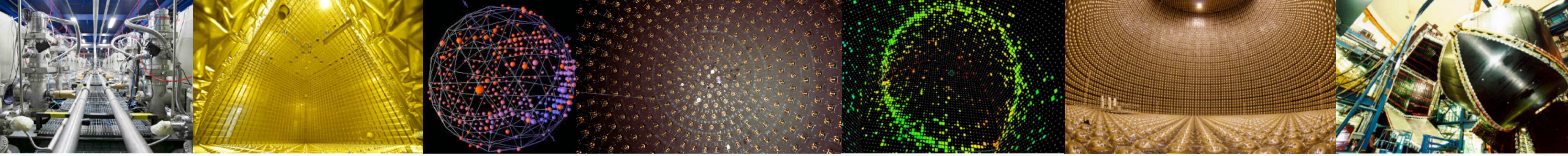


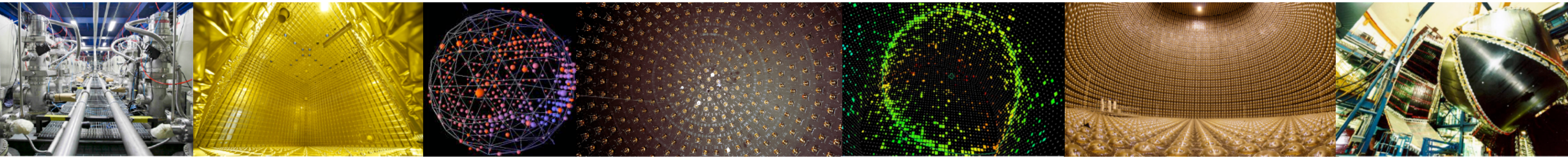
Achilles

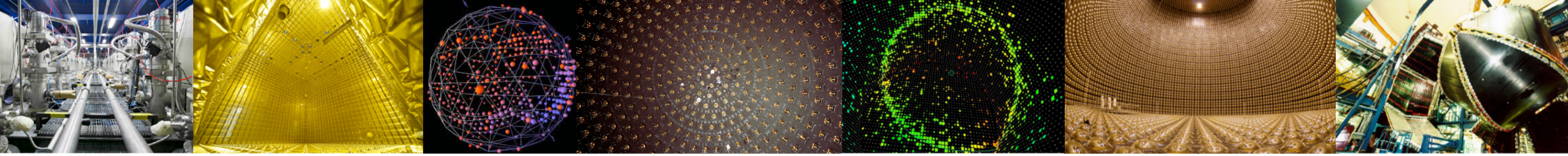
A CHIcagoLand Lepton Event Simulator

William Jay — MIT

with Joshua Isaacson, Alessandro Lovato, Pedro Machado, Noemi Rocco, and Luke Pickering

HEP Journal Club Seminar
University of Hawaii
3 October 2023

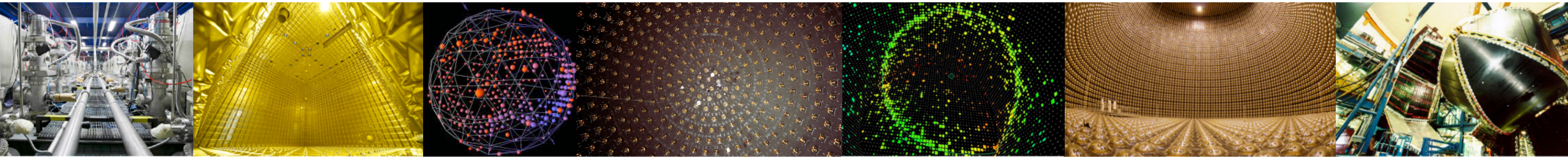


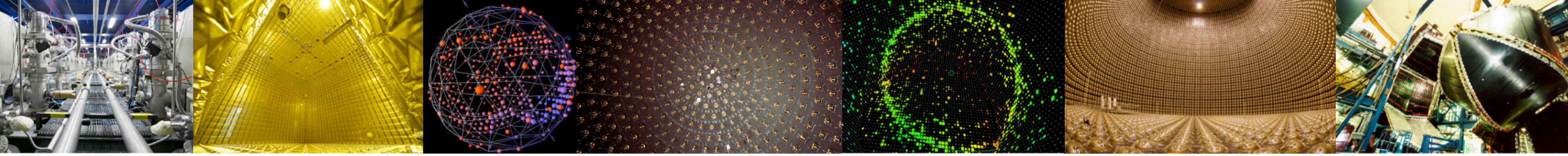


Based largely on:

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

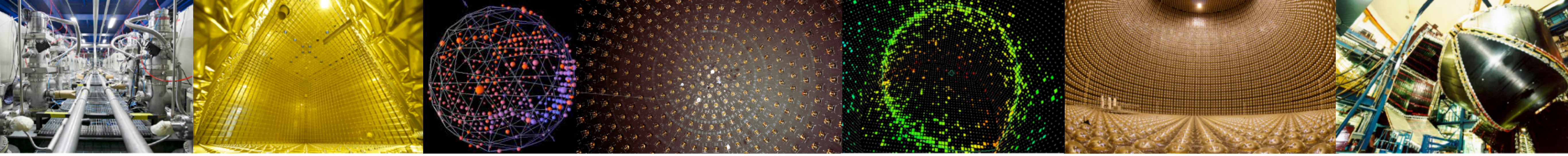
Isaacson [WJ] et al.
"Introducing a novel event generator for electron-nucleus and neutrino-nucleus scattering**"**
Phys.Rev.D **107 (2023) 3, 033007 [arXiv:2205.06378]**



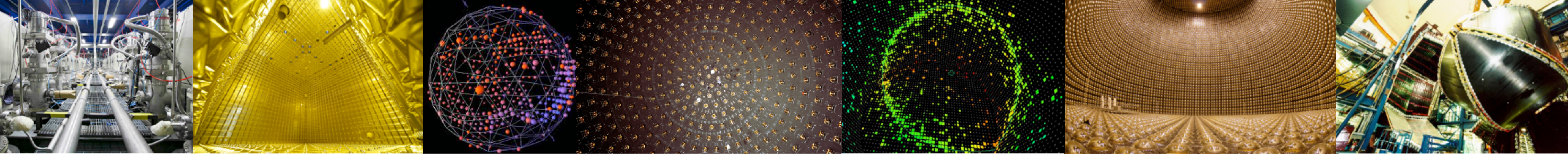


Outline

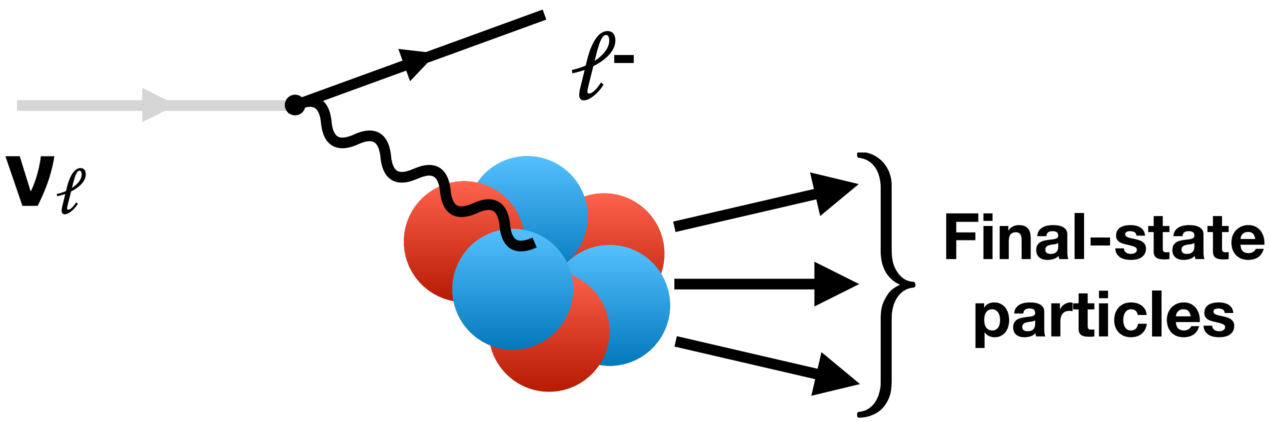
- Motivation
- Achilles overview
    - Theoretical setup
    - Implementation comments
    - Work in progress
- Recent results



Motivation

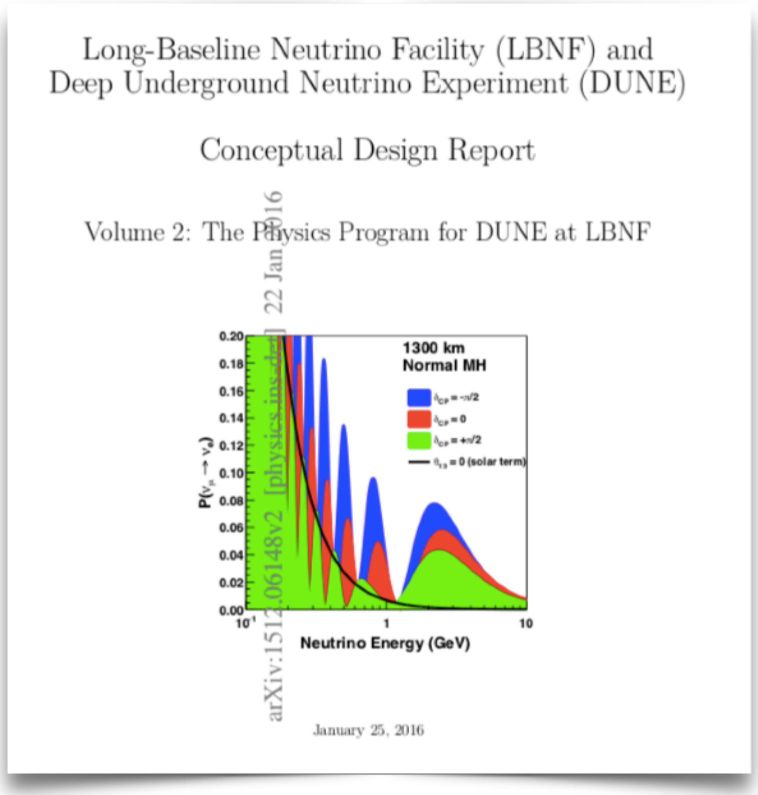


The Challenge
Lepton Event Simulation



- Neutrino experiments like DUNE and T2HK herald the start of the “precision era” for neutrino experiments
- Percent-level theoretical control of neutrino-nucleus scattering cross sections is needed

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

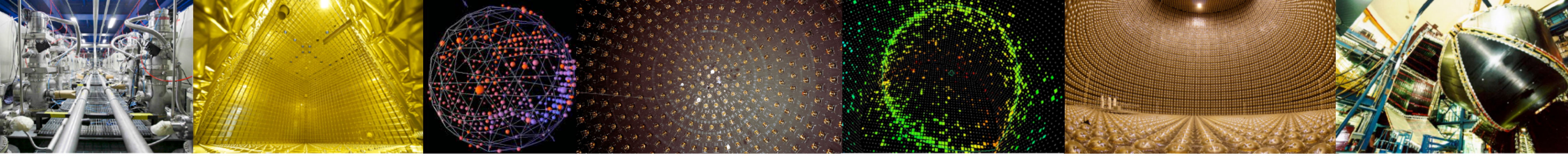

Long-Baseline Neutrino Facility (LBNF) and Deep Underground Neutrino Experiment (DUNE)

Conceptual Design Report

Volume 2: The Physics Program for DUNE at LBNF

January 25, 2016

arXiv:1512.06148v2 [physics.ins-det] 22 Jan 2016



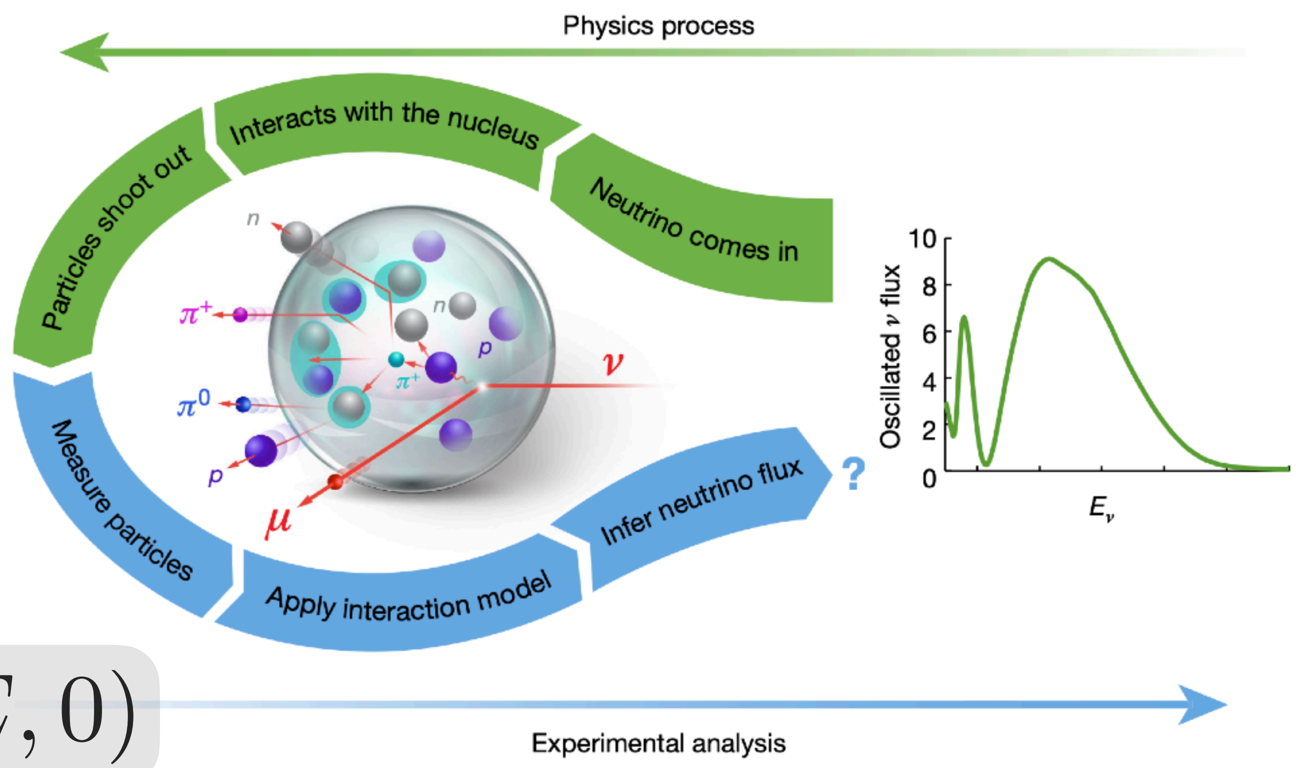
The Challenge

Lepton Event Simulation

Want: Mixing parameters, e.g, angle θ

$$P_{\nu_\mu \to \nu_e} \approx \sin^2(2\theta)\sin^2\left(\frac{\Delta m^2 L}{4E}\right)$$

$$\Phi_e(E,L) \propto P_{\nu_\mu \to \nu_e}(E,L)\Phi_\mu(E,0)$$



Neutrino fluxes. "Measurable."

"Smearing matrix"

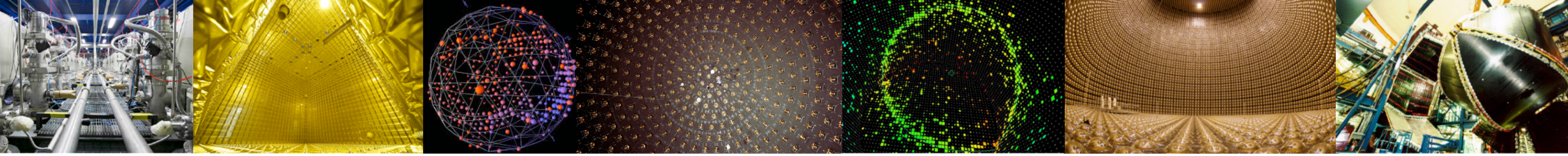
(Experimental + theoretical)

$$N_\alpha(E_{\rm rec},L) \propto \int dE\, \Phi_\alpha(E,L)\sigma(E) f_{\sigma_i}(E,E_{\rm rec})$$

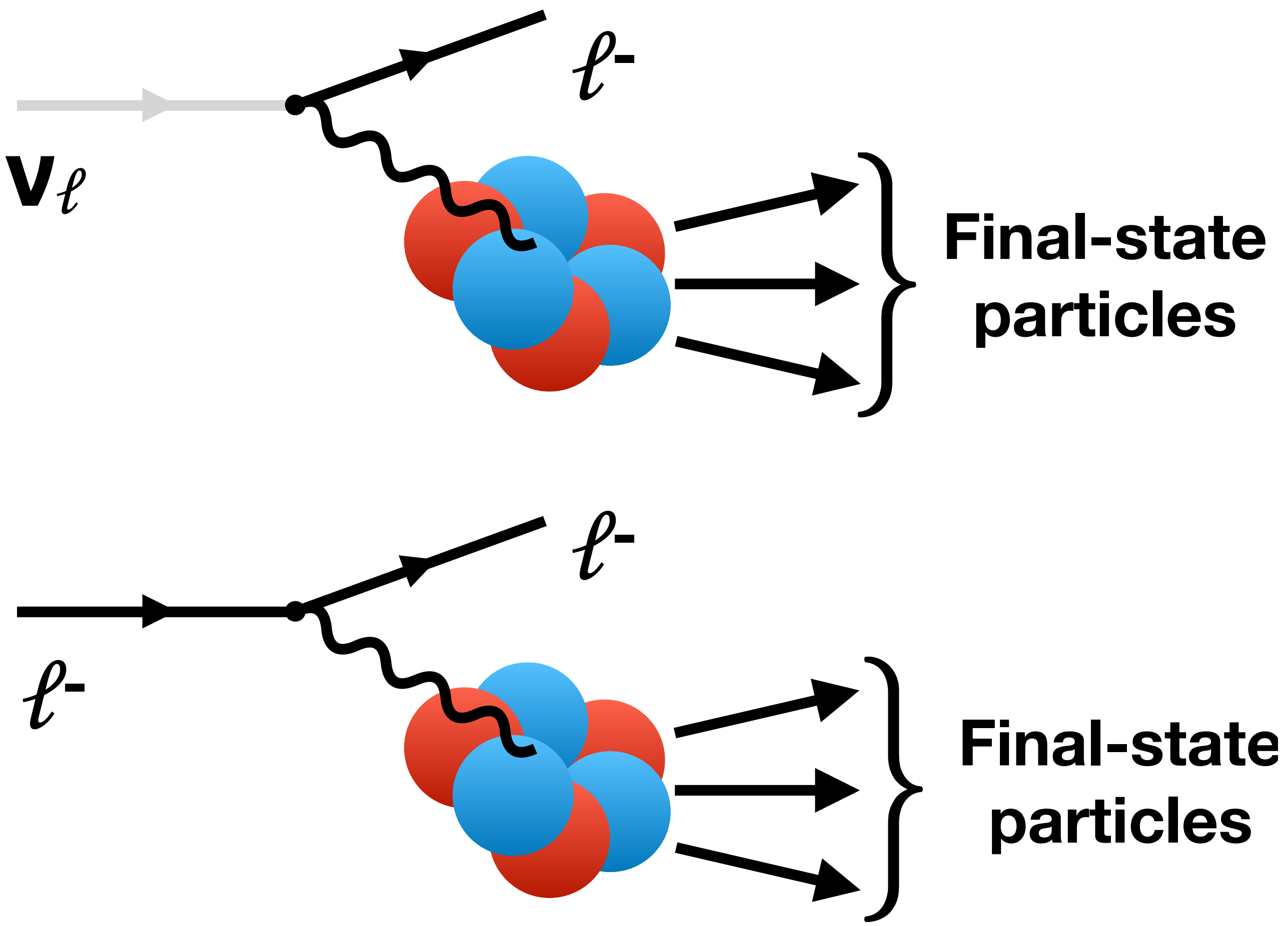
Event rate

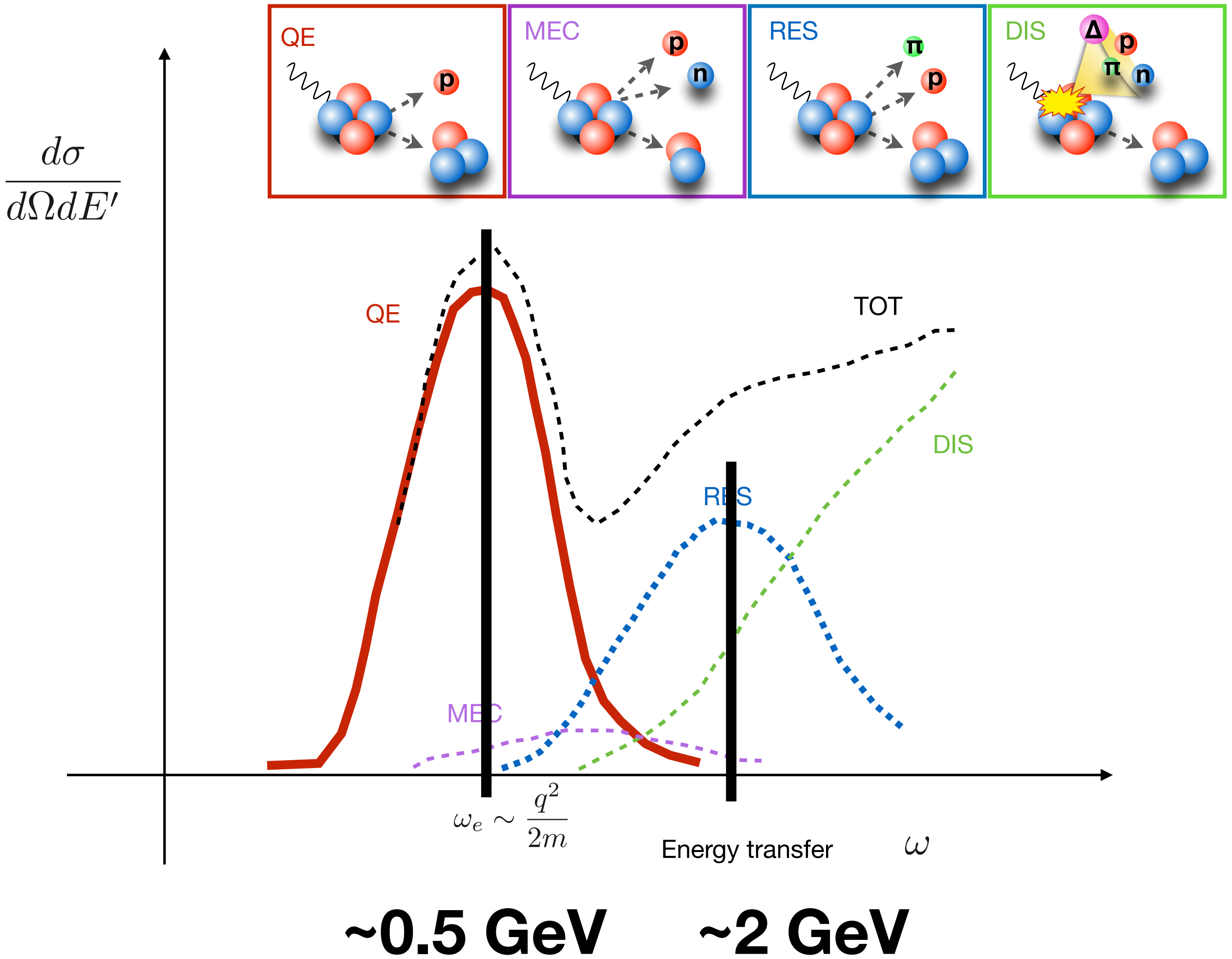
Interaction cross section

Figure credit:
M. Khachatryan et al. (e4v)
Nature 599, 565 (2021)

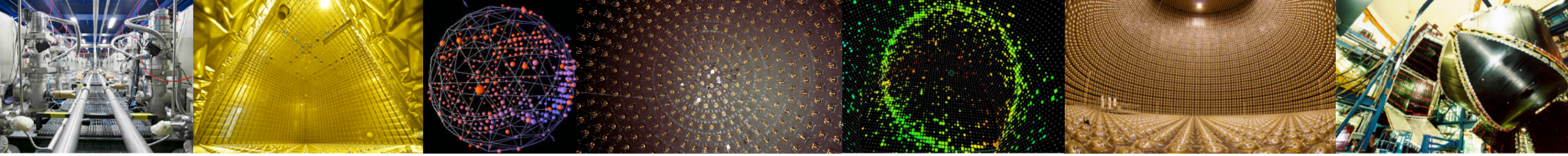


The Challenge
Lepton Event Simulation

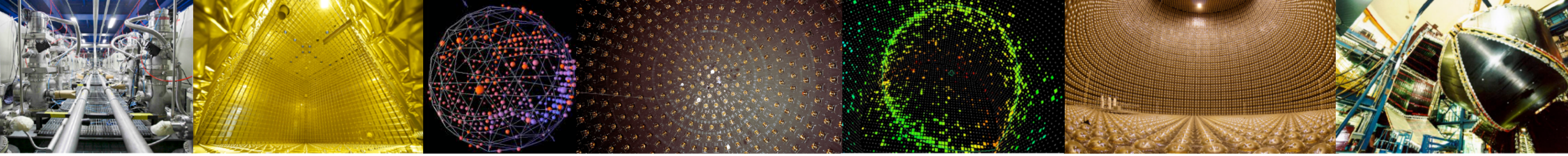




Achilles is a **theory-driven event generator** aiming to be responsive to **current and upcoming experimental needs**

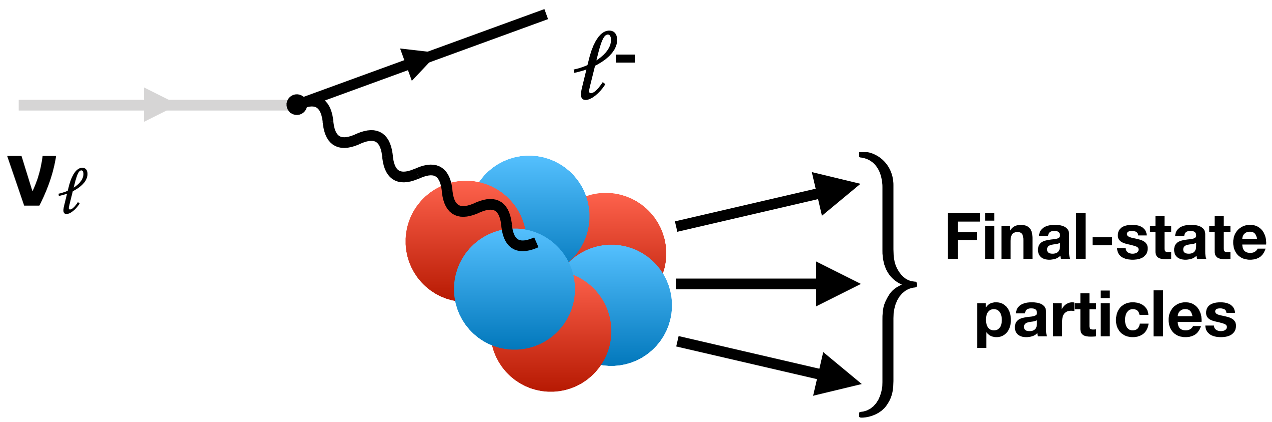


Achilles overview



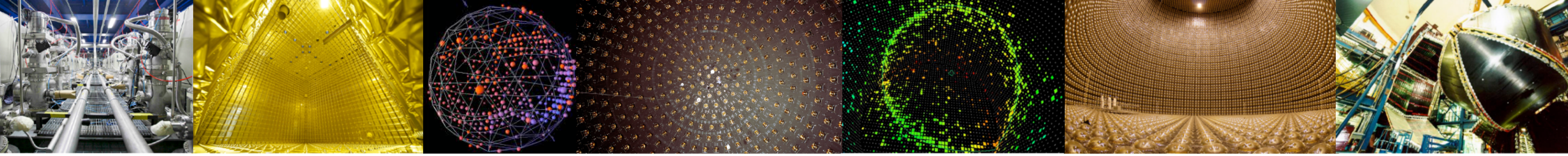
Achilles

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



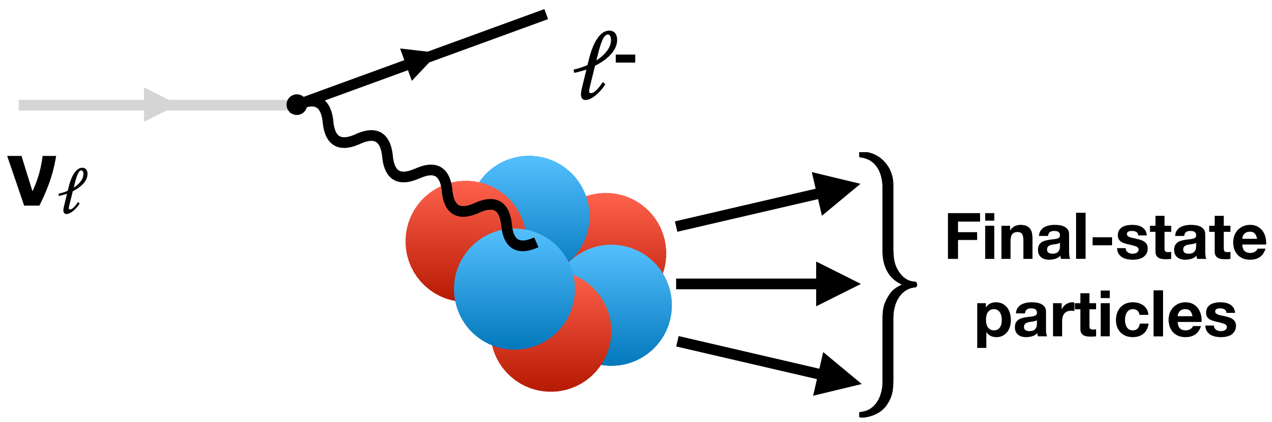
$$d\sigma = \left(\frac{1}{|v_A - v_\ell|}\frac{1}{4E_A^{\text{in}}E_\ell^{\text{in}}}\right) \times \left|\mathscr{M}\right|^2 \times \prod_f \frac{d^3p_f}{(2\pi)^3}(2\pi)^4\delta^4\left(k_A + k_\ell - \sum_f p_f\right)$$

$$d\sigma = (\text{flux}) \times (\text{matrix element}) \times (\text{phase space})$$



The Matrix Element

Approx. 1: Single gauge boson exchange



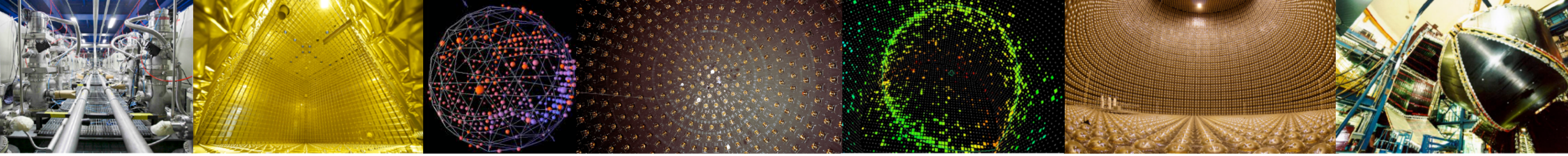
$$\left|\mathscr{M}\right|^2 = L_{\mu\nu}\,\frac{1}{P^2}\,W^{\mu\nu} \longrightarrow \langle\Psi_0|J^\dagger_\mu(q)|\Psi_f\rangle\langle\Psi_f|J_\nu(q)|\Psi_0\rangle$$

Leptonic tensor: Known analytically in SM or BSM scenario

Hadronic tensor: Complicated multi-scale objecting encoding all the hadronic/nuclear physics

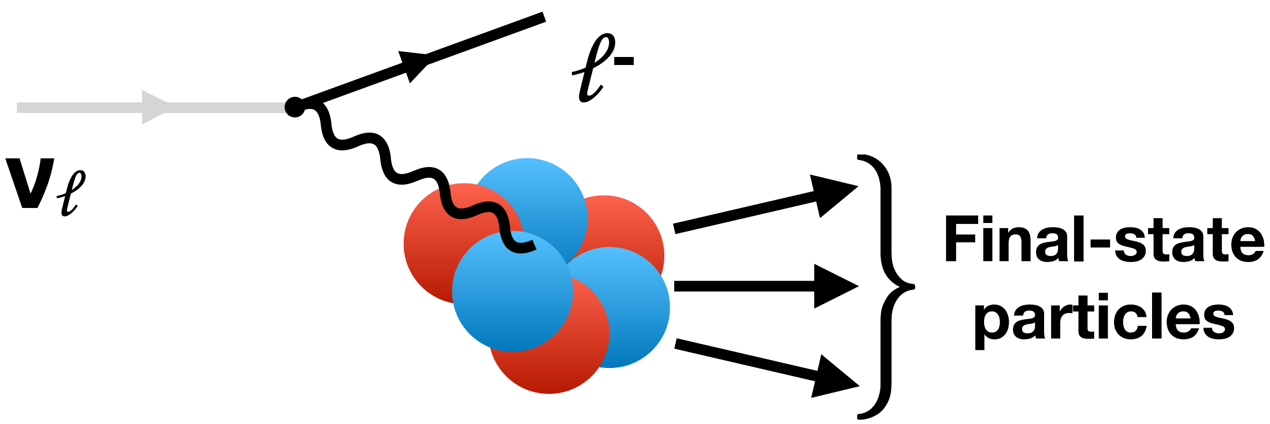
$|\Psi_0\rangle$: Initial state (say, ^{40}Ar or H_2O)

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



The Matrix Element

Approx. 2: Factorization of primary vertex



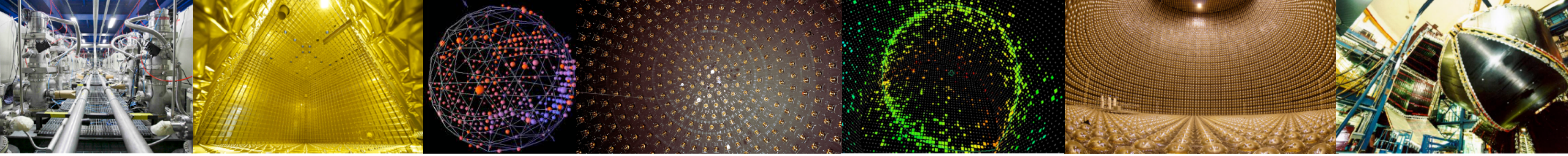
$\mathscr{V}$: Primary-interaction vertex

$\mathscr{P}$: Time evolution to produce observed final states

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

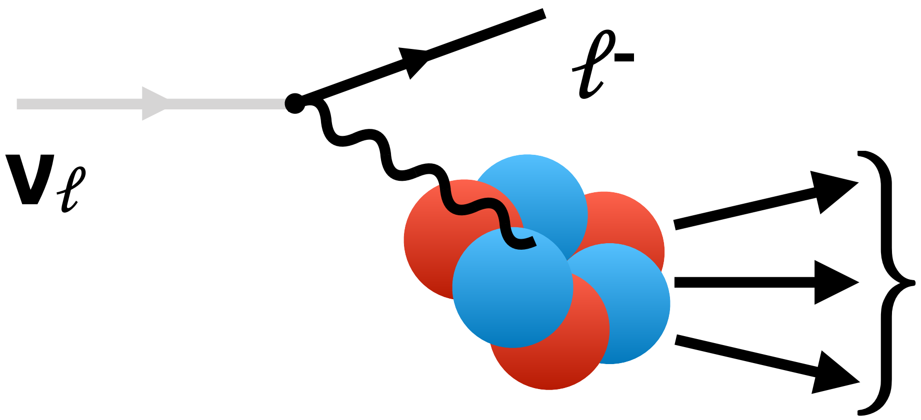
$$|\mathcal{M}(\{k\} \to \{p\})|^2 = \Big| \sum\!\!\!\!\!\!\int_{p'} \mathcal{V}(\{k\} \to \{p'\}) \times \mathcal{P}(\{p'\} \to \{p\})\Big|^2$$

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



The Matrix Element

Approx. 2: Factorization of primary vertex



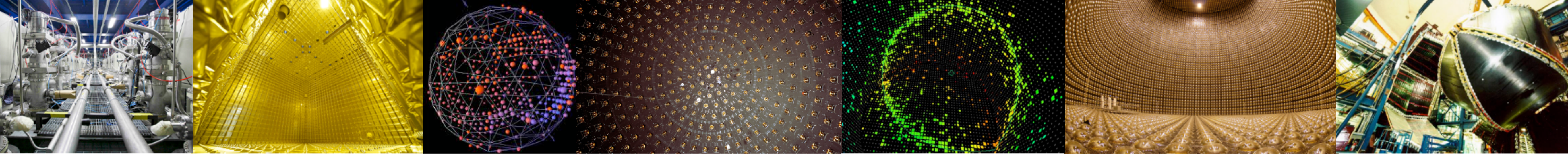
$\mathscr{V}$: Primary-interaction vertex

$\mathscr{P}$: Time evolution to produce observed final states

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

Treat the sum incoherently.
Handle constituents with theoretical care.

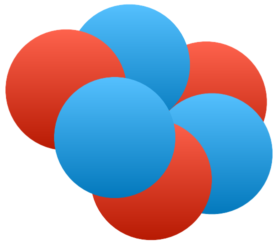
(For LHC crowd: similar to dressing hard-scattering cross sections with parton showers)



The Primary-interaction vertex

Approx. 3: Choose DOF, Factorization Scheme

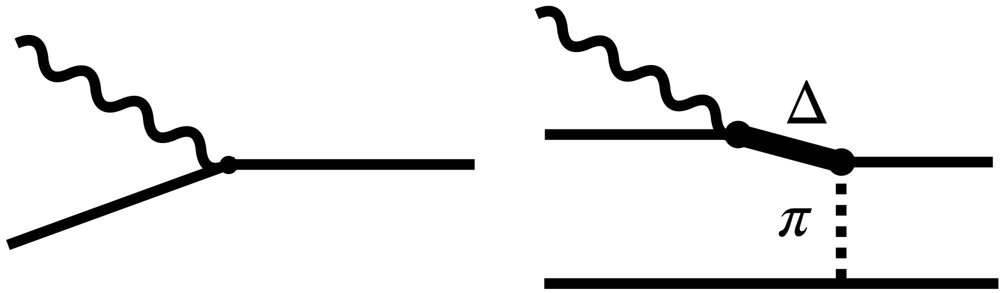
- Take nucleons as initial-state DOF



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

- Take electroweak currents from nuclear EFT:

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

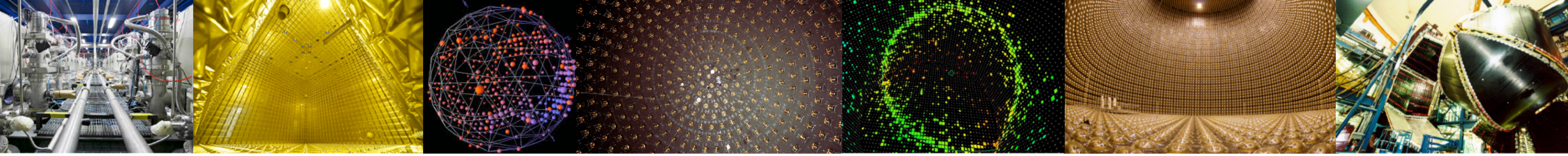


(among others)

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

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

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



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

$$W_{\mathrm{N}}^{\mu\nu} \propto S_n \otimes w_n^{\mu\nu}$$

Nuclear hadronic tensor

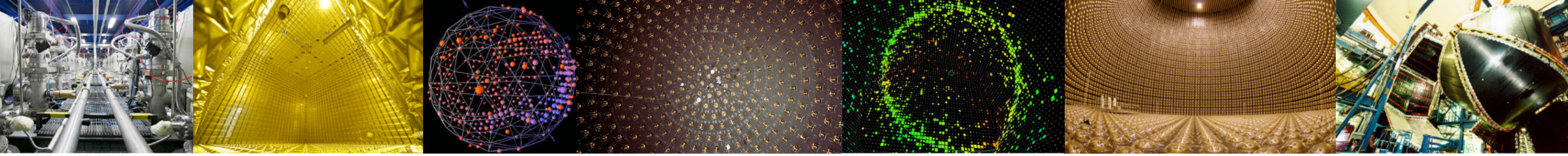
Nuclear spectral function (exactly calculable in nuclear many-body theory up to ~O16)

= "probability to find a nucleon with a given momentum inside the nucleus"

Nucleon hadronic tensor (experimentally measurable or calculable with lattice QCD)

For QE scattering:

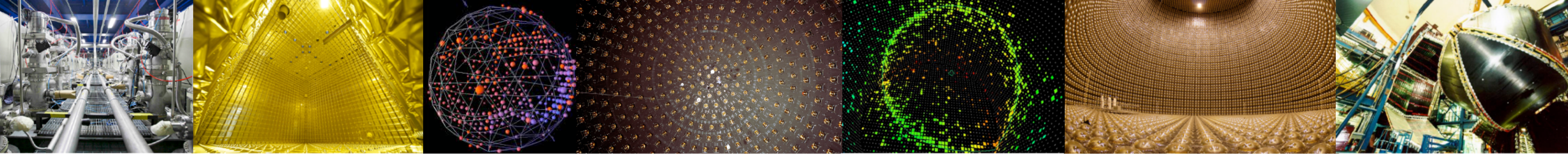
$$w_n^{\mu\nu} \sim |\text{form factor}|^2$$



Subsequent time evolution

Approx. 4: Intranuclear cascade

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



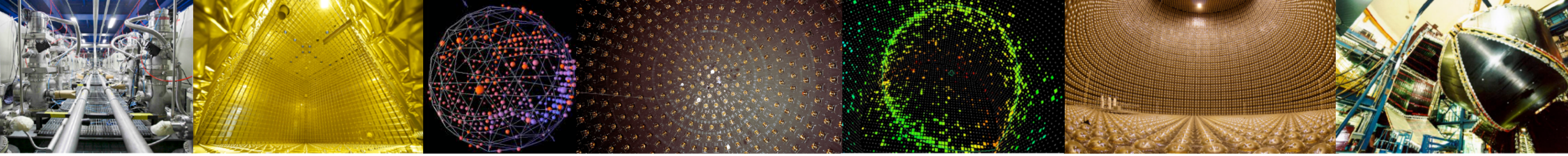
Subsequent time evolution

Approx. 4: Intranuclear cascade

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

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

(Neglect interference between successive scattering events in propagation)

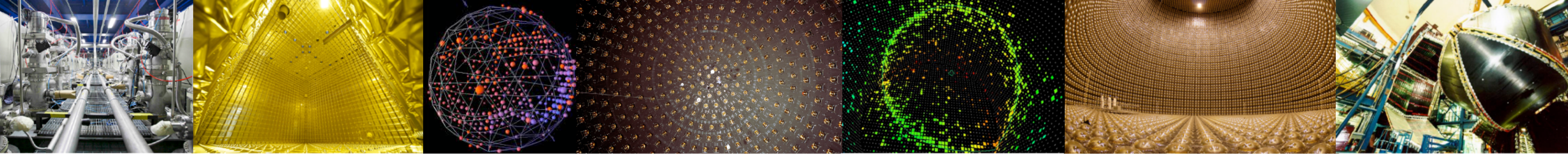


Subsequent time evolution

Approx. 3: Intranuclear cascade

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

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

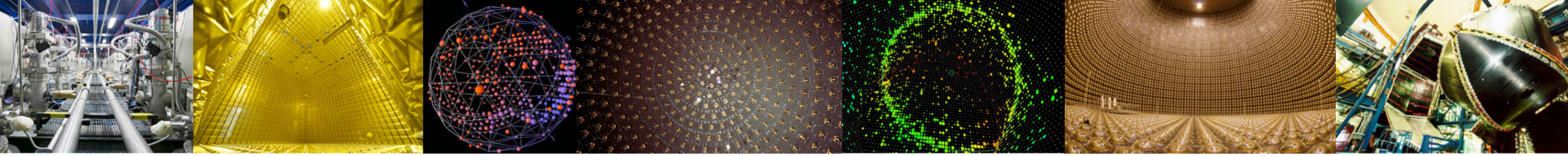


Subsequent time evolution
Approx. 3: Intranuclear cascade

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

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: $P(b) = \exp(-\pi b^2/\sigma)$
  - ☑ $\lambda^{-1} = \rho\sigma$ for the mean free path λ
  - ☑ Total probability integrates to the cross section σ
- Incorporates Pauli blocking and formation zone to constrain possible scatterings



Subsequent time evolution

Approx. 3: Intranuclear cascade

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

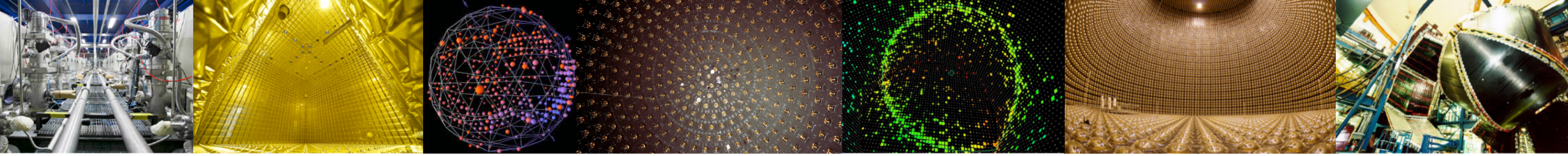
Classical propagation in the background nucleus creates an effective optical potential which induces two effects:

1. Short-distance: $$\frac{d\sigma}{d\Omega} \longrightarrow \left(\frac{d\sigma}{d\Omega}\right)_{\text{in medium}}$$

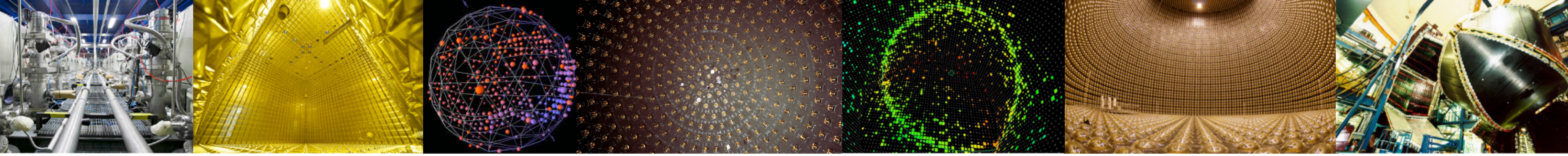
(In-medium corrections to NN interactions)

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)



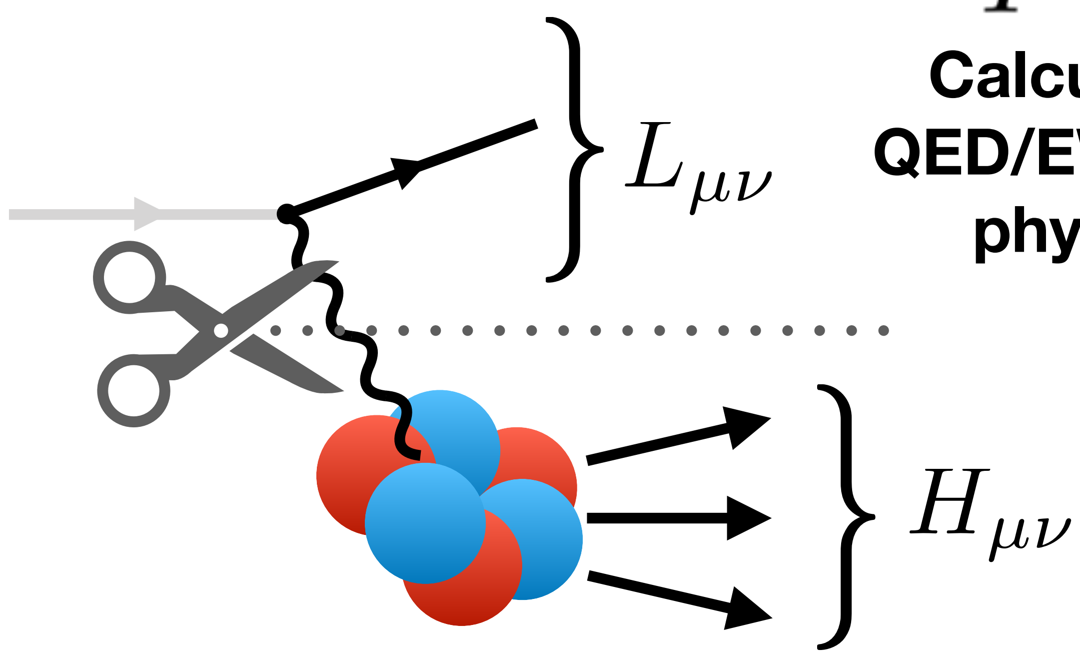
Isaacson et al.
PRD 105 (2022) 9, 096006
[arXiv:2110.15319]

Achilles — Recent updates

Factorization of leptonic and hadronic tensors

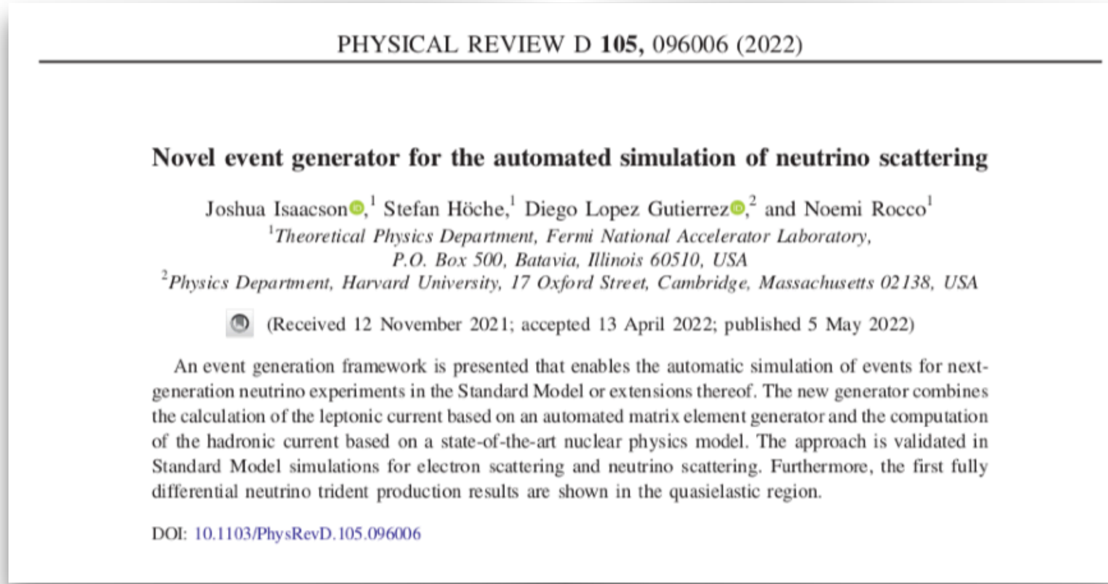
- Automated specification of leptonic tensor (including BSM possibilities)
- Key involvement: Diego Lopez Gutierrez [Undergrad @ Macalester → PhD @ Wash. U. St Louis]
- Uses tools developed by LHC event generation community: Sherpa, Comix, FeynRules, UFO files

$$|\mathcal{M}|^2 = L_{\mu\nu} W^{\mu\nu} \frac{1}{P^2}$$



Calculable QED/EW/BSM physics

Nuclear/hadronic physics of initial interaction and subsequent evolution


PHYSICAL REVIEW D **105,** 096006 (2022)

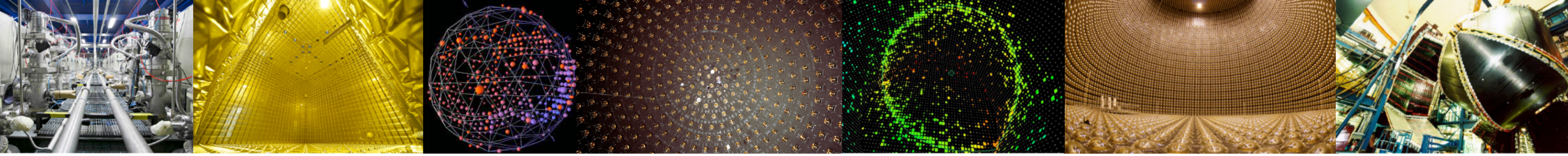
Novel event generator for the automated simulation of neutrino scattering

Joshua Isaacson,[1] Stefan Höche,[1] Diego Lopez Gutierrez,[2] and Noemi Rocco[1]
[1]*Theoretical Physics Department, Fermi National Accelerator Laboratory, P.O. Box 500, Batavia, Illinois 60510, USA*
[2]*Physics Department, Harvard University, 17 Oxford Street, Cambridge, Massachusetts 02138, USA*

(Received 12 November 2021; accepted 13 April 2022; published 5 May 2022)

An event generation framework is presented that enables the automatic simulation of events for next-generation neutrino experiments in the Standard Model or extensions thereof. The new generator combines the calculation of the leptonic current based on an automated matrix element generator and the computation of the hadronic current based on a state-of-the-art nuclear physics model. The approach is validated in Standard Model simulations for electron scattering and neutrino scattering. Furthermore, the first fully differential neutrino trident production results are shown in the quasielastic region.

DOI: 10.1103/PhysRevD.105.096006



Achilles — Recent updates

New API for nuclear models

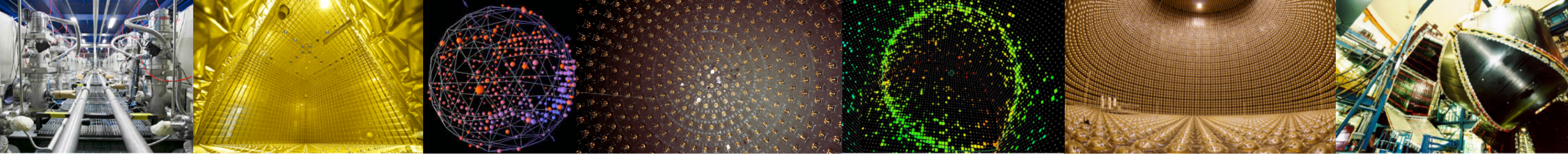
- We have new API/extendible interface for nuclear models
- The API supports models implemented in Fortran or CPP. Extension to models in python is straightforward if there is community interest
- Allows, e.g., for different nuclear spectral functions [Also more general]

$$W_{\mathrm{N}}^{\mu\nu} \propto S_n \otimes w_n^{\mu\nu}$$

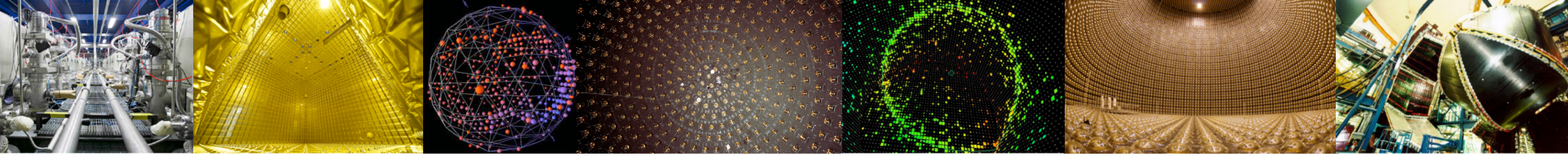
Nuclear hadronic tensor

Nuclear spectral function

Nucleon hadronic function



Recent results



Achilles: Comparison to experiment

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

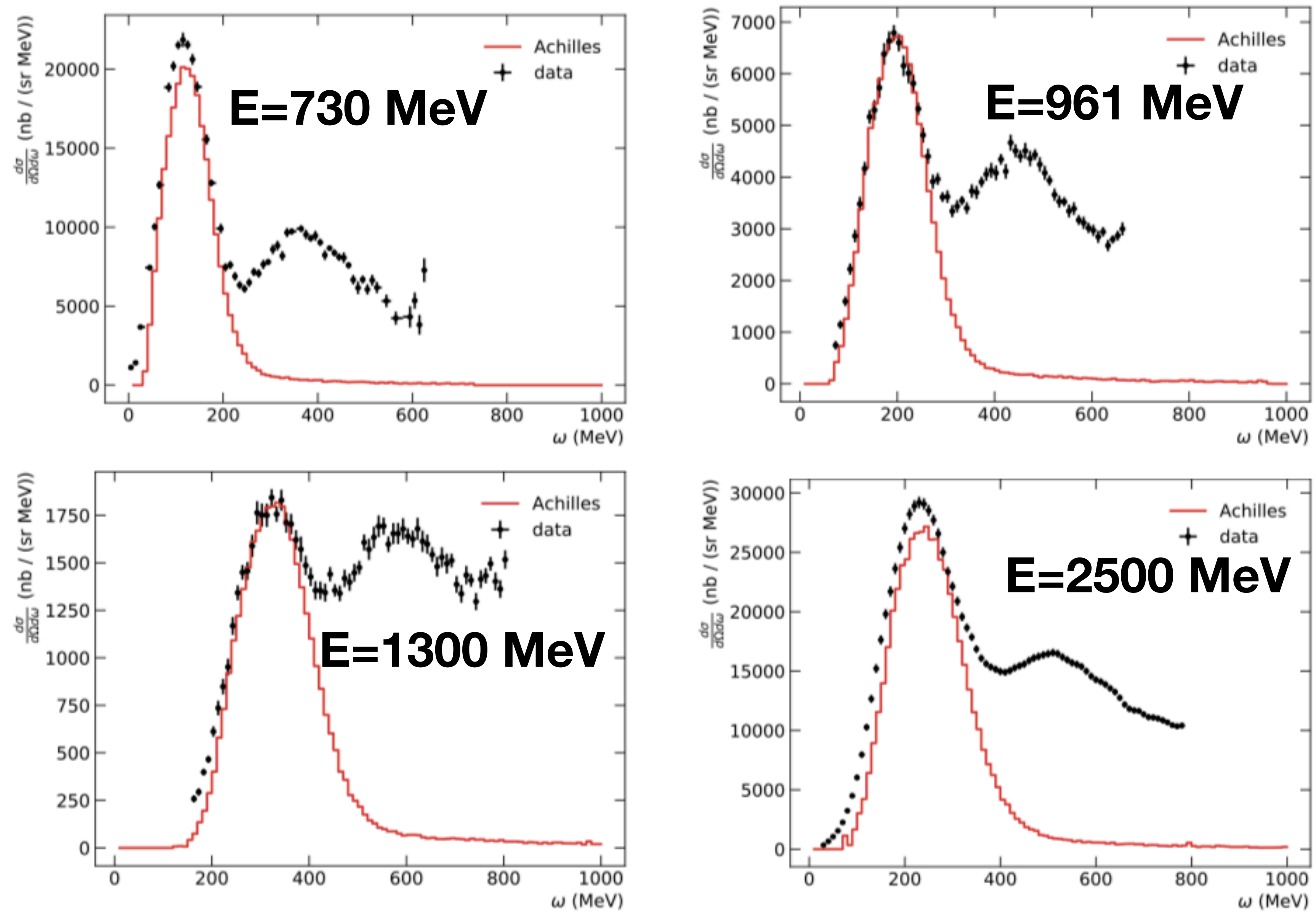
J. S. O'Connell *et al.*, Phys. Rev. C **35**, 1063 (1987).
R. M. Sealock *et al.*, Phys. Rev. Lett. **62**, 1350 (1989).
D. Zeller, Investigation of the structure of the C-12 nucleus by high-energy electron scattering, Other thesis, Karlsruhe University, 1973.

Inclusive e-C hadronic cross section

$$\frac{d\sigma}{d\Omega d\omega}$$

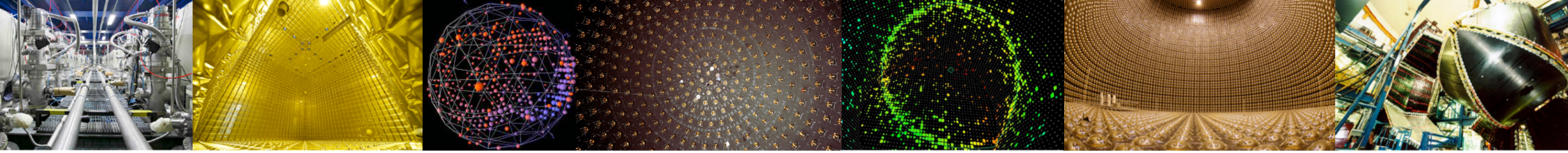
Fixed outgoing electron angle θ=37° to match experimental settings

Differential in outgoing electron energy ω



Beyond firsts peak: Neglected MEC and resonance contributions

Good agreement = Validation of initial model for QE interaction



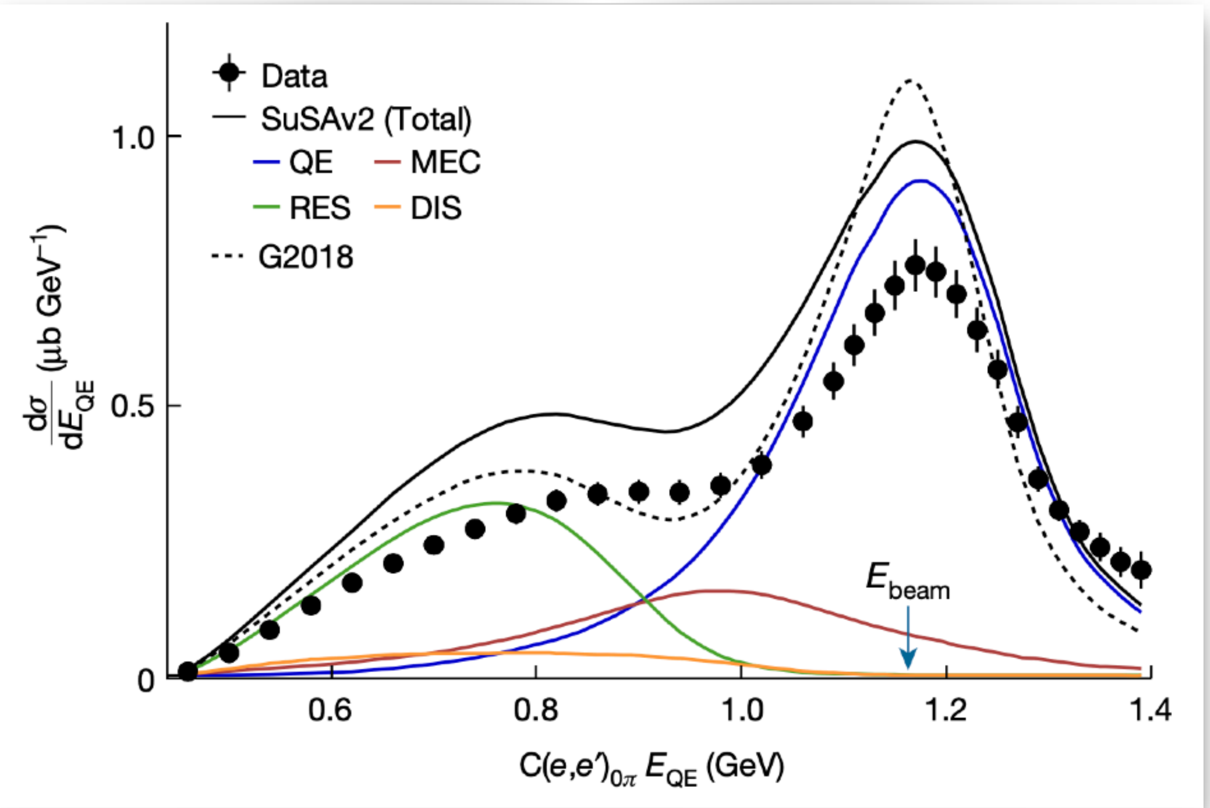
Achilles: Comparison to experiment

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

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

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

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



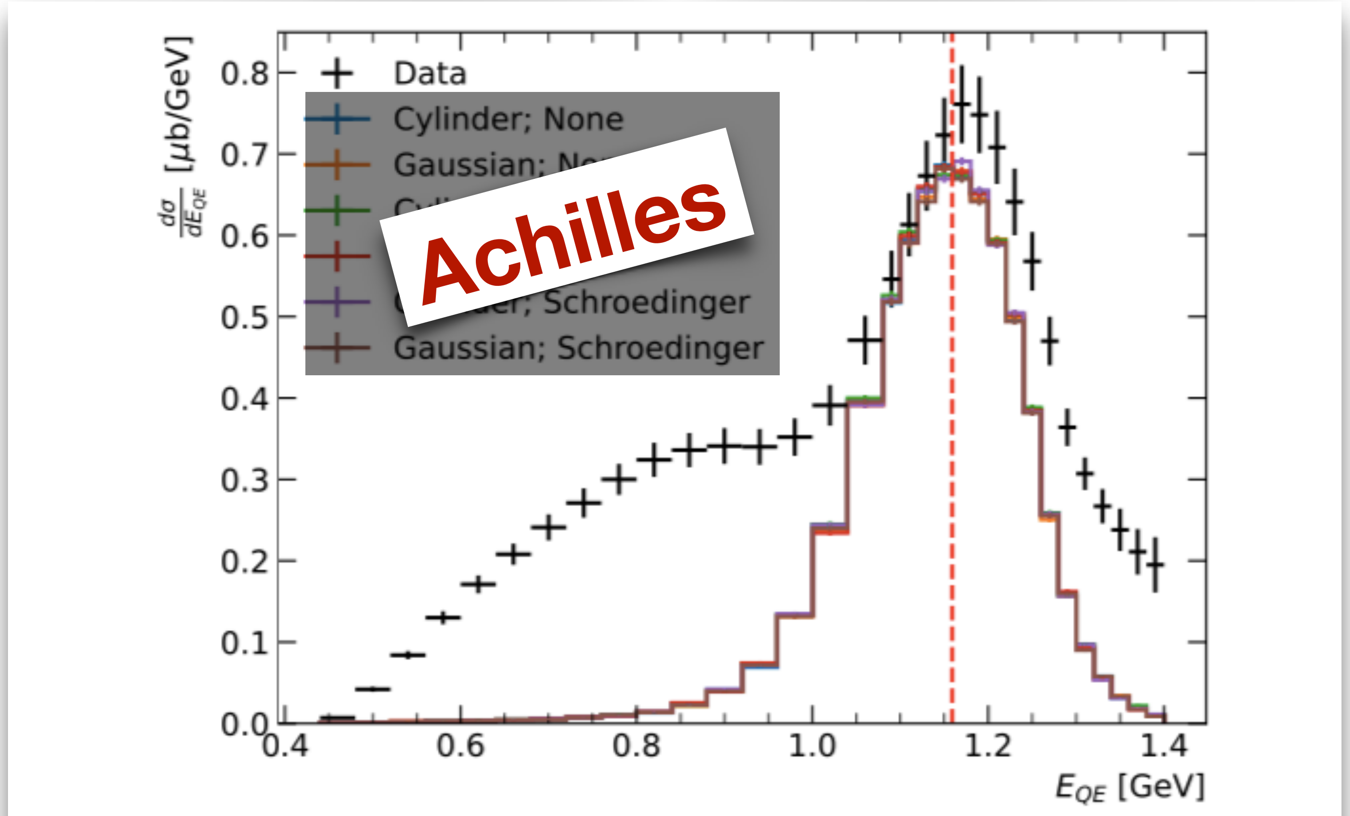
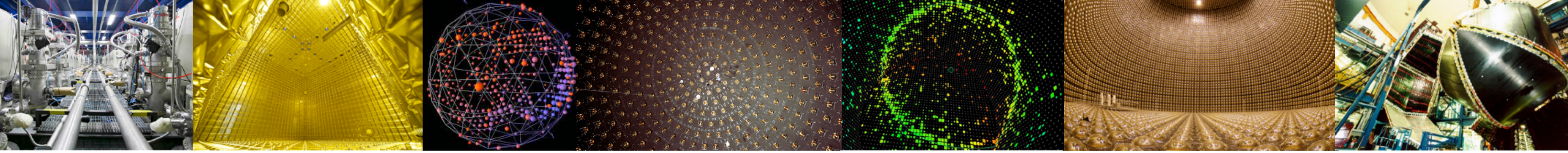


FIG. 4: Comparison of the quasielastic energy reconstructed for an electron beam of 1159 MeV. Data is taken from Ref. [69]. The definition of E_{QE} can be found in Eq. 31. The red dashed vertical line marks the true beam energy.

- **Low E_{QE}: MEC and resonance contributions**
- **High E_{QE}: interference effects (neglected)**



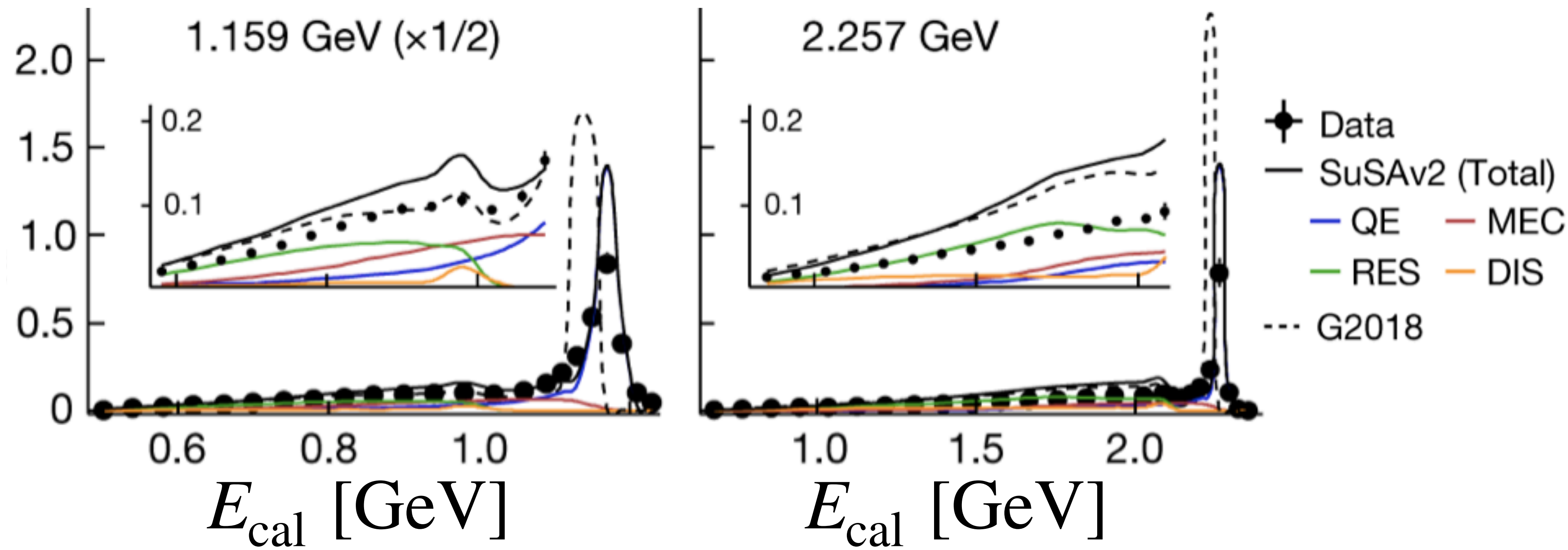
Achilles: Comparison to experiment

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

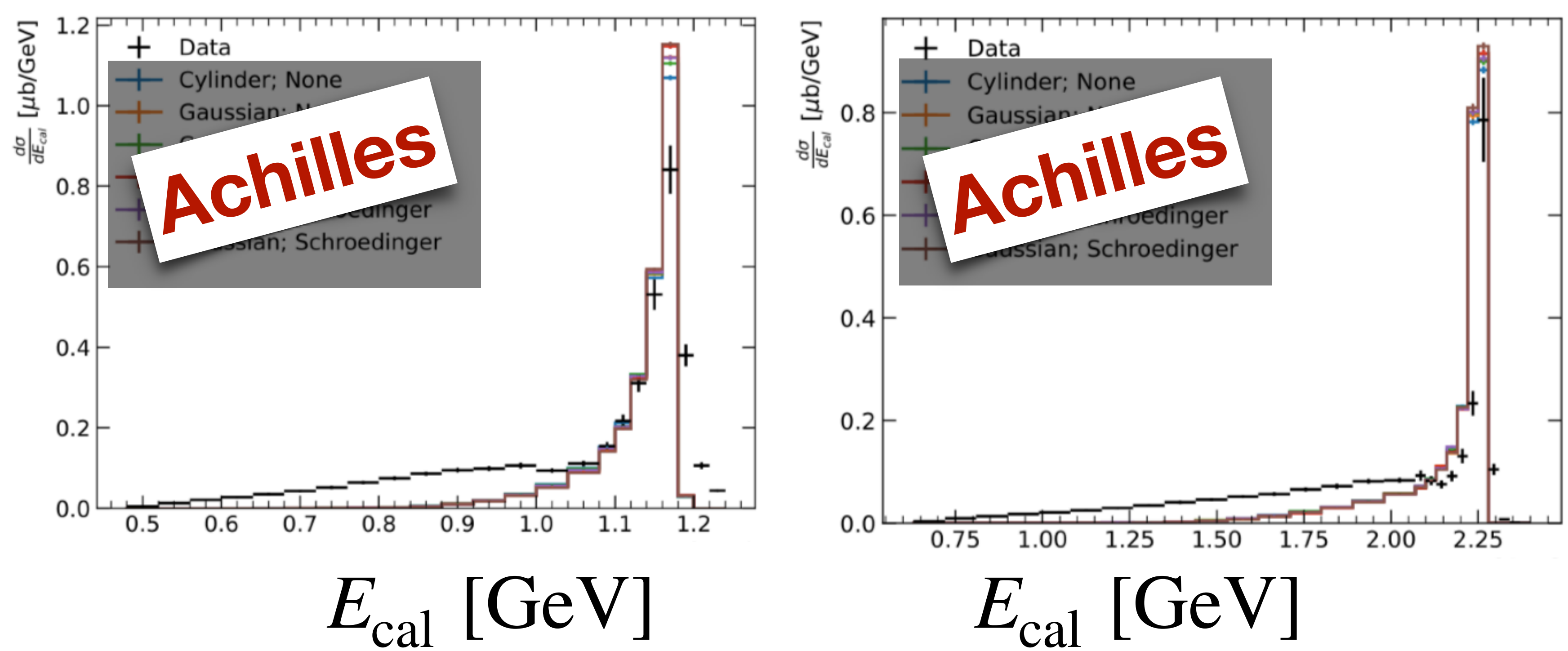
CLAS and e4v collaborations
Nature 599 (2021) 7886, 565-570

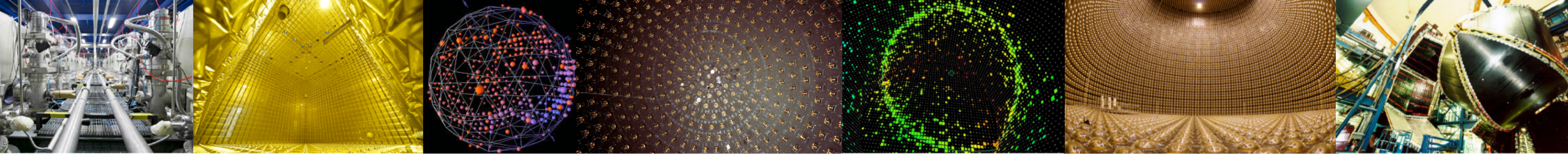
E_{cal} = “Calorimetric energy” = “sum of final-state energies”

Data + simulation from e4v paper $\dfrac{d\sigma}{dE_{\mathrm{cal}}}$



Same e4v data vs Achilles $\dfrac{d\sigma}{dE_{\mathrm{cal}}}$





Achilles: Recent Results

Isaacson et al. [arXiv:2303.08104]

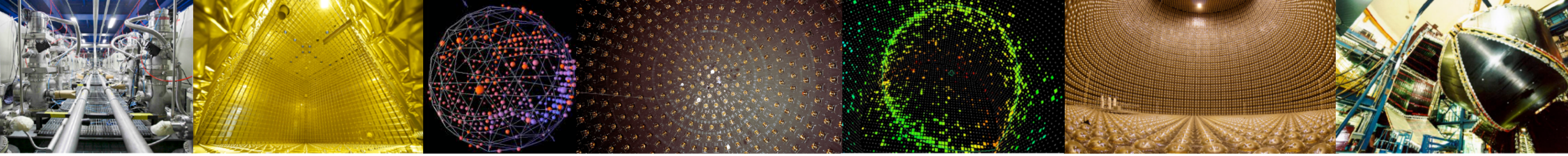
Application: Correlated decays in neutrino experiments

Motivation: ν_τ is perhaps the least understood elementary particle

- DUNE: O(few hundred) ν_τ events per year → Accurate theoretical predictions critical
- Outgoing/decaying τ is polarized → 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 ν_e, ν_μ → "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



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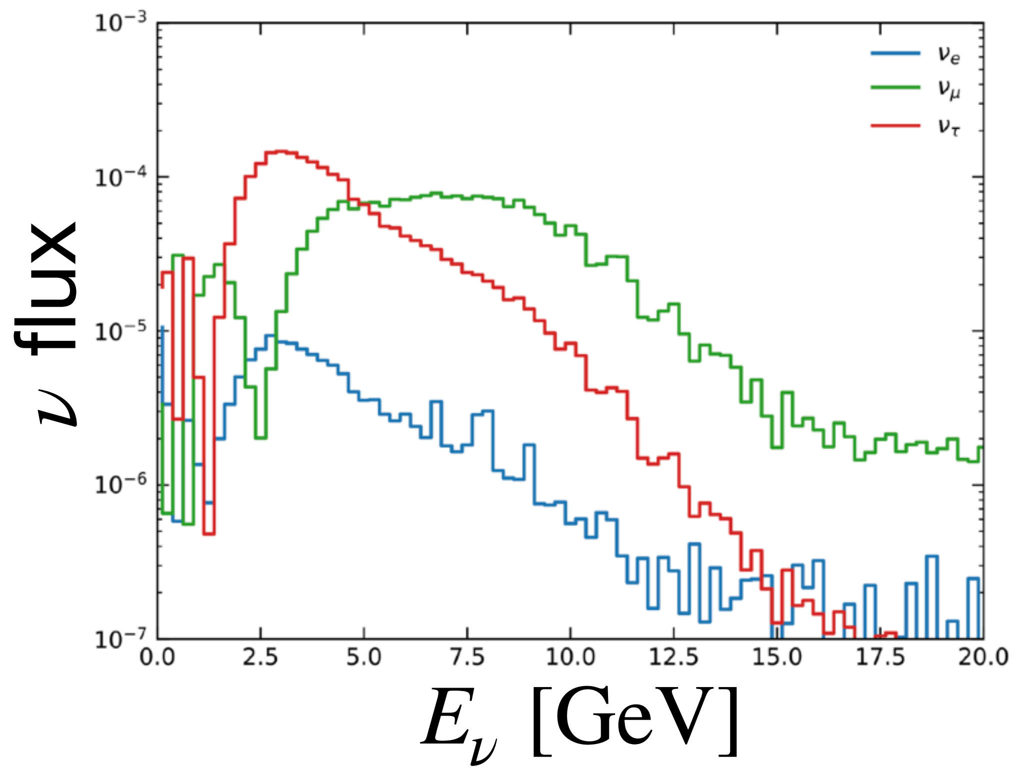


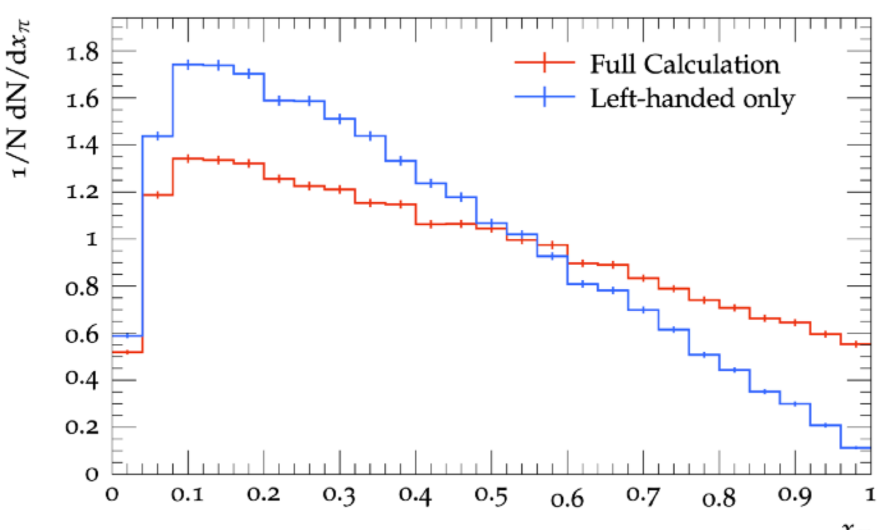
Momentum Fraction Distributions

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

$$\frac{1}{N}\frac{dN}{\boxed{dx_i}}$$

Momentum fraction

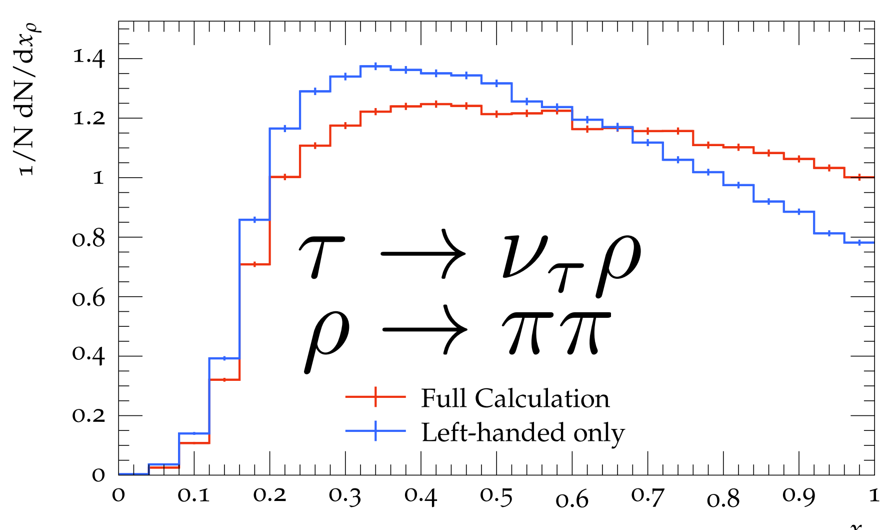
$x_i = E_i/E_\tau$



x_π

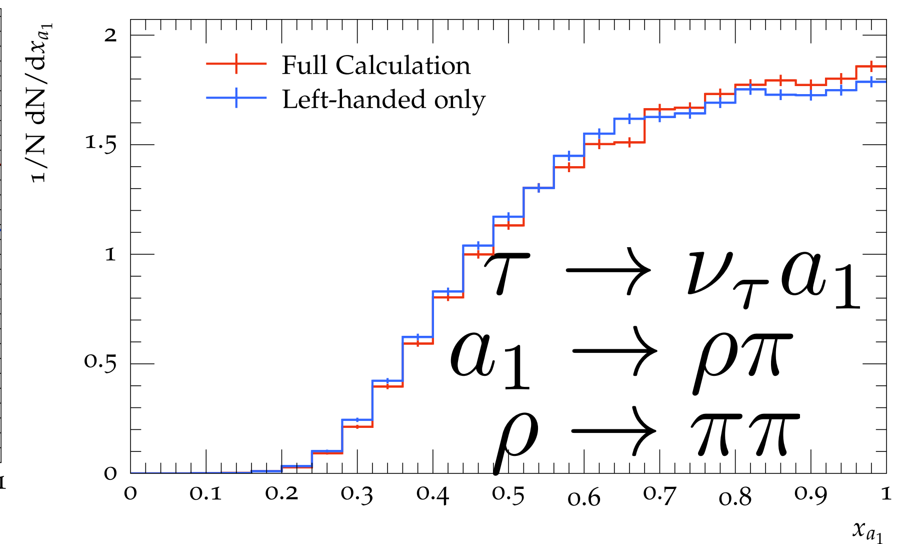
Clean at DUNE

$\mathscr{B}(1\pi) \sim 10\,\%$

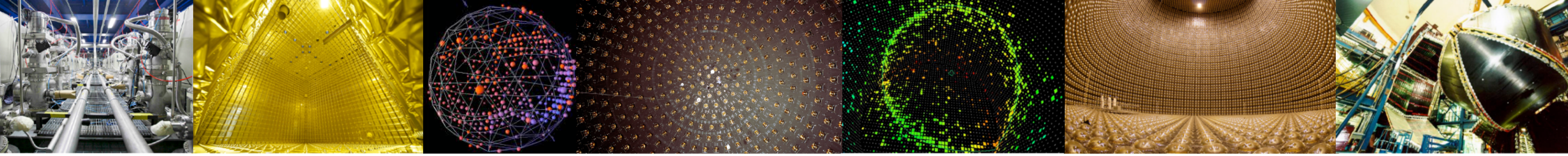


x_ρ

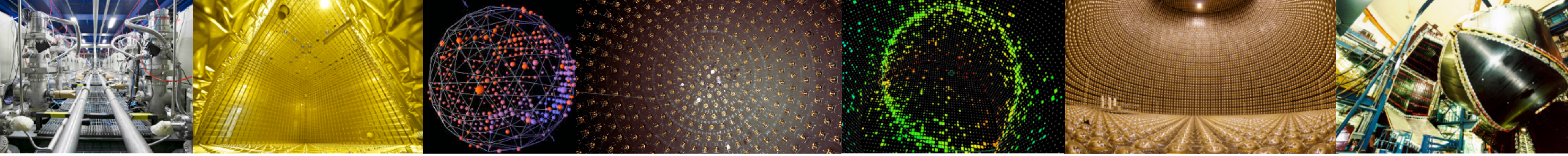
$\mathscr{B}(2\pi) \sim 25\,\%$



x_{a_1}



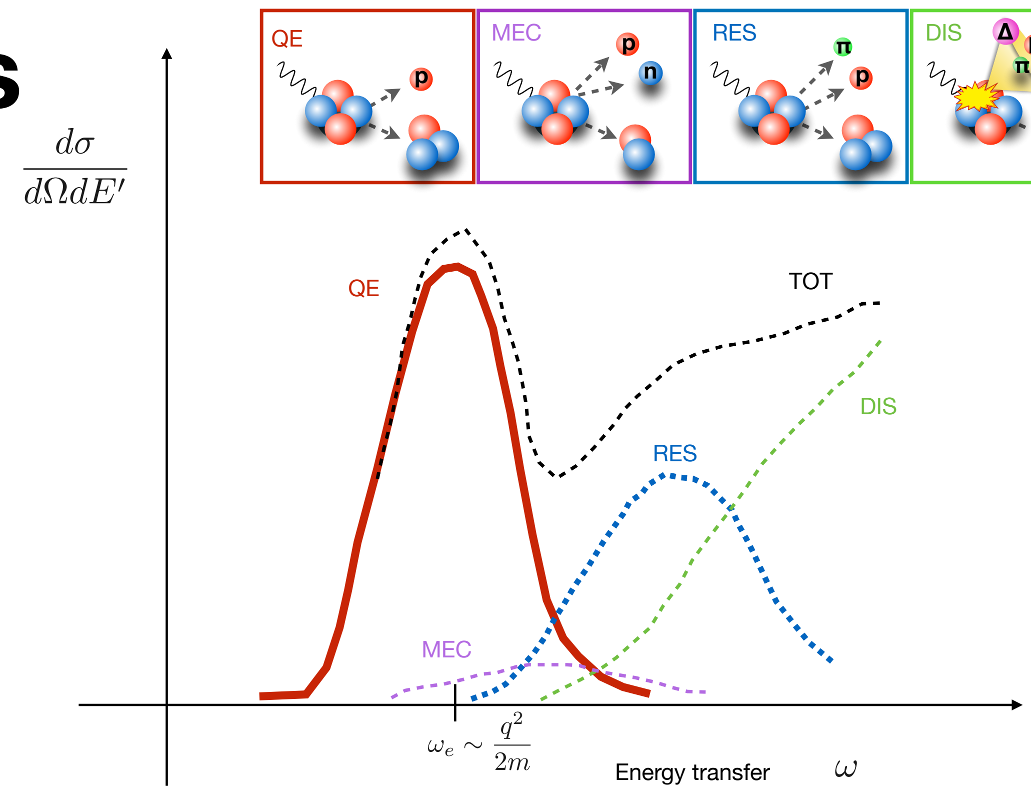
Conclusions



Achilles — What's next?

More production processes

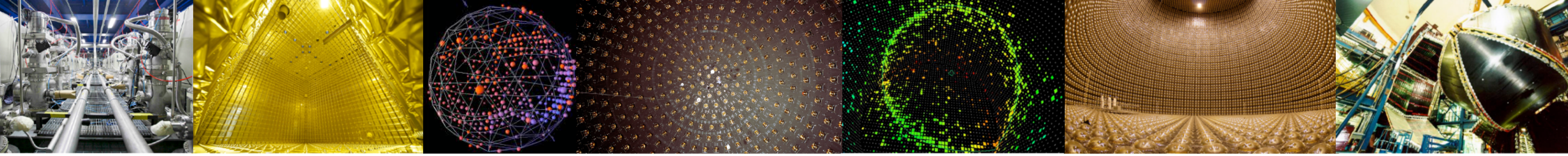
- Existing generator: QE scattering only
- Near-term goals: particle production (+decay) at the initial interaction and cascade
- Initial "hard interaction"
    - **Meson-exchange currents** in the spectral function formalism
    - **Resonant scattering** in the dynamical coupled channel formalism
 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



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

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

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



Achilles — Summary

- **Our Goal/Credo: 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
  - Theoretical uncertainties should be incorporated by event generators
- **Achilles employs a modular design to factorize physically different processes:**
  - Leptonic vs hadronic tensors,
  - Nuclear vs hadronic physics
  - "Hard interaction" vs intranuclear cascade
- Achilles currently supports quasi-elastic scattering (e.g., spectral function formalism)
- In the near term ($\lesssim$ year), we expect to implement MEC and resonant production mechanisms and particle production/decay in the intranuclear cascade