# QMC calculations of nuclear responses: beyond Carbon

Workshop on Software Infrastructure for Advanced Nuclear Physics Computing

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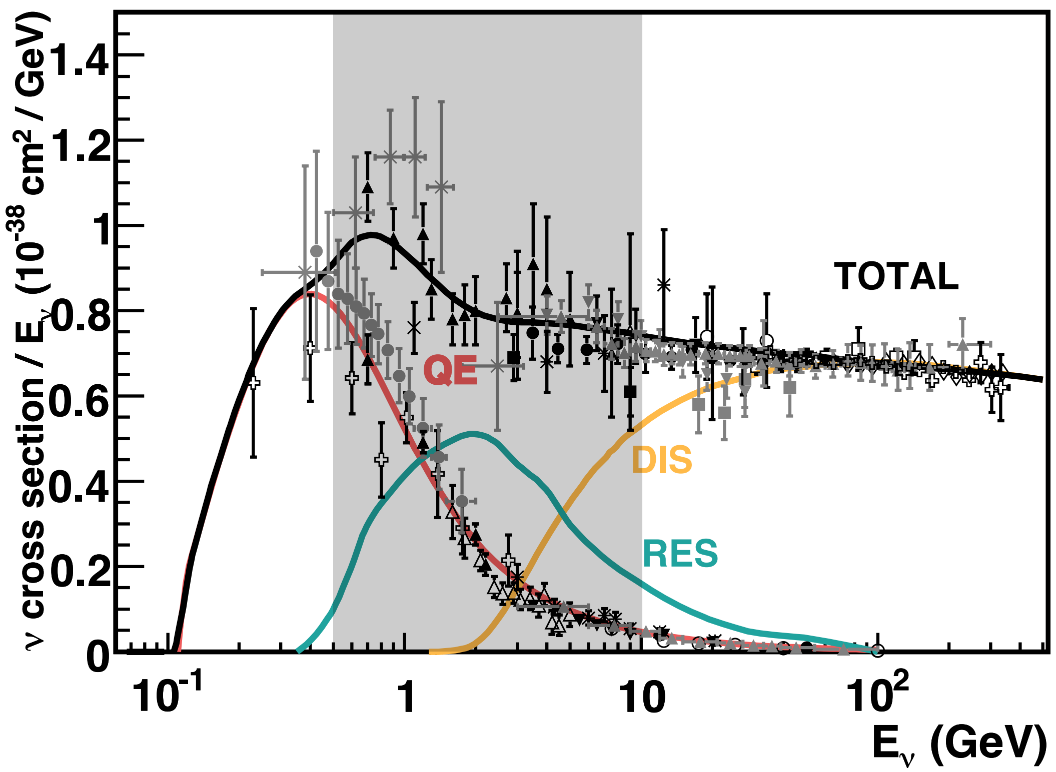
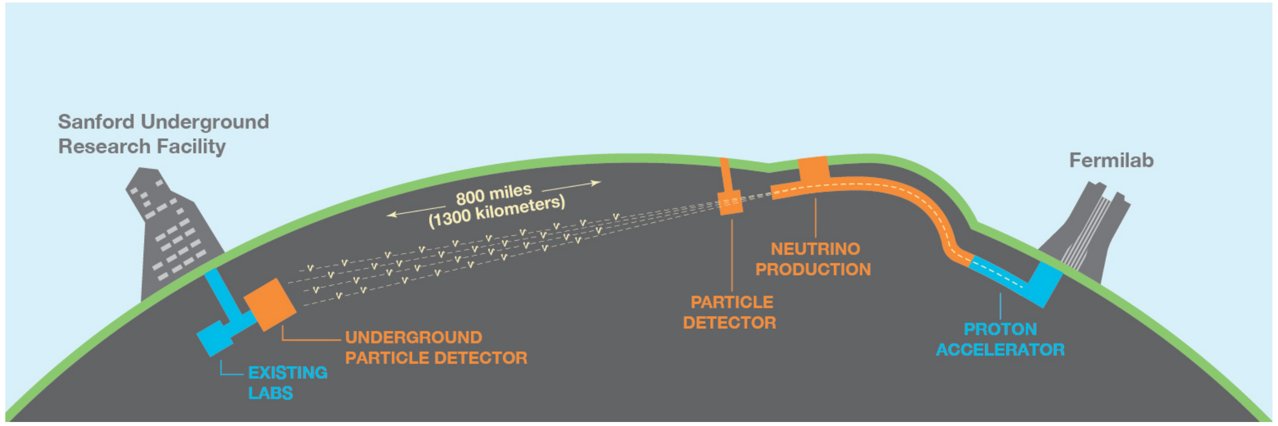
# Lepton-nucleus scattering

Theoretical understanding of **nuclear effects** is extremely important for **electron** and **neutrino** experimental programs: oscillation experiments require accurate calculations of cross sections




Electron scattering can be used to test our nuclear model:

- **same nuclear effects**
- **no need to reconstruct energies**
- **abundant experimental data**

# Lepton-Nucleus scattering: Inclusive Processes

Electromagnetic Nuclear Response Functions

$$R_\alpha(q,\omega) = \sum_f \delta(\omega + E_0 - E_f) |\langle f | O_\alpha(\mathbf{q}) | 0 \rangle|^2$$

Longitudinal response induced by $O_L = \rho$

Transverse response induced by $O_T = j$

$$\frac{d^2\sigma}{d\omega d\Omega} = \sigma_M [v_L R_L(\mathbf{q},\omega) + v_T R_T(\mathbf{q},\omega)]$$

One can exploit integral properties of the response functions to avoid explicit calculation of the final states: **GFMC** Euclidean response, **CC** LIT

# Short-time approximation

S. Pastore, J. Carlson, S. Gandolfi, R. Schiavilla, and R. B. Wiringa PRC101(2020)044612

Factorization scheme:

- describe electroweak scattering from $A \geq 12$ without losing **two-body physics**
- account for **exclusive processes**
- incorporate **relativistic effects**

# Short-time approximation: $^{12}C$

QMC Calculations of nuclear response **densities**, response **functions** and **cross sections** within the STA (quasielastic regime)

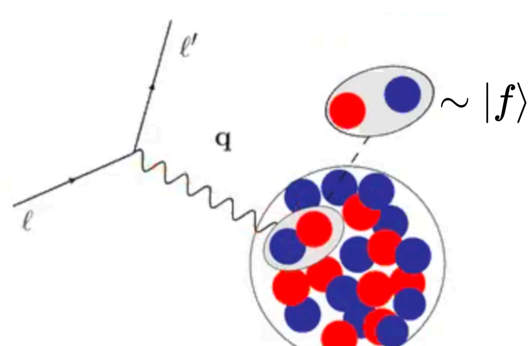
Correctly reproduces experimental data for electron energies from ~300 to 1600 MeV

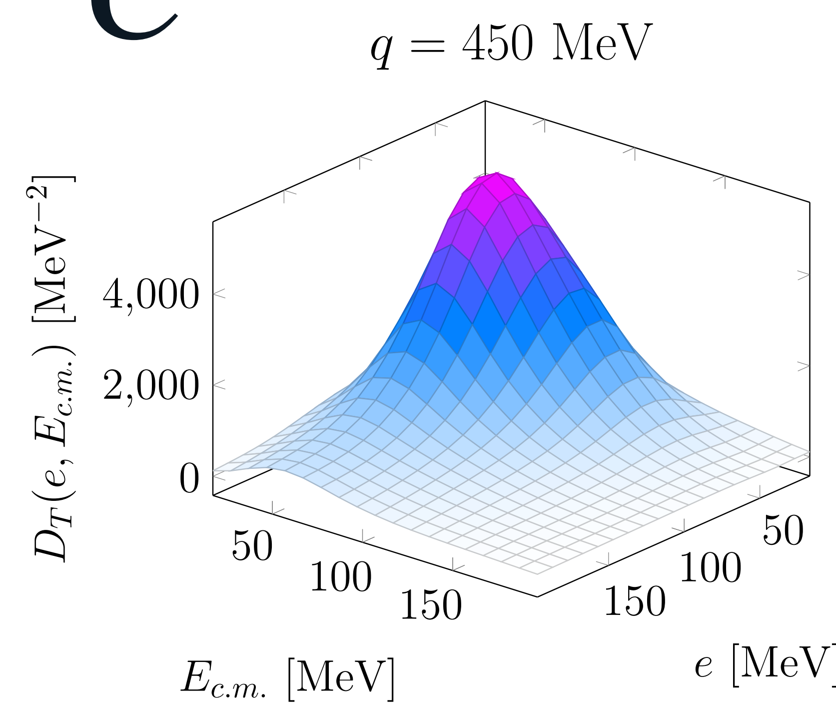
$$R_\alpha(q,\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i(\omega+E_i)t} \langle \Psi_i | O_\alpha^\dagger(\mathbf{q}) e^{-iHt} O_\alpha(\mathbf{q}) | \Psi_i \rangle$$

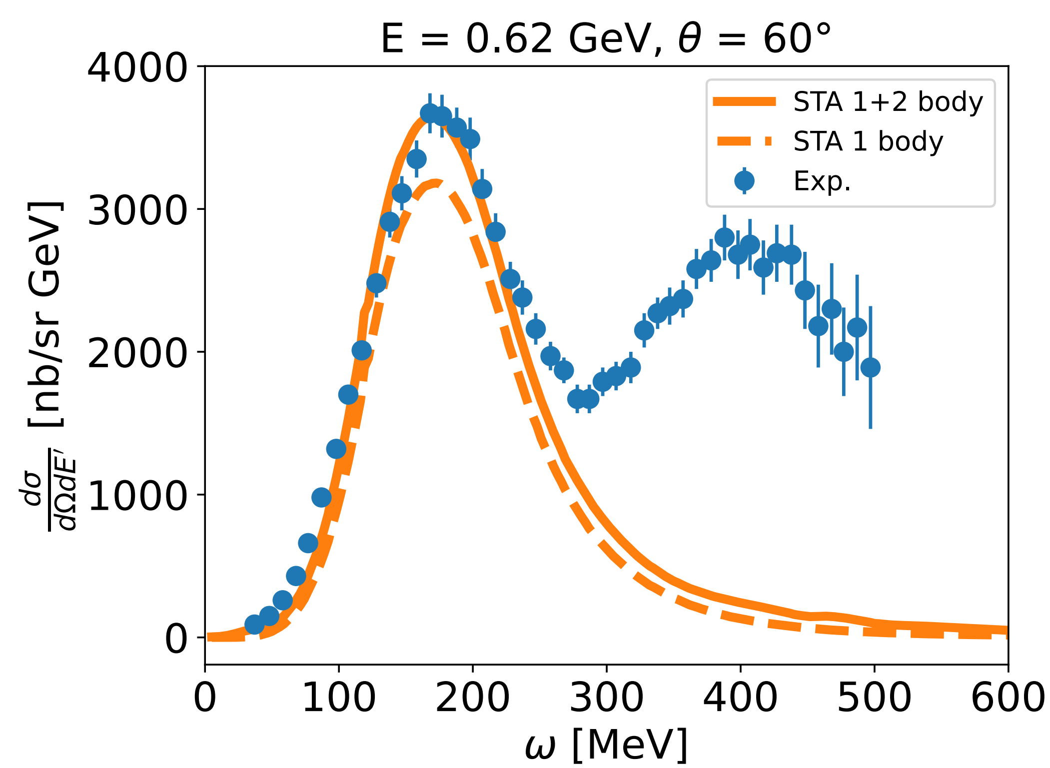
$$R^{\mathrm{STA}}(q,\omega) \sim \int \delta(\omega + E_0 - E_f) de\, dE_{cm} \mathcal{D}(e, E_{cm}; q)$$

$$\begin{aligned} O^\dagger e^{-iHt} O &= \left(\sum_i O_i^\dagger + \sum_{i<j} O_{ij}^\dagger\right) e^{-iHt} \left(\sum_{i'} O_{i'} + \sum_{i'<j'} O_{i'j'}\right) \\ &= \sum_i O_i^\dagger e^{-iHt} O_i + \sum_{i\neq j} O_i^\dagger e^{-iHt} O_j \\ &+ \sum_{i\neq j} \left( O_i^\dagger e^{-iHt} O_{ij} + O_{ij}^\dagger e^{-iHt} O_i \right. \\ &\left. + O_{ij}^\dagger e^{-iHt} O_{ij} \right) + \dots \end{aligned}$$

Interference






In preparation L. Andreoli et al.

# Many-body nuclear problem

Many-body Nuclear Hamiltonian in coordinate space:

$$H = \sum_i T_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk}$$

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A, s_1, s_2, \ldots, s_A, t_1, t_2, \ldots, t_A)$$

$\psi$ are complex spin-isospin vectors in $3A$ dimensions with components $2^A \times \dfrac{A!}{Z!(A-Z)!}$

$^4$He: 96

$^6$Li: 1280

$^8$Li: 14336

$^{12}$C: 540572

# Many-body nuclear problem

few node hours

$^{4}$He: 96

$^{6}$Li: 1280

$^{8}$Li: 14336

$^{12}$C: 540572


~100k node hrs

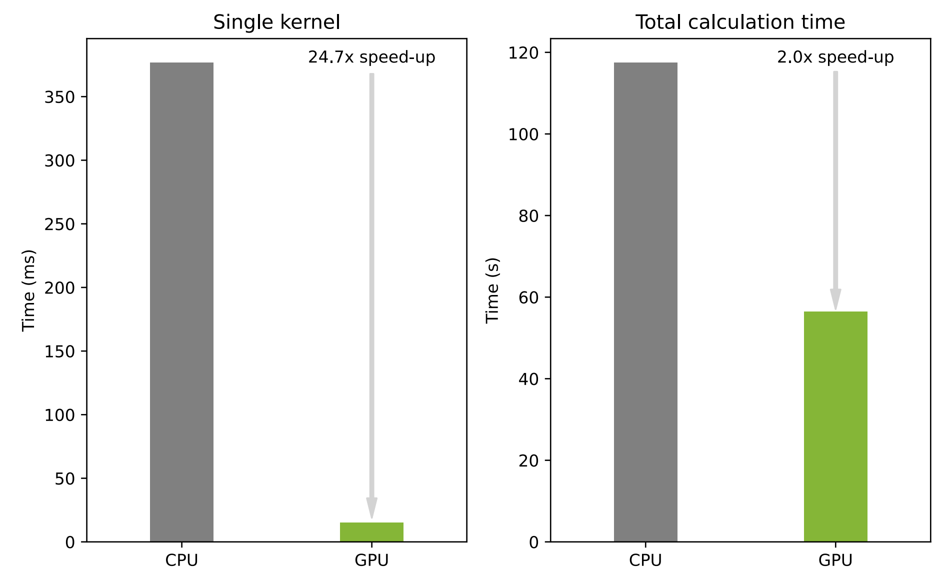

Beyond $^{12}C$:

- Getting ready for **Aurora**: refactoring of QMC codes, porting to GPU (see A. Flores' talk)
- STA with **AFDMC** (S. Gandolfi)

# Refactoring of QMC codes & GPU

**2023:**

- ALCF INCITE Hackathon, discrete success in porting to GPU calculation of wave function (tested on $^{12}C$)
- We realized that a major refactoring of the code was necessary




**2024:**

- Refactoring of VMC code in **final stages** (A. Flores, P.Fasano)
- The refactoring effort and porting to GPU will allow us to fully exploit next-generation HPC architectures
- STA can be easily adapted to the new code
- Codes have been moved to Perlmutter, thanks to the **NTNP** allocation at NERSC

# Thank you!

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