



# Updates on Quantum Monte Carlo Implementations for $\ell^4_2\text{He}$ and $\ell^{12}_6\text{C}$ Scattering in GENIE

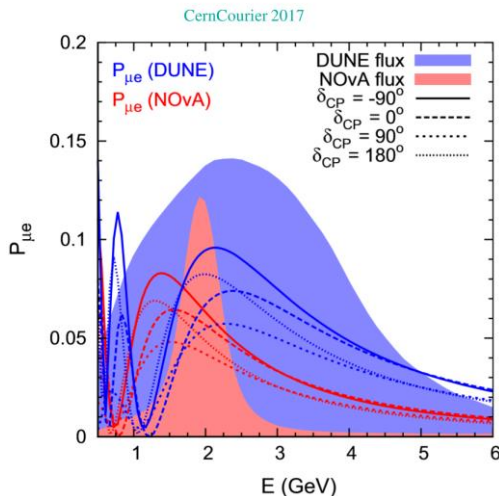
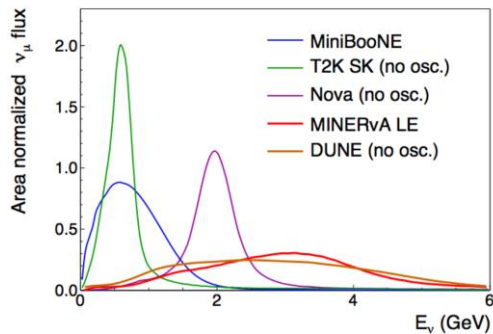
Steven Gardiner ([gardiner@fnal.gov](mailto:gardiner@fnal.gov)) and Joshua Barrow ([jbarrow@fnal.gov](mailto:jbarrow@fnal.gov))

Joint Theory/Experiment Meeting on Lepton-Nucleus Scattering

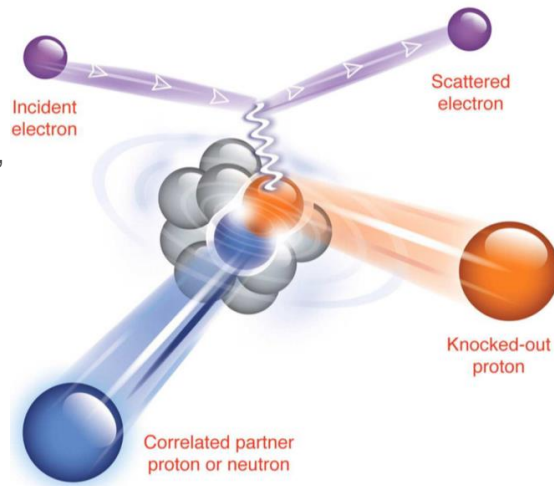
Tuesday, October 1<sup>st</sup>, 2019



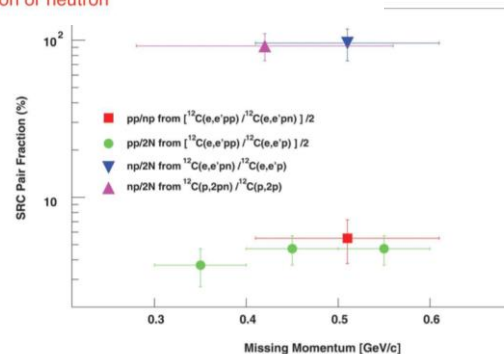
# The Need for Accurate and Precise $\ell$ Monte Carlo Generators



- See [Artur's talk](#), along with [Kendall](#) and [Joe](#)
- We require good  $\nu$  energy and position reconstruction to nail down SM  $\nu$  interactions
  - Understanding of in/exclusive cross sections, fluxes, etc.
  - PMNS matrix elements (flavor changing oscillations), associated  $\theta_{ij}$  values
  - Value of  $\delta_{CP}$
  - Supernovae  $\nu$ 's, masses, mass hierarchy, majorana-nature, etc., etc...



- The same can be said for limits on BSM interactions
  - Lorentz/CPT violation
- We require accurate simulations of *atmospheric neutrino backgrounds* for BSM searches
  - $p$ -decay,  $n \rightarrow \bar{n}$ , and other baryon number violating modes
  - Dark matter
- All of these require ample theoretical and computational study across large swaths of energy and momentum transfer



[Ghosh et al. Eur. Phys. J. C \(2016\)76](#)

JLab, Subedi et al. Science320(2008)1475

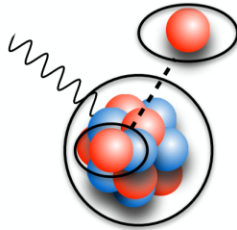


# A unified dynamical model for the nuclear response

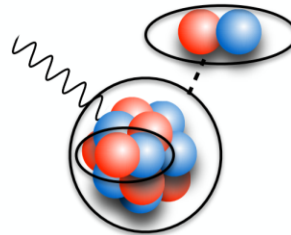
- Nuclear interactions are described by a realistic phenomenological Hamiltonian

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

CBF Spectral Function

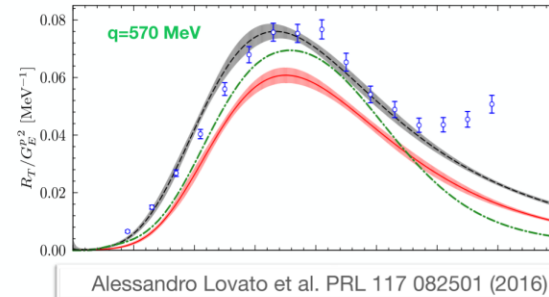
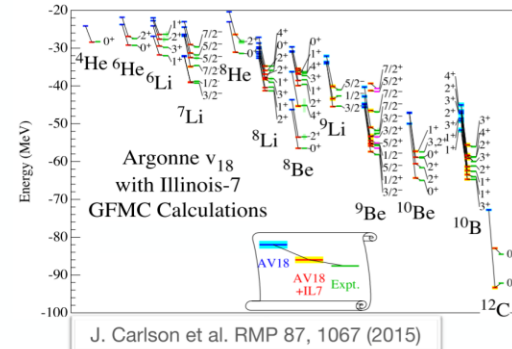


Short-time Approximation



Saori Pastore et al

The Green's Function Monte Carlo



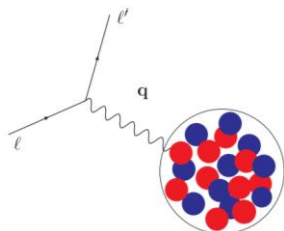
- Ab initio methods provide strict benchmarks valuable to constrain more approximate models at low  $|\mathbf{q}|$

# STA: The Inclusion of Two-Body Physics: Nuclear Response

- The second order correction to a Hamiltonian describing a system of bound nucleons comes from two-body interaction terms in a high-order expansion:

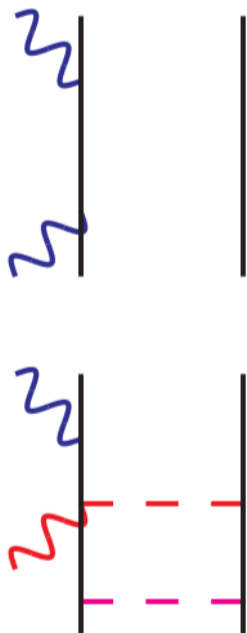
Considering the modes:  
responses  $\rho$  and  $\mathbf{j}$ , res

1b



– The total inclusive c

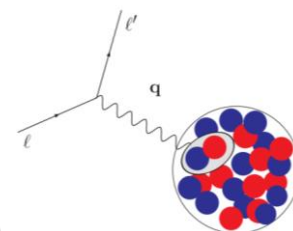
$$\frac{d^2\sigma}{dE'd\Omega'} = \sigma_M [\nu_L R_L(q^\mu$$



$$\langle \mathbf{j}_{1b}^\dagger \mathbf{j}_{1b} \rangle > 0$$

ial and transverse

2b



$$\langle \mathbf{j}_{1b}^\dagger \mathbf{j}_{2b} v_\pi \rangle \propto \langle v_\pi^2 \rangle > 0$$

response:

$$\cdot |\langle f | v_T O_T(q^\mu) | 0 \rangle|^2 = \dots$$

$$\dots = \sigma_M \int dt \left[ \langle 0 | O_L^\dagger(q^\mu) e^{i(\hat{H}-\omega)t} O_L(q^\mu) | 0 \rangle + \langle 0 | O_T^\dagger(q^\mu) e^{i(\hat{H}-\omega)t} O_T(q^\mu) | 0 \rangle \right]$$

# STA: The Inclusion of Two-Body Physics: 1b-1b, 1b-2b, 2b-1b, 2b-2b

- The nuclear response in a mode  $\alpha$  can be expanded to include two-body terms **for short times**, where

$$e^{i(\hat{H}-\omega)t} = e^{i(\sum_i t_i + \sum_{i<j} v_{i,j} - \omega)t} \approx \sum_i t_i + \sum_{i<j} v_{i,j} = P(t)$$

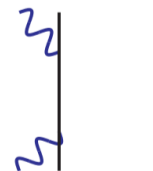
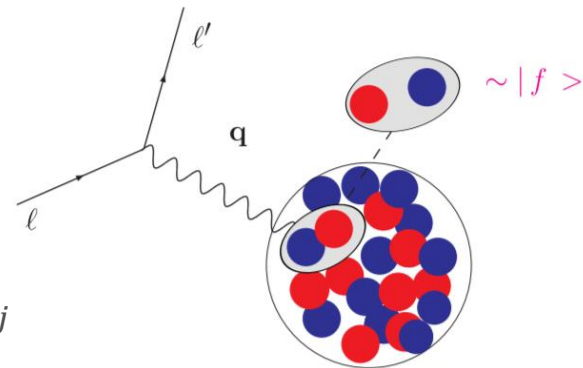
$$\Rightarrow R_\alpha(q^\mu) = \int dt \left[ \langle 0 | O_\alpha^\dagger(q^\mu) e^{i(\hat{H}-\omega)t} O_\alpha(q^\mu) | 0 \rangle \right] \approx \int dt \left[ \langle 0 | O_\alpha^\dagger(q^\mu) P(t) O_\alpha(q^\mu) | 0 \rangle \right]$$

$$\Rightarrow R_\alpha \sim O_{\alpha;i}^\dagger P(t) O_{\alpha;i} + O_{\alpha;i}^\dagger P(t) O_{\alpha;j} + O_{\alpha;i}^\dagger P(t) O_{\alpha;j} + O_{\alpha;i,j}^\dagger P(t) O_{\alpha;i,j}$$

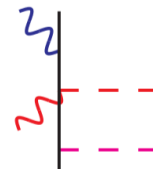
- This naturally leads us to consider lepton scattering off of pair objects

$$|f\rangle \sim \left| \psi_{p',P',J,M,L,S,T,M_T}(r,R) \right\rangle$$

- Correlated two-nucleon wave-functions allow for a full solve of the Schrödinger equation
- Retains all nuclear and electroweak interactions induced by an  $e$  or  $\nu$ 
  - Does not directly include  $\Delta$ -resonance



$$\langle j_{1b}^\dagger j_{1b} \rangle > 0$$



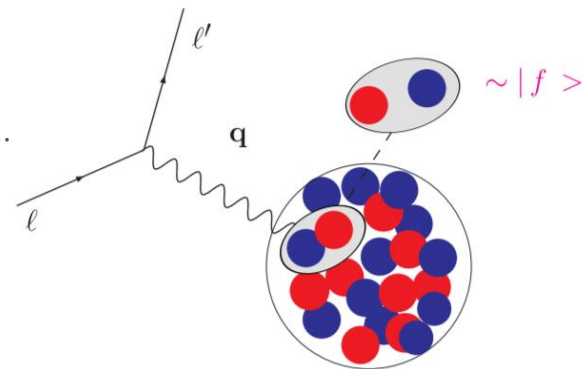
$$\langle j_{1b}^\dagger j_{2b} v_\pi \rangle \propto \langle v_\pi^2 \rangle > 0$$

# STA: The Inclusion of Two-Body Physics: Densities

- One can encode all of this structure within *response densities*,  $\mathcal{D}$

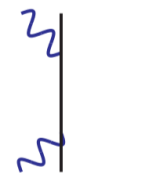
$$R_{\alpha}(q^{\mu}) \sim \int d\Omega_{P'} d\Omega_{p'} dP' dp' \delta(\omega + E_0 - E_f) \cdot \left[ p^{\mu'2} P^{\mu'2} \left\langle 0 \left| O_{\alpha}^{\dagger}(q^{\mu}) \right| p^{\mu'}, P^{\mu'} \right\rangle \left\langle p^{\mu'}, P^{\mu'} \left| O_{\alpha}^{\dagger}(q^{\mu}) \right| 0 \right\rangle \right] = \dots$$

$$\dots = \int dP' dp' \delta(\omega + E_0 - E_f) \cdot \mathcal{D}(p^{\mu'}, P^{\mu'}; q^{\mu})$$

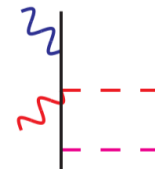


- Contains information about...

- ...the contents of the nucleus after the probe interacts with the pair
- “Exclusive” information on specific nucleon pair kinematics
- Correctly accounts for interference terms



$$\langle j_{1b}^{\dagger} j_{1b} \rangle > 0$$



$$\langle j_{1b}^{\dagger} j_{2b} v_{\pi} \rangle \propto \langle v_{\pi}^2 \rangle > 0$$

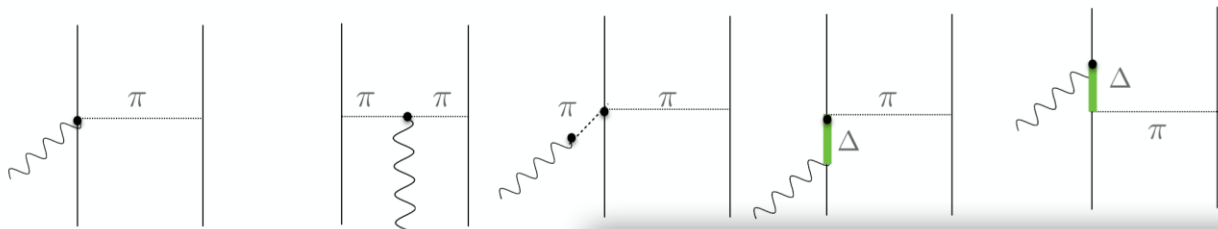


# (Anti)neutrino $^{12}\text{C}$ scattering cross sections

- We generalized the SF formalism to include vector and axial vector relativistic two-body currents

$$W_{2b}^{\mu\nu}(\mathbf{q}, \omega) \propto \int d\tilde{E} \frac{d^3k}{(2\pi)^3} d\tilde{E}' \frac{d^3k'}{(2\pi)^3} P_h(\mathbf{k}, \tilde{E}) P_h(\mathbf{k}', \tilde{E}') \sum_{ij} \langle k k' | j_{ij}^{\mu\dagger} | p p' \rangle \langle p p' | j_{ij}^{\nu} | k k' \rangle$$

- NN correlations are accounted for by the including the product of two one-hole spectral functions
- We extended the calculation to include vector and axial vector relativistic two-body currents



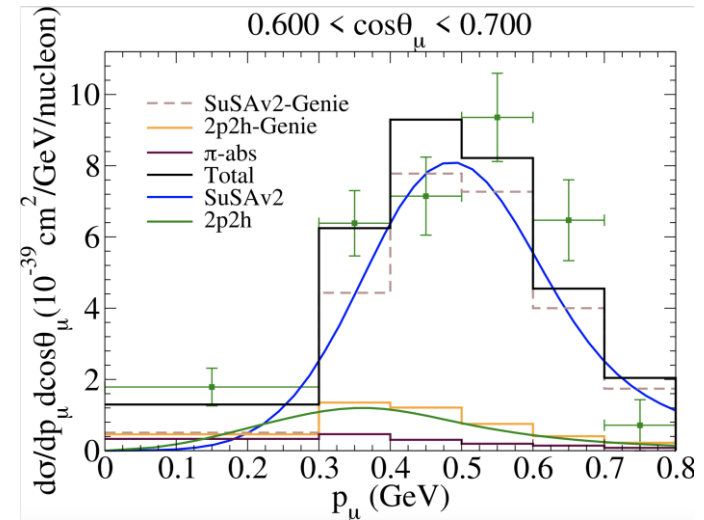
NR, C.Barbieri, O. Benhar, A. De Pace, A. Lovato, arXiv:1810.07647

- The calculation of the MEC current matrix is carried out automatically
- 9d-integral + use of realistic SFs implies dealing with a broader phase space: we developed an highly parallel Monte Carlo code, importance sampling procedure

# Hadron tensor framework & SuSAv2 implementation

- Hadronic tensor framework for GENIE
  - Based on Valencia CCMEC implementation in v2, generalized and expanded
  - SuSAv2 CCQE+MEC implementation under GENIE review, expected in next release (v3.2)
- Bilinear interpolation used to evaluate tensor elements in  $(\omega, |\vec{q}|)$  space
- Used by our STA implementation to select lepton kinematics
- Noemi has also provided tensor tables for 2-body contribution
  - QE cross section for SF approach computed directly within GENIE
- [HadronTensor framework technical note](#) now available

$$\frac{d^2\sigma}{dE'_\ell d\cos(\theta'_\ell)} = \frac{|\mathbf{k}'|}{|\mathbf{k}|} \frac{G_F^2}{2\pi} L_{\mu\nu} W^{\mu\nu}$$

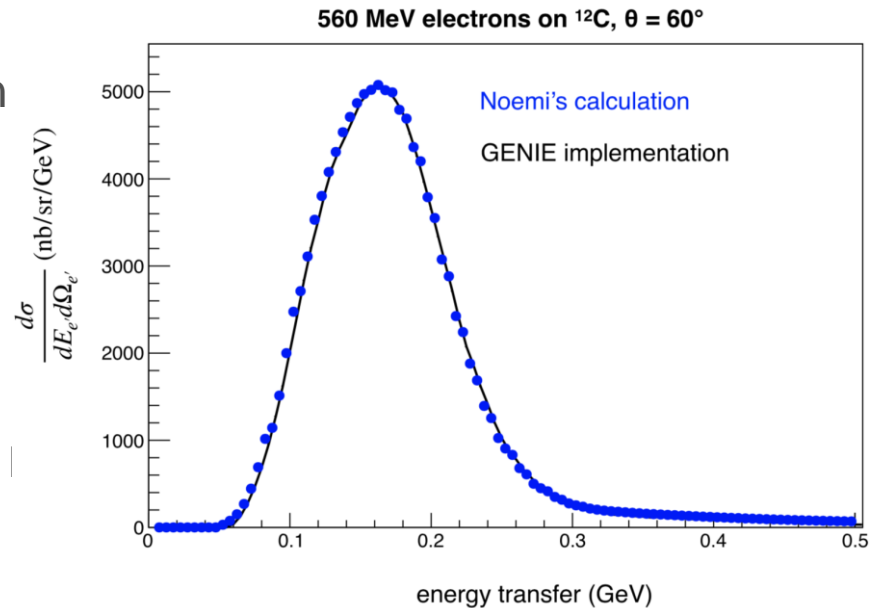


[SuSAv2 implementation note](#)



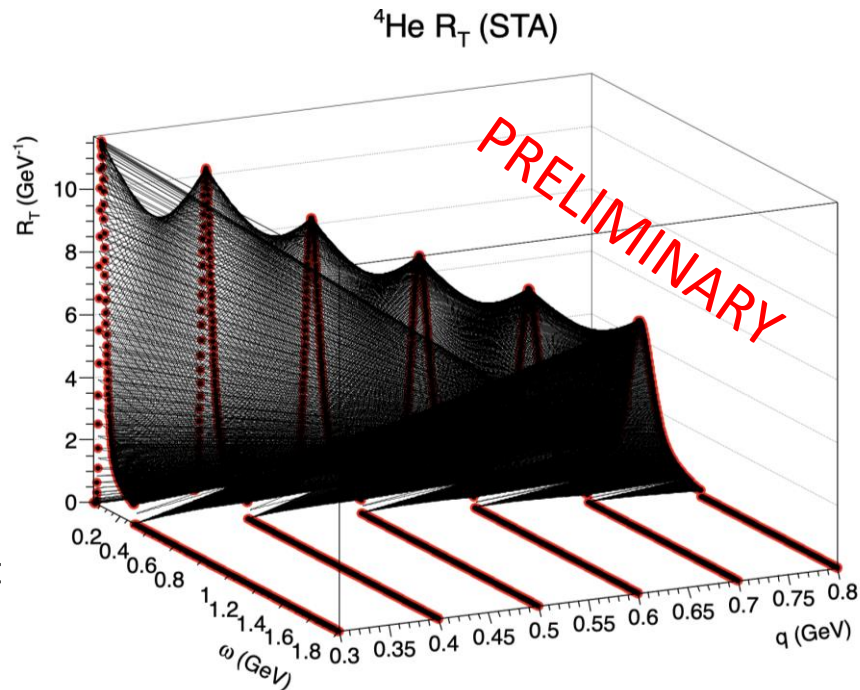
# GENIE spectral function implementation status

- Spectral function code & tabulated data for  $^{12}\text{C}$  updated to reflect latest calculation provided by Noemi
- Checks of GENIE QE differential cross section look good
  - EMQE example shown
  - Weak interactions show similar agreement
- Two-body EM hadronic tensor table in hand, testing in progress
  - Will employ the same code as Valencia, SuSav2
- Currently troubleshooting a problem with EM event generation
  - Maximum cross section estimate fails during sampling
  - Low  $Q^2$  cut needed to avoid divergence → appears related
- When resolved, will prepare for GENIE review soon



# Interpolation of STA responses

- Saori has provided STA tables to use for interpolation
  - Integrated responses (hadron tensor elements)
  - Response densities (for future use in sampling hadronic final states)
- Plots show current status of *bilinear interpolation*
  - Correct at the grid points, but  $q$  grid is too coarse
  - **Production of more tables underway**
    - Use of more sophisticated interpolation methods are also possible if number of tables becomes too unwieldy
- [STA/SF/GFMC technical note](#) is *developing*
  - Will eventually include...
    1. Full validation of cross section/response comparisons
    2. Writeup of (forthcoming) generator module processes



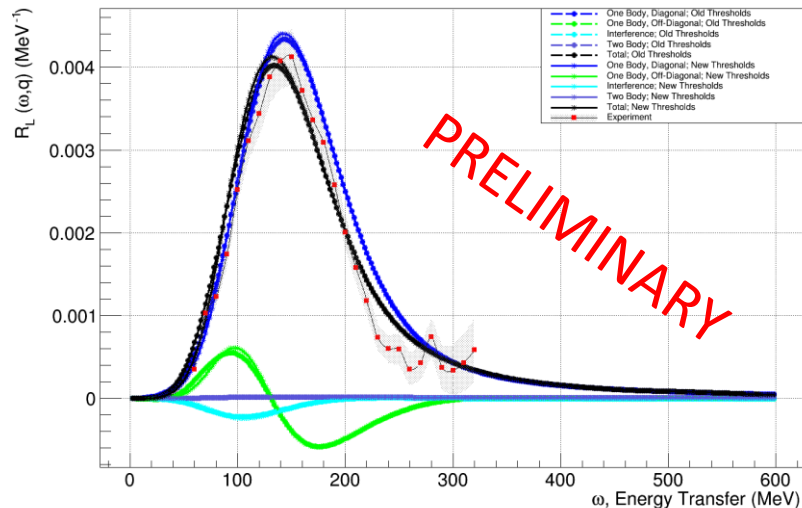
"Kinks" are an artifact of interpolation on a coarse grid

# Scripts for Comparisons Against World Data

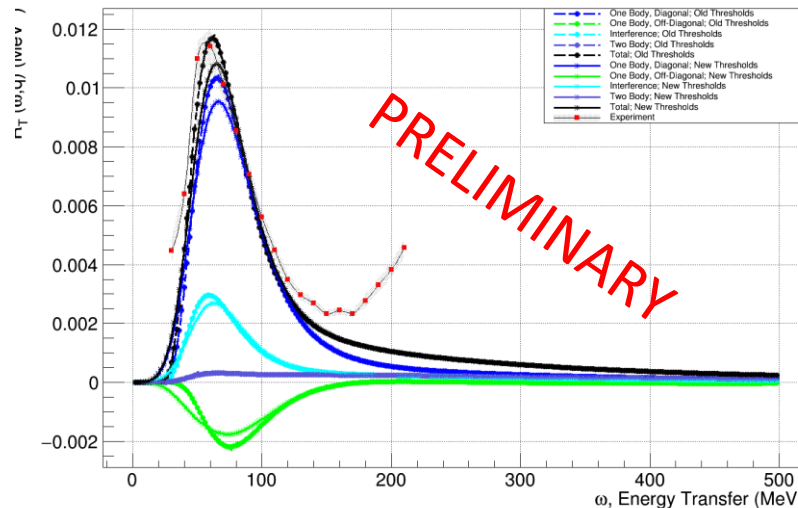
- Simple interfaces between GENIE's SuSAv2 HadronTensor framework have been made for easy plotting of interpolated cross sections
  - Some validation of Noemi's responses and their interpolation within GENIE to  $\frac{d^2\sigma}{dE' d\Omega'}(|\vec{q}|, \omega)$  still needs to be completed (unit checks?)
- [build XX.sh](#) and [test XX.cc](#) scripts run interpolations within the HadronTensor framework
  - Within SuSA fork: `./build_XX.sh`; `./test_XX`
- Create table outputs for input to simple [ValidationCode.C](#) plotter
  - Will compare all available outputted model cross sections for all targets to available [World Data](#): `root -l ValidationCode.C`;

# STA ${}^4_2\text{He}$ Responses Used in GENIE for Interpolation (GFMC coming soon!)

Longitudinal Response Comparisons,  $q = 500 \text{ MeV}$



Transverse Response Comparisons,  $q = 300 \text{ MeV}$



Dark Blue: one-body diagonal; Green: one-body off-diagonal; Light Blue: interference; Purple: two-body

Saori's STA is shown here component by component for two different shifts/thresholds.

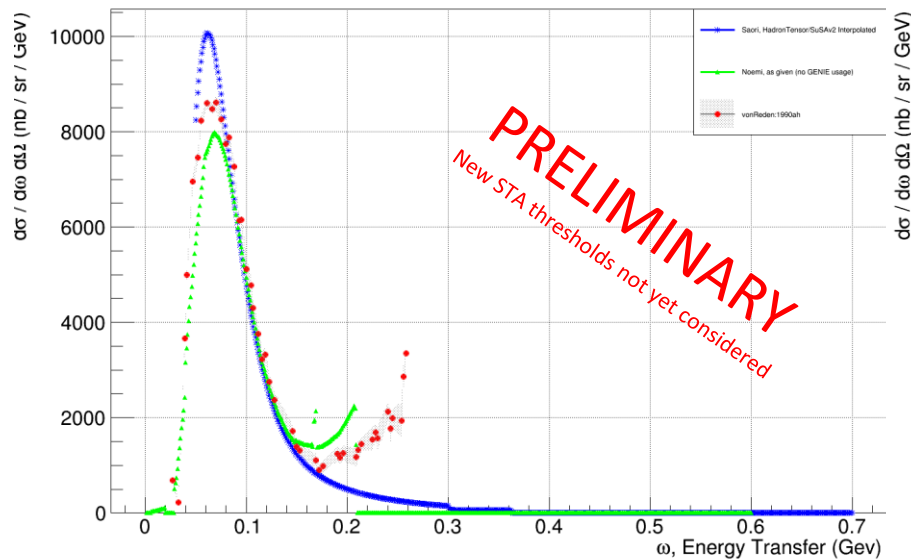
The *interference* and *one-body off-diagonal* terms show asymmetric and even destructive behavior to the total response (shown in black)

New threshold predominately effect the *transverse response*

Current experimental response data interpolated by Ingo Sick for  ${}^4_2\text{He}$  only, so far; some others exist (Dytman) and will integrated for comparisons

# Some simple, first-pass comparisons between models and data for ${}^4_2\text{He}$

$Z = 2, A = 4$ , Beam Energy = 0.36399999999999999 GeV, Angle =  $60^\circ$



**Green**-Noemi, GFMC (as given)

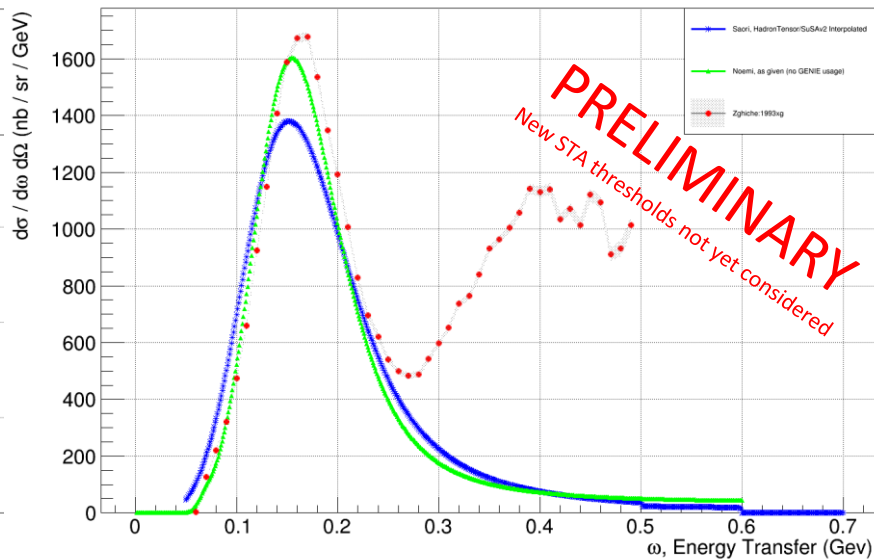
**Blue**-Saori, STA (GENIE interpolated)

**Red**-Cross section data, with uncertainty bands

*Elastic peak in STA needs to be removed still*

*Some of the resonant production seems to be included*

$Z = 2, A = 4$ , Beam Energy = 0.59999999999999998 GeV, Angle =  $60^\circ$



**Green**-Noemi, GFMC (as given)

**Blue**-Saori, STA (GENIE interpolated)

**Red**-Cross section data, with uncertainty bands

*No apparent resonant production from Noemi's model here?*

# Collaborators—Thank-you!

*The Roses  
Between  
The Thorns*



Saori Pastore, WUSTL



Steven Gardiner, FNAL



Joshua Barrow, UTK



Minerba Betancourt, FNAL



# Backup Slides

# Requirements Going Forward with GENIE

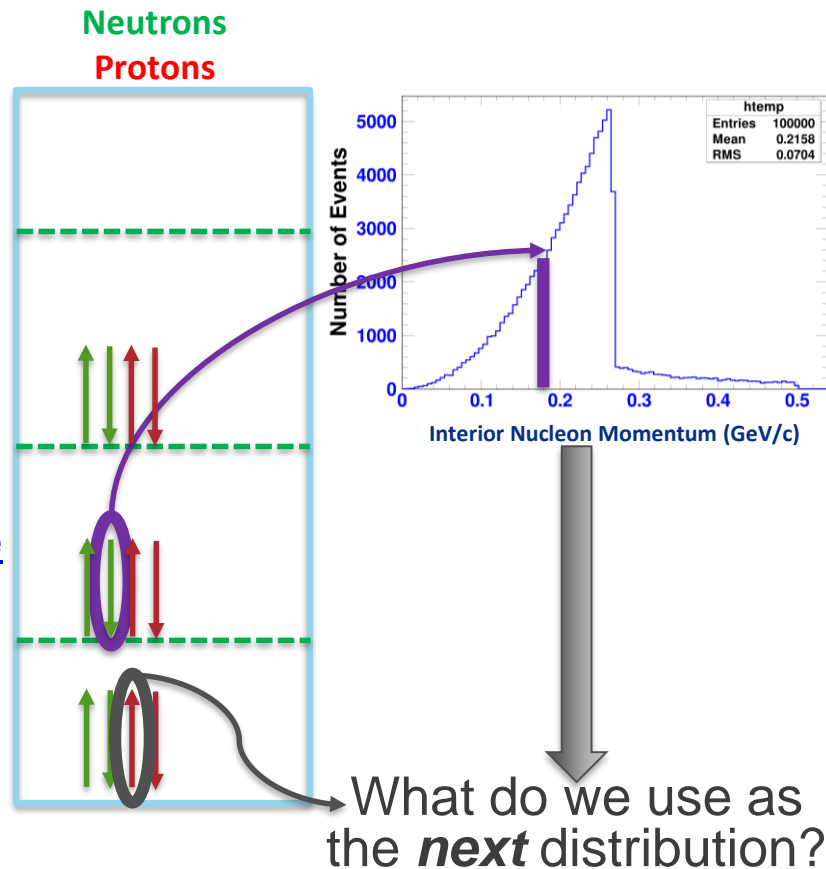
- An attempt at a general framework should be considered
  - When new response densities are ready for larger nuclei from future calculations, we should want to be able to simply “drop something in”
- Must streamline table reading, or avoid it altogether with another structure
- Must hand off two-nucleon configurations properly to GENIE...
  - Attain particle identities
  - Select all angles (currently integrated out)
  - Derive individual nucleon momenta
  - Track individual nucleons through the intranuclear cascade
    - Could be critically dependent upon initial positions and separations
    - One or both nucleons may not be emitted due to low momentum transfer
      - A phenomenological momentum cutoff must be considered for each struck nucleon

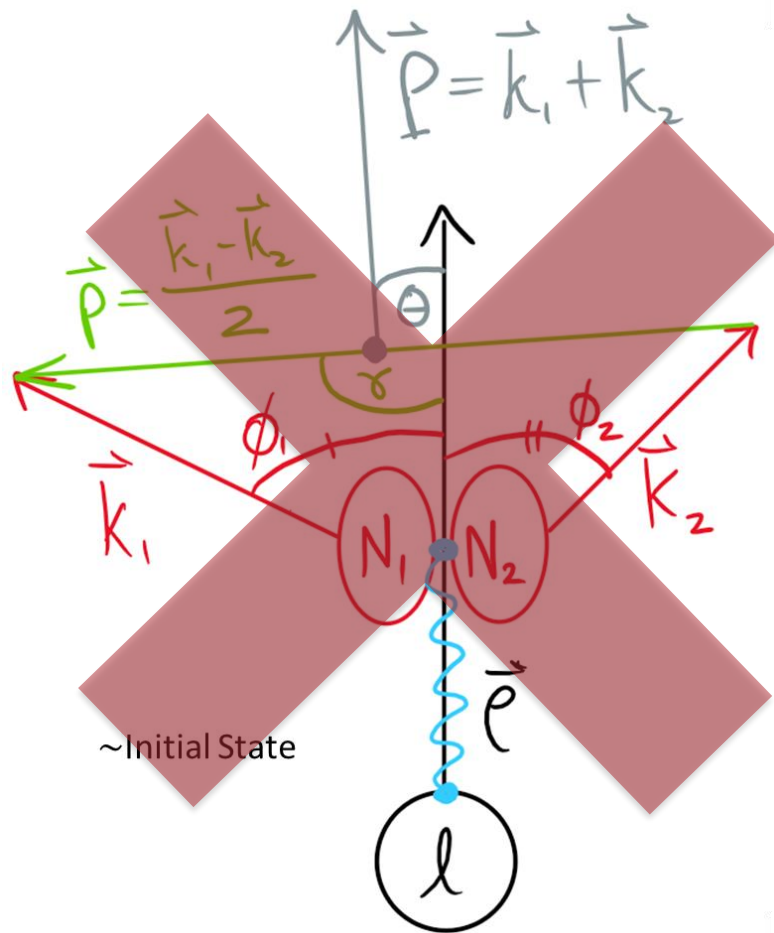
# Future Generator Validation

- Ample amounts of data are available for  $e_2^4\text{He}$  and  $e_6^{12}\text{C}$  scattering
  - Will serve as a good comparison for total inclusive cross sections
  - Will compare to other GENIE nuclear models
  - I would highly encourage everyone to investigate any BSM contributions your models could make to electron interactions
    - Can they already be constrained?
- Once the generator is complete, tested, and validated on  $e$  data, we will proceed to  $\nu$  generation
  - Will involve more response densities (five in total) for inclusion of CC interactions
  - Will similarly compare to data where available...
  - ...and other GENIE nuclear and interaction models
- Publication will follow soon after

# Nucleon Correlations: A Requirement for Future Simulations

- There are QM problems with the assumptions made when throwing momenta for *multiple* nucleons from *single* nucleon momentum distributions
  - By making a choice from a distribution of *all single nucleons*, we have ***changed the remaining distribution***
- Furthermore, it has been found that nucleons are choosey about their neighbors
  - Neutrons spend more time around protons in the nucleus
  - These pairs can have inextricably linked momenta
- More JLAB data interpretation on LAr coming? See also recent cross section measurements
- Can we use ~two body momentum distributions instead?***
  - Noemi et al.
- Or, can we deal solely with accurate semi-final states induced by vertex interactions?***
  - Saori et al.

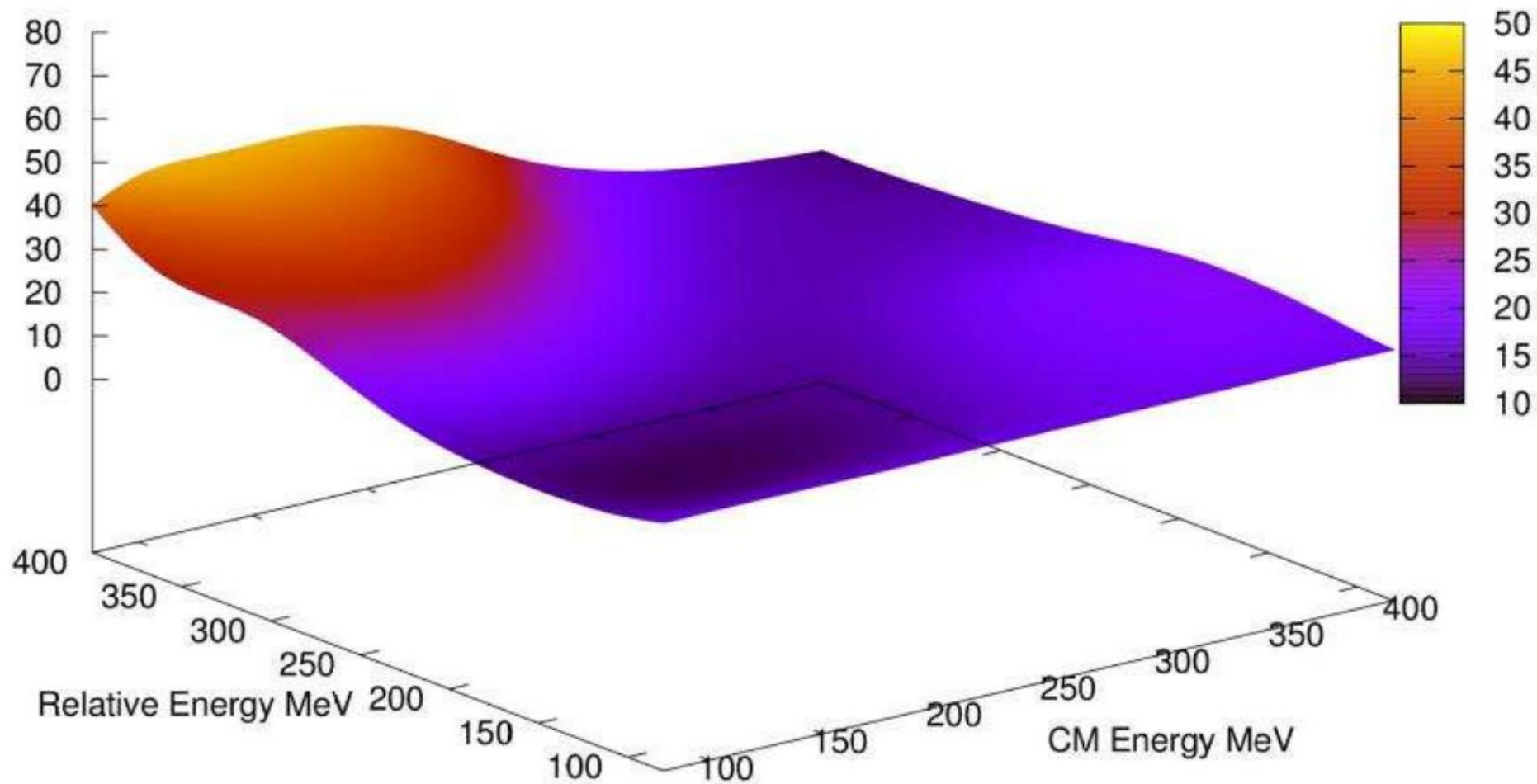




# Current QMC STA Outputs for $e_2^4\text{He}$

ep(i),	EP(j),	sldia,	sloff,	s2b,	sinterf				
-3.00	45.00	0.050	0.006	0.143	0.027	0.025	0.002	0.136	0.006
3.00	45.00	113.331	17.522	141.536	40.624	47.566	2.376	235.977	11.865
9.00	45.00	186.794	15.781	39.516	35.231	32.404	1.354	186.854	7.073
15.00	45.00	305.190	14.678	33.075	26.301	27.865	0.982	179.861	5.435
21.00	45.00	456.554	14.122	40.020	19.453	25.923	0.786	181.912	4.588
27.00	45.00	626.606	13.866	39.480	14.544	25.063	0.672	186.540	4.031
33.00	45.00	801.265	13.304	30.970	11.206	24.736	0.603	191.038	3.601
39.00	45.00	966.206	12.483	16.138	8.904	24.690	0.560	193.883	3.272
45.00	45.00	1108.040	11.633	-4.086	7.383	24.791	0.534	194.245	3.037
51.00	45.00	1216.391	10.926	-28.344	6.288	24.967	0.519	191.820	2.870
57.00	45.00	1285.269	10.560	-54.234	5.469	25.175	0.512	186.707	2.735
63.00	45.00	1313.351	10.540	-78.704	4.896	25.392	0.510	179.275	2.604
69.00	45.00	1303.386	10.610	-99.390	4.474	25.604	0.512	170.040	2.468
75.00	45.00	1261.053	10.500	-114.335	4.144	25.802	0.518	159.570	2.327
81.00	45.00	1193.636	10.104	-123.049	3.891	25.981	0.525	148.404	2.188
87.00	45.00	1108.799	9.454	-125.845	3.671	26.140	0.535	137.017	2.056
93.00	45.00	1013.675	8.642	-123.571	3.463	26.277	0.545	125.789	1.937
99.00	45.00	914.317	7.761	-117.278	3.298	26.391	0.557	115.006	1.831
105.00	45.00	815.467	6.888	-108.013	3.207	26.483	0.569	104.861	1.739
111.00	45.00	720.564	6.070	-96.720	3.174	26.553	0.582	95.470	1.659
117.00	45.00	631.888	5.331	-84.232	3.167	26.601	0.595	86.888	1.587
123.00	45.00	550.769	4.679	-71.279	3.168	26.628	0.608	79.123	1.522
129.00	45.00	477.807	4.111	-58.491	3.171	26.635	0.620	72.150	1.462
135.00	45.00	413.069	3.619	-46.390	3.177	26.622	0.633	65.924	1.408
141.00	45.00	356.263	3.199	-35.363	3.192	26.590	0.645	60.389	1.359
147.00	45.00	306.863	2.843	-25.640	3.229	26.539	0.657	55.484	1.319
153.00	45.00	264.214	2.545	-17.298	3.290	26.472	0.668	51.147	1.286
159.00	45.00	227.606	2.298	-10.273	3.362	26.387	0.679	47.321	1.262
165.00	45.00	196.324	2.094	-4.400	3.427	26.287	0.689	43.952	1.245
171.00	45.00	169.684	1.926	0.533	3.484	26.171	0.699	40.991	1.234
177.00	45.00	147.051	1.785	4.740	3.544	26.042	0.709	38.393	1.226
183.00	45.00	127.855	1.667	8.399	3.620	25.899	0.717	36.121	1.220
189.00	45.00	111.591	1.566	11.629	3.704	25.744	0.726	34.136	1.213
195.00	45.00	97.818	1.478	14.486	3.779	25.578	0.733	32.406	1.205
201.00	45.00	86.154	1.401	16.976	3.826	25.401	0.740	30.899	1.195
207.00	45.00	76.268	1.331	19.073	3.845	25.214	0.747	29.585	1.182





# The GENIE Generator

```
.000000.      00000000000000 000000      000 00000 000000000000
d8P' `Y8b      `888' `8 `888b.      `8' `888' `888' `8
888      888      8 `88b.      8 888 888
888      88800008      8 `88b. 8 888 88800008
888      00000 888      "      8 `88b.8 888 888      "
`88.      .88' 888      o 8      `888 888 888      o
`Y8bood8P'      o888000000d8 o8o      `8 o888o o888000000d8
```

GENIE GHEP Event Record [pr

Idx	Name	Ist
0	nu_mu	0
1	C12	0
2	neutron	11
3	C11	2
4	mu-	1
5	HadrSyst	12
6	proton	14
7	pi0	14
8	pi0	14
9	pi0	14
10	proton	1
11	pi0	1
12	proton	1
13	pi0	1
14	pi0	1
15	HadrBlob	15

Description	<i>GHepStatus_t</i>	As int
Undefined	<i>kIStUndefined</i>	-1
Initial state	<i>kIStInitialState</i>	0
Stable final state	<i>kIStStableFinalState</i>	1
Intermediate state	<i>kIStIntermediateState</i>	2
Decayed state	<i>kIStDecayedState</i>	3
Nucleon target	<i>kIStNucleonTarget</i>	11
DIS pre-fragm. hadronic state	<i>kIStDISPreFragmHadronicState</i>	12
Resonant pre-decayed state	<i>kIStPreDecayResonantState</i>	13
Hadron in the nucleus	<i>kIStHadronInTheNucleus</i>	14

Fin-Init:

Remnant nucleus

*kIStFinalStateNuclearRemnant* 15

Vertex: nu\_mu @ (x = 0.00000 m, y = 0.00000 m, z = 0.00000 m, t = 0.000000e+00 s)

Err flag [bits:15->0] : 0000000000000000 | 1st set: none  
 Err mask [bits:15->0] : 1111111111111111 | Is unphysical: NO | Accepted: YES

sig(Ev) = 4.45912e-38 cm^2 | d2sig(x,y;E)/dxdy = 2.09365e-37 cm^2 | Weight = 1.00000



UNIVERSAL NEUTRINO GENERATOR  
& GLOBAL FIT



# GENIE Implementation

- We will soon begin implementation of QMC STA within GENIE using semi-final states from tabulated response densities
- This will be tricky, to say the least...
  - GENIE's normal operating mode is almost always dependent on an predominately *single particle* paradigm
  - Initial state preparation—**avoidable?**
    - Single* nucleon lepton scattering
    - Single* nucleon momentum distributions in nuclear models
    - Single* nucleon initial positions
    - Some two-body dynamic options becoming available as we speak (SuSA), but initial correlations are only approximate
  - Final state preparation—**unavoidable!**
    - Propagation of *single* particles through the nucleus using an intranuclear cascade

```

.000000.      .000000000000 00000      .000000000000
d8P' `Y8b      `888' `8 `888b.      `8' `888' `888' `8
888      888      8 `88b.      8 888 888
888      88800008      8 `88b. 8 888 88800008
888      00000 888      "      8 `88b.8 888 888      "
`88.      .88' 888      o 8      `888 888 888      o
`Y8bood8P'      o888000000d8 o8o      `8 o888o o88800000d8
    
```

Idx	Name	Ist	PDG	Mother	Daughter	Px	Py	Pz	E	n
0	nu_mu	0	14	-1	-1	4	0.000	0.000	2.261	0.000
1	C12	0	1000060120	-1	-1	2	3	0.000	0.000	11.175
2	neutron	11	2112	1	-1	5	5	0.141	-0.119	0.919
3	C11	2	1000060110	1	-1	15	15	-0.141	0.105	10.256
4	nu-	1	13	0	-1	-1	-1	-0.006	-0.343	0.359
5	HadrSyst	12	2000000001	2	-1	6	9	0.147	0.238	2.160
6	proton	14	2212	5	-1	10	10	0.202	-0.123	0.958
7	pi0	14	111	5	-1	11	12	-0.006	-0.116	0.178
8	pi0	14	111	5	-1	13	13	0.001	0.227	0.589
9	pi0	14	111	5	-1	14	14	-0.049	0.018	0.618
10	proton	1	2212	6	-1	-1	-1	0.202	-0.123	0.958
11	pi0	1	111	7	-1	-1	-1	0.059	-0.028	0.044
12	proton	1	2212	7	-1	-1	-1	-0.028	0.173	-0.161
13	pi0	1	111	8	-1	-1	-1	0.001	0.227	0.589
14	pi0	1	111	9	-1	-1	-1	-0.049	0.018	0.618
15	HadrBlob	15	2000000002	3	-1	-1	-1	-0.178	0.076	0.229
Fin-Init:						0.000	0.000	0.000	0.000	
Vertex:						nu_mu @ (x = 0.00000 m, y = 0.00000 m, z = 0.00000 m, t = 0.000000e+00 s)				
Err flag [bits:15->0] : 0000000000000000						1st set:				
Err mask [bits:15->0] : 1111111111111111						Is unphysical:	NO	Accepted:	YES	none
sig(Ev) = 4.45912e-38 cm^2						d2sig(x,y;E)/dxdy = 2.09365e-37 cm^2	Weight = 1.00000			

Description	GHEPStatus	t	As int
Undefined	kIstUndefined		-1
Initial state	kIstInitialState		0
Stable final state	kIstStableFinalState		1
Intermediate state	kIstIntermediateState		2
Decayed state	kIstDecayedState		3
Nucleon target	kIstNucleonTarget		11
DIS pre-fragm. hadronic state	kIstDISPreFragmHadronicState		12
Resonant pre-decayed state	kIstPreDecayResonantState		13
Hadron in the nucleus	kIstHadronInTheNucleus		14

Remnant nucleus *kIstFinalStateNuclearRemnant* 15



# Summary

- Neutrino generators must grow and evolve their capabilities as we enter the precision and intensity frontiers
  - One step in this evolution is implementation of a generator dependent only upon semi-final states
  - Avoids phenomenological nuclear models of initial states in MC
- A new series of total inclusive lepton scattering cross section calculations for  $\omega \in (300, 800] \text{ MeV}$  are now available for  $\ell^4_2\text{He}$  and  $\ell^{12}_6\text{C}$  responses
  - Employs two-body physics in an inherent way
- Implementation of this model is beginning for GENIE
  - Will likely depend on many developments from Steven Gardiner (SuSAv2)
  - Efficient table reading implementation is necessary, or another structure
  - Will pass much of the particle information to the intranuclear cascade for transport