Quantum Monte Carlo calculations of electron scattering for A≤12 nuclei in the Short-Time Approximation

Joint Group Meeting

Quantum Monte Carlo Group @ WashU

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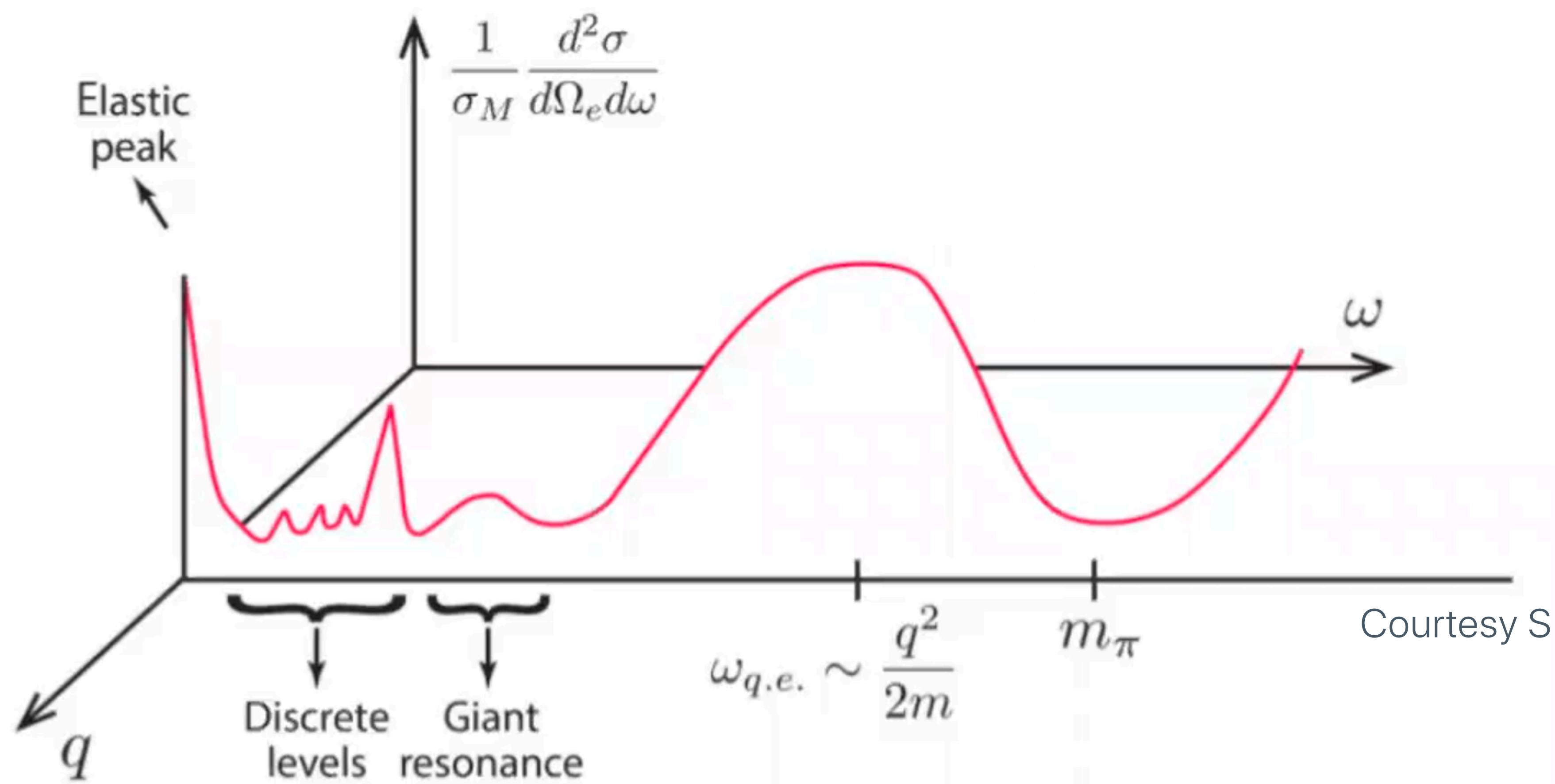
Electron-nucleus scattering

Theoretical understanding of nuclear effects is extremely important for experimental programs



Courtesy S. Pastore

Ab-initio description of nuclei

- Nuclear interaction
- Electroweak interaction of leptons with nucleons
- Computational method

Many-body nuclear interaction

Many-body Nuclear Hamiltonian: Argonne v_{18} + Urbana IX

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

Quantum Monte Carlo methods:
Use nuclear wave functions that minimize the expectation value of E

$$E_V = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \geq E_0$$

The evaluation is performed using Metropolis sampling

Nuclear Wave Functions

Variational wave function for nucleus in J state

$$|\psi\rangle = \mathcal{S}\prod_{i<j}^{A}\left[1 + U_{ij} + \sum_{k\neq i,j}^{A} U_{ijk}\right]\left[\prod_{i<j} f_c(r_{ij})\right]|\Phi(JMTT_3)\rangle$$

Two-body spin- and isospin-dependent correlations

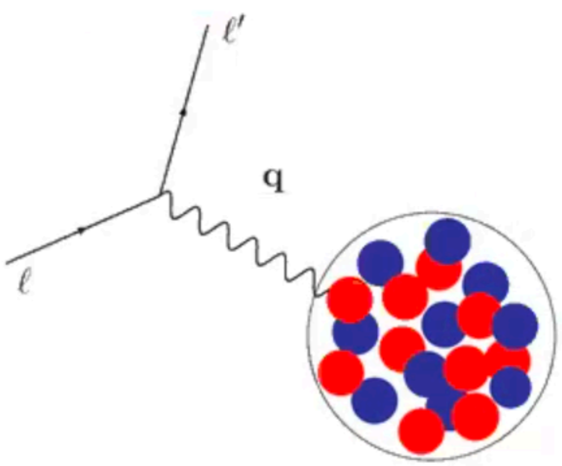
$$U_{ij} = \sum_p f^p(r_{ij})\, O^p_{ij}$$

$$O^p_{ij} = [1, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}] \otimes [1, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j]$$

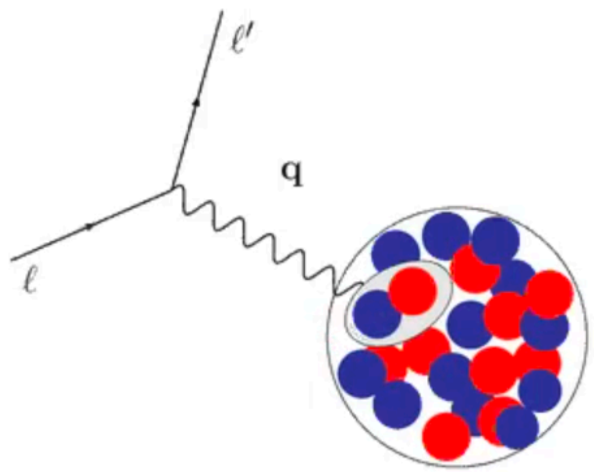
$$U_{ijk} = \epsilon v_{ijk}(\bar{\boldsymbol{r}}_{ij}, \bar{\boldsymbol{r}}_{jk}, \bar{\boldsymbol{r}}_{ki})$$

Electromagnetic interactions

The interaction with external probes is described in terms on one- and two-body charge and current operators



one-body



two-body

Charge operators

$$\rho = \sum_{i=1}^{A} \rho_i + \sum_{i<j} \rho_{ij} + \dots$$

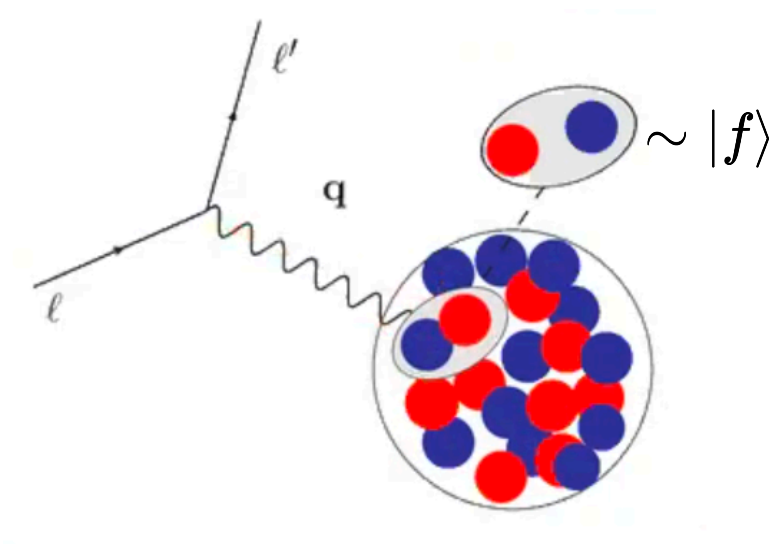
Current operators

$$\mathbf{j} = \sum_{i=1}^{A} \mathbf{j}_i + \sum_{i<j} \mathbf{j}_{ij} + \dots$$

Short-time approximation

Pastore et al. PRC101(2020)044612

Quasilastic scattering cross sections are expressed in terms of response function



The sum over all final states is replaced by a two nucleon propagator

Response functions

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

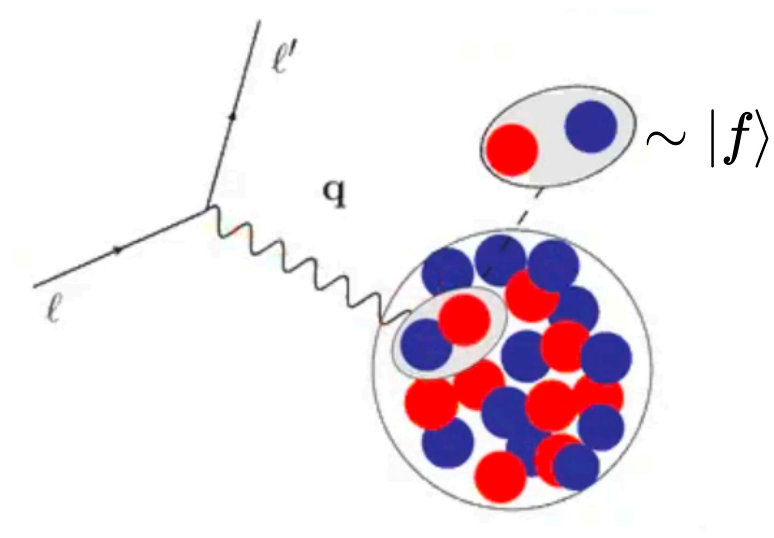
$$R_\alpha(q,\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i(\omega+E_i)t} \left\langle \Psi_i \middle| O_\alpha^\dagger(\mathbf{q}) e^{-iHt} O_\alpha(\mathbf{q}) \middle| \Psi_i \right\rangle$$

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

Short-time approximation

Pastore et al. PRC101(2020)044612

Quasilastic scattering cross sections are expressed in terms of response function



Response functions

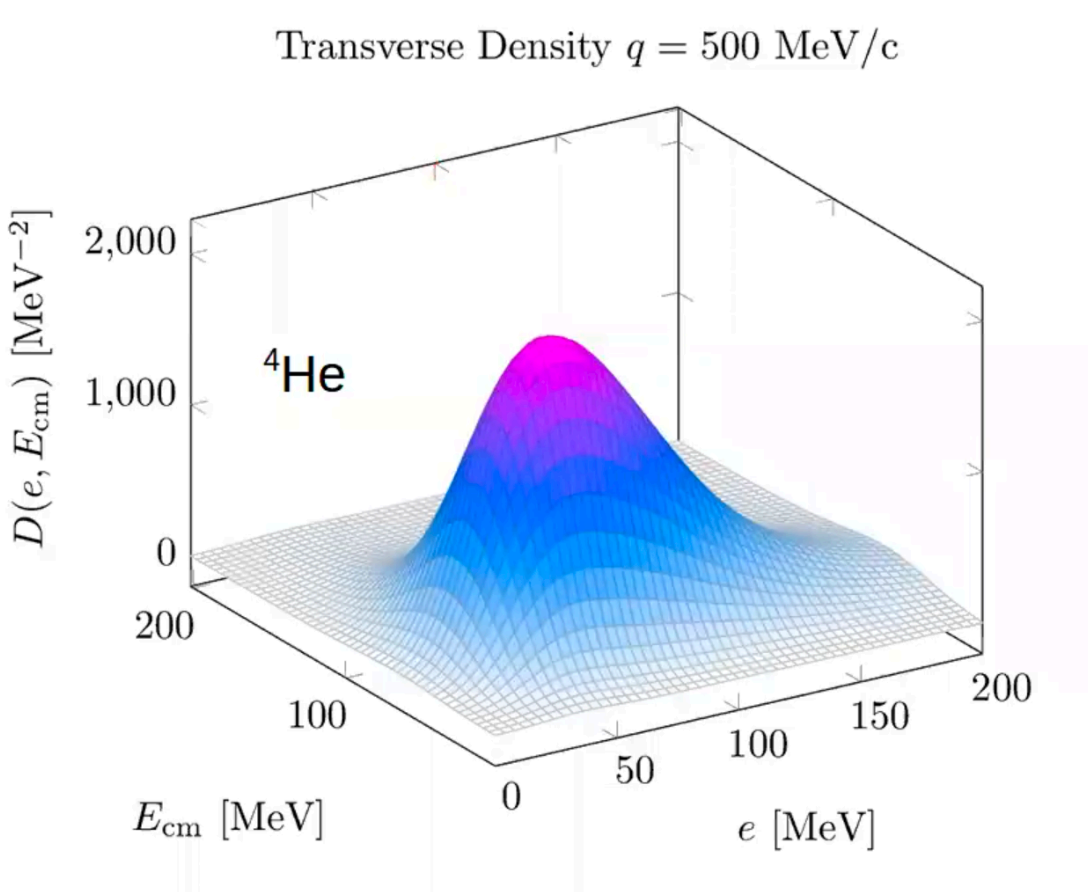
$$R_\alpha(q,\omega) = \sum_f \delta(\omega + E_0 - E_f) |\langle f | O_\alpha(\mathbf{q}) | 0 \rangle|^2$$

Response densities

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

STA: scattering of a correlated pair of nucleons inside a nucleus

Transverse response density

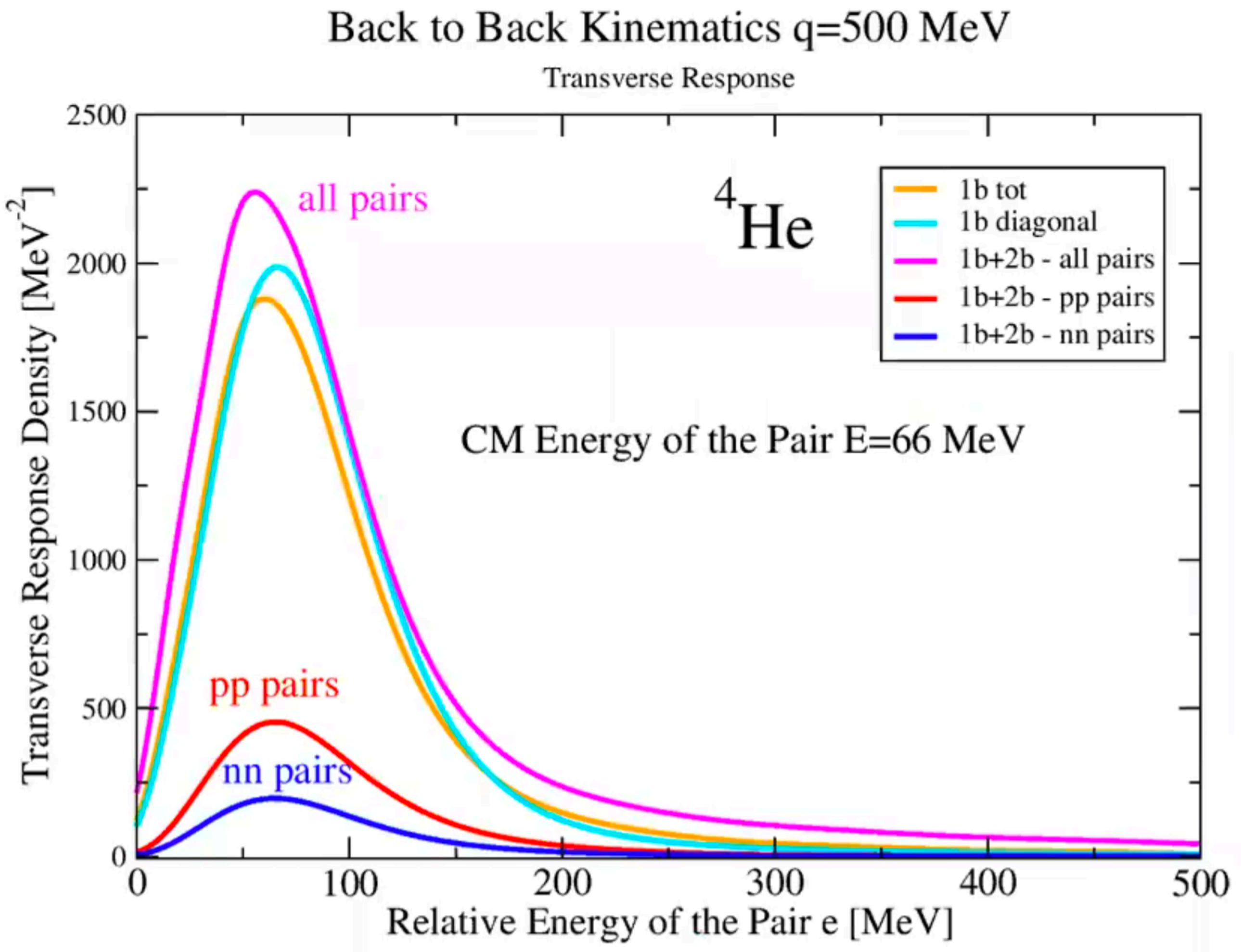


Electron scattering from $^4\mathrm{He}$:

- Response density as a function of (E,e)
- Give access to particular kinematics for the struck nucleon pair

Pastore et al. PRC101(2020)044612

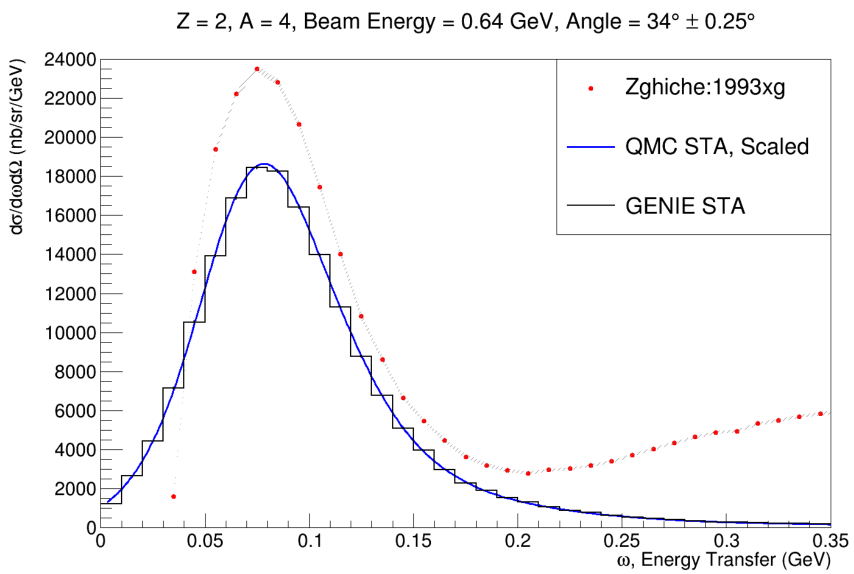
Back-to-back kinematic

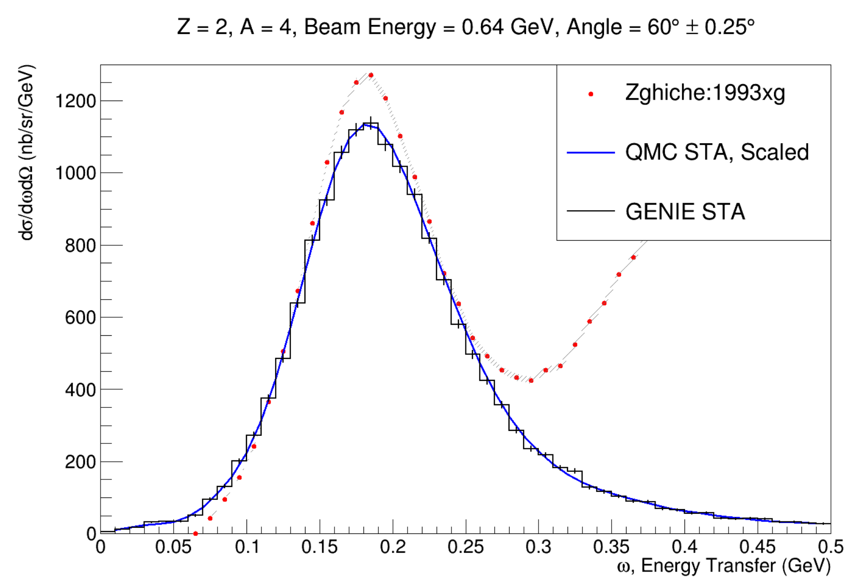


We can select a particular kinematic, and assess the contributions from different particle identities

Pastore et al. PRC101(2020)044612

STA + GENIE





- Response densities as input to event generators
- Consistent two body physics
- 1+2 body interference terms

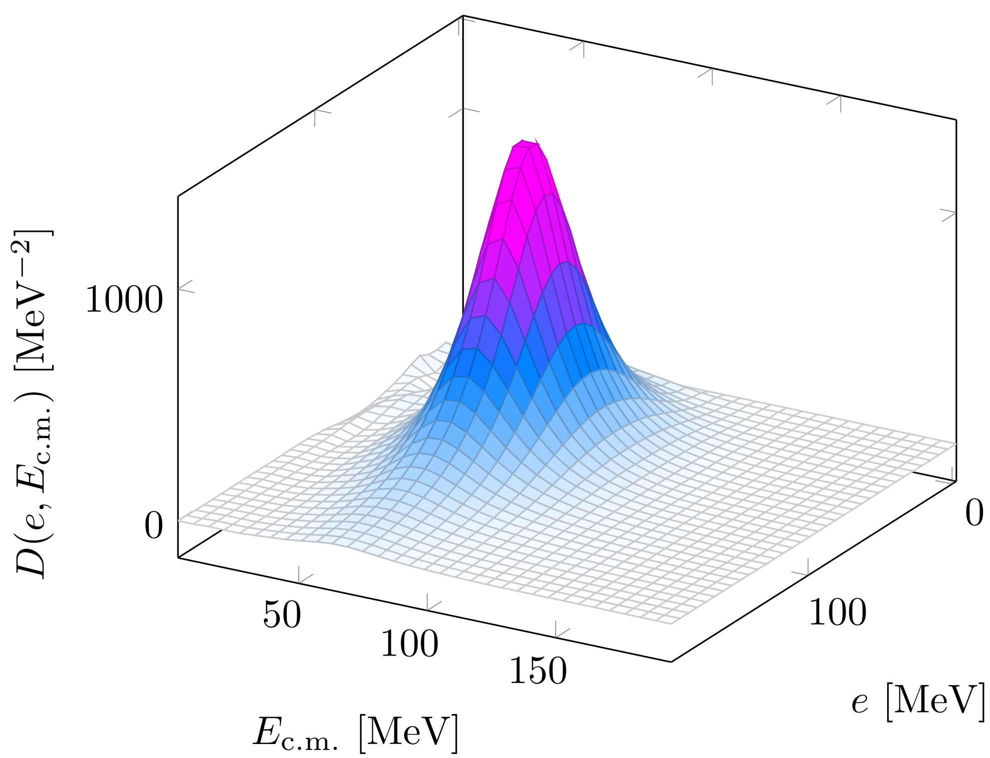
J. L. Barrow, S. Gardiner, S. Pastore, M. Betancourt, J. Carlson. arxiv.org/abs/2010.04154

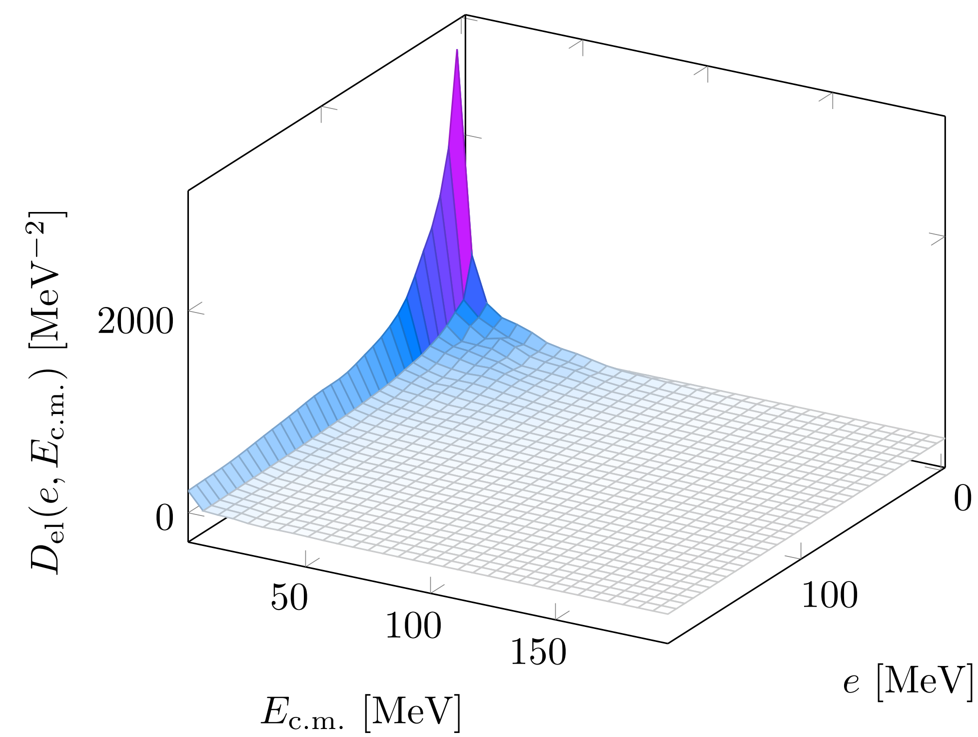
Elastic contribution

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

$$\mathcal{D}(e, E_{\mathrm{cm}}) - \mathcal{D}_{\mathrm{el}}(e, E_{\mathrm{cm}})$$

$$\mathcal{D}_{el}(\mathbf{q}, \mathbf{p}', \mathbf{P}') = |\langle\Psi_0|J(\mathbf{q})|\Psi_0\rangle|^2 \times \sum_{\beta}\langle\Psi_0 \mid \Psi_2(\mathbf{p}', \mathbf{P}', \beta)\rangle\langle\Psi_2(\mathbf{p}', \mathbf{P}', \beta) \mid \Psi_0\rangle$$





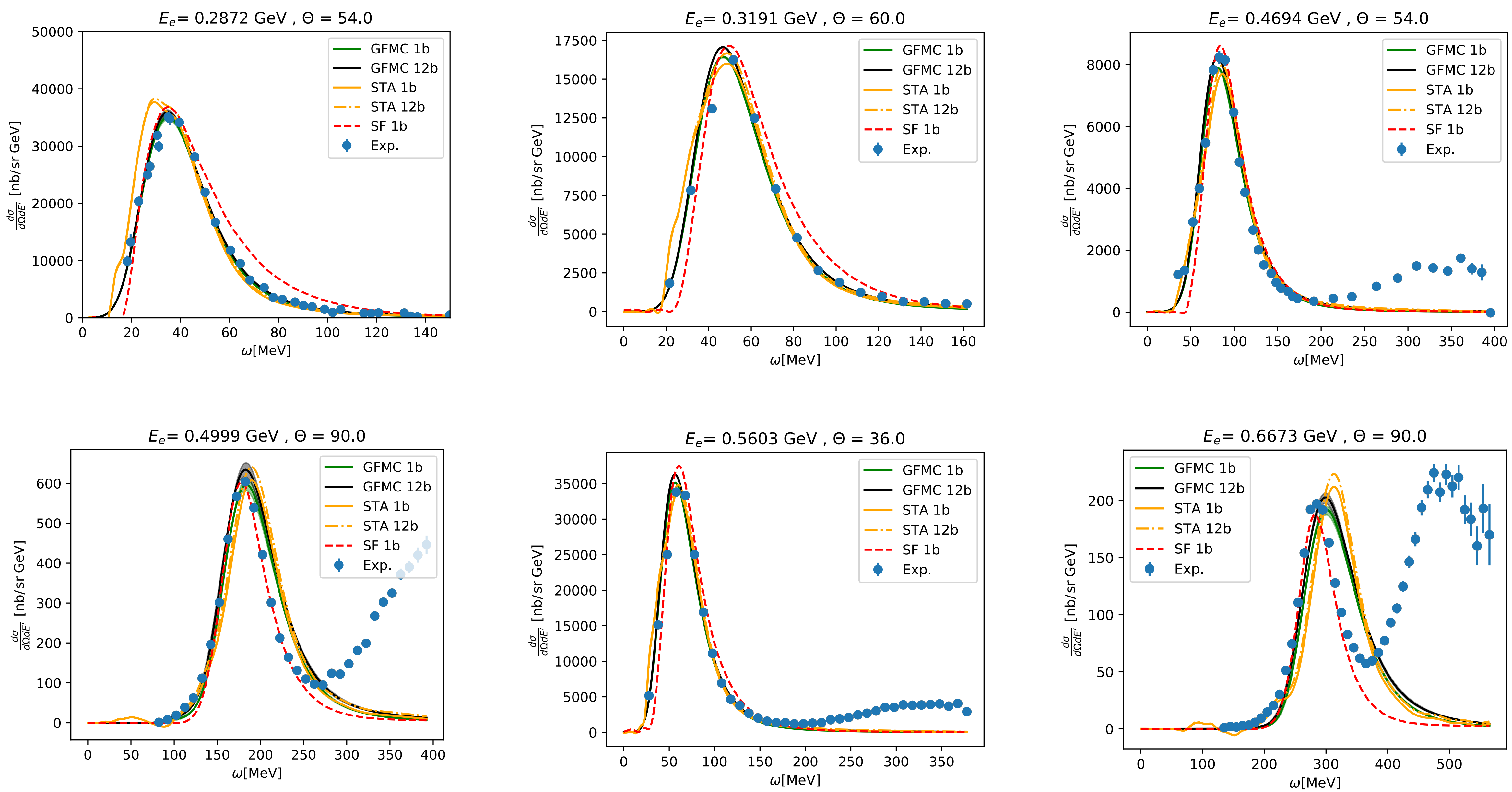
^{3}H Longitudinal response at 300 MeV

L.A., J. Carlson, A. Lovato, S. Pastore, N. Rocco, R. B. Wiringa. arXiv:2108.10824

Cross sections

LA et al. arXiv:2108.10824

^{3}He

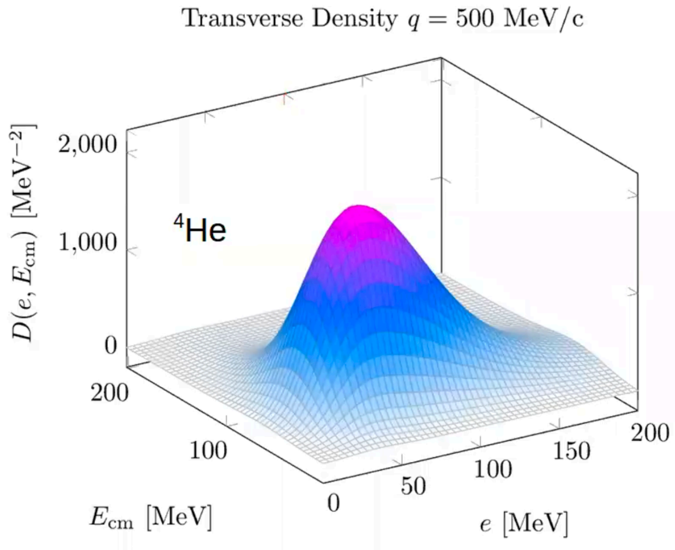


Heavier nuclei

Computational complexity of response functions and densities:

Wave-function		^{4}He	^{12}C
Spin	2^A	16	4096
Isospin	$\dfrac{A!}{Z!(A-Z)!}$	6	924
Pairs	$A(A-1)/2$	6	66

Response densities: E, e grid



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

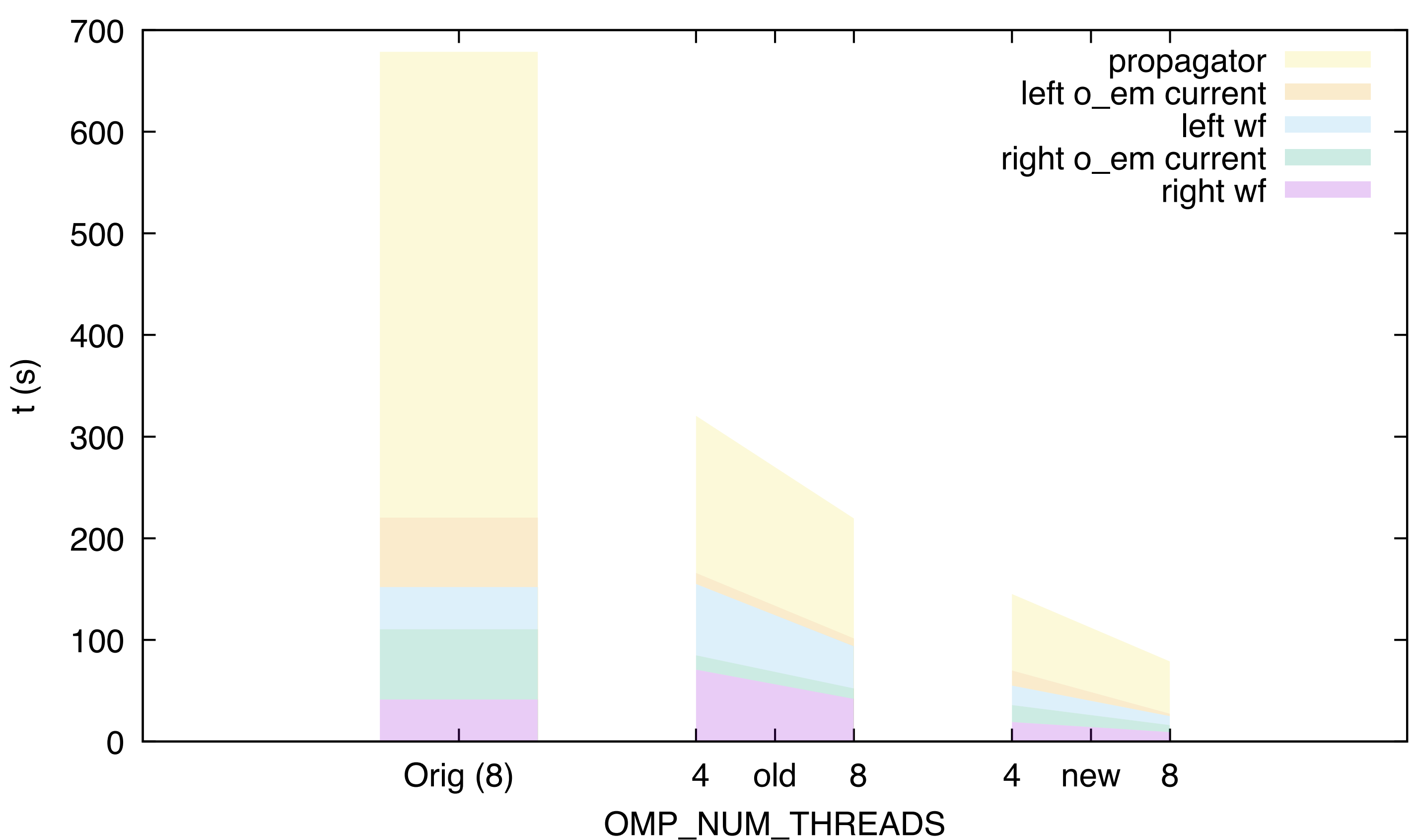
Heavier nuclei

Optimization was necessary to tackle heavier nuclei

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

- Parallelization – MPI and OpenMP:
  Variational Monte Carlo is almost perfectly parallelizable, but with increased system size memory becomes a constrain
- Refactoring of the code
- Computational algorithms and approximations

Progress on ^{12}C



Optimization specific to ^{12}C was needed in oder to perform full response densities calculations:

- **parallelization**
- **refactoring of the code**

Recent progress in em currents and wave function evaluation

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

Heavier nuclei

Comparison for ^3H, 72k MC configurations, 40x40 points in r, R integration

Original:

- ~15k core hours
  (LA et al arXiv:2108.10824)

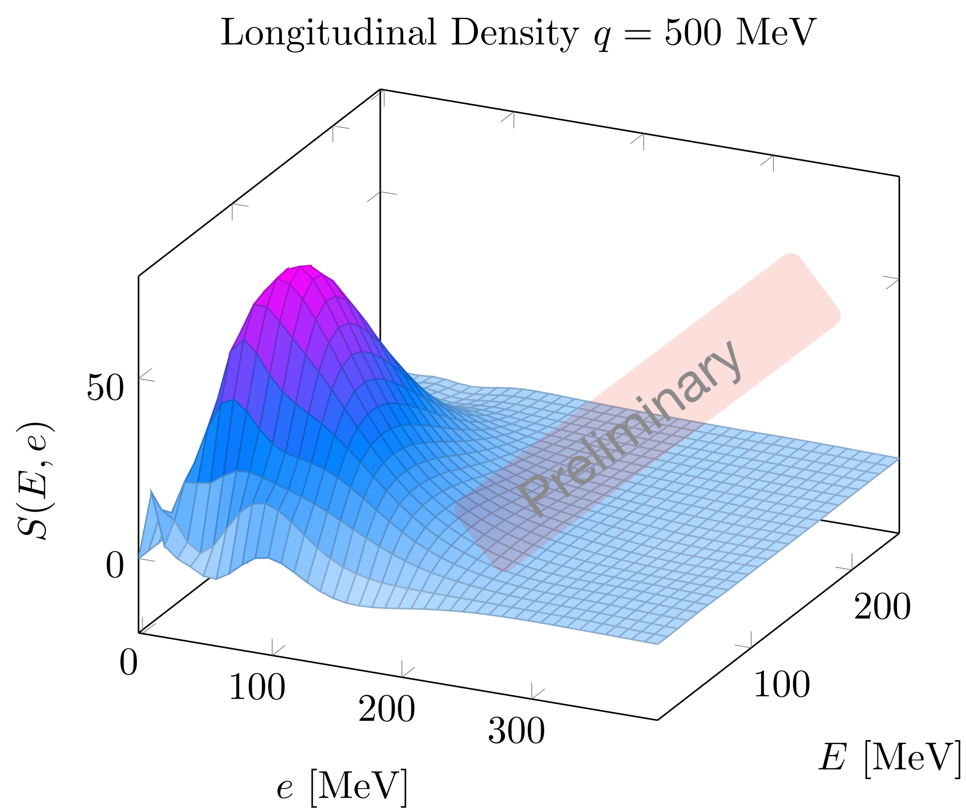
After optimization:

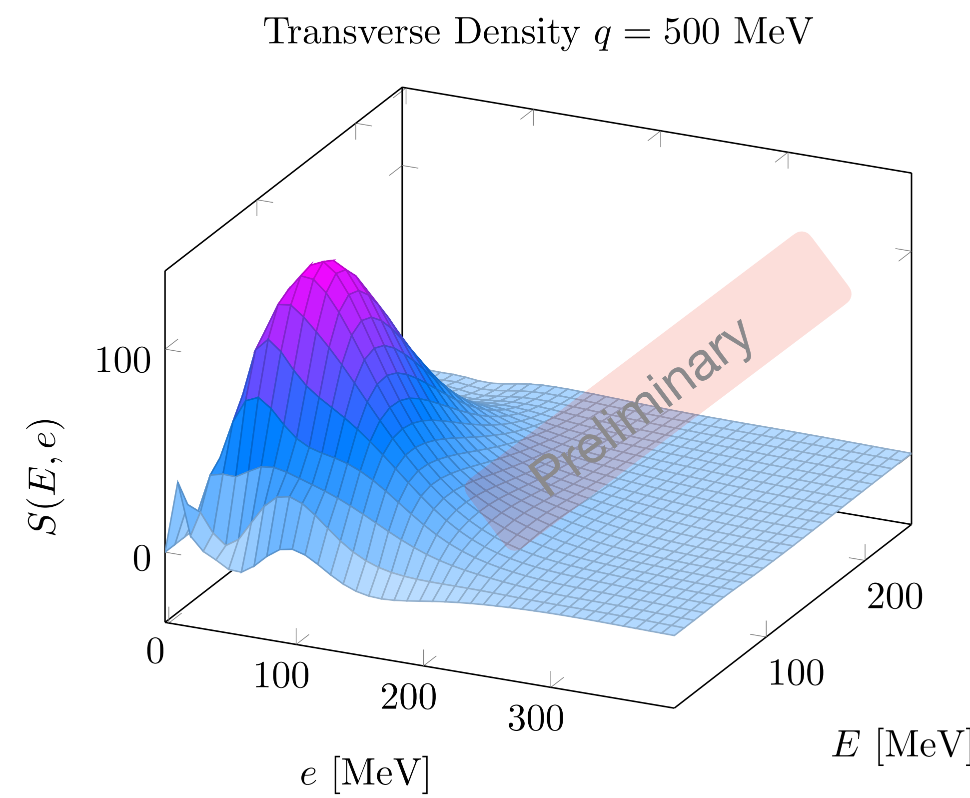
- ~1.8k core hours

Debug queue on Theta

Additional approximations reduce the computation time:
r, *R* integration up to 8, 5 fm
reduction of grid spacing in relative energy *e*

Response densities for ^{12}C





Preliminary results for longitudinal and transverse response densities in ^{12}C

Conclusions

- STA + QMC methods reproduce the quasi-elastic response of light nuclei at momentum transfers for q=300-600 MeV (Pastore et al. PRC101(2020)044612)
- Agreement with experiments and previous QMC calculations (LA et al arXiv:2108.10824)
- Incorporates the relevant two-nucleon physics
- Computationally less expensive that e.g. GFMC
- Full results for ^{12}C coming soon

Collaborators: J. Carlson, A. Lovato, N. Rocco, R. B. Wiringa

Thank you!

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U.S. Department of Energy INCITE Leadership Computing

Argonne National Laboratory

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