Achilles ACHIcagoLand Lepton Event Simulator

Current Capabilities & Future Plans for Lepton Scattering Modeling and Associated Uncertainties

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Version: (:56}] Authors: Joshua Isaacson, William Jay, Alessandro Lovato, Pedro A. Machado, Noeni Rocco

Undergraduate Student Contributions: Diego Lopez Gutierrez, Sherry Wang, Russell Farnsworth







Based largely on:

Isaacson [WJ] et al. *"New approach to intranuclear cascades with quantum Monte Carlo configurations" Phys.Rev.C* 103 (2021) 1, 015502 [arXiv:2007.15570]

Isaacson [WJ] et al. *"Introducing a novel event generator for electron-nucleus and neutrino-nucleus scattering" Phys.Rev.D* 107 (2023) 3, 033007 [arXiv:2205.06378]

+ unpublished work in progress



Outline

- Motivation
- Achilles overview
 - Theoretical setup
 - Work in progress
- Recent results



Motivation

The Challenge Lepton Event Simulation



"Uncertainties exceeding 1% for signal and 5% for backgrounds may result in substantial degradation of the sensitivity to CP violation and the mass hierarchy."



- neutrino experiments
- Percent-level theoretical control of neutrinonucleus scattering cross sections is needed





The Challenge Lepton Event Simulation



Achilles is a **theory-driven event generator** aiming to be responsive to **current and upcoming experimental needs**



Achilles overview

For contrast / context, see other talks

- Steven Gardiner (W 10:40) [MARLEY]
- Yoshinari Hayato (Th 15:00) [NEUT]
- Ulrich Mosel (Th 16:20) [GiBUU]
- Marco Roda (F 09:00) [GENIE]
- Kajetan Niewczas (F 10:10) [NuWro]

Achilles

Theory-driven: break the problem into well-defined theoretical pieces

$$d\sigma = \left(\frac{1}{|v_{A} - v_{\ell}|} \frac{1}{4E_{A}^{\text{in}}E_{\ell}^{\text{in}}}\right) \times \left|\mathscr{M}\right|^{2} \times \prod_{f} \frac{d^{3}p_{f}}{(2\pi)^{3}} (2\pi)^{4} \delta^{4} \left(k_{A} + k_{\ell} - \sum_{f} p_{f}\right)$$
$$d\sigma = (\text{flux}) \times (\text{matrix element}) \times (\text{phase space})$$

The Matrix Element

Approx. 1: Factorization of leptonic & hadronic tensors



Leptonic tensor: Known analytically in SM or BSM scenario

Hadronic tensor:

Complicated multi-scale objecting encoding all the hadronic/nuclear physics $|\Psi_0
angle$: Initial state (say, 40 Ar or H_2O)

 $|\Psi_f\rangle$: Final state (nuclear remnant + outgoing pions, kaons, etc...)

The Matrix Element Approx. 2: Factorization of primary vertex



 \mathscr{V} : Primary-interaction vertex \mathscr{P} : Time evolution to produce observed final states

"Sum coherently over all possible intermediate states p'." -Quantum mechanics

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

This is exact, but exponentially hard. Factorize the problem again.

The Matrix Element Approx. 2: Factorization of primary vertex



 \mathscr{V} : Primary-interaction vertex \mathscr{P} : Time evolution to produce observed final states

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

Treat the sum incoherently. Handle constituents with theoretical care.

Similar to dressing hard-scattering cross sections with parton showers in LHC context

See talk by Stephen Mrenna (M 15:40) Uncertainties in LHC Physics Modelling

The Primary-interaction vertex Approx. 3: Choose DOF, Factorization Scheme

- Take nucleons as initial-state DOF
- Take electroweak currents from nuclear EFT:

$$J^{\mu}(q) = \sum_{i} j^{\mu}_{i}(q) + \sum_{i < j} j^{\mu}_{ij}(q) + \cdots$$

• Choose a factorization scheme: the *impulse approximation*:

$$|\Psi_f\rangle = |\mathbf{p}\rangle \otimes |\Psi_f^{A-1}\rangle$$

"For momentum transfer $|\mathbf{q}| \gtrsim 400 \text{ MeV}$, external probes resolve individual nucleons."

Compare with talks by Lovato (T 09:00), Adreoli (T 9:40), Steinberg (T 11:10), Sobczyk (T 10:40), González Jiménez (T 14:20),





Spatial distribution from nuclear many-body theory: QMC. Quasi-exact.



(among others)

The Primary-interaction vertex Approx. 3: Choose DOF, Factorization Scheme

 $W_{N}^{\mu\nu} = \langle \Psi_{0} | J^{\mu\dagger}(q) | \Psi_{f} \rangle \langle \Psi_{f} | J^{\nu}(q) | \Psi_{0} \rangle$

With the impulse approximation $|\Psi_f\rangle = |\mathbf{p}\rangle \otimes |\Psi_f^{A-1}\rangle$,



See talks by R. Gupta (M 14:10) A. Meyer (M 14:40)

The Hadronic Tensor and Lattice QCD A brief detour $n \quad J^{\mu}(t) \quad J^{\nu}(0) \quad n$





- Would provide a vital bounding constraint, grounded in QCD for shallow inelastic kinematics, on exclusive models used in generators
- Complementary to QCD on $\langle N | J_{\mu} | N\pi \rangle$ form factors for Δ -resonance physics
 - See also: A. Grebe's talk (T 15:00) Towards lattice QCD calculations of pion production
- Key technical point: scattering happens in real time

 $W_n^{\mu\nu}(t,\mathbf{q}) \propto$

 \implies Cross sections / inclusive structure functions need analytic continuation $t \rightarrow \omega + i\epsilon$

The Hadronic Tensor and Lattice QCD A brief detour $n J^{\mu}(\tau) J^{\nu}(0) n$



DETOUR

• Key technical point: scattering happens in real time

 \implies Cross sections / inclusive structure functions need analytic continuation $t \rightarrow \omega + i\epsilon$

• Inverse Laplace transform
$$w_n^{\mu\nu}(\tau, \mathbf{q}) = \int \frac{d\omega}{2\pi} w_n^{\mu\nu}(\omega, \mathbf{q}) e^{-\omega\tau}$$

- Recent work on rigorous bounding of uncertainties (from complex analysis, with a theorem!)
 - See T. Bergamaschi, WJ, P.R. Oare PRD 108 (2023) 7, 074516 [arXiv:2305.16190] + refs therein
 - Close connection to Euclidean response functions in nuclear theory community

The Hadronic Tensor and Lattice QCD A brief detour

Lattice QCD calculations occur in Euclidean time:



DETOUR



The Hadronic Tensor and Lattice QCD A brief detour



R. Nevanlinna Ann. Acad. Sci. Fenn. Ser. A 13 (1919) Ann. Acad. Sci. Fenn. Ser. A 32 (1929)

- The problem of analytic continuation is amenable to techniques from Nevanlinna-Pick interpolation
- Theorem (Nevanlinna, 1919/1929): Computes the <u>space of functions</u> in the upper half-plane which
 - 1. Interpolate the given set of Euclidean data and
 - 2. Are analytic in the upper-half plane.
- Applicability to field-theory problems first recognized by Fey, Yeh, and Gull [arXiv:2010.04572]
- Existence of rigorous error bounds first recognized in our [arXiv:2305.16190]

The Hadronic Tensor and Lattice QCD A brief detour



DETOUR

- Energies rescaled to line in unit interval \implies lattice units with $a \approx 0.07$ fm, so $am_{\rho} \approx 0.25$
- ✓ Spectral peaks from $\rho(770)/\omega(782)$ and $\phi(1020)$ cleary visible in reconstructions
- Exact answer is contained within the rigorous bounding envelope of the "Wertevorrat"



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

END

DETOUR



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

- Intranuclear Cascade (INC)
 - Scatter nucleons quantum mechanically
 - Propagate nucleons classically, with in-medium corrections

(Neglect interference between successive scattering events in propagation)

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

- The initial configuration of nucleons is taken from:
 - Spatial distribution: quantum Monte Carlo, retaining correlations
 - Momenta: local Fermi gas model

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

The quantum mechanical scattering model:

- Utilizes measured NN cross sections, e.g., from from SAID database with GEANT4 or NASA parameterization
- Scatters probabilistically according to the impact parameter: $P(b) = \exp(-\pi b^2/\sigma)$

 $\mathbf{\mathfrak{S}} \lambda^{-1} = \rho \sigma$ for the mean free path λ

 ${\ensuremath{\,\overline{\!\!\mathcal O\!}}}$ Total probability integrates to the cross section σ

• Incorporates Pauli blocking and formation zone to constrain possible scatterings

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

Classical propagation in the background nucleus creates an effective optical potential which induces two effects:

$$\frac{d\sigma}{d\Omega} \longrightarrow \left(\frac{d\sigma}{d\Omega}\right)_{\text{in medium}}$$

(In-medium corrections to NN interactions)

2. Long-distance:

$$\dot{\mathbf{p}} = -\partial_{\mathbf{q}}H \quad \dot{\mathbf{q}} = +\partial_{\mathbf{p}}H$$

(Classical evolution in background potential)



Achilles overview (A few recent developments)

Achilles – Recent updates

Isaacson et al. PRD 105 (2022) 9, 096006 [arXiv:<u>2110.15319]</u>

Factorization of leptonic and hadronic tensors

- Automated specification of leptonic tensor (including BSM possibilities)
- Key involvement: Diego Lopez Gutierrez [Undergrad @ Macalester → PhD @ Wash. U. St Louis]
- Uses tools developed by LHC event generation community: Sherpa, Comix, FeynRules, UFO files



Achilles — Work in progress New API for nuclear models

- We have new API/extendible interface for nuclear models
- The API supports models implemented in Fortran or CPP. Extension to models in python is straightforward if there is community interest
- Allows, e.g., for different nuclear spectral functions



Achilles — Work in progress Resonant production

- First Achilles paper focused on QE scattering: $2 \rightarrow 2$ scattering
- Resonant scattering (e.g., $\ell N \rightarrow \ell N \pi$) is $2 \rightarrow 3$ scattering
- Preliminary implementation [Noemi Rocco] of the dynamical coupled channel (DCC) model of resonant scattering.
 - See Rocco et al., PRC 100 (2019) 4, 045503 [arXiv:1907.01093]
 - Fundamental input to Achilles: DCC $\rightarrow \langle N | J_{\mu} | N \pi \rangle$ matrix elements with fully exclusive kinematics
- Working on cascade model including pion production

Achilles — Work in progress New "process grouping" for multiple processes

- Accommodates charged-currents and neutral-current scattering in the same run with correct event fractions
- Handles different beam particles (e.g., different neutrino flavors and/or charged leptons from detector environment)
- Allows for different scattering mechanisms (e.g, QE and resonance) in the same run with correct event fractions

NuHepMC

S. Gardener, J. Isaacson, L. Pickering [arXiv:2310.13211]

Standardized event record format for neutrino event generators

- NuHepMC is the default output format for Achilles
- NuHepMC gives a framework for uncertainty quantifications via the "Generator Run metadata"
 - Example: G.R.7 Event Weights Can specify a vector of event weights. These can be used with "in situ parameter variation" to constrain model uncertainties.
 - See talk by Stephen Mrenna (M 15:40) for how this used already by LHC event generators like Pythia
- NuHepMC streamlines the pipeline for data/theory comparisons using the NUISANCE framework



"This comparison was made with the NUISANCE framework, which before this implementation of NuHepMC would have to have been built against GENIE, NEUT, and NuWro binaries of compatible versions to be able to generate the predictions shown in the figure."

See talk by Steven Gardiner (W 10:40)



Recent results

Achilles: Comparison to experiment

PRD 107 (2023) 3, 033007 [arXiv:2205.06378]

J. S. O'Connell *et al.*, Phys. Rev. C **35**, 1063 (1987). R. M. Sealock *et al.*, Phys. Rev. Lett. **62**, 1350 (1989). D. Zeller, Investigation of the structure of the C-12 nucleus by high-energy electron scattering, Other thesis, Karlsruhe University, 1973.



Beyond firsts peak: Neglected MEC and resonance contributions

Good agreement = Validation of initial model for QE interaction

W.I. Jay - MIT

Achilles: Comparison to experiment

CLAS and e4v collaborations Nature 599 (2021) 7886, 565-570

PRD 107 (2023) 3, 033007 [arXiv:2205.06378]

- Inclusive e-C hadronic cross section
- Analysis by e4v to mimic kinematic setup for QE vA scattering

$$E_{\rm QE} = \frac{2m_N\epsilon + 2m_N E_\ell - m_\ell^2}{2\left(m_N - E_\ell + p_\ell \cos\theta_\ell\right)}$$





FIG. 4: Comparison of the quasielastic energy reconstructed for an electron beam of 1159 MeV. Data is taken from Ref. [69]. The definition of E_{QE} can be found in Eq. 31. The red dashed vertical line marks the true beam energy.

- Low EQE: MEC and resonance contributions
- High EQE: interference effects (neglected)

Achilles: Comparison to experiment

CLAS and e4v collaborations Nature 599 (2021) 7886, 565-570

PRD 107 (2023) 3, 033007 [arXiv:2205.06378]

E_{cal} = "Calorimetric energy" = "sum of final-state energies"



Achilles: Recent Results

Application: Correlated decays in neutrino experiments

J. Isaacson et al. [arXiv:2303.08104]

Key involvement: Sherry Wang [Undergrad @ Northwestern]

Motivation: ν_{τ} is perhaps the least understood elementary particle

- DUNE: O(few hundred) ν_{τ} events per year \rightarrow Accurate theoretical predictions critical
- Outgoing/decaying τ is polarized \rightarrow Induces correlations in final-state particles
- Standard Model predicts:
 - τ polarization perpendicular to the lepton-scattering plane vanishes
 - τ polarization components within the lepton-scattering plane do <u>not</u> vanish
- Other generators have often treated ν_{τ} interactions as for $\nu_e, \nu_{\mu} \rightarrow$ "outgoing τ as LH only"

Results

- First fully differential predictions for ν_{τ} scattering at DUNE energies, including all spin correlations and all τ decay channels
- Calculated using generic interface between Achilles and Sherpa
- Correlations between production and decay are automatically maintained

Achilles: Recent Results

Application: Correlated decays in neutrino experiments

Momentum Fraction Distributions

- Benchmarking done against analytic results in collinear ($p_{\tau} \rightarrow \infty$) limit, monochromatic beams
- Final results calculated using realistic DUNE fluxes



J. Isaacson et al. [arXiv:2303.08104]



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Achilles — What's next?

More production processes

- Published generator: QE scattering only
- Near-term goals: particle production (+decay) at the initial interaction and cascade
- Initial "hard interaction"
 - Meson-exchange currents in the spectral function formalism
 - **Resonant scattering** in the dynamical coupled channel formalism (coming very soon!)
 - Longer term: consistent treatment of DIS



Cascade

 $d\sigma$

- **Pion production**
- **Propagation/decay of** Δ

 $NN \to N\Delta \to NN\pi$

(Can take from data. Lattice calculations will always help.)

Achilles – Summary

- Achilles aspires to be a theory-driven event generator, with consistent treatment
 of known theoretical uncertainties
- Observations:
 - Robustly quantifying systematic errors is generally a tough problem
 - Once chosen, correctly propagating systematics errors is comparatively easy
 - For uncertainties in the "hard interaction" the theoretical uncertainty amounts to an uncertainty in the overall event weight, which is straightforward to propagate

• Achilles employs a modular design to factorize physically different processes:

- Leptonic vs hadronic tensors,
- Nuclear vs hadronic physics
- Primary interaction vertex vs intranuclear cascade
- Achilles currently supports quasi-elastic scattering (e.g., spectral function formalism)
- Support for more processes is coming soon!



Backup

Cascade – Algorithm



Effective Background Potentials

- Three-parameter non-relativistic potential
- Parameters obtained by a fit to single-particle energy of nuclear matter (Urbana v₁₄ + TNI Hamiltonian)
- Consistent with variational ground-state calculations of Wiringa, Fiks, and Fabrocini

$$U(p',r) = \alpha[\rho(r)] + \frac{\beta[\rho(r)]}{1 + (p'/\Lambda[\rho(r)])^2} \qquad \begin{aligned} \alpha(\rho) &= 15.52(\rho/\rho_0) + 24.93(\rho/\rho_0)^2 \text{ MeV}, \\ \beta(\rho) &= -116(\rho/\rho_0) \text{ MeV}, \\ \Lambda(\rho) &= 3.29 - 0.373(\rho/\rho_0) \text{ fm}^{-1}, \\ \rho_0 &= 0.16 \text{ fm}^{-3} \end{aligned}$$

- [102] A. Nikolakopoulos, R. González-Jiménez, N. Jachowicz, K. Niewczas, F. Sánchez, and J. M. Udías, (2022), arXiv:2202.01689 [nucl-th].
- [103] R. B. Wiringa, Phys. Rev. C 38, 2967 (1988).
- [104] R. B. Wiringa, V. Fiks, and A. Fabrocini, Phys. Rev. C 38, 1010 (1988).

Effective Background Potentials

- Potential fitted from proton-nucleus cross section data to determine global proton-nucleus optical potentials for energies between 20 - 1040 MeV for several nuclear targets
- Taken from work by Cooper, Hama, and Clark

[97] E. D. Cooper, S. Hama, and B. C. Clark, Phys. Rev. C 80, 034605 (2009).

In-medium corrections

[107] V. R. Pandharipande and S. C. Pieper, Phys. Rev. C 45, 791 (1992).

$$\begin{aligned} \frac{d\sigma'}{d\Omega} &= \frac{|\mathbf{p}_1' - \mathbf{p}_2'|}{m} \left| \frac{\mathbf{p}_1'}{m^*(p_1', \rho)} - \frac{\mathbf{p}_2'}{m^*(p_2', \rho)} \right|^{-1} \frac{m^* \left(\sqrt{(p_3'^2 + p_4'^2)/2}, \rho \right)}{m} \frac{d\sigma}{d\Omega} \\ m^*(p', \rho) &= p' \left(\frac{p'}{m} + \frac{dU(p', \rho)}{dp'} \right)^{-1} \end{aligned}$$

Analytic Continuation Conformal maps

- Recall: analytic functions are defined by convergent power series in an open set around each nonsingular point
- Radius of convergence is determined by the location of the nearest pole

So change coordinates!



Analytic Continuation The technical problem

- Recall: analytic functions are defined by convergent power series in an open set around each nonsingular point
- Radius of convergence is determined by the location of the nearest pole
- The Cayley transform maps the problem to the unit disk.
- Given Euclidean data

$$\{i\omega_{\ell}\} \to \zeta_{\ell} \subset \mathbb{D},$$

 $\{G(i\omega_{\ell})\}\mapsto w_{\ell}\subset \mathbb{D},$

construct an analytic function $f(\zeta)$

on the disk such that $f(\zeta_{\ell}) = w_l$.



Analytic Continuation Nevanlinna's Theorem

R. Nevanlinna Ann. Acad. Sci. Fenn. Ser. A 13 (1919) Ann. Acad. Sci. Fenn. Ser. A 32 (1929)

- Theorem (Nevanlinna, 1919/1929):
 - Any solution to the interpolation problem with N points can be written in the form

$$f(\zeta) = \frac{P_N(\zeta)f_N(\zeta) + Q_N(\zeta)}{R_N(\zeta)f_N(\zeta) + S_N(\zeta)}$$

where the coefficient functions P_N , Q_N , R_N , S_N are calculable using an inductive formula in terms of the input data $\{\zeta_{\ell}\}$ and $\{w_{\ell}\}$ and an arbitrary analytic function $f_N(\zeta) : \mathbb{D} \to \mathbb{D}$.

Derivation: See our preprint [arXiv:2305.16190], which follows modern treatment by mathematician Nicolau [https://mat.uab.cat/~artur/data/nevanlinna-pick.pdf]

- P_N , Q_N , R_N , $S_N \iff$ "Nevanlinna coefficients"
- Arbitrary function $f_N(\zeta) \iff$ "Freedom to specify further Euclidean data to constrain the interpolating function"

Analytic Continuation The full space of solutions

- Question: For fixed N and ζ , what are the possible values that an interpolating function $f(\zeta)$ can take, by varying possible values of the arbitrary function $f_N(\zeta) \in \mathbb{D}$?
- Answer: The space of possible values is given by the *Wertevorrat* $\Delta_N(\zeta)$, which is the disk of radius $r_N(\zeta)$ and centered at $c_N(\zeta)$.

$$c_{N} = \frac{P_{N}(-R_{N}/S_{N}) + Q_{N}}{R_{N}(-R_{N}/S_{N}) + S_{N}} \qquad r_{N} = \frac{|P_{N}S_{N} - Q_{N}R_{N}|}{|S_{N}|^{2} - |R_{N}|^{2}}$$

• The Wertevorrat $\Delta_N(\zeta)$ rigorously contains the full infinite family of all possible analytic continuations at each point $\zeta \in \mathbb{D}$.

Analytic Continuation The Wertevorrat and rigorous bounds on $\rho^{\epsilon}(\omega)$

• Finally we need to map the Wertevorrat back to the upper half plane. Use the inverse Cayley transform $z = C^{-1}(\zeta)$.



$$\rho^{\epsilon}(\omega) = \frac{1}{\pi} \operatorname{Im} G(\omega + i\epsilon)$$

$$\delta \rho^{\epsilon}(\omega) = \frac{1}{\pi} \left[\max \operatorname{Im} \partial D_{N}(\omega + i\epsilon) - \min \operatorname{Im} \partial D_{N}(\omega + i\epsilon) \right]$$