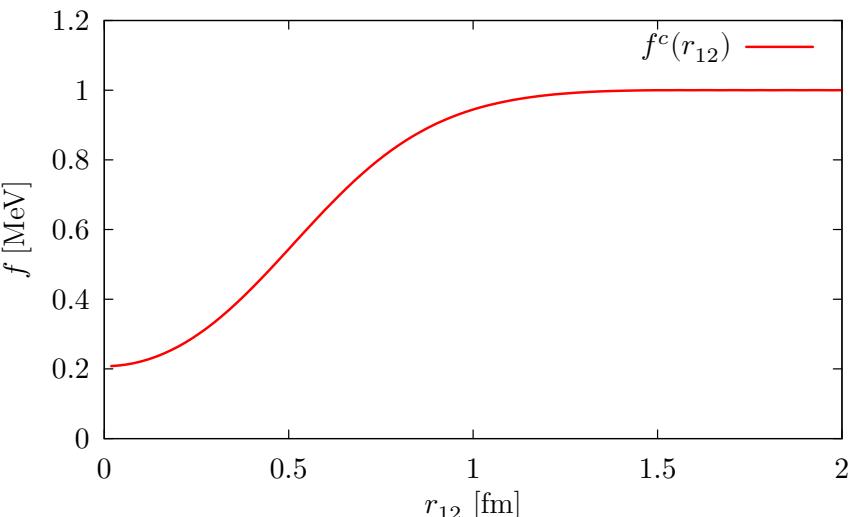
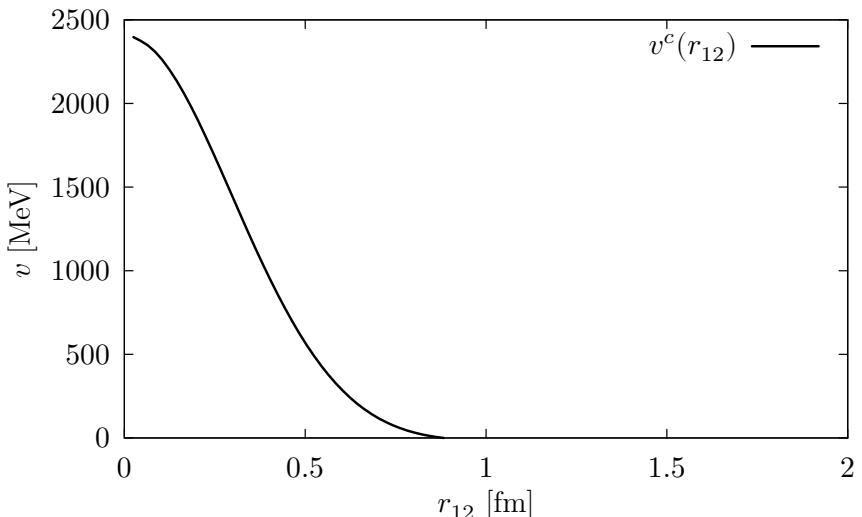


VARIATIONAL MONTE CARLO

The variational Moment Carlo wave function has correlations built in

$$|\Psi_T\rangle = \left(1 + \sum_{ijk} F_{ijk}\right) \left(\mathcal{S} \prod_{i < j} F_{ij}\right) |\Phi_{J,T_z}\rangle \quad \leftrightarrow \quad E_T = \langle \Psi_T | H | \Psi_T \rangle \geq E_0$$

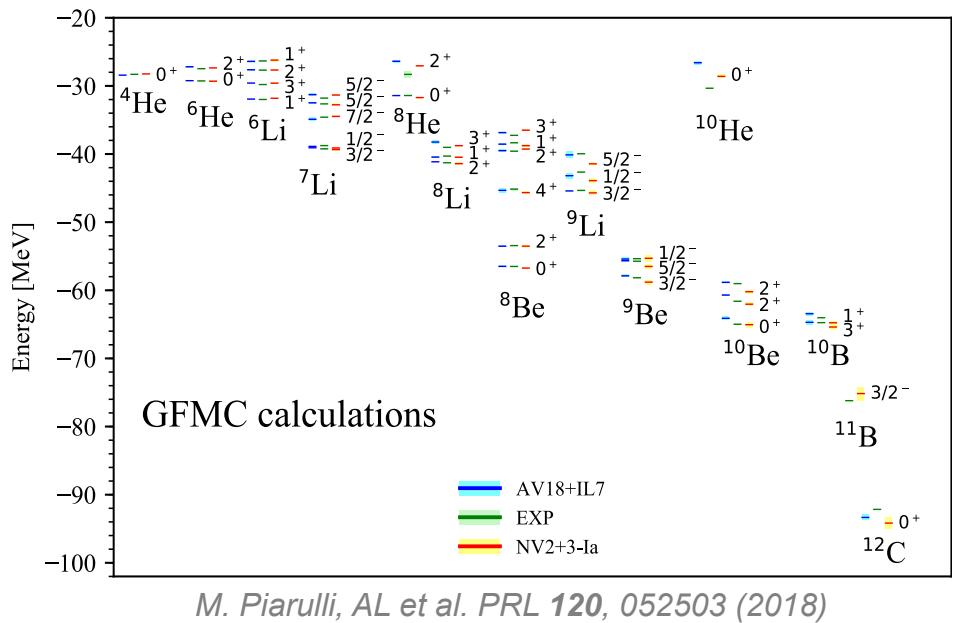
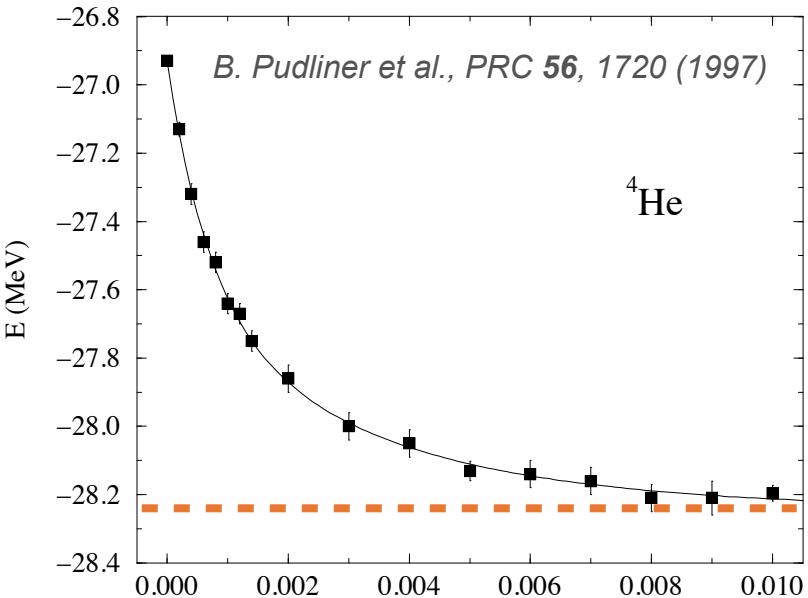
The correlations are consistent with the underlying nuclear interaction



GREEN'S FUNCTION MONTE CARLO

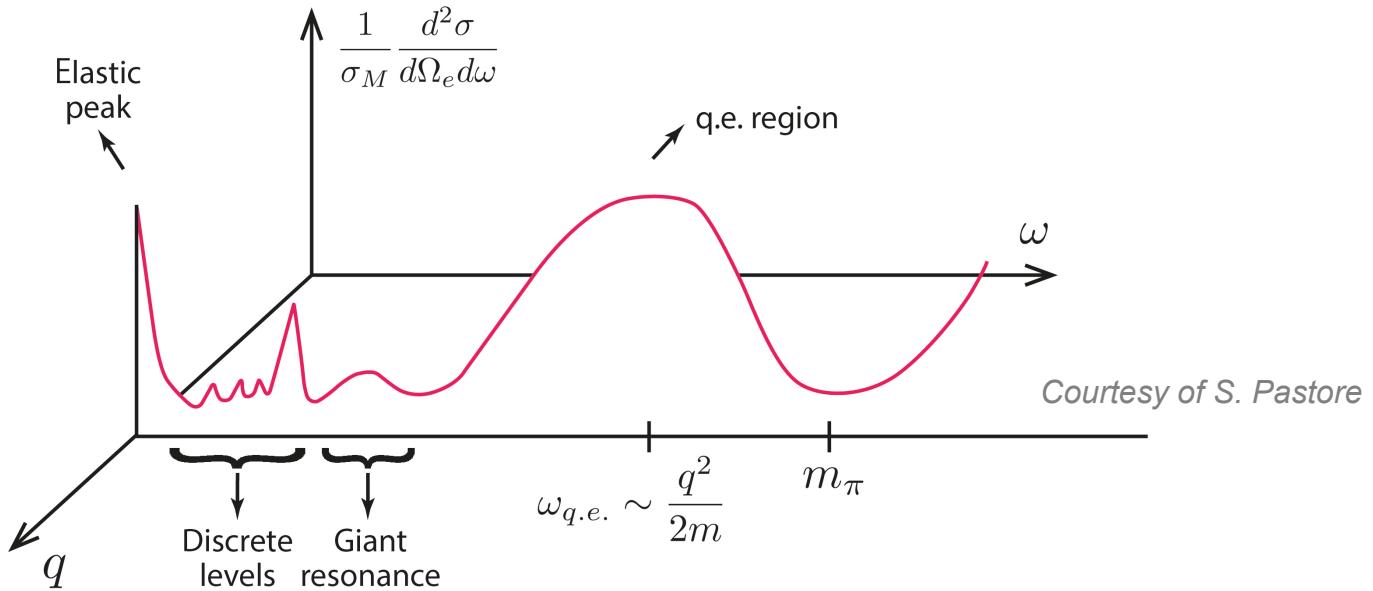
The GFMC performs an imaginary-time projection to extract the ground-state from the trial wave function

$$\lim_{\tau \rightarrow \infty} e^{-(H-E_0)\tau} |\Psi_T\rangle = \lim_{\tau \rightarrow \infty} \sum_n c_n e^{-(E_n-E_0)\tau} |\Psi_n\rangle = c_0 |\Psi_0\rangle$$



NEUTRINO-NUCLEUS SCATTERING

The inclusive cross section is characterized by a variety of reaction mechanisms



The response functions contain all nuclear-dynamics information

$$R_{\alpha\beta}(\omega, \mathbf{q}) = \sum_f \langle \Psi_0 | J_\alpha^\dagger(\mathbf{q}) | \Psi_f \rangle \langle \Psi_f | J_\beta(\mathbf{q}) | \Psi_0 \rangle \delta(\omega - E_f + E_0)$$

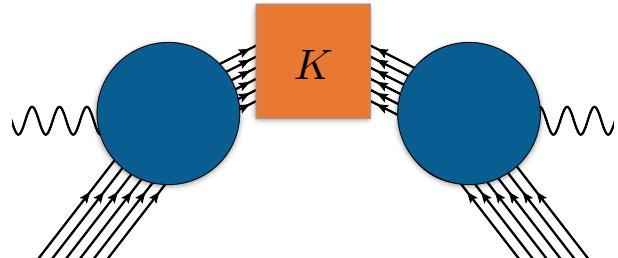
EUCLIDEAN RESPONSES

The integral transform of the response function is defined as

$$\begin{aligned} E_{\alpha\beta}(\sigma, \mathbf{q}) &\equiv \int d\omega K(\sigma, \omega) R_{\alpha\beta}(\omega, \mathbf{q}) \\ &= \sum_f \int d\omega K(\sigma, \omega) \langle \Psi_0 | J_\alpha^\dagger(\mathbf{q}) | \Psi_f \rangle \langle \Psi_f | J_\beta(\mathbf{q}) | \Psi_0 \rangle \delta(\omega - E_f + E_0) \end{aligned}$$

Using the completeness of the final states, it is expressed as a ground-state expectation value

$$E_{\alpha\beta}(\sigma, \mathbf{q}) = \langle \Psi_0 | J_\alpha^\dagger(\mathbf{q}) K(\sigma, H - E_0) J_\beta(\mathbf{q}) | \Psi_0 \rangle$$

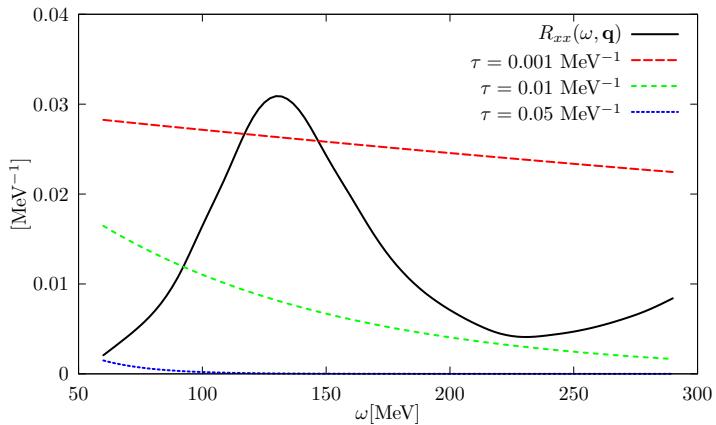


EUCLIDEAN RESPONSES

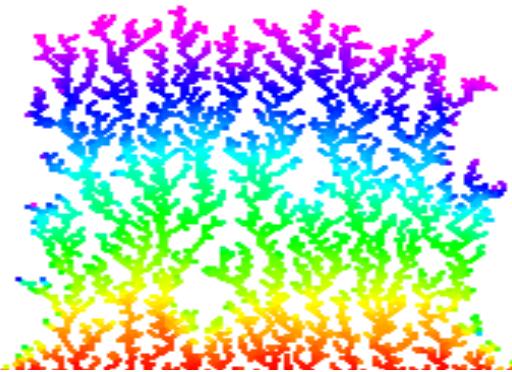
Our GFMC calculations rely on the Laplace kernel

$$E_{\alpha\beta}(\tau, \mathbf{q}) \equiv \int d\omega e^{-\omega\tau} R_{\alpha\beta}(\omega, \mathbf{q})$$

At finite imaginary time the contributions from large energy transfer are quickly suppressed



The system is first heated up by the transition operator. Its cooling determines the Euclidean response of the system



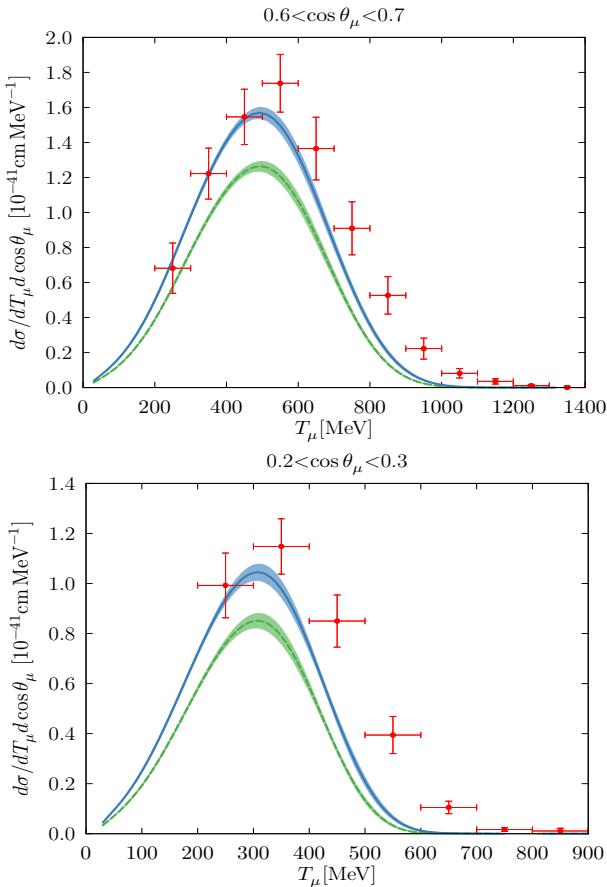
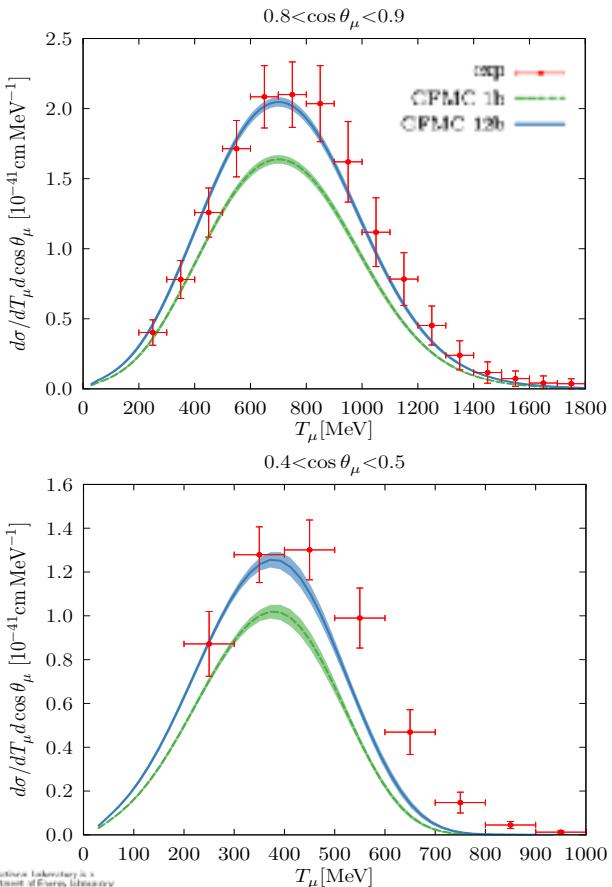
$$E_{\alpha\beta}(\tau, \mathbf{q}) = \langle \Psi_0 | J_\alpha^\dagger(\mathbf{q}) e^{-(H - E_0)\tau} J_\beta(\mathbf{q}) | \Psi_0 \rangle$$



$$\sum_f |\Psi_f\rangle\langle\Psi_f|$$

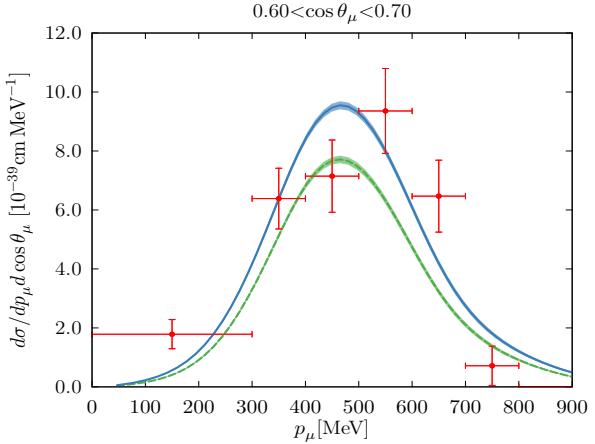
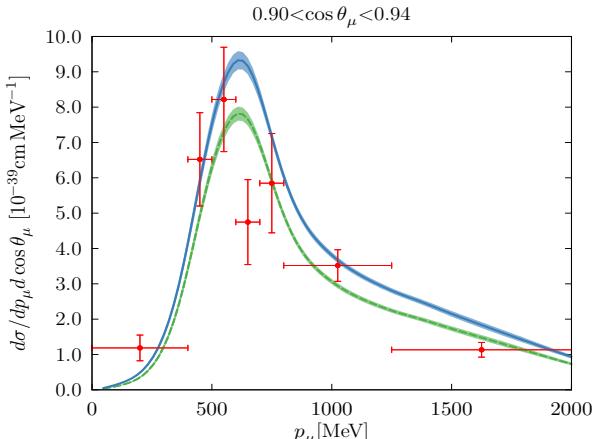
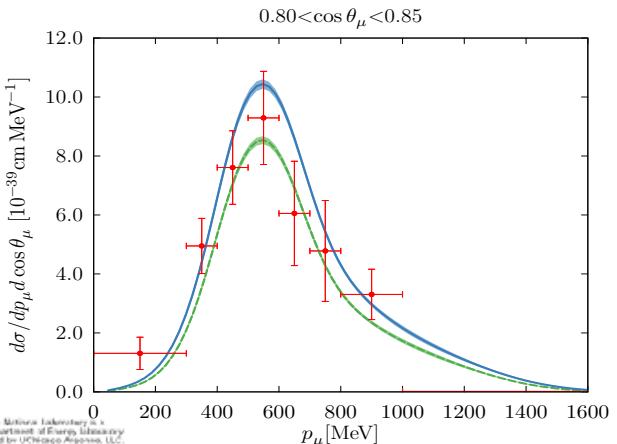
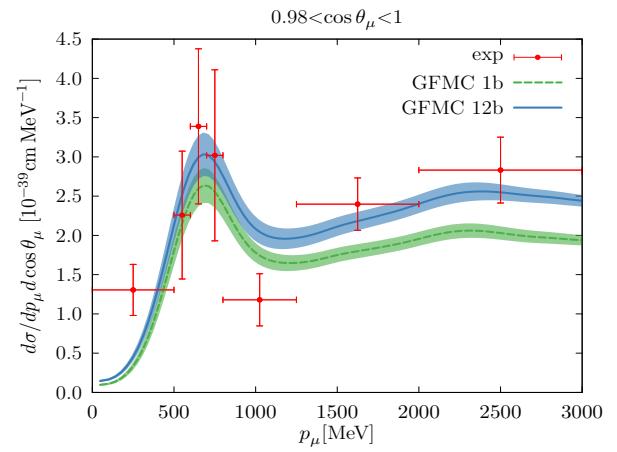
MINIBOONE CROSS SECTIONS

AL et al., PRX 10, 031068 (2020)



T2K CROSS SECTIONS

AL et al., PRX 10, 031068 (2020)

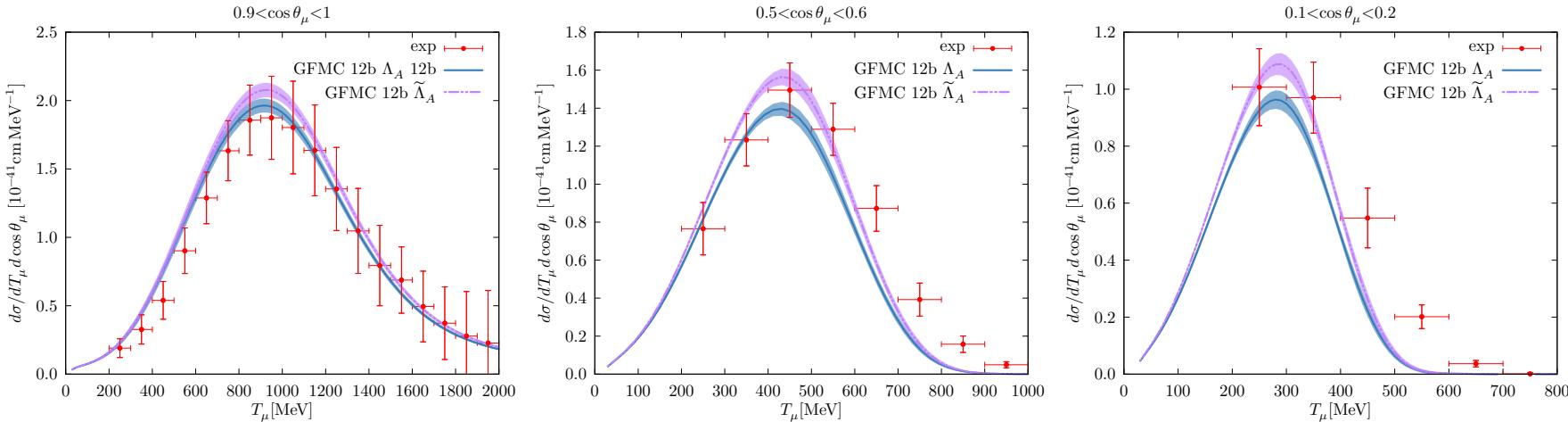


AXIAL FORM FACTOR

AL et al., PRX 10, 031068 (2020)

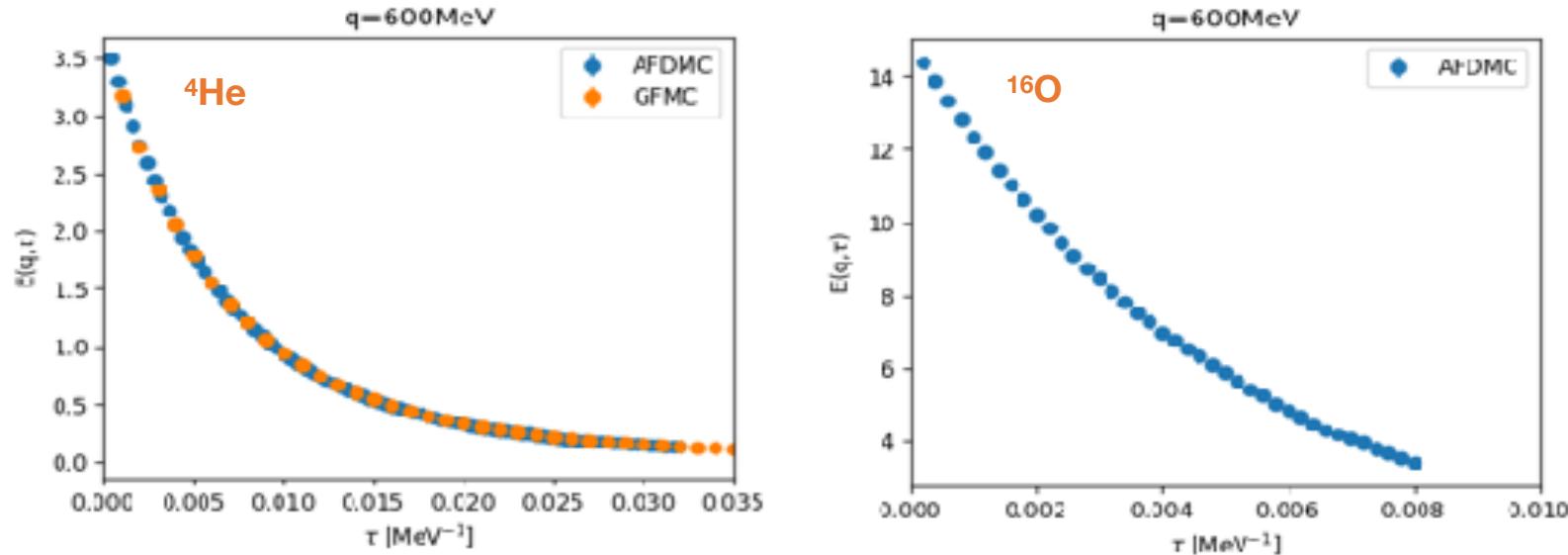
A precise knowledge of the **nucleon's axial-current form factors** is crucial for modeling neutrino-nucleus interactions;

We employ a dipole parametrization with $M_A=1$ GeV, and $M_A=1.15$ GeV, more in line with LQCD determinations;



BEYOND ^{12}C : AFDMC AND MACHINE LEARNING

The auxiliary-field diffusion Monte Carlo method allows to treat ^{16}O and beyond by sampling the spin-isospin degrees of freedom

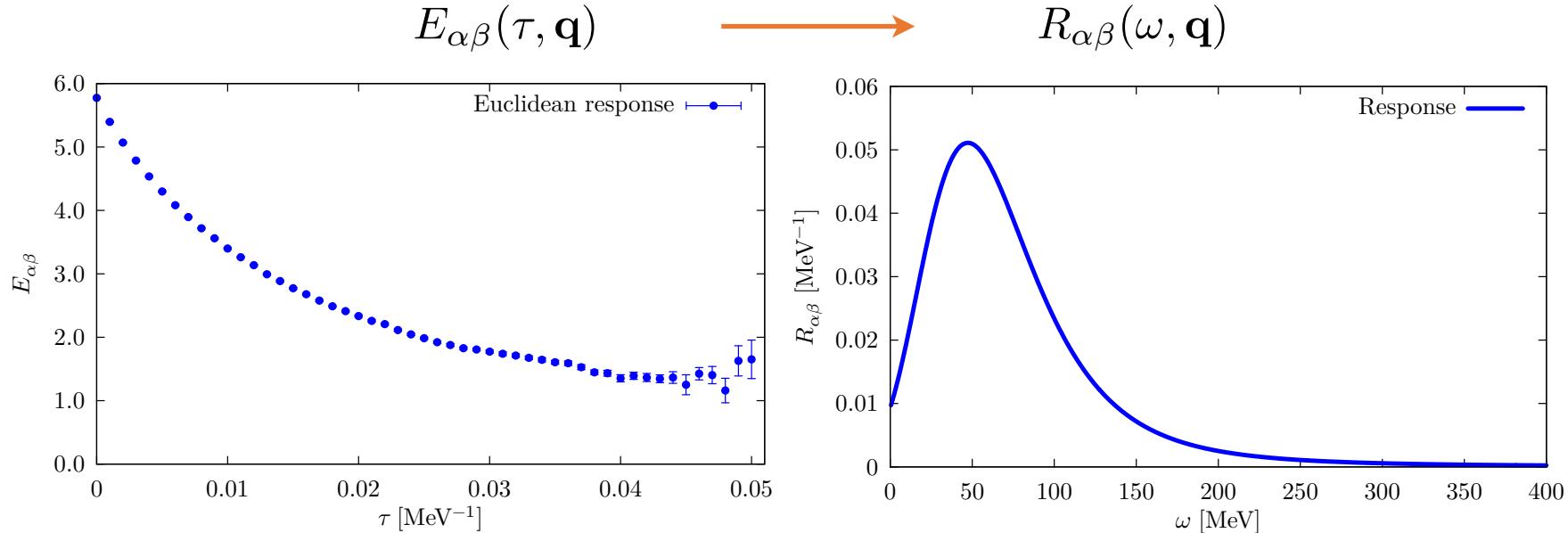


N. Rocco, AL et al., in preparation

- Excellent agreement with the GFMC in the ^4He case;
- Somewhat noisier estimates in ^{16}O because of the fermion-sign problem;

BEYOND ^{12}C : AFDMC AND MACHINE LEARNING

Inverting the Euclidean response is an ill posed problem: any set of observations is limited and noisy and the situation is even worse since the kernel is a smoothing operator.



We find Maximum-entropy techniques to be reliable enough for quasi-elastic responses

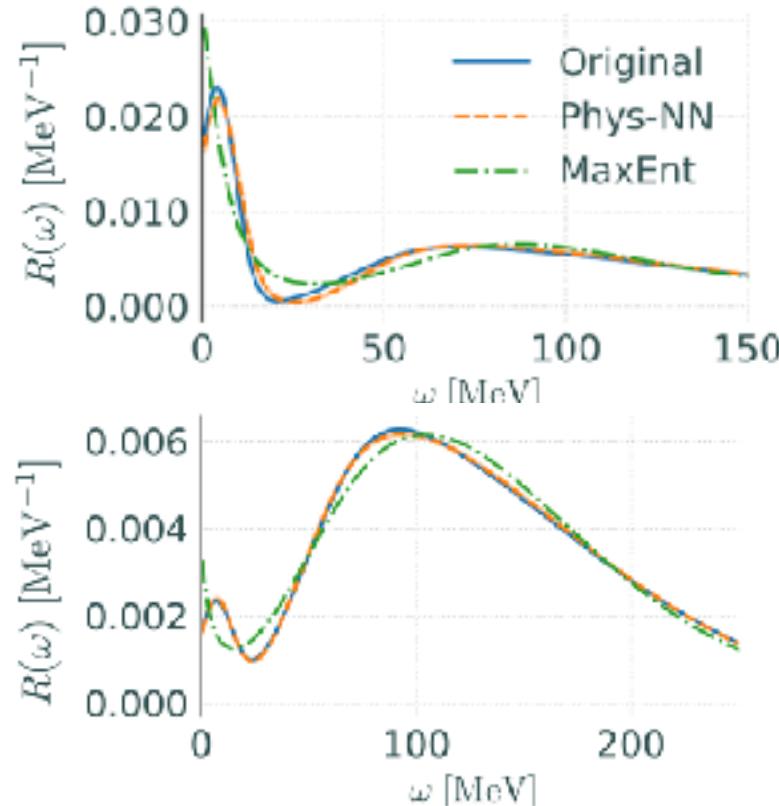
BEYOND ^{12}C : AFDMC AND MACHINE LEARNING

Inverting the Euclidean response functions of medium-mass nuclei is non-trivial:

- High noise due to unconstrained imaginary-time propagation;
- Rich structures at low energy due to transitions to low-lying states and collective modes;

We developed a physics-informed artificial neural network (“Phys-NN”) suitable to reliably invert the Laplace transform;

Phys-NN outperforms Maximum entropy, particularly in the low-energy transfer region;

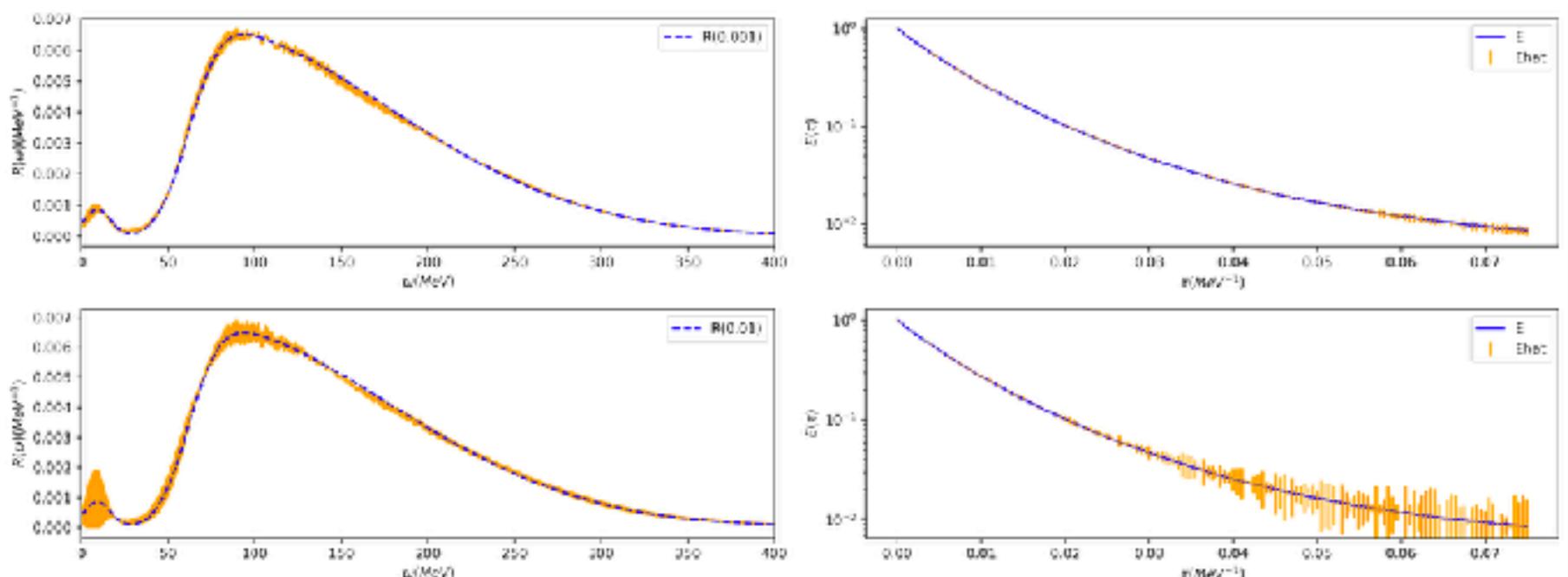


K. Raghavan, et al. PRC 103, 035502 (2021)

BEYOND ^{12}C : AFDMC AND MACHINE LEARNING

We developed an artificial-neural network approach suitable to invert the Laplace transform that:

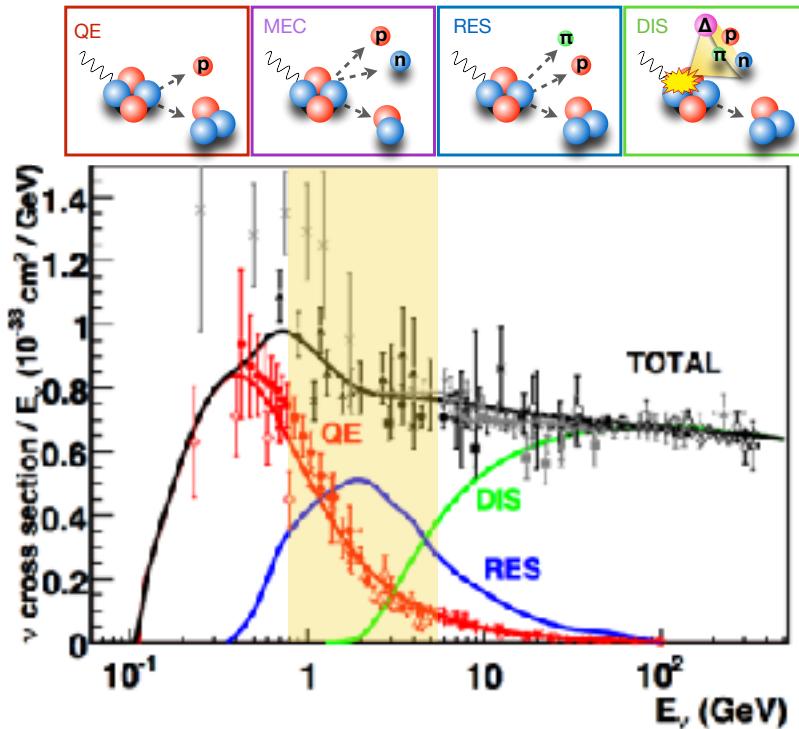
- Provides robust estimates of the uncertainty of the inversion;



ACCELERATOR NEUTRINO EXPERIMENTS

Achieving a robust description of the reaction mechanisms at play in accelerator-neutrino experiments is a **formidable nuclear-theory challenge**

- Realistic description of nuclear correlations
- Relativistic effects in the current operators and kinematics
- Description of resonance-production and DIS region



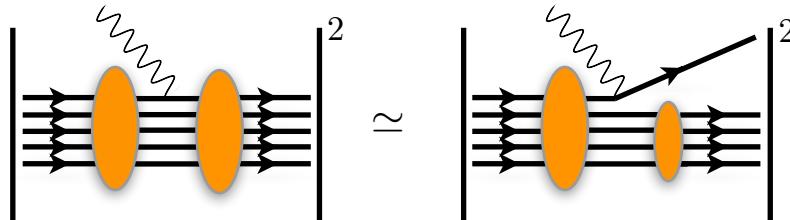
FACTORIZATION SCHEME

At large momentum transfer, the scattering reduces to the sum of individual terms

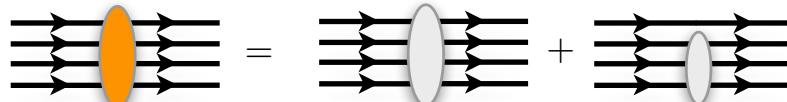
$$J^\mu \rightarrow \sum_i j_i^\mu \quad |\psi_f^A\rangle \rightarrow |p\rangle \otimes |\psi_f^{A-1}\rangle \quad E_f = E_f^{A-1} + e(\mathbf{p})$$

The incoherent contribution of the one-body response reads

$$R_{\alpha\beta} \simeq \int \frac{d^3k}{(2\pi)^3} dE P_h(\mathbf{k}, E) \sum_i \langle k | j_\alpha^i | k + q \rangle \langle k + q | j_\beta^i | k \rangle \delta(\omega + E - e(\mathbf{k} + \mathbf{q}))$$



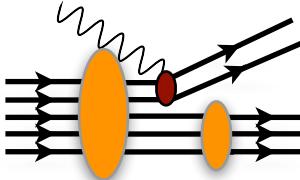
We include excitations of the A-1 final state with two nucleons in the continuum



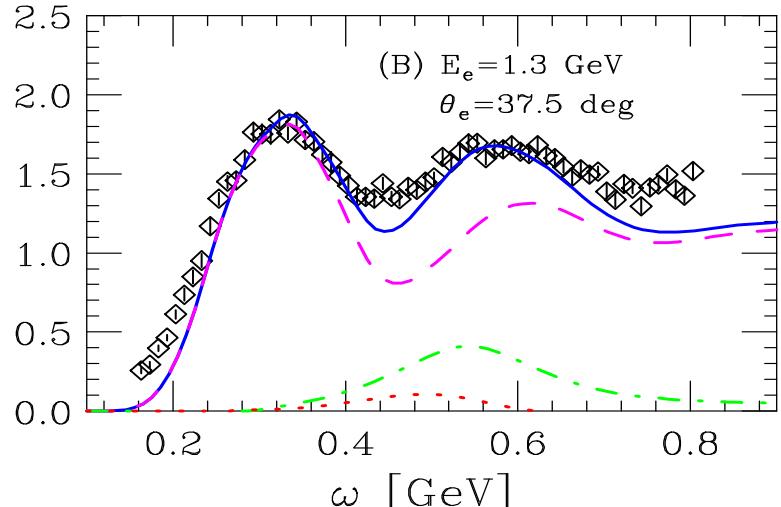
EXTENDED FACTORIZATION SCHEME

Using relativistic MEC requires extending the factorization scheme to two-nucleon emissions

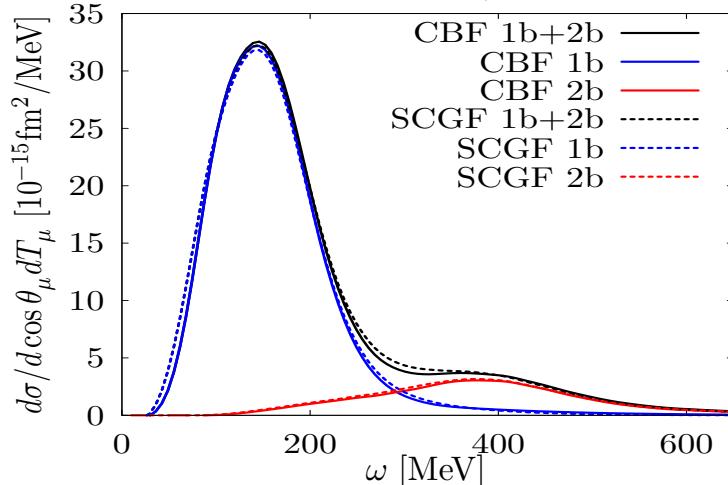
$$|\Psi_f^A\rangle \rightarrow |p_1 p_2\rangle \otimes |\Psi_f^{A-2}\rangle \quad \leftrightarrow$$



We compute electron and neutrino inclusive cross sections using CBF and SCGF spectral functions



N. Rocco, et al. PRL 116 192501 (2016)

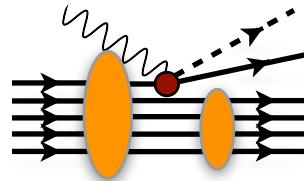


N. Rocco, et al. PRC 99 025502 (2019)

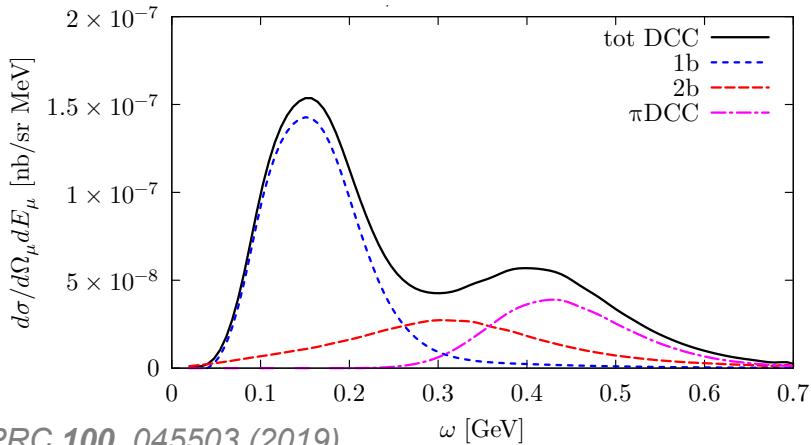
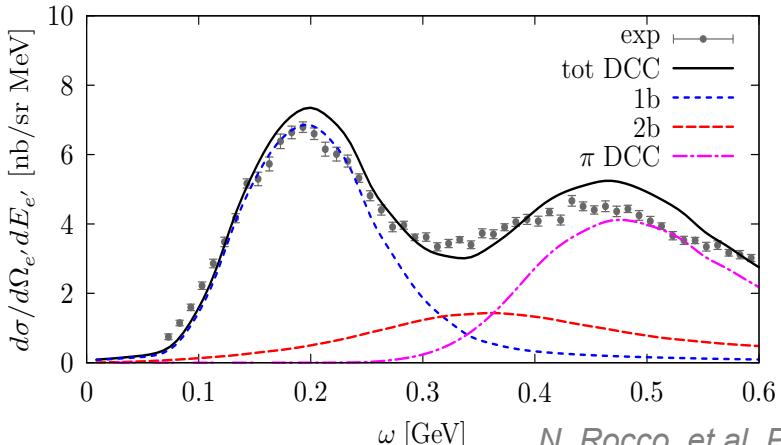
EXTENDED FACTORIZATION SCHEME

The factorization scheme can be further extended to include real pions in the final state

$$|\Psi_f^A\rangle \rightarrow |p_1, p_\pi\rangle \otimes |\Psi_f^{A-1}\rangle$$



The DCC model, suitable to accurately describe single-nucleon pion-production, is folded with a realistic spectral function

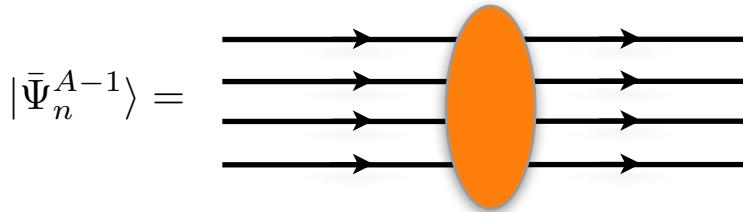


QMC-BASED SPECTRAL FUNCTION

The hole spectral function is a sum of two contributions

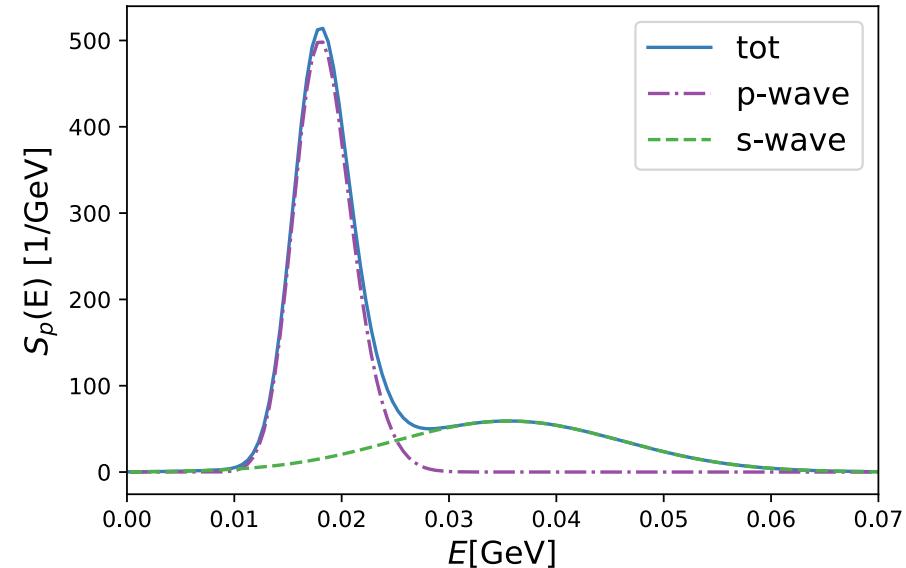
$$P_h(\mathbf{k}, E) = \sum_n |\langle \Psi_0^A | [k] \times |\Psi_n^{A-1} \rangle|^2 \delta(E + E_0^A - E_n^{A-1}) = P_h^{MF}(\mathbf{k}, E) + P_h^{corr}(\mathbf{k}, E)$$

Mean-field component



$$P_h^{MF}(\mathbf{k}, E) = \sum_n |\langle \Psi_0^A | [k] \times |\bar{\Psi}_n^{A-1} \rangle|^2$$
$$\times \delta\left(E - B_0^A + B_n^{A-1} - \frac{k^2}{2M^{A-1}}\right)$$

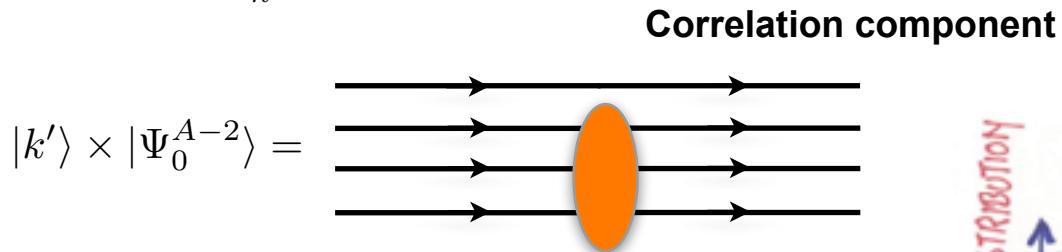
Computed using VMC spectroscopic overlaps



QMC-BASED SPECTRAL FUNCTION

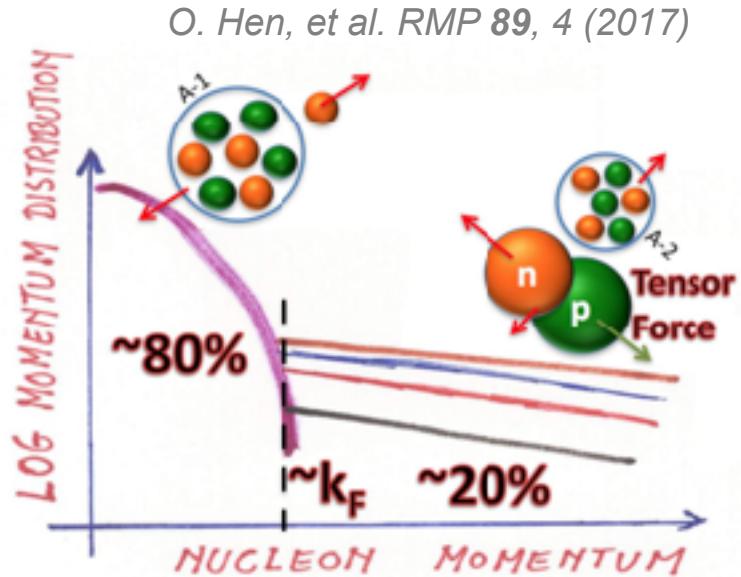
The hole spectral function is a sum of two contributions

$$P_h(\mathbf{k}, E) = \sum_n |\langle \Psi_0^A | [k] \times |\Psi_n^{A-1} \rangle|^2 \delta(E + E_0^A - E_n^{A-1}) = P_h^{MF}(\mathbf{k}, E) + P_h^{corr}(\mathbf{k}, E)$$



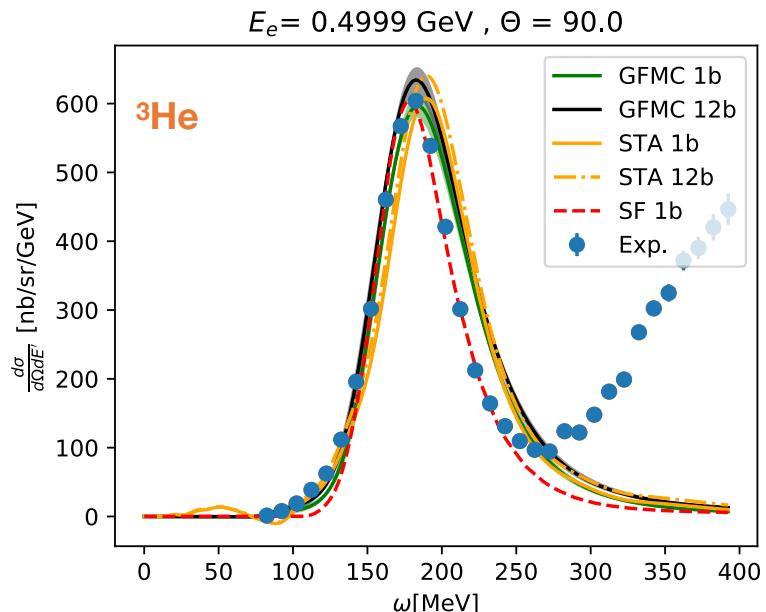
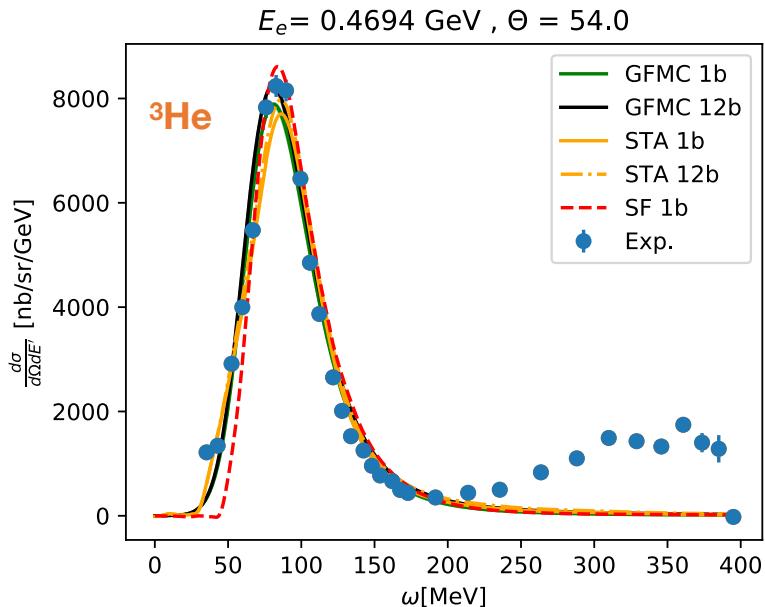
$$\begin{aligned} P_h^{corr}(\mathbf{k}, E) &\simeq \sum_{k'} |\langle \Psi_0^A | [kk'] \times |\bar{\Psi}_0^{A-2} \rangle|^2 \\ &\times \delta\left(E - B_0^A - e(k') + B_0^{A-2} - \frac{(\mathbf{k} + \mathbf{k}')^2}{2M^{A-2}}\right) \end{aligned}$$

Computed from the short-range contributions
of VMC two-body momentum distributions



QMC-BASED SPECTRAL FUNCTION

We compare the inclusive electron- ${}^3\text{He}$ cross section obtained with the QMC spectral functions and those computed within the GFMC and STA approaches

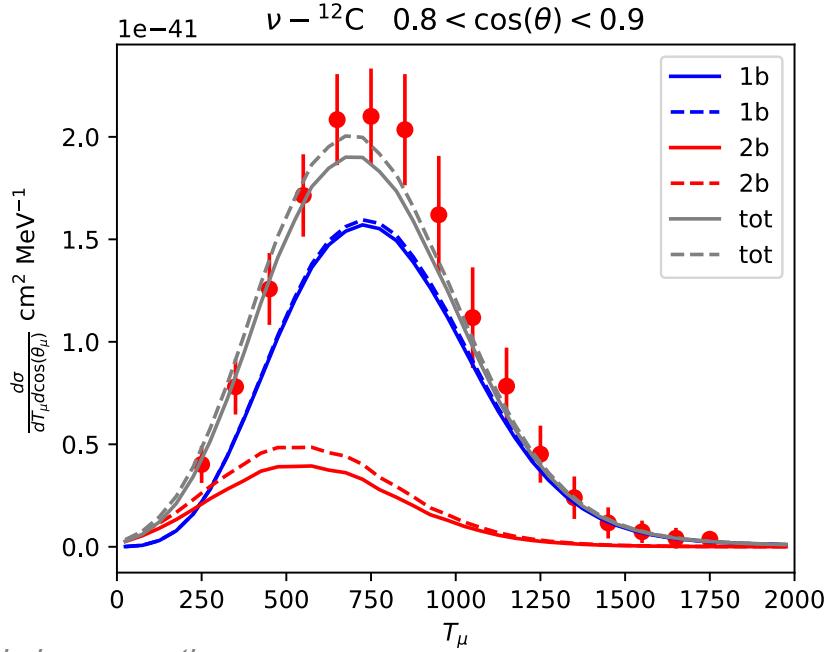
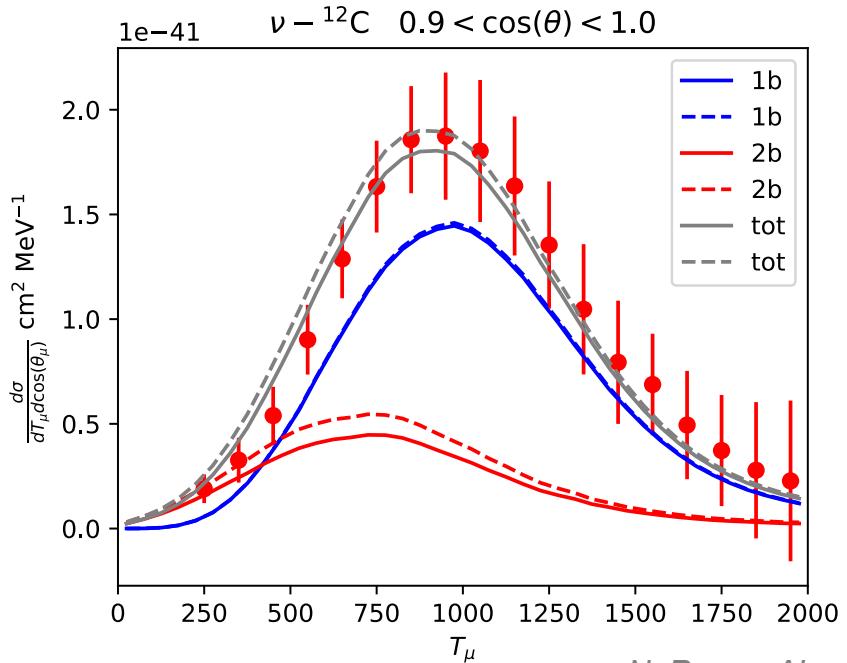


L. Andreoli, AL, et al. PRC 105, 014002 (2022)

We are using the same strategy to compute the spectral function of ${}^{12}\text{C}$.

QMC-BASED SPECTRAL FUNCTION

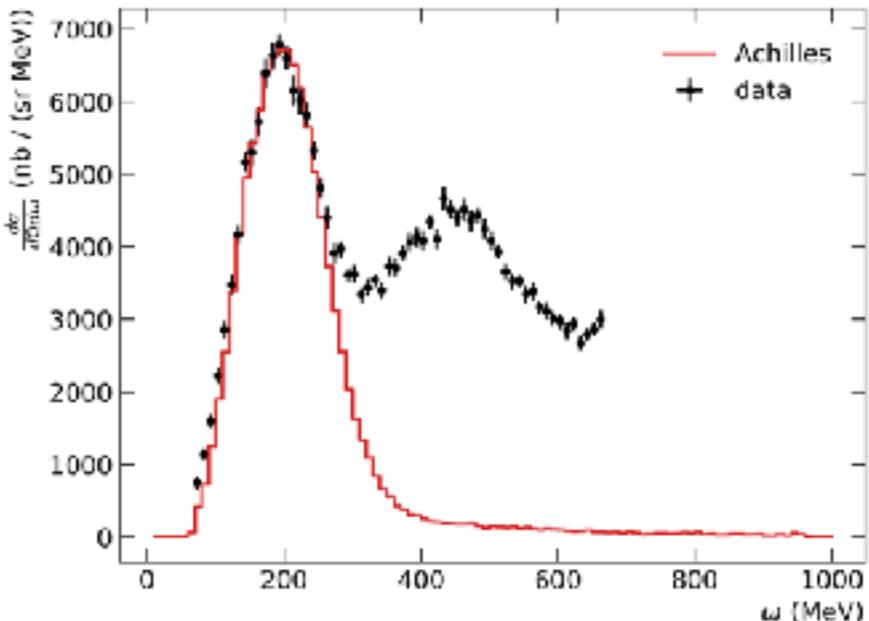
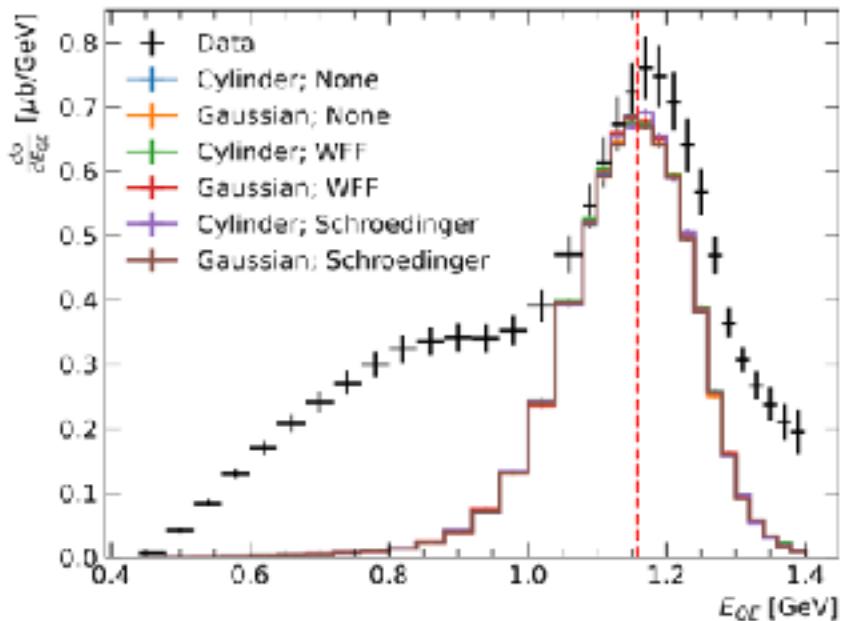
Using the QMC-based spectral function, we computed the flux-folded doubly-differential cross section of $\nu - {}^{12}\text{C}$ scattering and compared with MiniBooNE data.



N. Rocco, AL, et al., in preparation

QMC-BASED EVENT GENERATORS

We have developed “ACHILLES”: an theory-driven, event generator for lepton-nucleus scattering based on state of the art nuclear-theory approaches;



J. Isaacson, AL, et al. arXiv:2205.06378

SUMMARY AND OUTLOOK

Inclusive scattering from quantum Monte Carlo

- Validated our approach on electron- ^{12}C scattering
- Two-body currents enhance electromagnetic and charged-current responses
- Good agreement with MiniBooNE and T2K inclusive data  First ab-initio results!
- Use the AFDMC and ML methods to reach ^{16}O (and beyond)

Extended factorization scheme

- Two-body currents and pion-production are essential to reproduce electron-scattering data
- Need to treat two-pion production and deep-inelastic scattering regions;
- Using VMC to construct an “ab initio” spectral function;

QMC-based event generator

- Developed “ACHILLES”: an theory-driven, event generator;
- Josh Isaacson’s talk

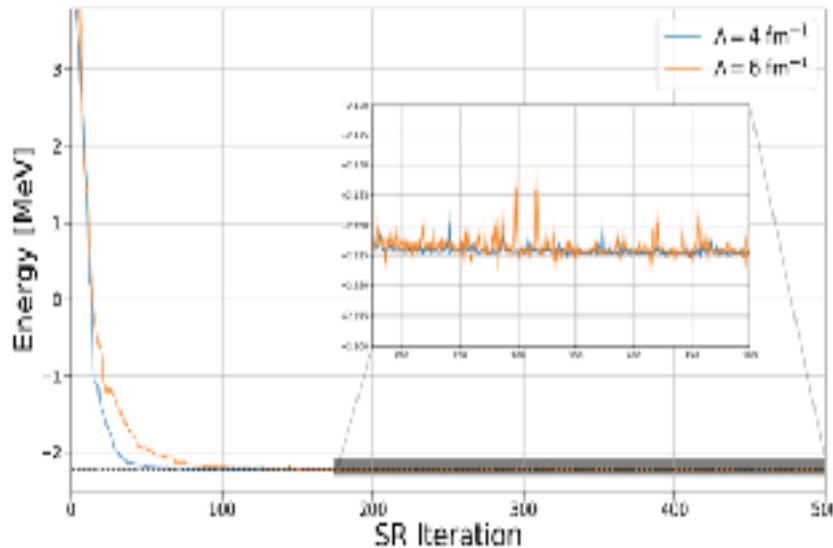
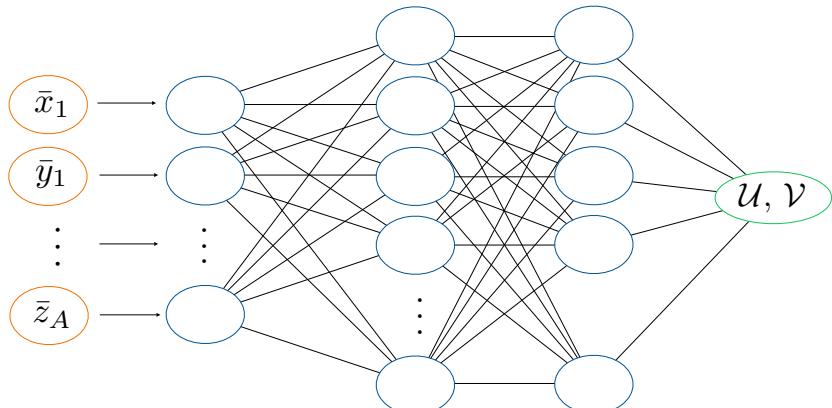
BACKUP SLIDES

SOME PERSPECTIVES

Machine learning methods allows to devise accurate nuclear wave functions suitable for quantum Monte Carlo calculations that do not scale exponentially with the number of nucleons;

We developed neural quantum states suitable to solve the nuclear many-body problem

$$|\Psi_V^{\text{ANN}}\rangle = e^{\mathcal{U}(\mathbf{r}_1, \dots, \mathbf{r}_A)} \tanh[\mathcal{V}(\mathbf{s}_1, \mathbf{r}_1, \dots, \mathbf{r}_A, \mathbf{s}_A)] |\Phi\rangle$$

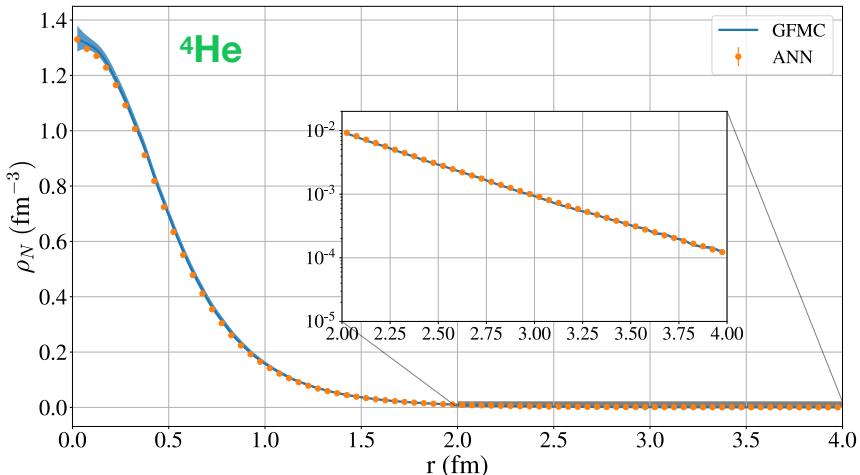


SOME PERSPECTIVES

For a LO pionless-EFT Hamiltonian the ANN outperforms conventional Variational Monte Carlo ansatz and perfectly reproduces the density profile of the nucleus, including the slow decaying tails;

	Λ	VMC-ANN	VMC-JS	GFMC	GFMC _e
² H	4 fm ⁻¹	-2.224(1)	-2.223(1)	-2.224(1)	-
	6 fm ⁻¹	-2.224(4)	-2.220(1)	-2.225(1)	-
³ H	4 fm ⁻¹	-8.26(1)	-7.80(1)	-8.38(2)	-7.82(1)
	6 fm ⁻¹	-8.27(1)	-7.74(1)	-8.38(2)	-7.81(1)
⁴ He	4 fm ⁻¹	-23.30(2)	-22.54(1)	-23.62(3)	-22.77(2)
	6 fm ⁻¹	-24.47(3)	-23.44(2)	-25.06(3)	-24.10(2)

The small differences with the exact GFMC result are to be resolved by spin-dependent backflow correlations

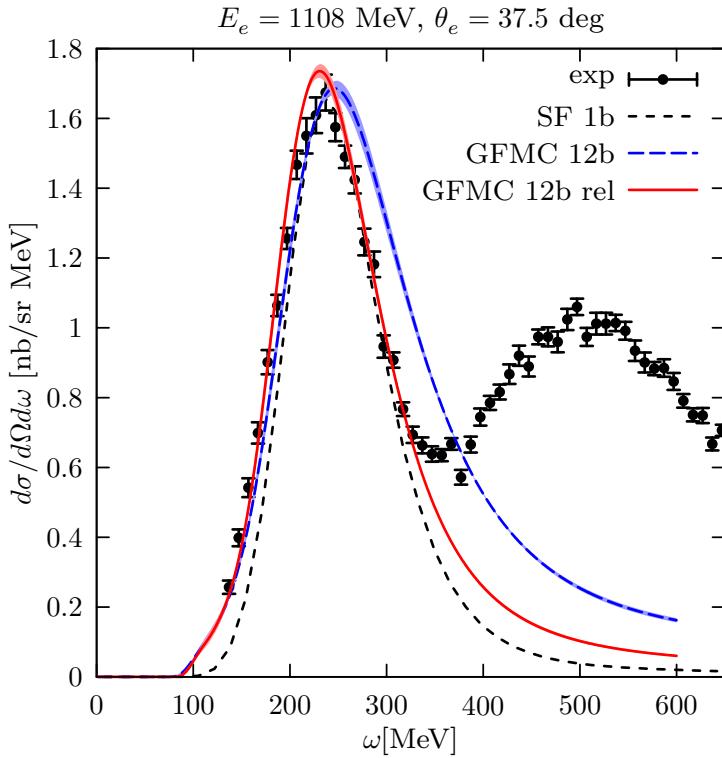
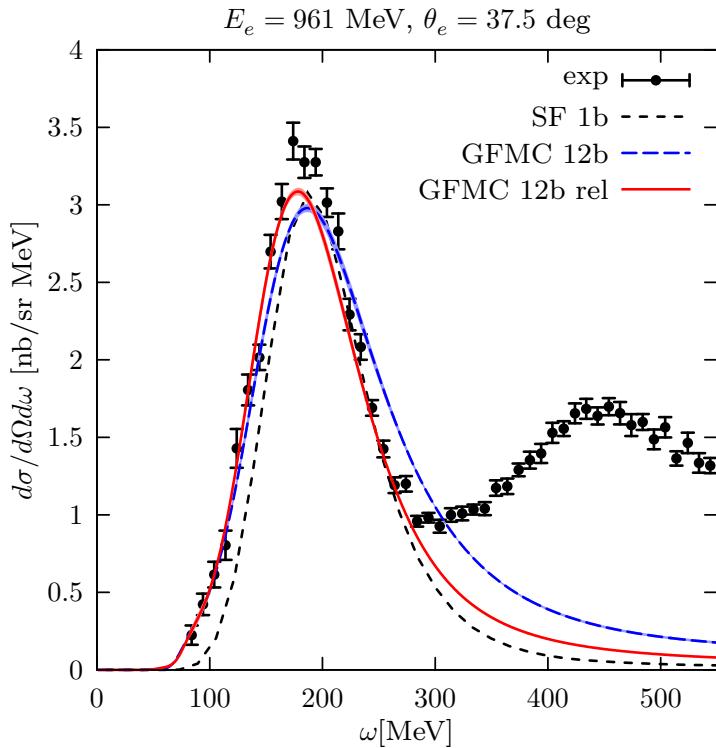


This algorithm exhibits a favorable polynomial scaling and it is amenable to compute real-time dynamics;

$$i \frac{\partial \Psi_V^{ANN}}{\partial t} = H \Psi_V^{ANN}$$

Time-dependent VMC
algorithm

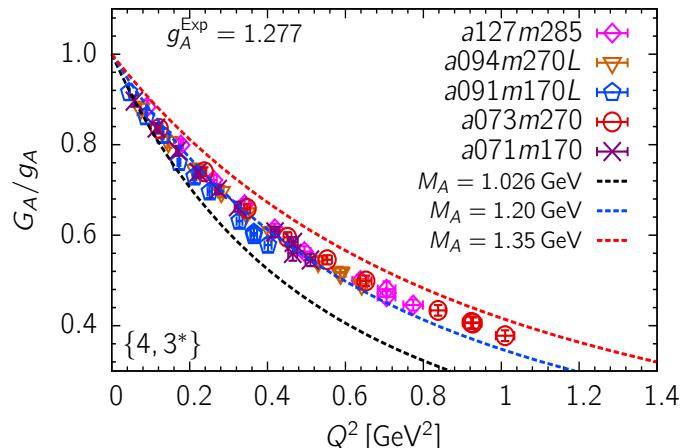
RELATIVISTIC EFFECTS



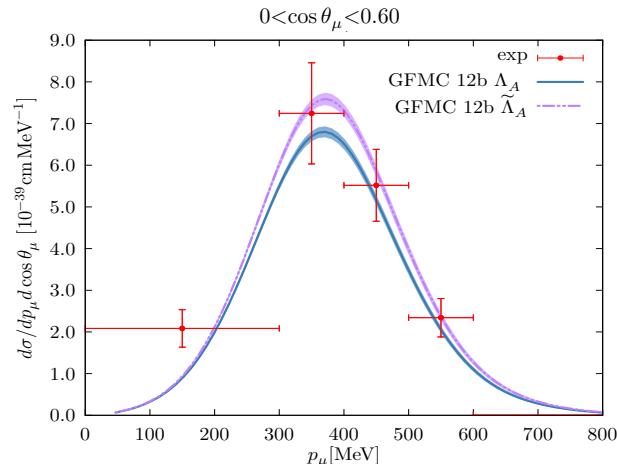
LQCD INPUTS

The success of the neutrino-oscillation program relies on accurate estimates of neutrino-nucleus interactions.

- Need for prompt comparisons between nuclear-theory prediction and experiments



NME collaboration (preliminary)



AL et al., Phys. Rev. X 10, 031068 (2020)