Achilles: A Modern Theorist-Driven Event Generator

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Based on: 2007.15570, 2110.15319, 2205.06378

Cross Theory Generator Working Group Meeting

7 June 2022

Achilles: A CHIcago Land Lepton Event Simulator

Project Goals:

- Theory driven
- Develop modular neutrino event generator
- Provide means for easy extension by end users
- Provide automated BSM calculations for neutrino experiments
- Evaluate theory uncertainties

Why a new generator?

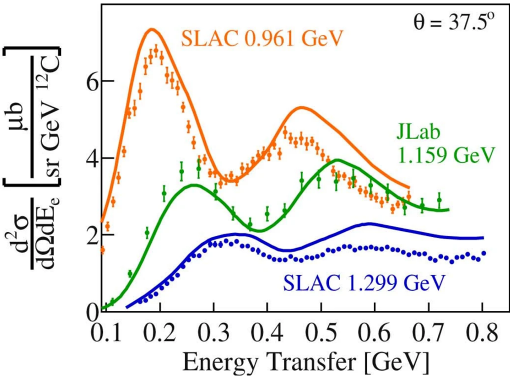
Oscillation Measurements

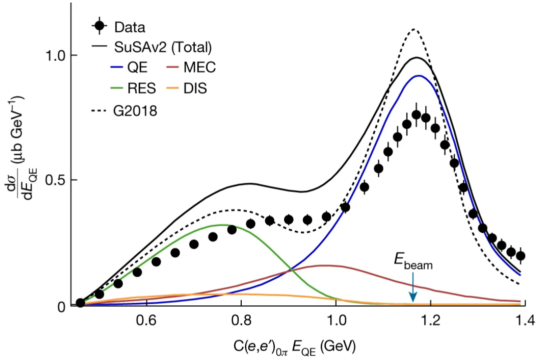
- $P_{\nu_\mu \to \nu_e} \sim \sin^2 2\theta \sin^2\left(\frac{\Delta m^2 L}{4E}\right) \to \Phi_e(E, L)/\Phi_\mu(E, 0)$
- Only measure events and not fluxes directly: $N(E_{reco}, L) \propto \sum_i \Phi(E, L)\sigma_i(E) f_{\sigma_i}(E, E_{reco})$
- Fit oscillation parameters by taking ratio of number of events in E_{reco} bins
- Cross sections do not exactly cancel in ratio, thus they are crucial
- Requires fully differential predictions

Other Measurements

- DUNE and HyperK near detectors are general purpose
- Leverage them for BSM searches
- Requires both SM and BSM fully differential predictions

Why a new generator? ($e4\nu$)





- State of the art is ok for inclusive
- Exclusive results need significant work

[Nature 599, 565–570 (2021)]

Why a new generator? (NOvA)

Source of Uncertainty	ν_e signal (%)	Total beam background (%)
Cross-section and FSI	7.7	8.6
Normalization	3.5	3.4
Calibration	3.2	4.3
Detector response	0.67	2.8
Neutrino flux	0.63	0.43
ν_e extrapolation	0.36	1.2
Total systematic uncertainty	9.2	11
Statistical uncertainty	15	22
Total uncertainty	18	25

Table 1: Effect of 1σ variations of the systematic uncertainties in the total ν_e signal and background predictions in the NOvA experiment[2]. The systematic uncertainties are from the latest NOvA results with $8.85\text{x}10^{20}$ protons on target.

- Cross section uncertainty one of dominant uncertainties
- Unclear if correctly fully estimated
- NOvA systematics and statistical uncertainty equal
- DUNE and HyperK will have significantly more events

Separating Primary Interaction and Cascade

General Lepton-Nucleus Scattering Cross Section

$$\mathrm{d}\sigma = \left(\frac{1}{|v_A - v_\ell|}\frac{1}{4E_A^{\mathrm{in}}E_\ell^{\mathrm{in}}}\right)|\mathcal{M}|^2\prod_f \frac{\mathrm{d}^3 p_f}{(2\pi)^3}(2\pi)^4\delta^4\left(k_A + k_\ell - \sum_f p_f\right)$$

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Matrix Element Schematically

$$|\mathcal{M}\left(\{k\} \to \{p\}\right)|^2 = \Big|\sum\!\!\!\!\!\!\int_{p'} \mathcal{V}(\{k\} \to \{p'\}) \times \mathcal{P}(\{p'\} \to \{p\})\Big|^2$$

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- Primary interaction

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- Primary interaction
- Evolution out of nucleus

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- Primary interaction
- Evolution out of nucleus
- Approximate as incoherent product of primary interaction and cascade

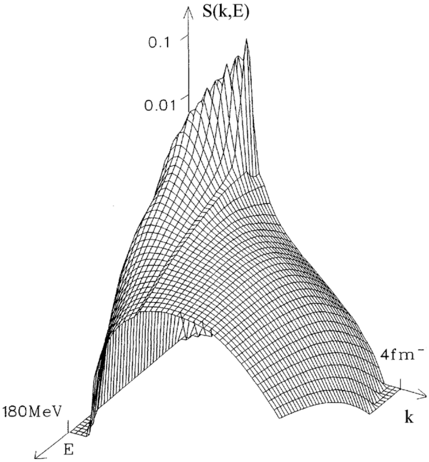
Factorization

- For Quasielastic scattering, factorize primary interaction as: $|\Psi_f\rangle = |p\rangle \otimes |\Psi_f^{A-1}\rangle$
- Initial state given via spectral function (probability distribution of removing a “hole” nucleon):

$$S_h(\mathbf{k}_h, E') = \sum_{f_{A-1}} |\langle \Psi_0 | k\rangle \otimes |\Psi_f^{A-1}\rangle|^2 \delta(E' + E_0^A - E_f^{A-1})$$

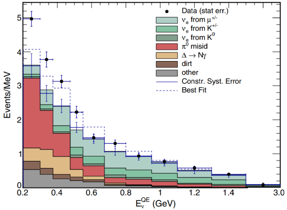
- Here we use spectral function obtained from correlated basis function theory [Phys. A 579, 493 (1994)]
- Spectral function normalized as:

$$\int \frac{\mathrm{d}k_h}{(2\pi)^3} \mathrm{d}E' S_h(\mathbf{k}_h, E') = \begin{cases} Z, & h = \mathrm{p}, \\ A - Z, & h = \mathrm{n}. \end{cases}$$

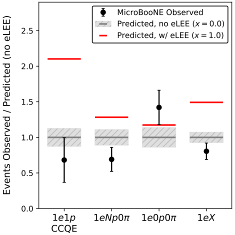


[Rev. Mod. Phys. 80, 189 (2008)]

BSM Motivation: MiniBooNE and MicroBooNE

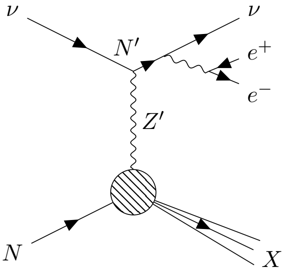


[PRL 121, 221801]



[arXiv:2110.14054]

- MiniBooNE sees excess of events
- MicroBooNE does not see excess of single electron events
- Excess can be from multiple lepton final states
- Event generators can not simulate these processes



Using Currents

Using tensors:

$$\frac{d\sigma}{d\Omega} = \sum_{i,j} L^{(ij)}_{\mu\nu} W^{(ij)\mu\nu} = L^{(\gamma\gamma)}_{\mu\nu} W^{(\gamma\gamma)\mu\nu} + L^{(\gamma Z)}_{\mu\nu} W^{(\gamma Z)\mu\nu} + L^{(Z\gamma)}_{\mu\nu} W^{(Z\gamma)\mu\nu} + L^{(ZZ)}_{\mu\nu} W^{(ZZ)\mu\nu} + \cdots$$

Using Currents:

$$\frac{d\sigma}{d\Omega} = \left| \sum_i L^{(i)}_{\mu} W^{(i)\mu} \right|^2$$

Interferences handled automatically using currents

Interface to tensors provided for nuclear calculations that **must** be expressed using tensors.

Handling Form Factors

Nuclear one-body current operators:

$$\mathcal{J}^\mu = \left(\mathcal{J}_V^\mu + \mathcal{J}_A^\mu\right)$$

$$\mathcal{J}_V^\mu = \gamma^\mu \mathcal{F}_1^a + i\sigma^{\mu\nu} q_\nu \frac{\mathcal{F}_2^a}{2M}$$

$$\mathcal{J}_A^\mu = -\gamma^\mu \gamma_5 \mathcal{F}_A^a - q^\mu \gamma_5 \frac{\mathcal{F}_P^a}{M}$$

Coherent Form Factors (spin-0 nucleus):

$$\mathcal{J}^\mu = (p_{\text{in}} + p_{\text{out}})^\mu \mathcal{F}_{\text{coh}}$$

Standard Model Form Factors:

$$\mathcal{F}_i^{\gamma(p,n)} = F_i^{p,n}, \qquad \mathcal{F}_A^\gamma = 0$$

$$\mathcal{F}_i^{W(p,n)} = F_i^p - F_i^n, \qquad \mathcal{F}_A^W = F_A$$

$$\mathcal{F}_i^{Z(p)} = \left(\frac{1}{2} - 2\sin^2\theta_W\right) F_i^p - \frac{1}{2} F_i^n,$$

$$\mathcal{F}_i^{Z(n)} = \left(\frac{1}{2} - 2\sin^2\theta_W\right) F_i^n - \frac{1}{2} F_i^p$$

$$\mathcal{F}_A^{Z(p)} = \frac{1}{2} F_A, \qquad \mathcal{F}_A^{Z(n)} = -\frac{1}{2} F_A$$

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Straight-forward to extend to BSM if CVC is valid

Recursive Matrix Element Generation

$$\mathcal{J}_\alpha(\pi) = P_\alpha(\pi) \sum_{\mathcal{V}_\alpha^{\alpha_1,\alpha_2}} \sum_{\mathcal{P}_2(\pi)} \mathcal{S}(\pi_1,\pi_2) V_\alpha^{\alpha_1,\alpha_2}(\pi_1,\pi_2) \mathcal{J}_{\alpha_1}(\pi_1) \mathcal{J}_{\alpha_2}(\pi_2)$$

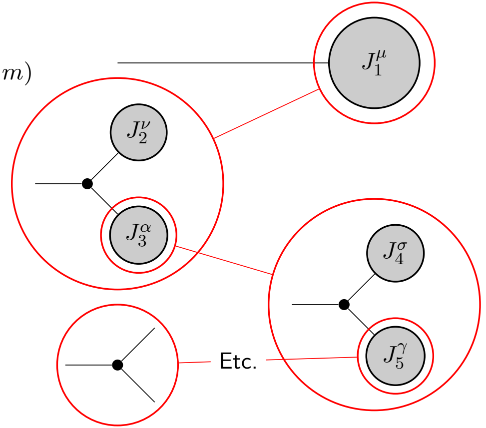
$$L_\mu^{(i)}(1,\ldots,m) = \mathcal{J}_\mu^{(i)}(1,\ldots,m)$$

$$L_{\mu\nu}^{(i,j)}(1,\ldots,m) = \mathcal{J}_\mu^{(i)}(1,\ldots,m)\mathcal{J}_\nu^{(j)\dagger}(1,\ldots,m)$$

Berends-Giele Recursion

- Reuse parts of calculation
- Most efficient for high multiplicity
- Reduces computation from $\mathcal{O}(n!)$ to $\mathcal{O}(3^n)$

[Nucl. Phys. B306(1988), 759]



Phase Space Generation

$$d\Phi_n\left(a,b;1,\ldots,n\right) = \delta^{(4)}\left(p_a + p_b - \sum_{i=1}^{n} p_i\right)\left[\prod_{i=1}^{n} \frac{d^4 p_i}{(2\pi)^3}\delta\left(p_i^2 - m_i^2\right)\Theta\left(p_{i_0}\right)\right]$$

The above phase space definition does not contain the handling of initial states.

Algorithms for n-body phase space generation

- Rambo [Comput. Phys. Commun. **40**(1986) 359]
- Multi-channel techniques [hep-ph/9405257]
- Recursive Phase Space [arXiv:0808.3674]

Results

Processes Considered:

- Electron-Carbon Scattering
- Neutrino-Carbon Scattering
- Neutrino Tridents
- Dirac/Majorana Heavy Neutral Lepton [1807.09877]

Experimental Setup:

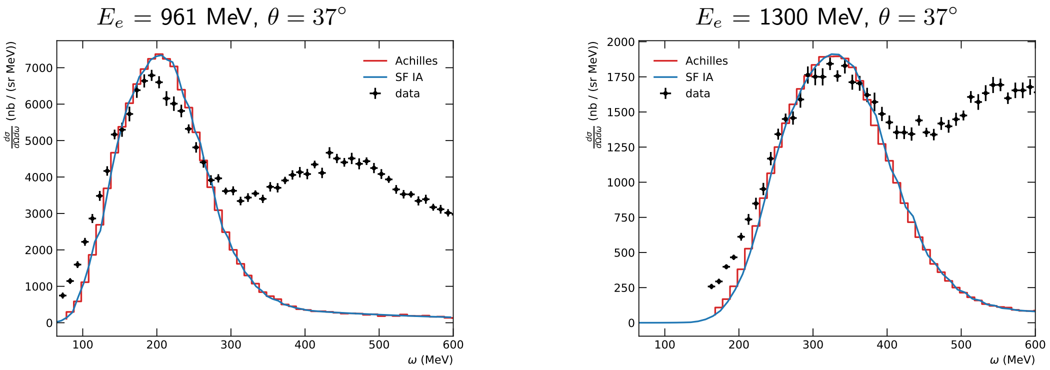
- Target Nucleus: Carbon (Argon for HNL)
- Electron: 961 MeV and 1299 MeV
- Neutrino: 1000 MeV
- Validating beam fluxes

NOTE: All processes are fully differential

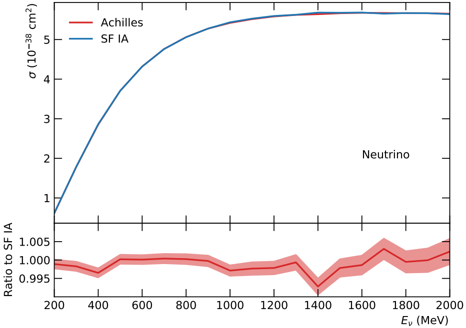
Parameters:

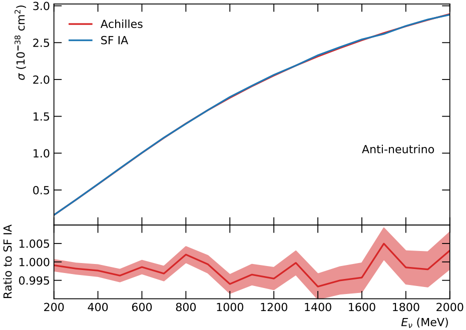
- Only quasielastic scattering (coherent for HNL) is included and no FSI
- EM Form Factors: Kelly [PRC 70, 068202 (2004)]
- Coherent Form Factor: Lovato [1305.6959]
- Axial Form Factor:
  - Dipole
  - $M_A = 1.0$ GeV
  - $g_A = 1.2694$
- $\alpha = 1/137$
- $G_F = 1.16637 \times 10^{-5}$
- $M_Z = 91.1876$ GeV

Electron Scattering



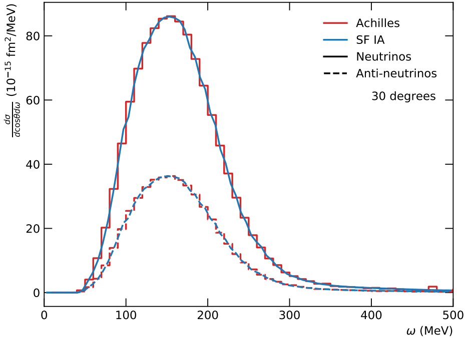
Neutrino Total Cross Section



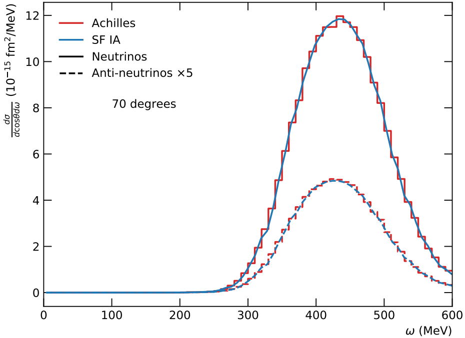


Neutrino Differential Cross Section

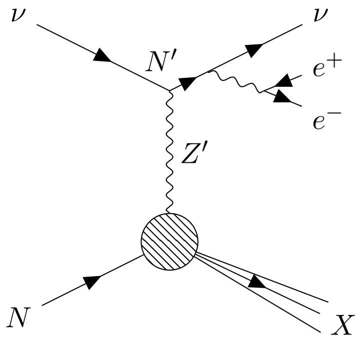
$E_\nu = 1000$ MeV, $\theta = 30^\circ$



$E_e = 1000$ MeV, $\theta = 70^\circ$



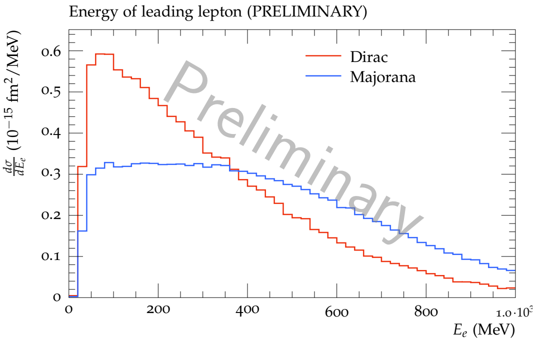
Heavy Neutral Lepton

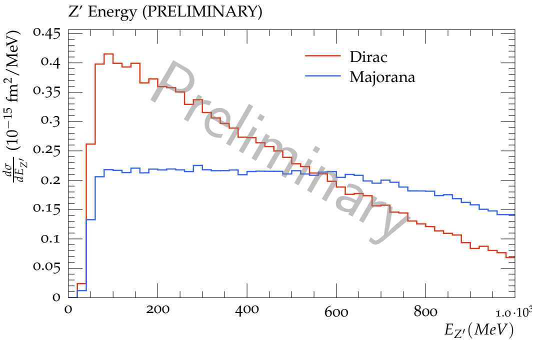


Parameters:

- $m_{N'} = 420$ MeV
- $m_{Z'} = 30$ MeV
- $\alpha_D = 0.25$
- $\alpha\epsilon^2 = 2 \times 10^{-10}$
- $|U^{\mu}_{42}| = 9 \times 10^{-7}$
- Widths of N' and Z' automatically calculated based on input parameters
- Handles both Dirac and Majorana fermions
- Results are flux-averaged over the MiniBooNE / MicroBooNE neutrino flux

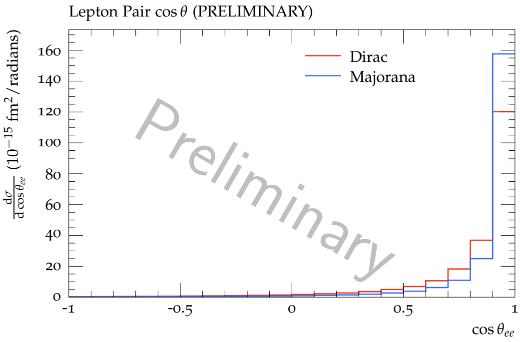
Heavy Neutral Lepton

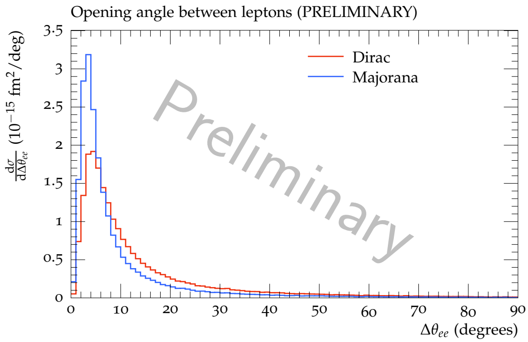




Heavy Neutral Lepton

- No cuts applied yet
- Typical opening angle around 5-6 degrees
- Working on scanning parameter space





- Need to include background to compare to MiniBooNE data
- Simulate possible MicroBooNE limits

MicroBooNE Simulation

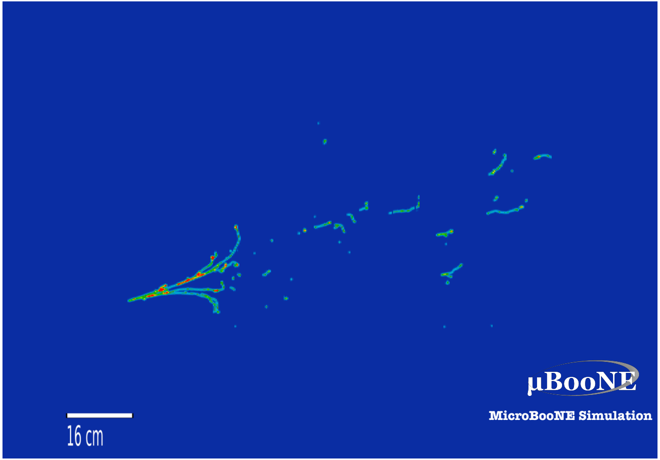


Image generated by the MicroBooNE collaboration using Achilles

- Working on implementing into MicroBooNE Pipeline
- Developing interface to LArSoft

Final State Interactions

Modify Primary Interaction:

- Captures rate change from FSI
- Loses all information about hadronic final state
- Primarily done using folding functions

Intranuclear Cascade:

- Unitary process (*i.e.* no rate change)
- Contains information about hadronic final state
- Primarily done via Monte Carlo methods

Note: Both approaches attempt to capture effects from nuclear potential. Therefore, can only use one or the other to avoid double counting effects.

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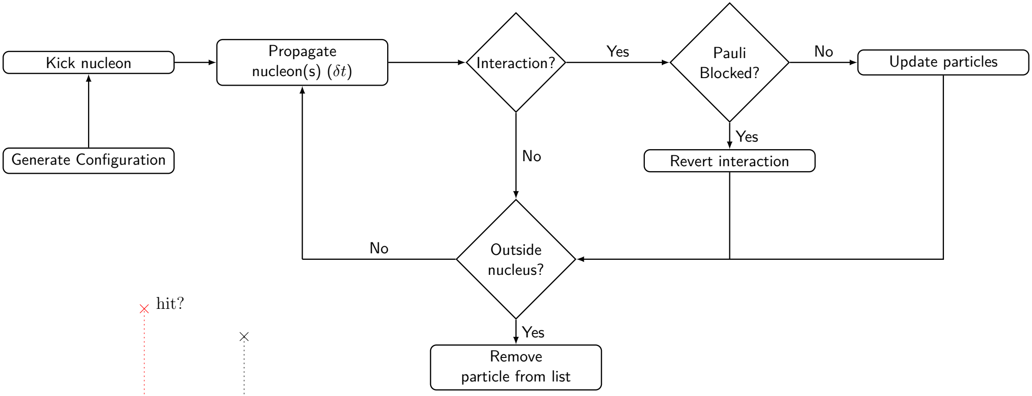
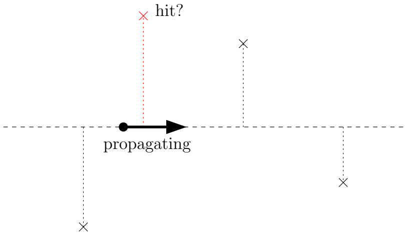
Matrix Element Schematically Approximation

$$|\mathcal{M}\left(\{k\} \to \{p\}\right)|^2 = \sum_{p'} |\mathcal{V}(\{k\} \to \{p'\})|^2 \times |\mathcal{P}(\{p'\} \to \{p\})|^2$$

Algorithm Overview

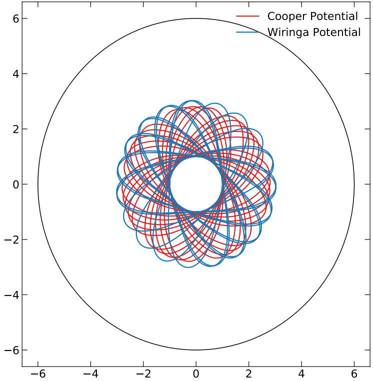




[Phys.Rev.C 103 (2021) 1, 015502]

Propagation with Potential

Initial Momentum: 250 MeV



- Propagation using symplectic integrator for non-separable Hamiltonians [1609.02212]
- Energy is conserved to a high degree of precision
- Extremely stable

- Blue: Non-relativistic potential $(E = \sqrt{p^2 + m^2} + V)$
  [Phys. Rev. C. 38, 2967]
- Red: Relativistic potential $(E = \sqrt{p^2 + (m+S)^2} + V)$
  [Phys. Rev. C. 80, 034605]

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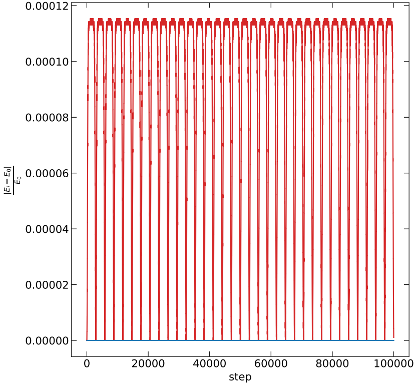

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CLAS/e4v Comparison

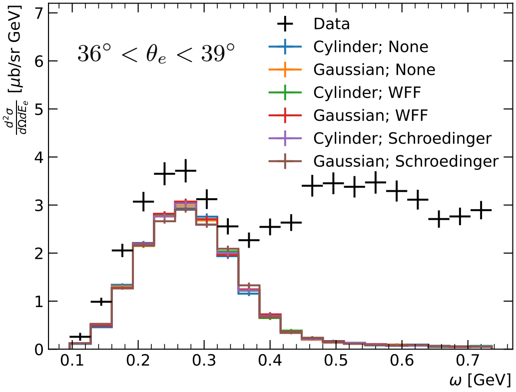
CLAS/e4v cuts:

- Select 1p0π events
- Protons: $p_p > 300$ MeV, $12^\circ < \theta_p$.
- electrons: $E_e > 0.4, 0.55, 1.1$ GeV, $\theta_e^i > \theta_0^i + \frac{\theta_1^i}{p_e[\mathrm{GeV}]}$, $\theta_0^i = 17^\circ, 16^\circ, 13.5^\circ$, $\theta_1^i = 7^\circ, 10.5^\circ, 15^\circ$ for $E_{\mathrm{beam}} = 1.159, 2.257, 4.453$ GeV respectively.

Simulation details:

- ACHILLES only has Quasielastic channel so far
- Events are reweighted by Q^4/GeV^4 (as done in the analysis)

Inclusive Results:



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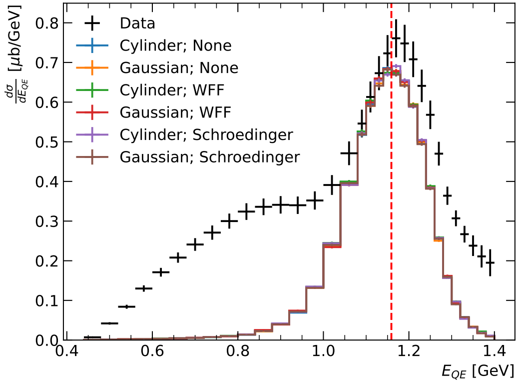
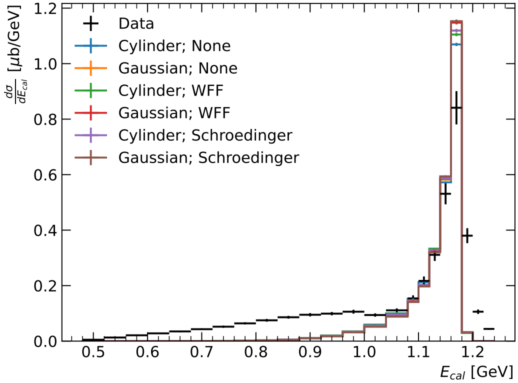
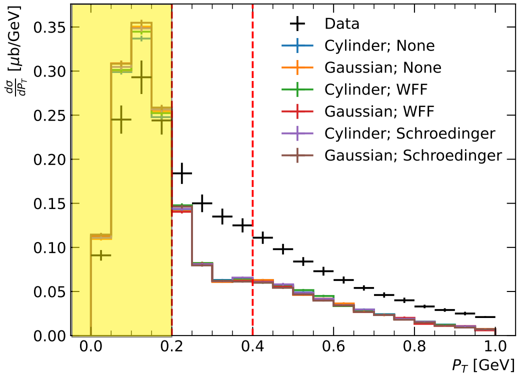


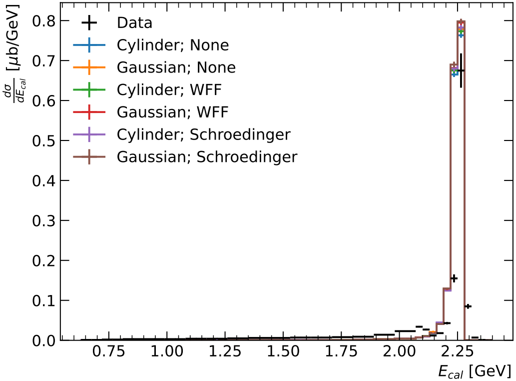


- $E_{QE} = \frac{2m_N\epsilon+2m_NE_\ell-m_\ell^2}{2(m_N-E_\ell+p_\ell\cos\theta_\ell)}$
- $\epsilon = 21$ MeV
- Mimics Cherenkov detectors

- $E_{\rm cal} = \sum_i (E_i + \epsilon_i)$
- Mimics LArTPC detectors

CLAS/e4v Comparison





$$\mathbf{p}^T = \mathbf{p}_e^T + \mathbf{p}_p^T$$

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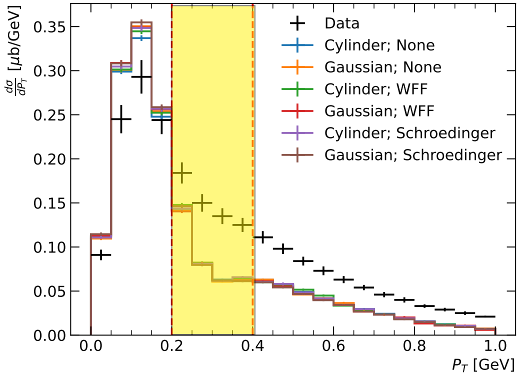
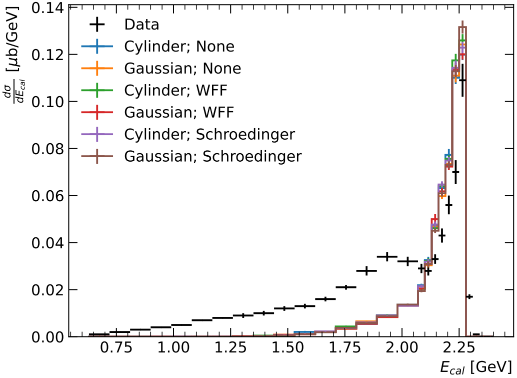
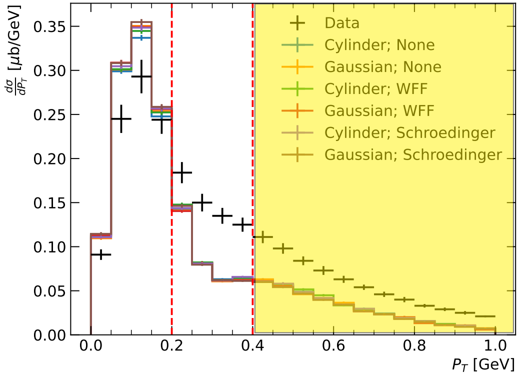
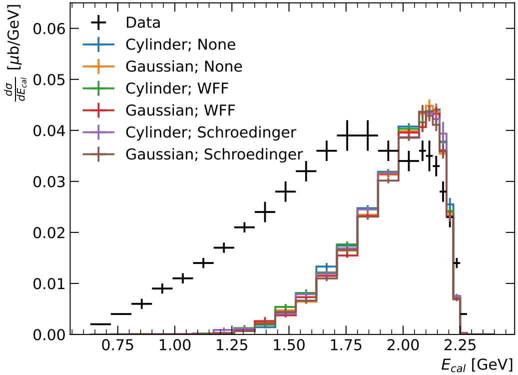




$$\mathbf{p}^T = \mathbf{p}_e^T + \mathbf{p}_p^T$$

CLAS/e4v Comparison





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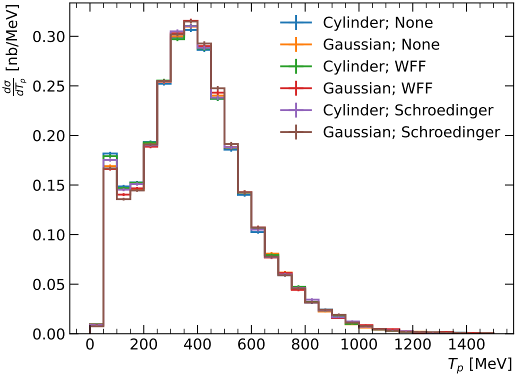
New Observables

New Observables:

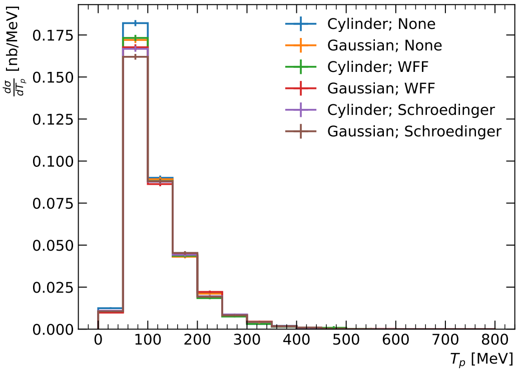
- Momentum of 1st proton



New Observables

New Observables:

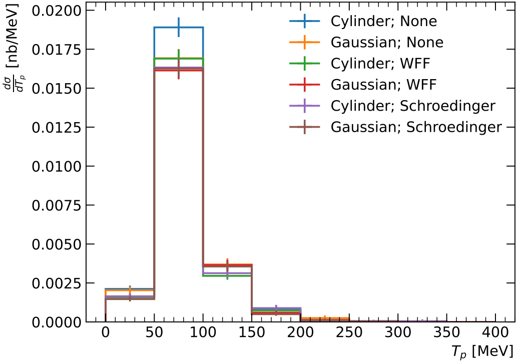
- Momentum of 1st proton
- Momentum of 2nd proton



New Observables

New Observables:

- Momentum of 1st proton
- Momentum of 2nd proton
- Momentum of 3rd proton

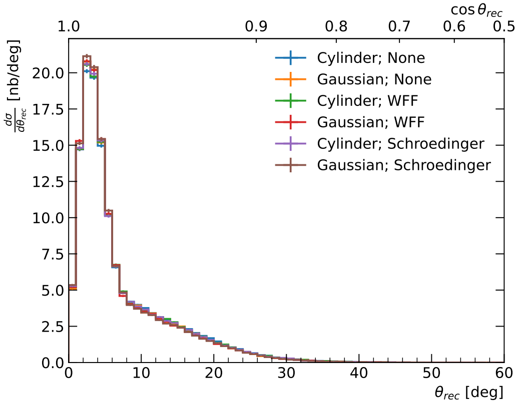


New Observables

New Observables:

- Momentum of 1st proton
- Momentum of 2nd proton
- Momentum of 3rd proton
- Reconstructed beam direction:

$$\cos\theta_{\text{rec}} \equiv \frac{\hat{\mathbf{k}}_e \cdot \mathbf{p}_{\text{out}}}{|\mathbf{p}_{\text{out}}|}$$



Conclusions

Current Status:

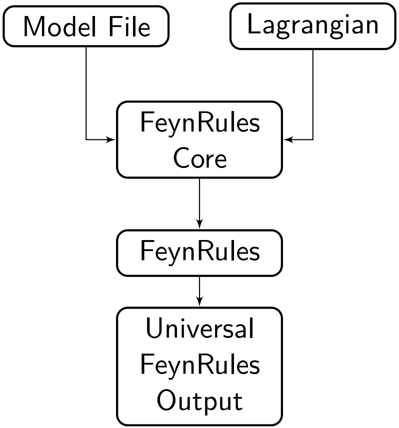
- DUNE and HK will require precision neutrino event generators
- ACHILLES aims to be a modular theory driven generator to address these needs
- BSM important for the current and next generation neutrino experiments
- Robust BSM program requires automating theory calculations
- Comparison of cascade results with CLAS/e4v experiment

Future Steps:

- Implement QED showers to handle radiative corrections
- Interface with LArSoft
- Implement MEC, Resonance, and DIS processes
- Continue to improve cascade modeling

- *Mathematica* Program
- Takes model file and Lagrangian as input
- Calculates the Feynman rules
- Outputs in Universal FeynRules Output (UFO) format

[arXiv:0806.4194, arXiv:1310.1921]



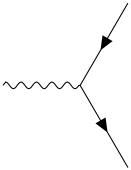
Universal FeynRules Output (UFO)

Example QED ($e^+e^-\gamma$ Vertex):

- Python output files
- Contains model-independent files and model-dependent files
- Contains all information to calculate any tree level matrix element
- Has parameter file to adjust model parameters to scan allowed regions

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\psi}\left(iD^\mu\gamma_\mu - m\right)\psi$$

$$V_{e^+e^-\gamma} = ie\gamma^\mu = \gamma$$



[arXiv:1108.2040]

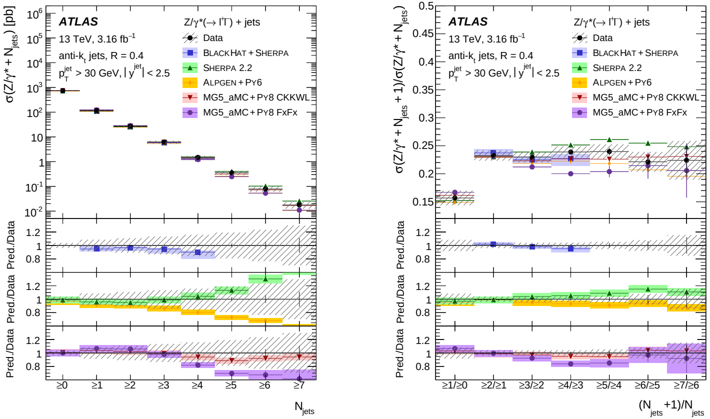
Universal FeynRules Output (UFO)

Example for photon-electron vertex

```
e__minus__ = Particle(pdg_code=11, name='e-', antiname='e+',
                      spin=2, color=1, mass=Param.ZERO,
                      width=Param.ZERO, texname='e-',
                      antitexname='e+', charge=-1,
                      GhostNumber=0, LeptonNumber=1,
                      Y=0)
V_77 = Vertex(name='V_77',
              particles=[ P.e__plus__, P.e__minus__, P.a ],
              color=[ '1' ], lorentz=[ L.FFV1 ],
              couplings={(0,0):C.GC_3})
FFV1 = Lorentz(name='FFV1', spins=[ 2, 2, 3 ],
               structure='Gamma(3,2,1)')
GC_3 = Coupling(name='GC_3', value='-(ee*complex(0,1))',
                order={'QED':1})
```

Tree Level Matrix Element Generators

- ALPGEN [arXiv:hep-ph/0206293]
- AMEGIC [arXiv:hep-ph/0109036]
- COMIX [arXiv:0808.3674]
- CALCHEP [arXiv:1207.6082]
- HERWIG [arXiv:0803.0883]
- MADGRAPH [arXiv:1405.0301]
- WHIZARD [arXiv:0708.4233]
- etc.



[arXiv:1702.05725]

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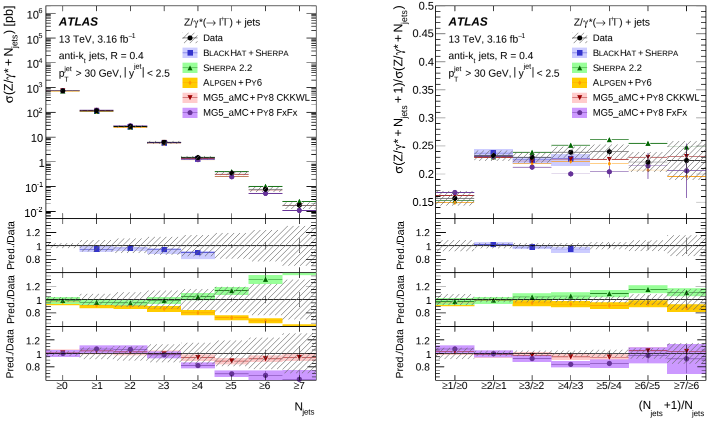

[arXiv:1702.05725]

$2 \to 2$ Phase Space Example

Consider $l + {}^{12}C \to l' + N + X$ in the quasielastic regime.

$$d\sigma \propto \; d\Phi_2(a, b; 1, 2) \;\; d^4 p_a \;\; d^3 p_b$$

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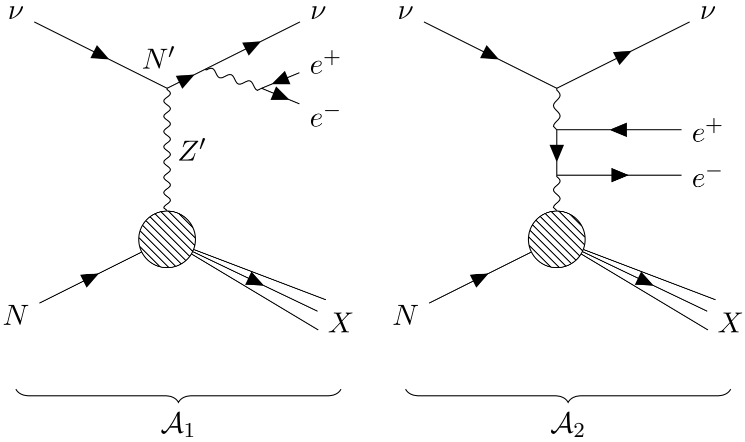
Quasielastic Delta Function: $\delta(E_b - E_1 - E_r + m - E_2)$
Phase Space Delta Function: $\delta(E_a + E_b - E_1 - E_2)$
Define initial nucleon energy as $E_a = m - E_r$. Allows use of phase space tools developed at LHC.

Multi-channel Integration



- Both diagrams contribute to cross section
- They have different pole structures
- Need method to sample these structures efficiently (i.e. $|\mathcal{A}_1 + \mathcal{A}_2|^2$)

Multi-channel Integration and VEGAS

Multi-channel Integration

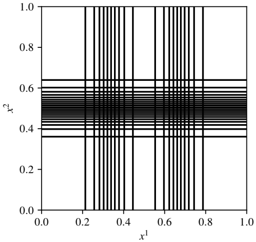
- Generate PS efficiently for $|\mathcal{A}_1|^2$ or $|\mathcal{A}_2|^2$
- Do not know how to efficiently sample $2Re(\mathcal{A}_1\mathcal{A}_2^\dagger)$
- Define channels: C_1 and C_2
- Generate events according to distributions g_i for channel i

$$\int d\vec{x} f(\vec{x}) = \sum_i \alpha_i \int d\vec{x} g_i(\vec{x}) \frac{f(\vec{x})}{g_i(\vec{x})}$$

- Optimize α_i to minimize variance

VEGAS

- Adaptive importance sampling
- Use this to get interference terms more accurately



VEGAS grid for $\int_0^1 d^4x \left(e^{-100(\vec{x}-\vec{r_1})^2} + e^{-100(\vec{x}-\vec{r_2})^2}\right)$

[J.Comput.Phys. 27 (1978) 291, 2009.05112]

Recursive Phase Space Decomposition

Phase space can be decomposed as:

$$\mathrm{d}\Phi_n(a,b;1,\ldots,n) = \mathrm{d}\Phi_{n-m+1}(a,b;m+1,\ldots,n)\frac{\mathrm{d}s_\pi}{2\pi}\mathrm{d}\Phi_m(\pi;1,\ldots,m)$$

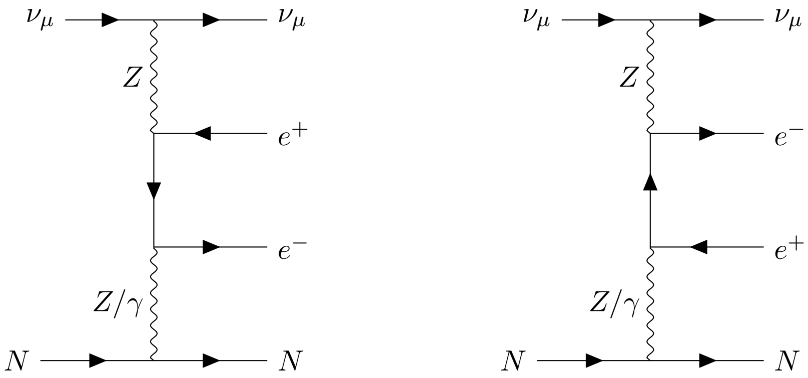
Iterate until only $1 \to 2$ phase spaces remain.
Basic building blocks:

$$S_\pi^{\rho,\pi\setminus\rho} = \frac{\lambda(s_\pi, s_\rho, s_{\pi\setminus\rho})}{16\pi^2\, 2\, s_\pi}\,\mathrm{d}\cos\theta_\rho\,\mathrm{d}\phi_\rho$$

$$T_{\alpha,b}^{\pi,\overline{\alpha b \pi}} = \frac{\lambda(s_{\alpha b}, s_\pi, s_{\overline{\alpha b \pi}})}{16\pi^2\, 2 s_{\alpha b}}\,\mathrm{d}\cos\theta_\pi\,\mathrm{d}\phi_\pi$$

Momentum conservation: $(2\pi)^4\mathrm{d}^4p_{\overline{\alpha b}}\delta^{(4)}(p_\alpha + p_b - p_{\overline{\alpha b}})$

Neutrino Tridents



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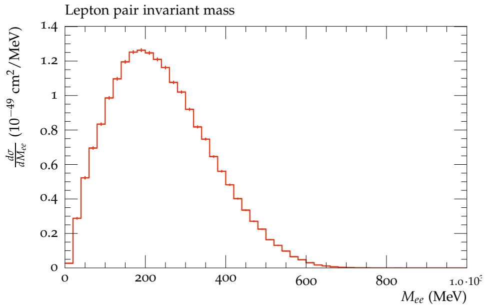

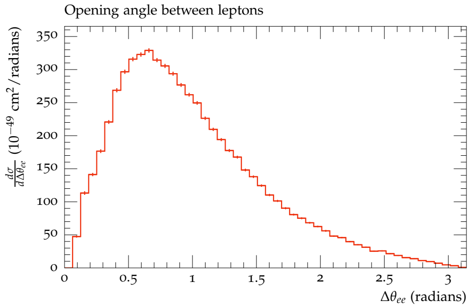

Symplectic Integration for non-separable Hamiltonians

- Create copy of Hamiltonian:

$$\overline{H}(q,p,x,y) \equiv H_A(q,y) + H_B(x,p) + \omega H_C(q,p,x,y)$$
$$H_C(q,p,x,y) = |q-x|^2/2 + |p-y|^2/2$$

- Time step for each Hamiltonian:

$$\phi^\delta_{H_A}: \begin{bmatrix} q \\ p \\ x \\ y \end{bmatrix} \to \begin{bmatrix} q \\ p - \delta\partial_q H(q,y) \\ x + \delta\partial_y H(q,y) \\ y \end{bmatrix}, \phi^\delta_{H_B}: \begin{bmatrix} q \\ p \\ x \\ y \end{bmatrix} \to \begin{bmatrix} q + \delta\partial_p H(x,p) \\ p \\ x \\ y - \delta\partial_x H(x,p) \end{bmatrix},$$

$$\phi^\delta_{H_C}: \begin{bmatrix} q \\ p \\ x \\ y \end{bmatrix} \to \frac{1}{2}\begin{bmatrix} \begin{pmatrix} q+x \\ p+y \end{pmatrix} + R(\delta)\begin{pmatrix} q-x \\ p-y \end{pmatrix} \\ \begin{pmatrix} q+x \\ p+y \end{pmatrix} - R(\delta)\begin{pmatrix} q-x \\ p-y \end{pmatrix} \end{bmatrix},$$

- Full second order time step:

$$\phi^\delta_2 = \phi^{\delta/2}_{H_A} \circ \phi^{\delta/2}_{H_B} \circ \phi^\delta_{\omega H_C} \circ \phi^{\delta/2}_{H_B} \circ \phi^{\delta/2}_{H_A}.$$