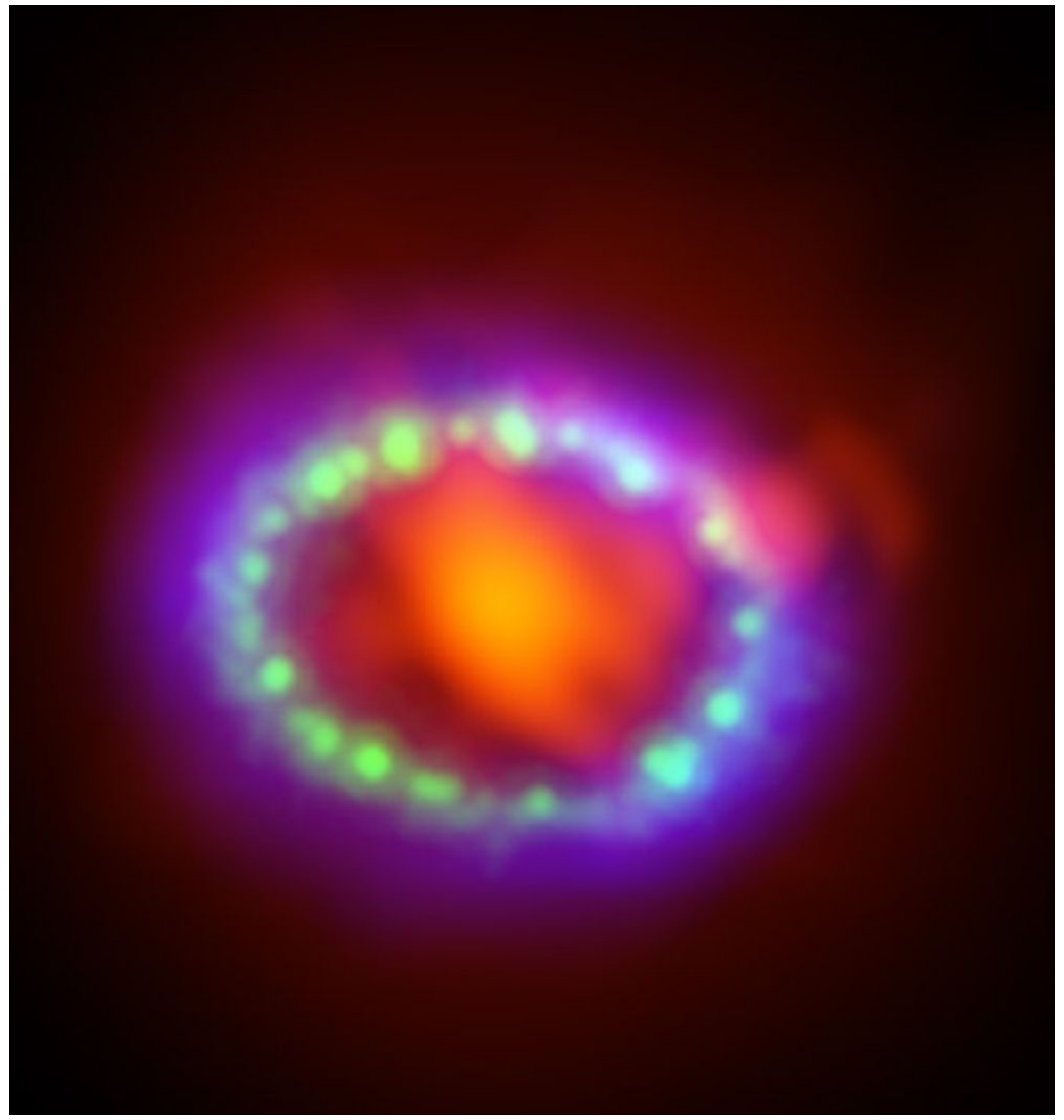
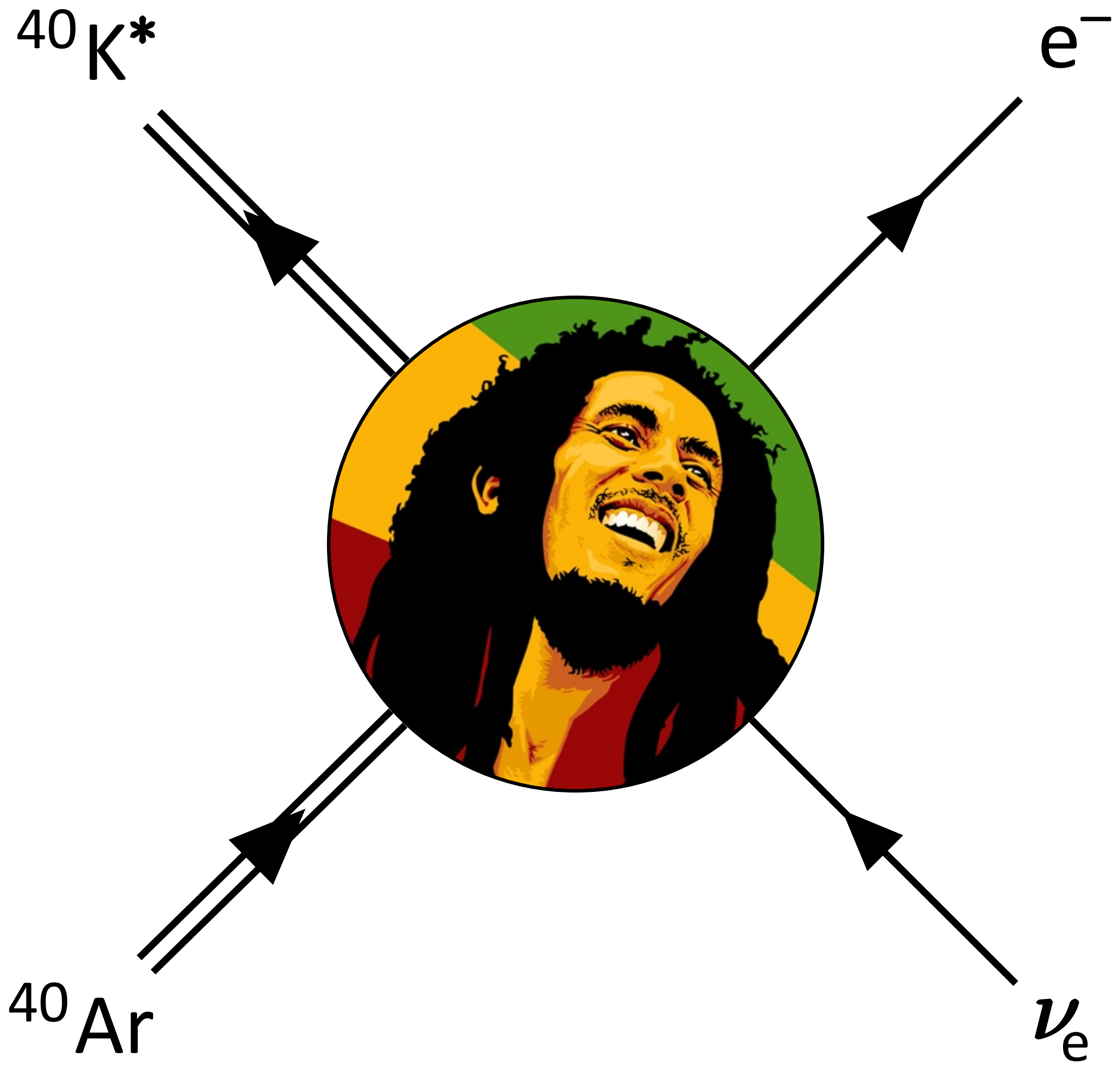
(Prospects for) Uncertainty quantification in MARLEY





Steven Gardiner (gardiner@fnal.gov)
Event Generators Group, Fermilab Physics Simulation Department

Theoretical Physics Uncertainties to Empower Neutrino Experiments (INT-23-86W)

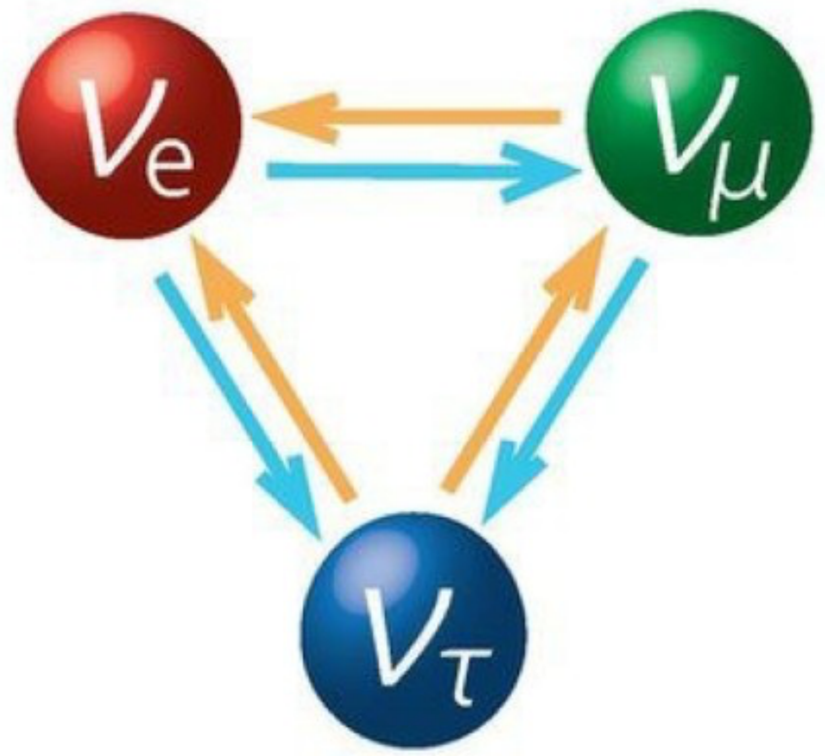
1 November 2023

Overview

- Motivation in context of DUNE
- ν-A modeling at O(10 MeV)
  - Compare & contrast to higher energies
- The MARLEY event generator
- Model uncertainties, both easy and hard
  - Brief NuHepMC cameo
- First study for DUNE:
  [Phys. Rev. D 107, 112012 (2023)]

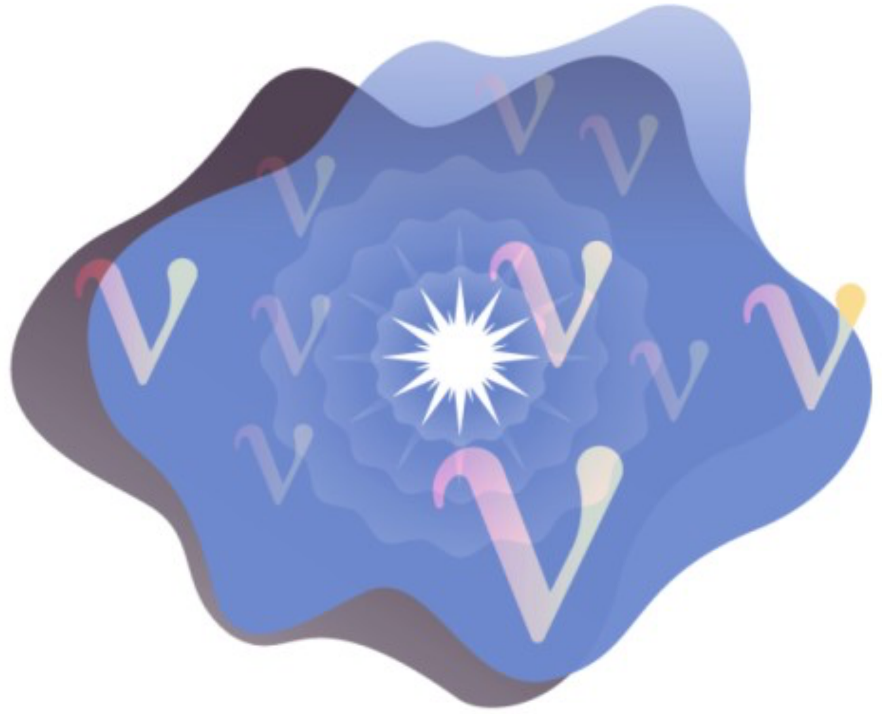
Bob sighting @ Golden Oldies Records, Seattle

Primary science goals of DUNE



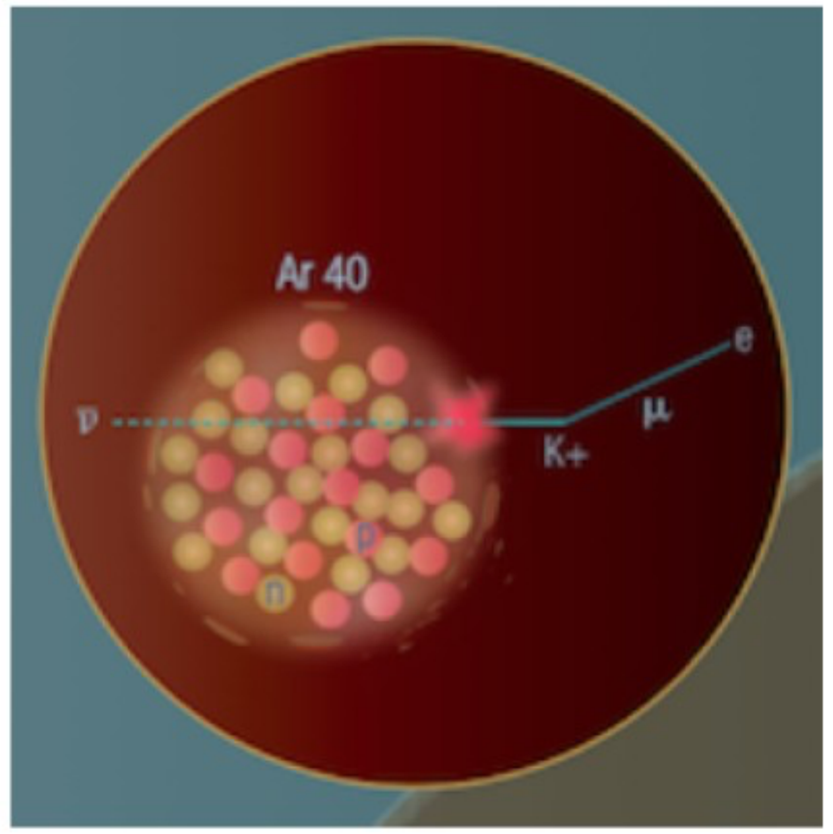
Accelerator neutrino oscillations

- Search for CP violation ($\delta^{CP} \neq 0,\pi$)
- Neutrino mass ordering
- Precision mixing parameters



Supernova physics

- Measure O(10 MeV) neutrinos from a galactic supernova
- Unique sensitivity to ν_e component, rich physics potential



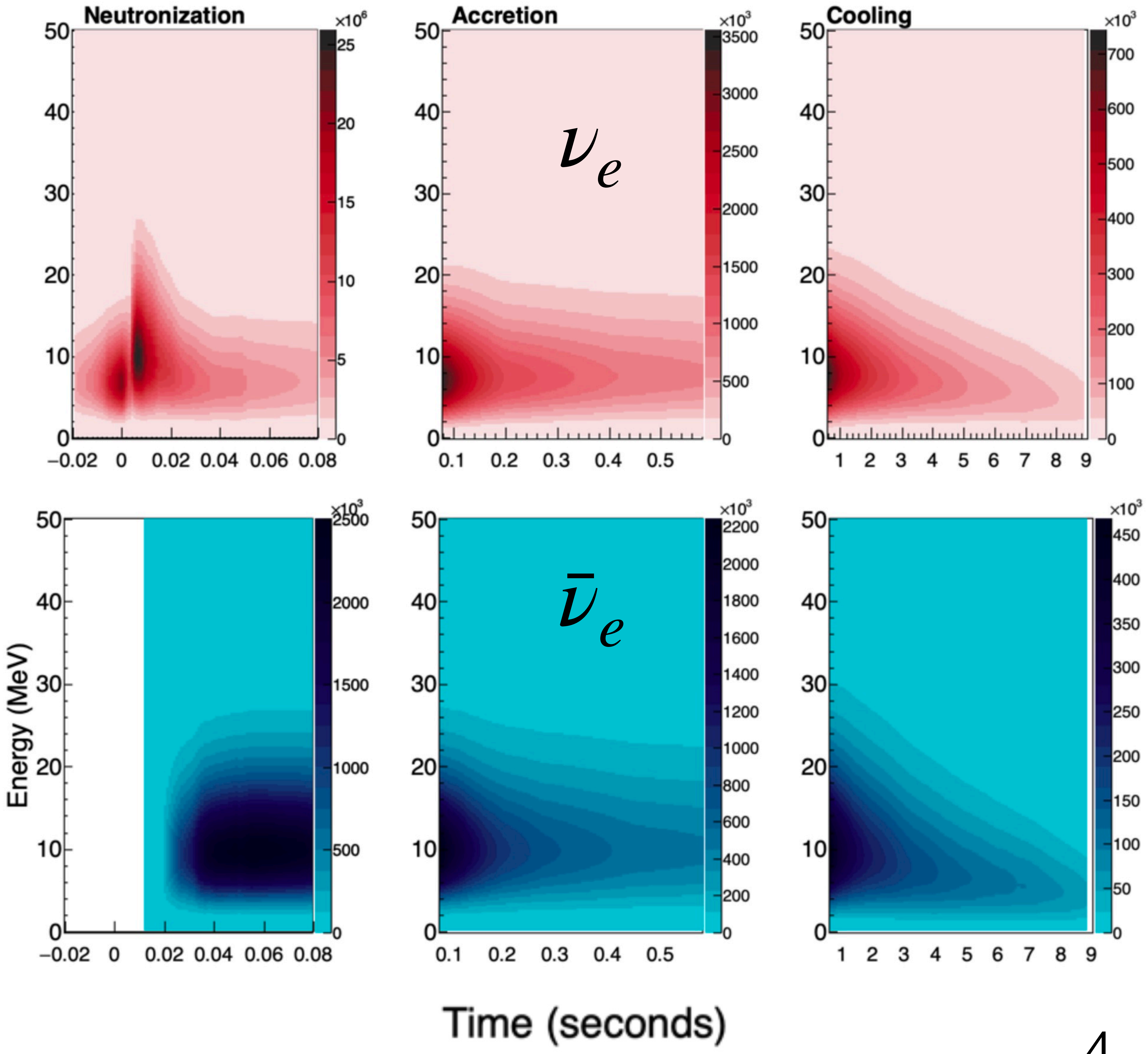
Explore physics beyond the Standard Model

- Proton decay, other baryon number violating processes
- Heavy neutral leptons, boosted dark matter
- Various other exotic physics scenarios

Observables for a supernova neutrino analysis

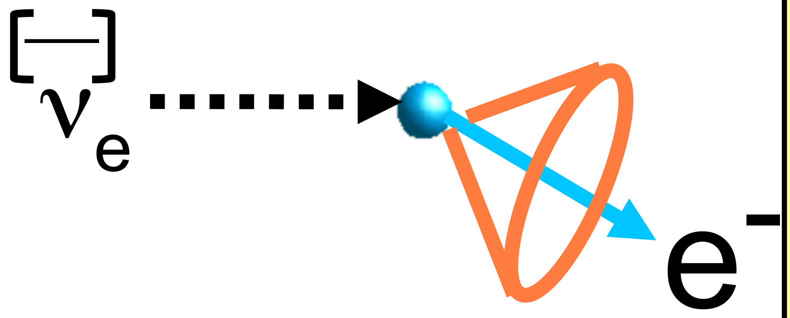
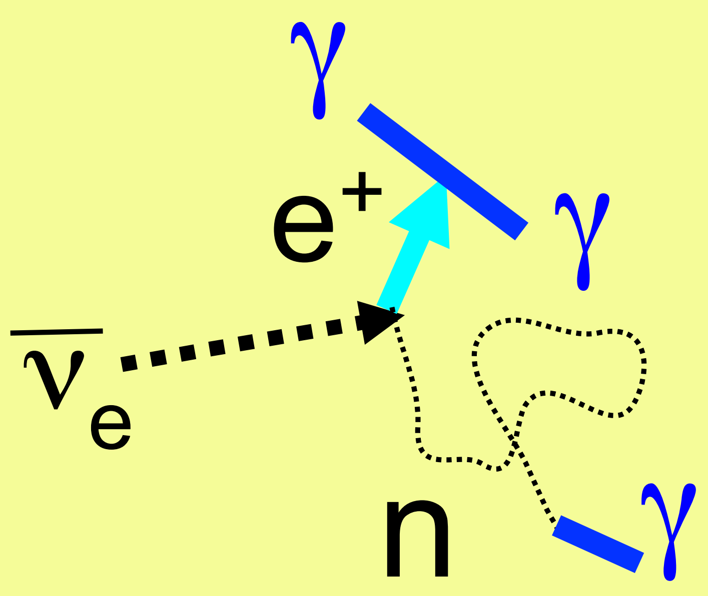
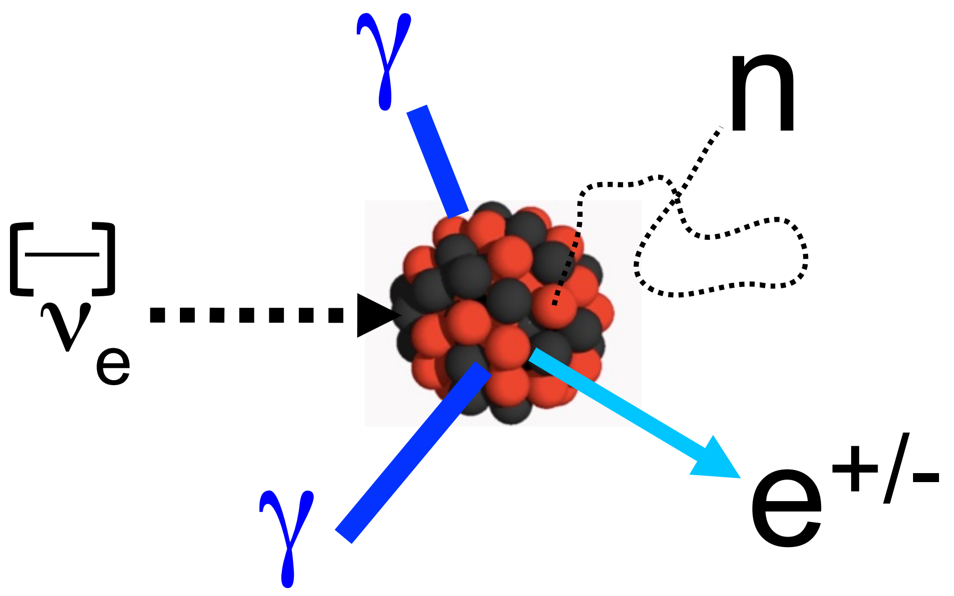
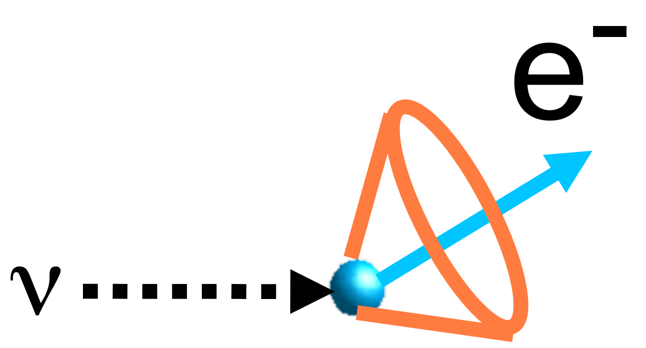
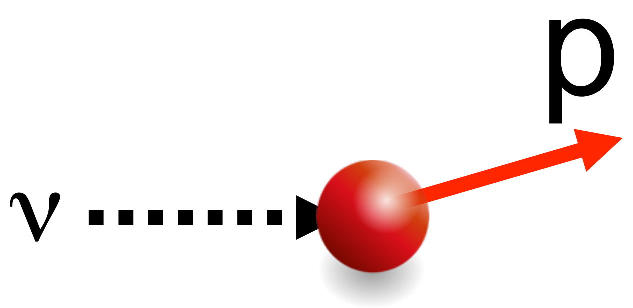
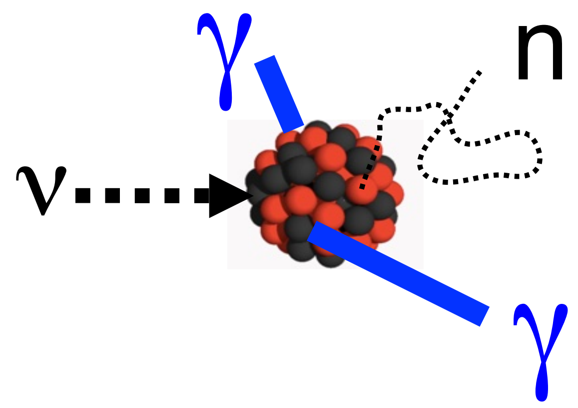
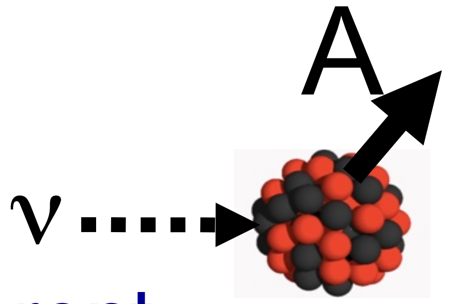
- Physics signatures imprinted on time-dependent flux
  - Core-collapse dynamics, mass ordering, collective oscillations, BSM, …
- Measure **energy**, flavor, and time
  - Low **tens-of-MeV** set by supernova temperature
- Distinct information from ν_e, $\bar{\nu}_e$, ν_x
  - Detection of all highly desirable

Eur. Phys. J. C 81, 423 (2021)



Supernova-relevant neutrino interactions

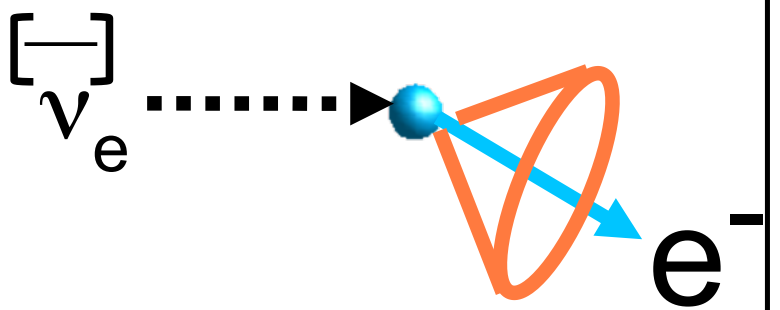
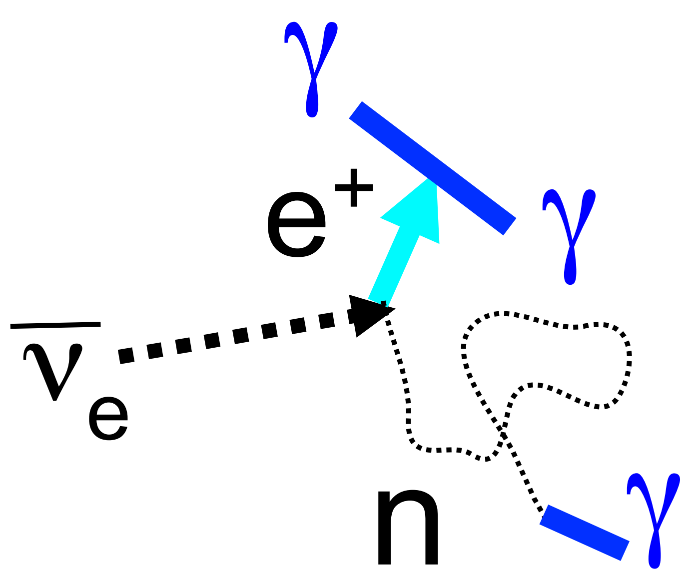
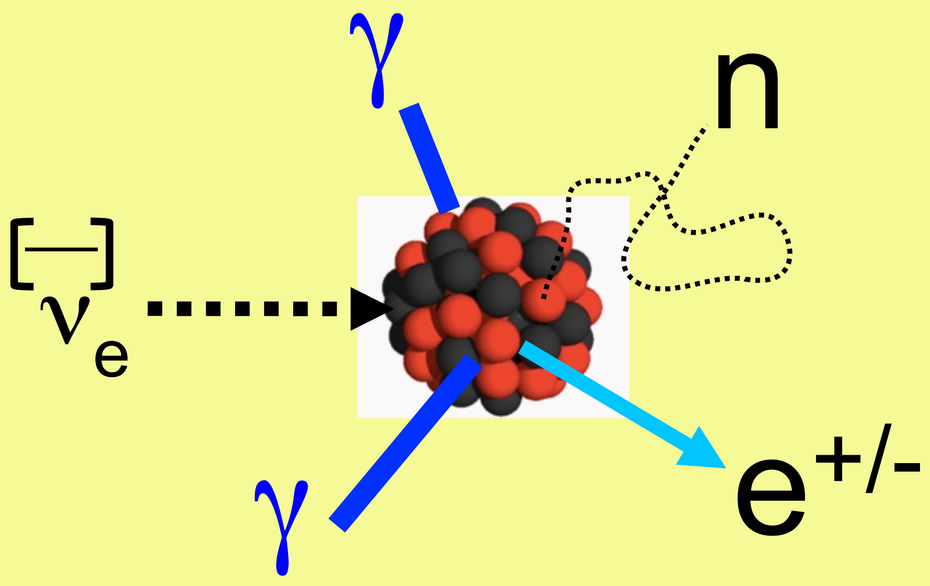
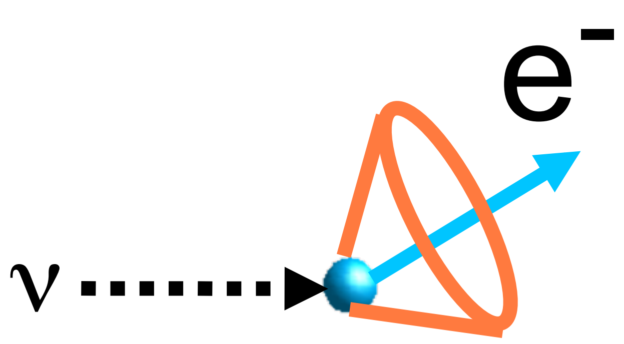
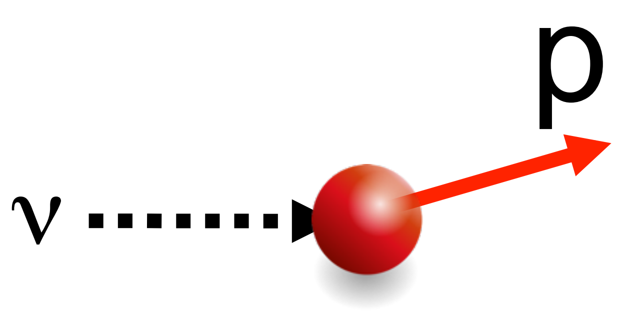
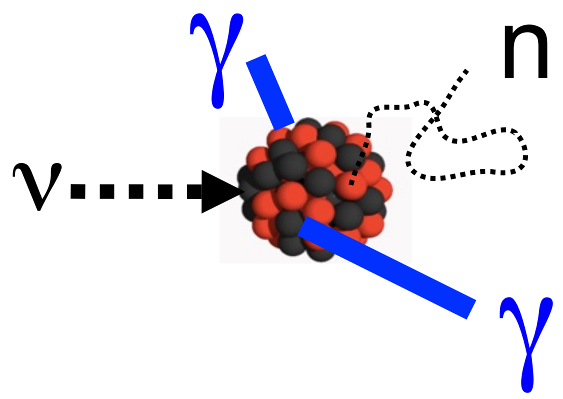
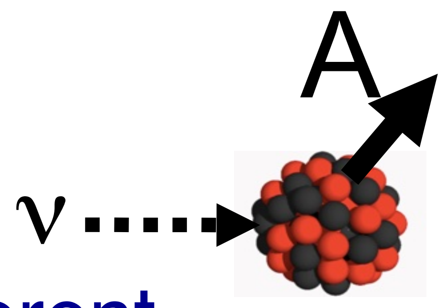
K. Scholberg

	Electrons	Protons	Nuclei
Charged current	Elastic scattering $\nu + e^- \rightarrow \nu + e^-$ 	Inverse beta decay $\bar{\nu}_e + p \rightarrow e^+ + n$ 	$\nu_e + (N, Z) \rightarrow e^- + (N-1, Z+1)$ $\bar{\nu}_e + (N, Z) \rightarrow e^+ + (N+1, Z-1)$  Various possible ejecta and deexcitation products
Neutral current	 Useful for pointing	Elastic scattering  very low energy recoils	$\nu + A \rightarrow \nu + A^*$   $\nu + A \rightarrow \nu + A$ Coherent elastic (CEvNS)

IBD (electron *anti*neutrinos) dominates for current detectors

Supernova-relevant neutrino interactions

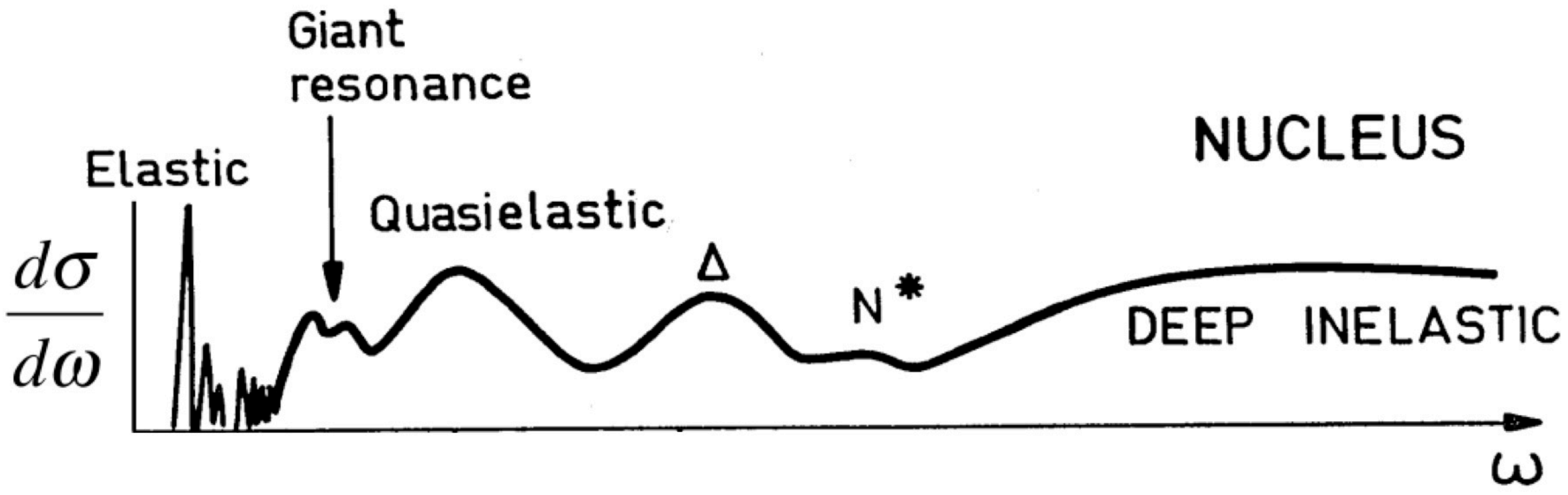
K. Scholberg

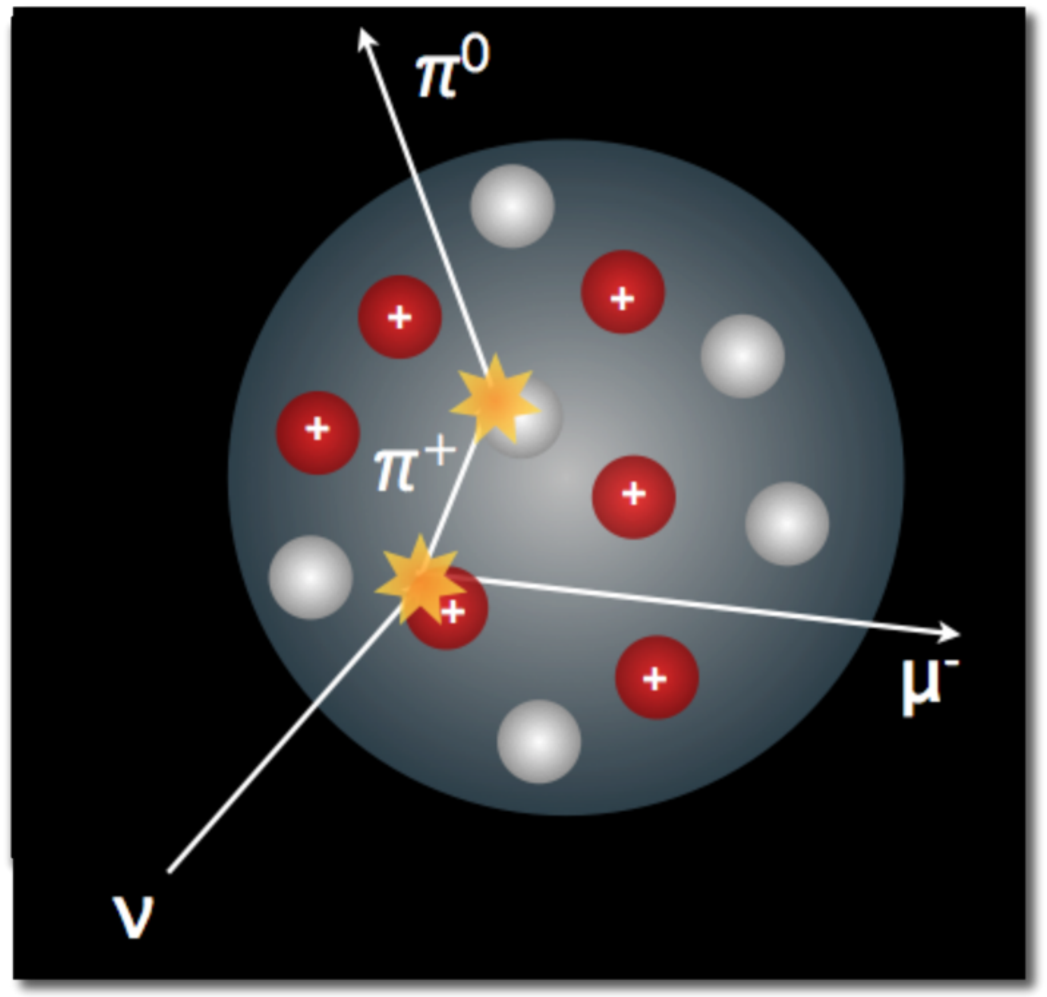
	Electrons	Protons	Nuclei
Charged current	Elastic scattering $\nu + e^- \to \nu + e^-$ 	Inverse beta decay $\bar{\nu}_e + p \to e^+ + n$ 	$\nu_e + (N,Z) \to e^- + (N-1, Z+1)$ $\bar{\nu}_e + (N,Z) \to e^+ + (N+1, Z-1)$  Various possible ejecta and deexcitation products
Neutral current	 Useful for pointing	Elastic scattering  very low energy recoils	$\nu + A \to \nu + A^*$   $\nu + A \to \nu + A$ Coherent elastic (CEvNS)

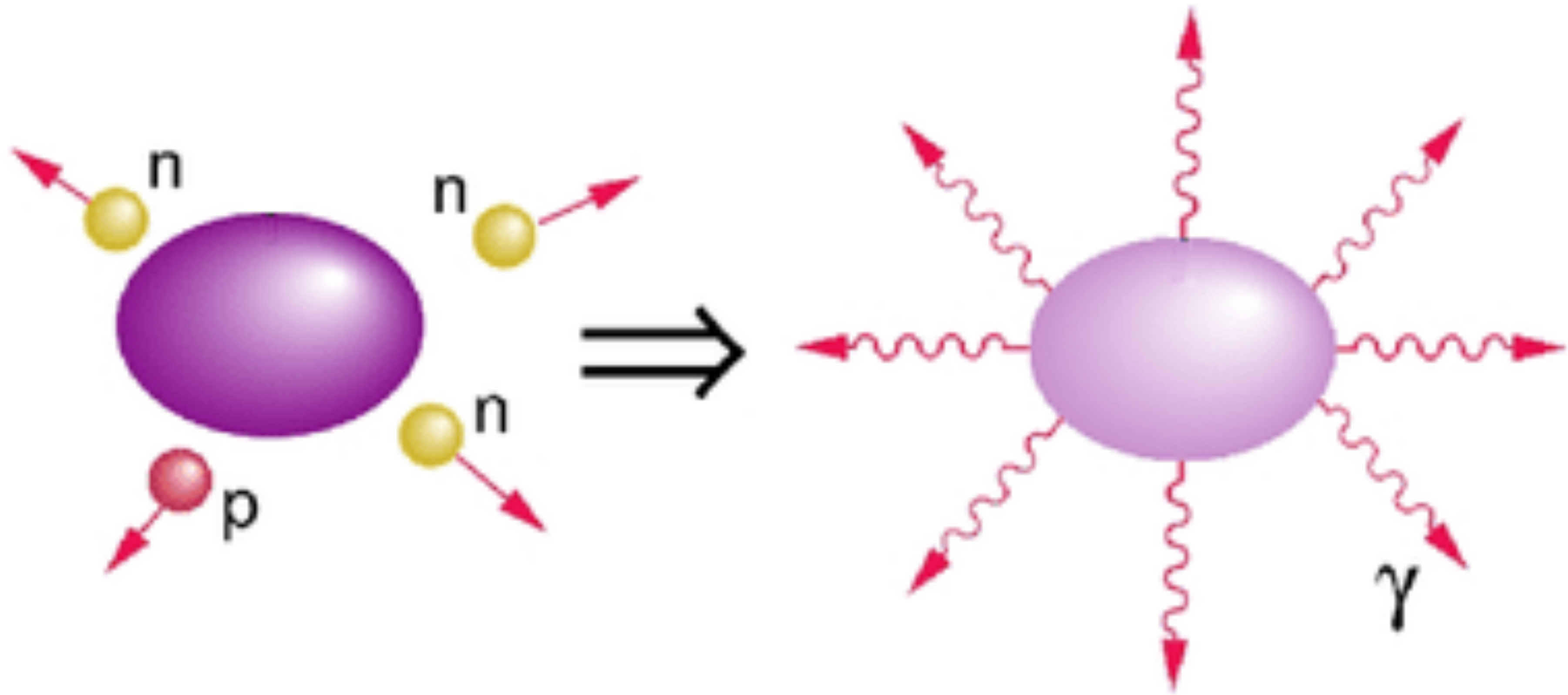
Nuclear target needed to isolate electron neutrino flux!

Modeling differences in the low-energy regime

- **Inclusive** cross sections sensitive to nuclear structure details
  - Discrete levels, giant resonances
- **Exclusive** predictions describe hadronic system very differently
- **Direct knockout** picture used at high energies
  - Dynamical models: BUU, INC
- **Compound nucleus** picture used at low energies
  - Statistical models: Hauser-Feshbach, SMM

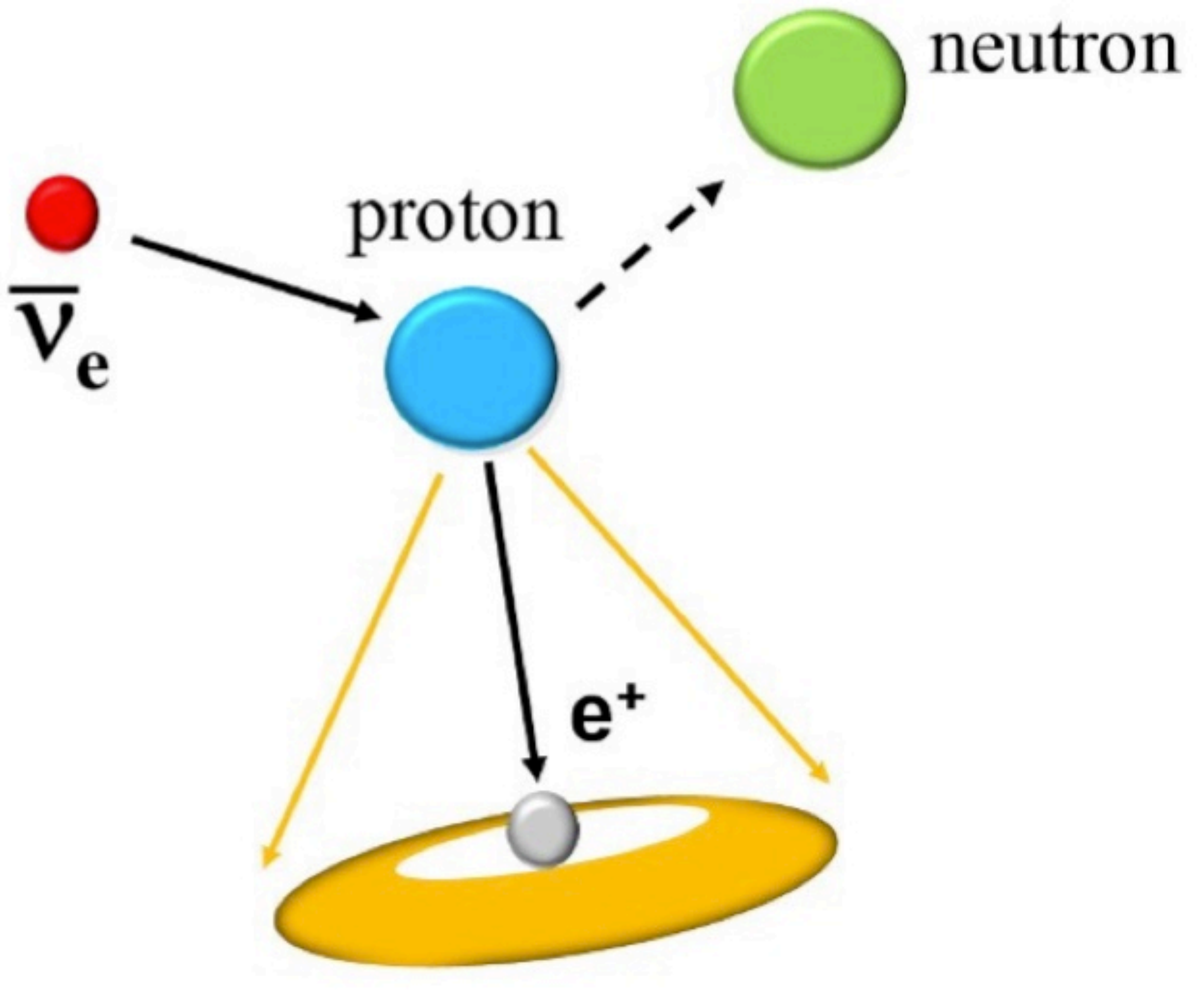






Neutrino calorimetry still main driver of modeling needs

IBD: e^+ sufficient to infer E_ν

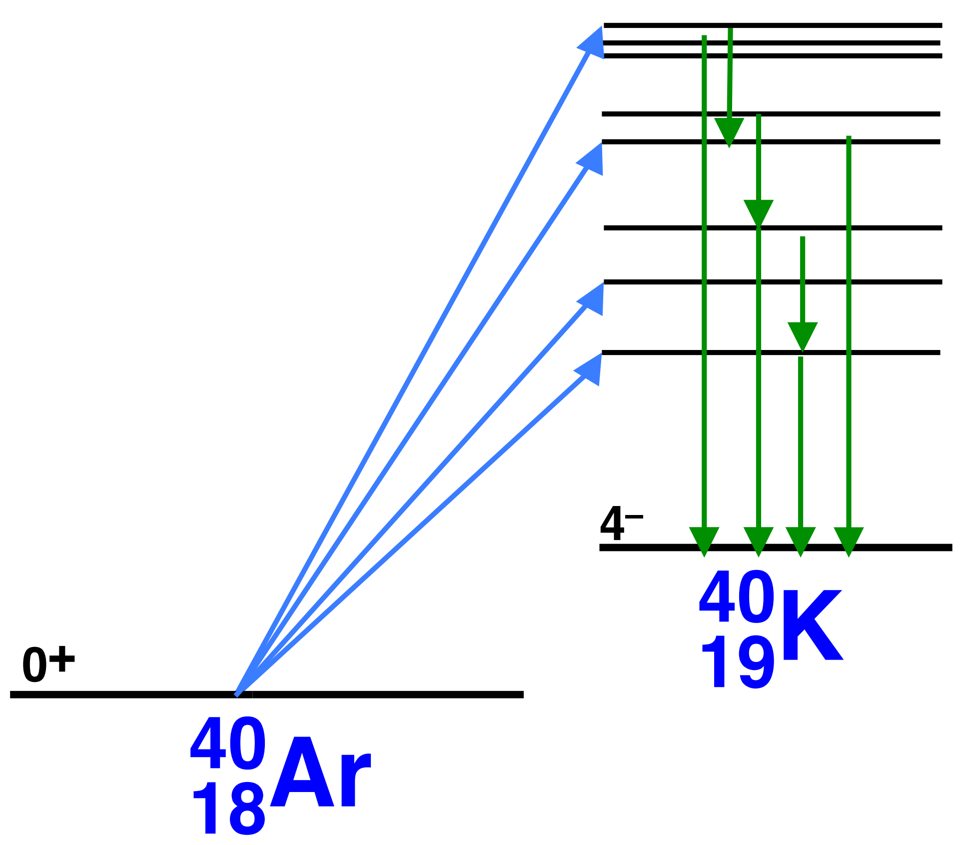


inverse beta decay

Outgoing e^+ energy — Neutron proton mass difference — Recoil energy of neutron (negligible)

$$E_{\bar{\nu}} = E_e + \Delta + K_{\text{recoil}}$$

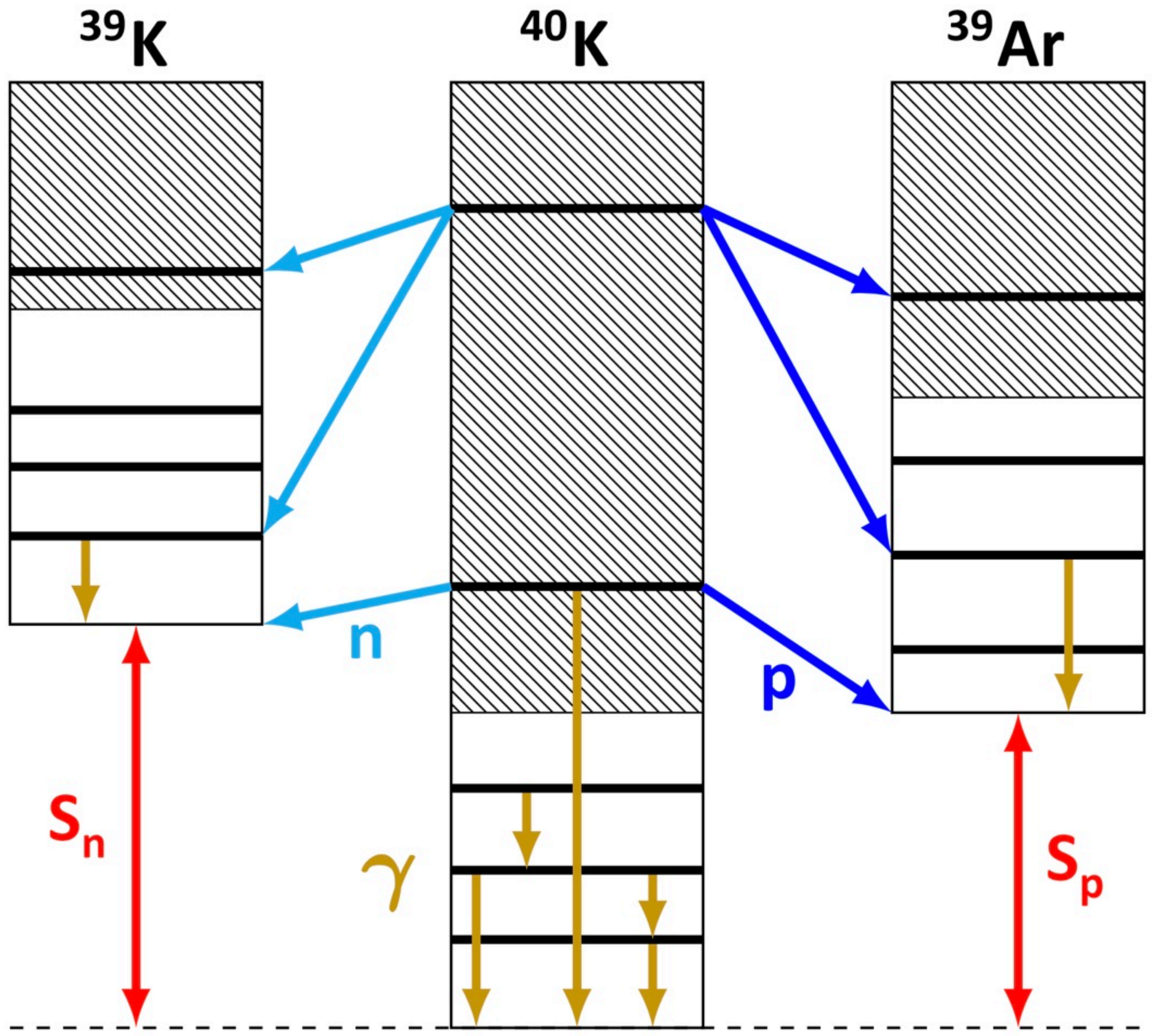
$$\nu_e + {}^{40}\text{Ar} \rightarrow {}^{40}\text{K}^* + e^-$$



ν-A is much more complex

Outgoing e^- Energy — Energy donated to transition — Recoil Energy of Nucleus (negligible)

$$E_\nu = E_e + Q + K_{\text{recoil}}$$

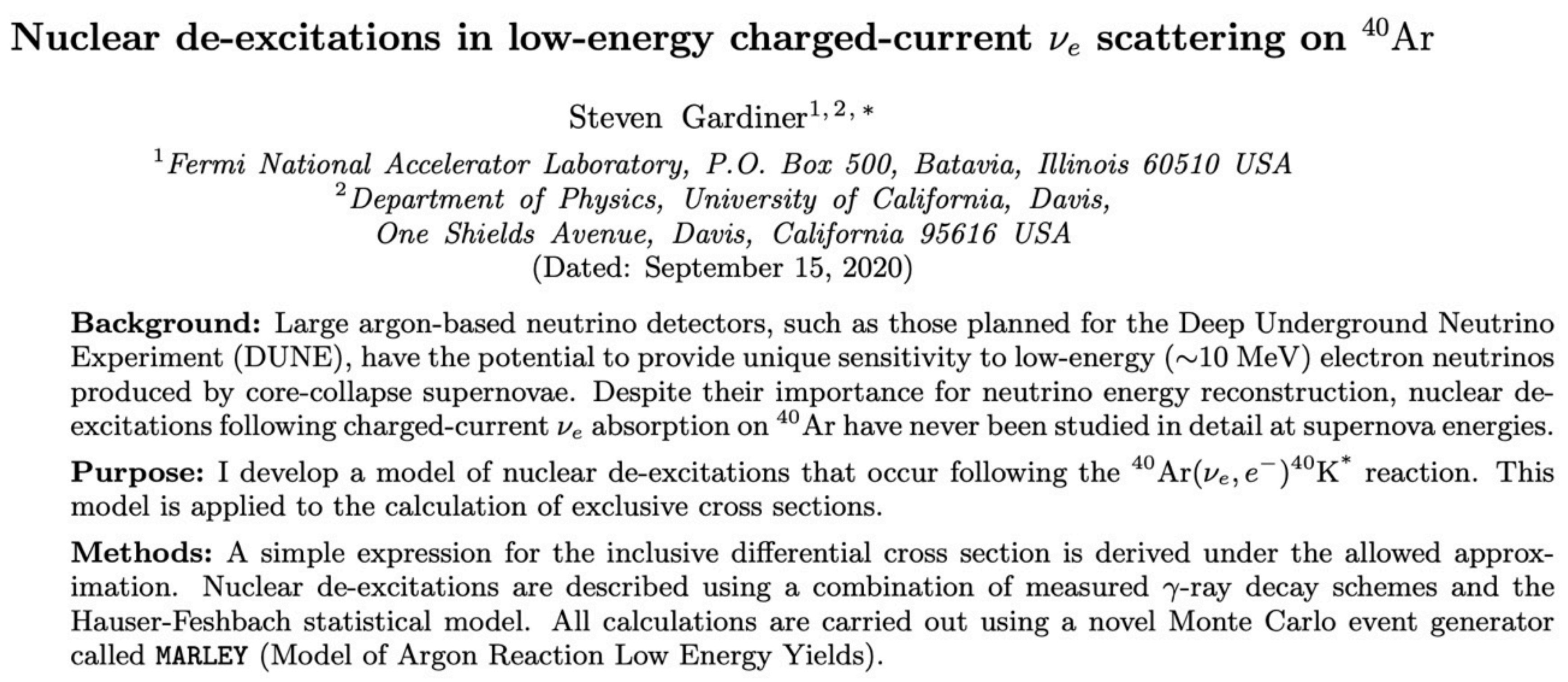


Two-step approach

1. Nuclear transitions
2. De-excitations

MARLEY overview

- Event generator focused specifically on neutrino energies below ~100 MeV
- “Model of Argon Reaction Low Energy Yields”
  - Emphasizes ν_e CC on ^{40}Ar, extensible to other channels
- Two dedicated publications so far:
  - Physics models: **[Phys. Rev. C 103, 044604 (2021)]**
  - Numerical implementation: **[Comput. Phys. Commun. 269, 108123 (2021)]**
- Written in C++14, few dependencies



Nuclear de-excitations in low-energy charged-current ν_e scattering on ^{40}Ar

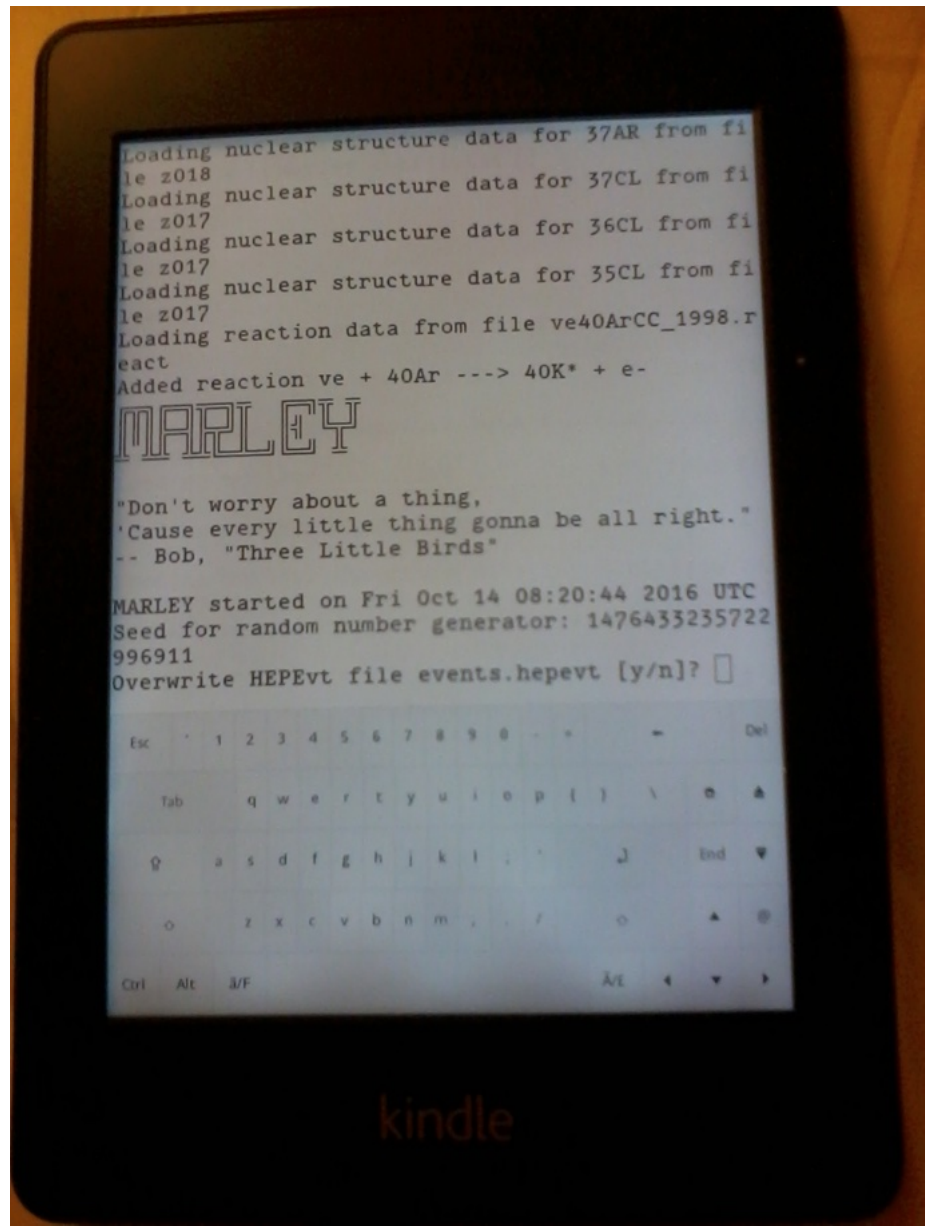
Steven Gardiner[1,2,*]

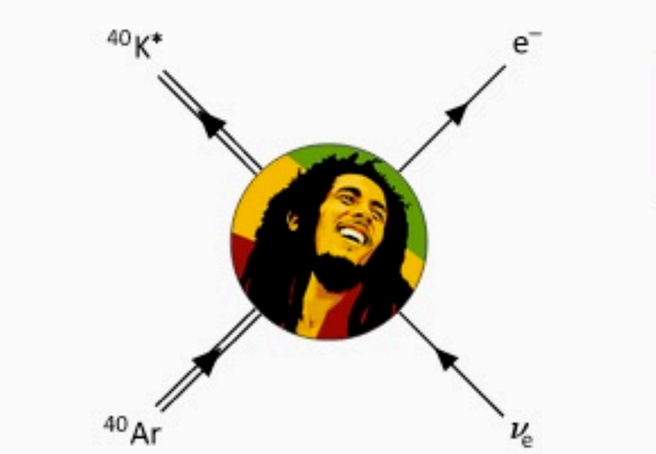
[1] Fermi National Accelerator Laboratory, P.O. Box 500, Batavia, Illinois 60510 USA
[2] Department of Physics, University of California, Davis, One Shields Avenue, Davis, California 95616 USA
(Dated: September 15, 2020)

Background: Large argon-based neutrino detectors, such as those planned for the Deep Underground Neutrino Experiment (DUNE), have the potential to provide unique sensitivity to low-energy (~10 MeV) electron neutrinos produced by core-collapse supernovae. Despite their importance for neutrino energy reconstruction, nuclear de-excitations following charged-current ν_e absorption on ^{40}Ar have never been studied in detail at supernova energies.

Purpose: I develop a model of nuclear de-excitations that occur following the $^{40}\mathrm{Ar}(\nu_e, e^-)^{40}\mathrm{K}^*$ reaction. This model is applied to the calculation of exclusive cross sections.

Methods: A simple expression for the inclusive differential cross section is derived under the allowed approximation. Nuclear de-excitations are described using a combination of measured γ-ray decay schemes and the Hauser-Feshbach statistical model. All calculations are carried out using a novel Monte Carlo event generator called MARLEY (Model of Argon Reaction Low Energy Yields).





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Overview

MARLEY (Model of Argon Reaction Low Energy Yields) is a Monte Carlo event generator for neutrino-nucleus interactions at energies of tens-of-MeV and below. The current version computes inclusive neutrino-nucleus cross sections employing the *allowed approximation*: the nuclear matrix elements are evaluated while neglecting Fermi motion and applying the long-wavelength (zero momentum transfer) limit. De-excitations of the final-state nucleus emerging from the primary interaction are simulated using a combination of tabulated γ-ray decay schemes and an original implementation of the Hauser-Feshbach statistical model.

Input files are provided with the code that are suitable for simulating the charged-current process

$$\nu_e + {}^{40}\mathrm{Ar} \rightarrow e^- + {}^{40}\mathrm{K}^*,$$

coherent elastic neutrino-nucleus scattering (CEvNS) on spin-zero target nuclei, and neutrino-electron elastic scattering on any atomic target. Inclusion of additional reactions and targets is planned for the future.

The material presented here focuses on the practical aspects of MARLEY: installing the code, configuring and running simulations, and analyzing the output events. For more details on the MARLEY physics models, please see the references in the online bibliography.

MARLEY follows an open-source development model and welcomes contributions of new input files and code improvements from the community. A partial list of potential projects for future MARLEY development is available on the developer documentation webpage.

https://www.marleygen.org

MARLEY inclusive cross section model

Phys. Rev. C 103, 044604 (2021)

Inclusive scattering on the nucleus is simulated using this differential cross section:

$$\frac{d\sigma}{d\cos\theta_\ell} = \frac{G_F^2}{2\pi}\mathscr{F}_{CC}\left[\frac{E_i E_f}{s}\right] E_\ell\,|\mathbf{p}_\ell|\left[\left(1+\beta_\ell\cos\theta_\ell\right)B(\mathrm{F}) + \left(1-\frac{1}{3}\beta_\ell\cos\theta_\ell\right)B(\mathrm{GT})\right]$$

Charged current factor

Recoil factor

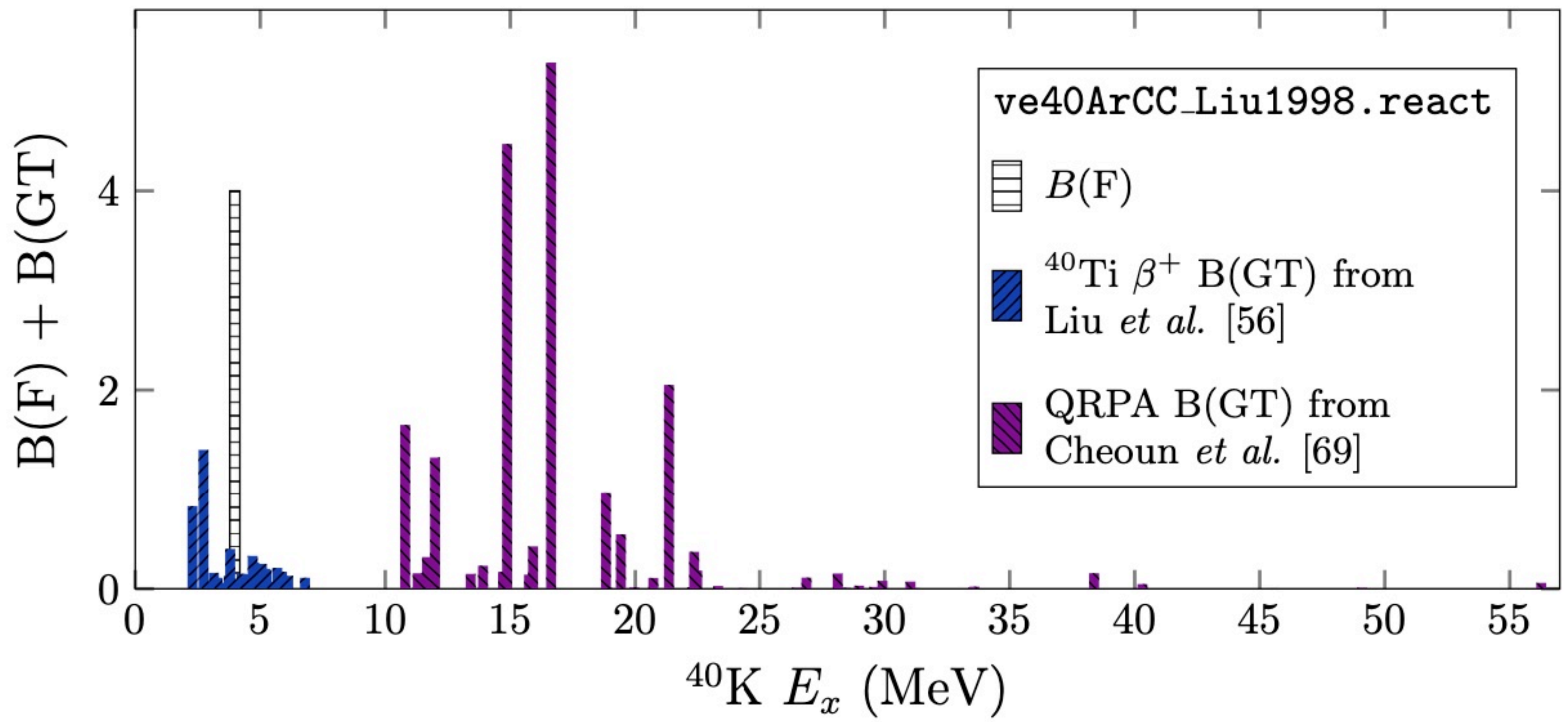
Allowed nuclear matrix elements

Expression above obtained under the impulse approximation and the **allowed approximation**

Long-wavelength limit: $q \to 0$

Slow nucleon limit: $\frac{|\mathbf{p}_{N_i}|}{m_N} \to 0$

Nuclear matrix elements must be supplied as input. For ^{40}Ar, they are based on a combination of **indirect measurements** (e.g., mirror β decay) and a **QRPA calculation**



MARLEY inclusive cross section model

Phys. Rev. C 103, 044604 (2021)

Charged-current factor contains CKM matrix element and a Coulomb correction factor F_C. MARLEY handles Coulomb corrections using a combination of the Fermi function and the Modified Effective Momentum Approximation (MEMA).

$$\mathcal{F}_{CC} \equiv \begin{cases} |V_{ud}|^2 F_C & \text{CC} \\ 1 & \text{NC} \end{cases}$$

See J. Engel, Phys. Rev. C 57, 2004 (1998)

The code can handle **allowed matrix elements** for ν_e CC, $\bar{\nu}_e$ CC, and NC, but only inputs for ν_e CC are currently provided "out of the box"

$$\mathcal{O}_\text{F} \equiv \begin{cases} \sum_{n=1}^{A} t_\pm(n) & \text{CC} \\ Q_W/2 & \text{NC} \end{cases}$$

$$B(\text{F}) \equiv \frac{g_V^2}{2J_i+1}\left|\langle J_f \,\|\, \mathcal{O}_\text{F} \,\|\, J_i\rangle\right|^2$$

$$B(\text{GT}) \equiv \frac{g_A^2}{2J_i+1}\left|\langle J_f \,\|\, \mathcal{O}_\text{GT} \,\|\, J_i\rangle\right|^2$$

$$\mathcal{O}_\text{GT} \equiv \begin{cases} \sum_{n=1}^{A} \boldsymbol{\sigma}(n)\, t_\pm(n) & \text{CC} \\ \sum_{n=1}^{A} \boldsymbol{\sigma}(n)\, t_3(n) & \text{NC} \end{cases}$$

Hauser-Feshbach Model

W. Hauser and H. Feshbach, Physical Review **87**, 366 (1952)

- Successfully used for many years to describe low-energy nuclear cross sections

- Two key assumptions:
  1. compound nucleus
  2. reciprocity theorem (time-reversal invariance)

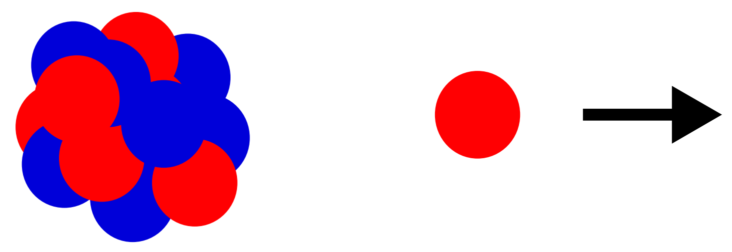
- Transmission coefficient $T_{\ell j}$ = probability for fragment to escape the nucleus

- Compound nucleus + time-reversal symmetry = $T_{\ell j}$ via "reciprocity"

- Optical model is used to compute $T_{\ell j}$ for time-reversed process

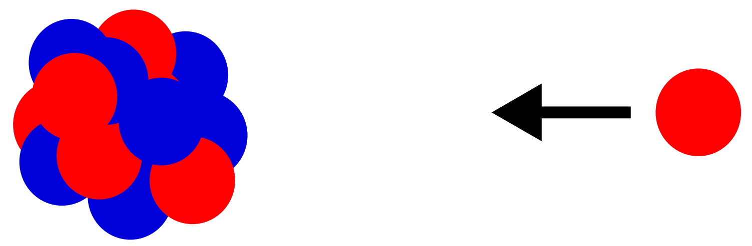
- Numerical solution of Schrödinger equation via Numerov's method

The fragment emission width of a compound nucleus



$A \to \alpha + B$

is related to its formation cross section



$\alpha + B \to A$

MARLEY nuclear de-excitation model

Phys. Rev. C 103, 044604 (2021)

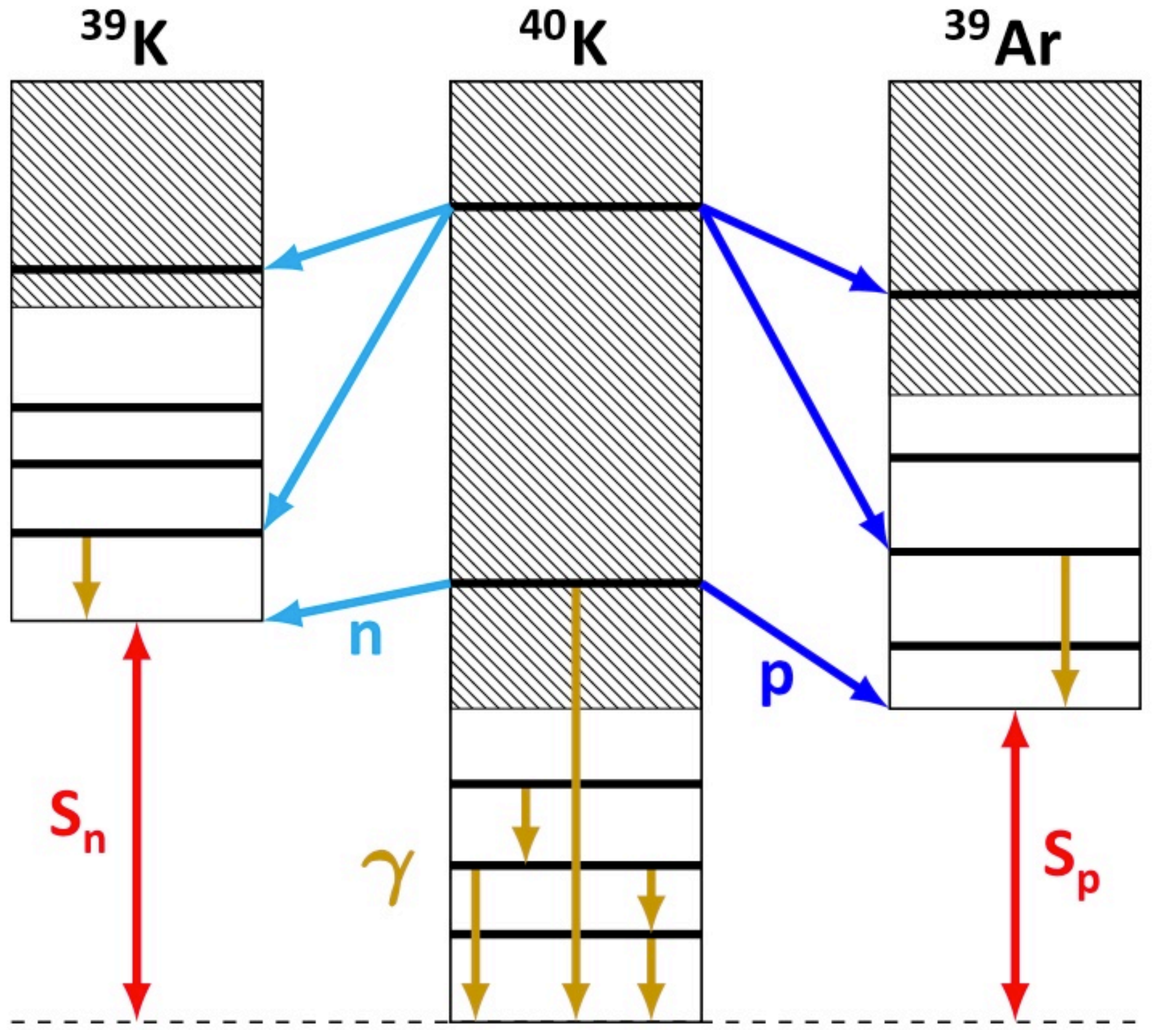
In the second step, the nucleus de-excites via a series of binary decays. Decay widths for **unbound states** are computed according to the Hauser-Feshbach formalism:

Differential decay width for emission of a nuclear fragment α (A ≤ 4 considered)

$$\frac{d\Gamma_\alpha}{dE_x'} = \frac{1}{2\pi\rho_i(E_x, J, \Pi)} \sum_{\ell=0}^{\ell_{\max}} \sum_{j=|\ell-s|}^{\ell+s} \sum_{J'=|J-j|}^{J+j} T_{\ell j}(\varepsilon)\, \rho_f(E_x', J', \Pi')$$

Differential decay width for emission of a γ-ray

$$\frac{d\Gamma_\gamma}{dE_x'} = \frac{1}{2\pi\rho_i(E_x, J, \Pi)} \sum_{\lambda=1}^{\lambda_{\max}} \sum_{J'=|J-\lambda|}^{J+\lambda} \sum_{\Pi'\in\{-1,1\}} T_{X\lambda}(E_\gamma)\, \rho_f(E_x', J', \Pi')$$



Level density model: Back-shifted Fermi gas (RIPL-3), Nucl. Data Sheets 110, 3107–3214 (2009)

Nuclear optical model: Koning & Delaroche, Nucl. Phys. A 713, 231–310 (2003)

Gamma-ray strength function model: Standard Lorentzian (RIPL-3), Nucl. Data Sheets 110, 3107–3214 (2009)

Supplemented with tabulated discrete levels and γ-rays for **bound states** (taken from TALYS 1.6). Transitions from continuum to all accessible levels are explicitly treated.

MARLEY v1.2.0 predictions for ^{40}Ar

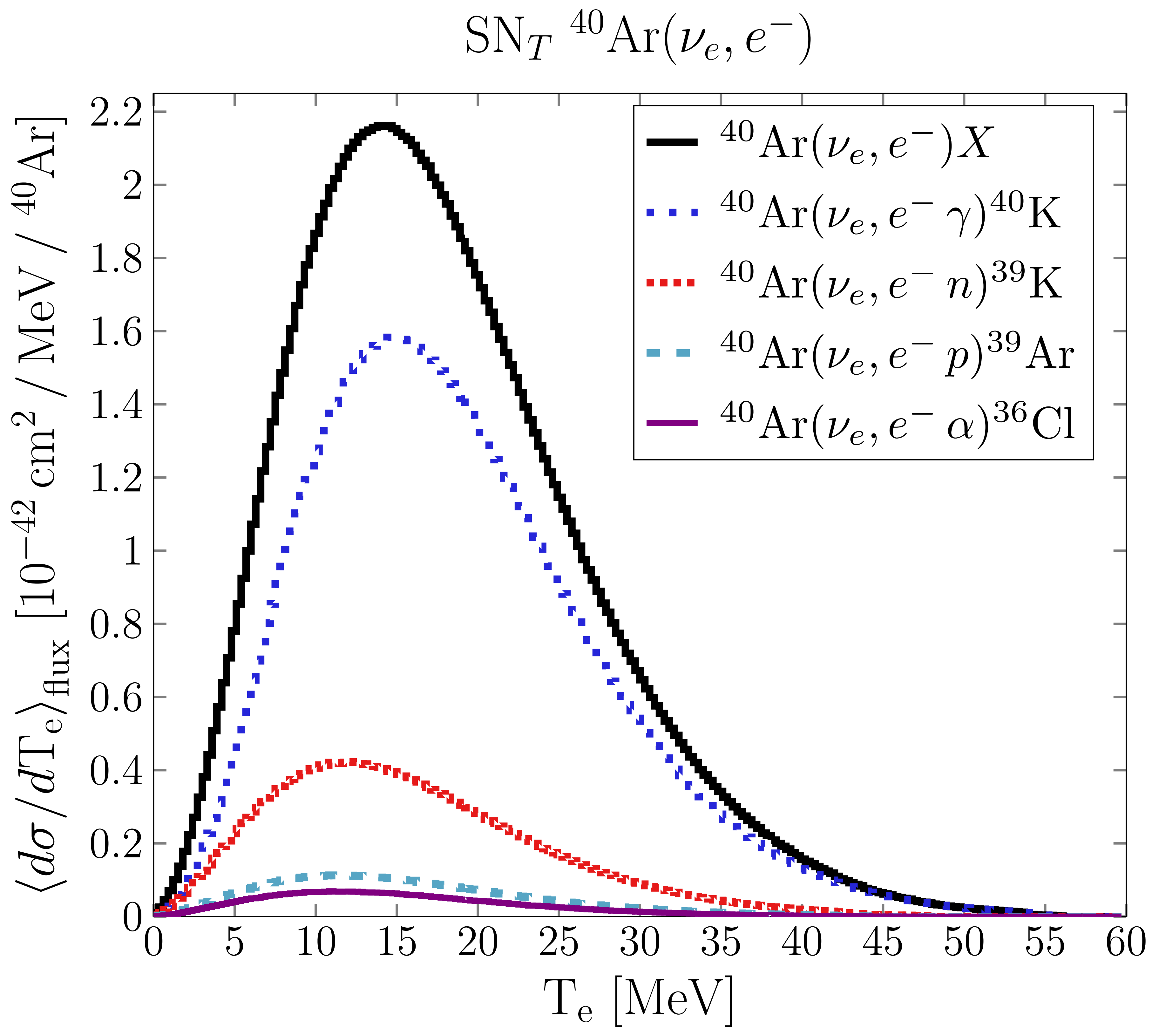
Phys. Rev. C 103, 044604 (2021)

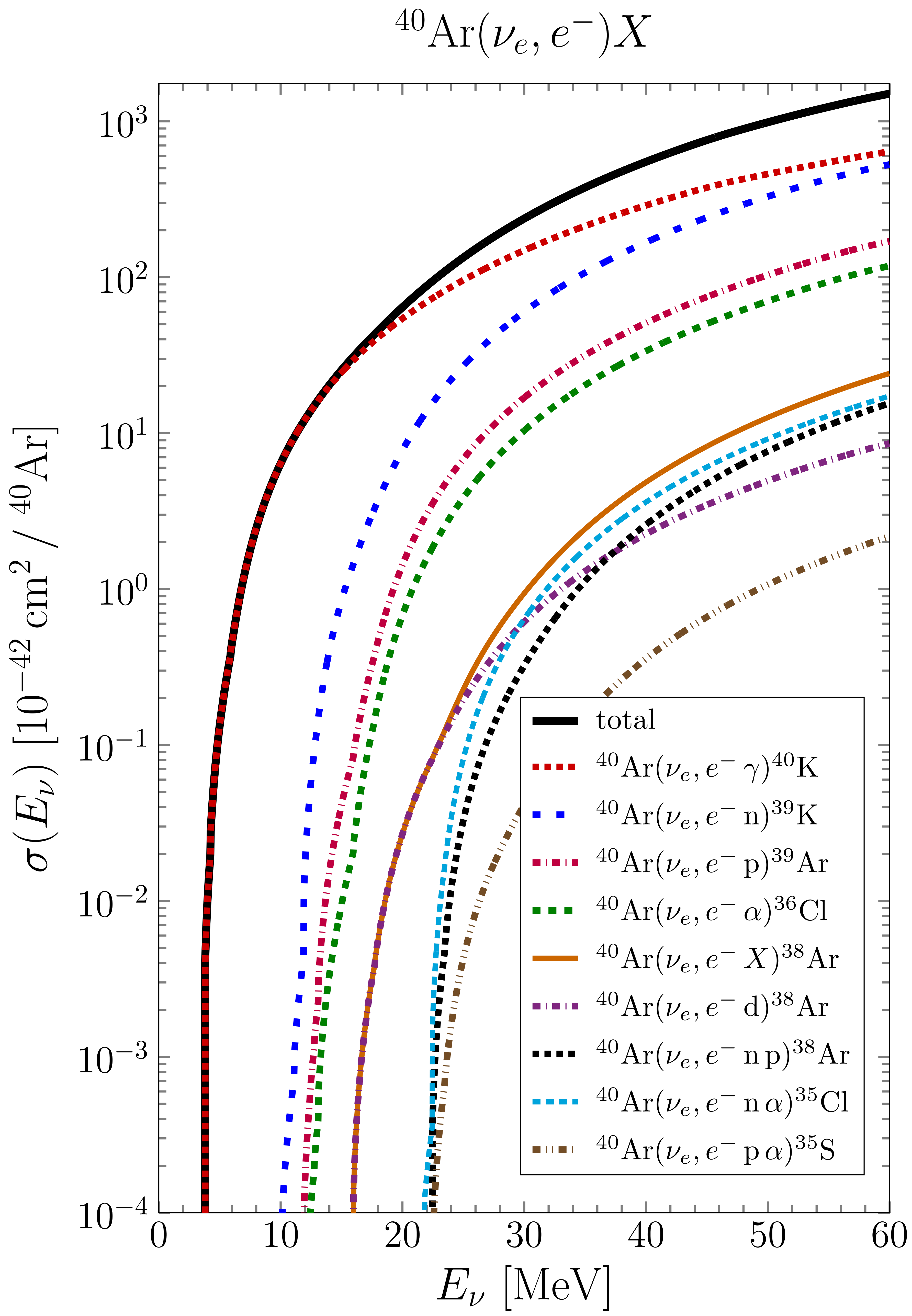
- First calculation of cross sections for **exclusive final states** of the reaction

$$\nu_e + {}^{40}\mathrm{Ar} \rightarrow e^- + X$$

at tens-of-MeV energies.

- Flux-averaged differential cross sections shown here are for the supernova model described in Phys. Rev. D 97, 023019 (2018).





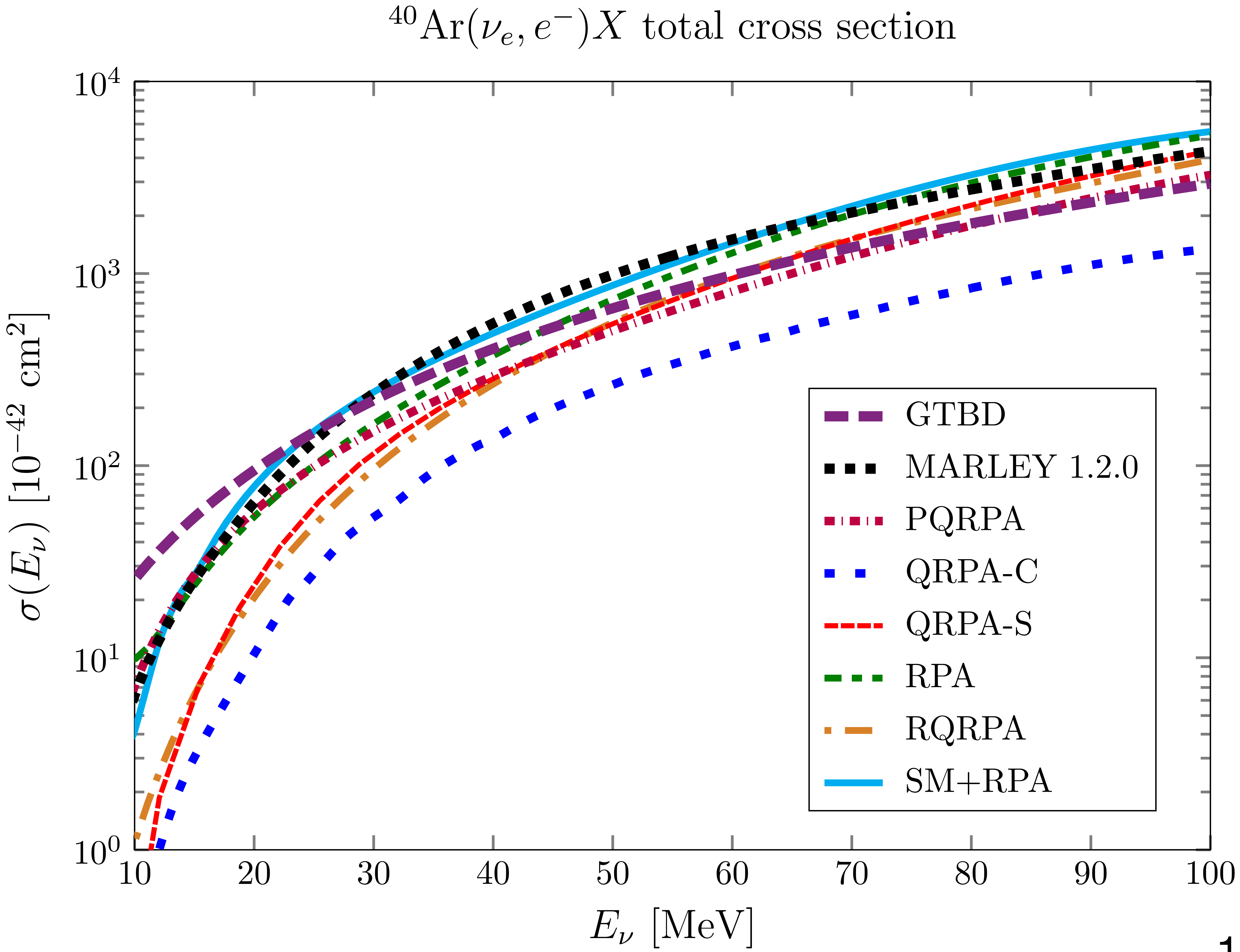
Uncertainties overview

- Limited out-of-the-box support
  - Handful of configurable parameters
  - Edits to input data
- **Shortcuts** in model choices biggest concern
  - Easier to quantify on model ingredients
- **Reweighting** is standard approach
  - Will point out where this is tricky
- More attention needed from both theory & experiment

Other perspectives welcome!

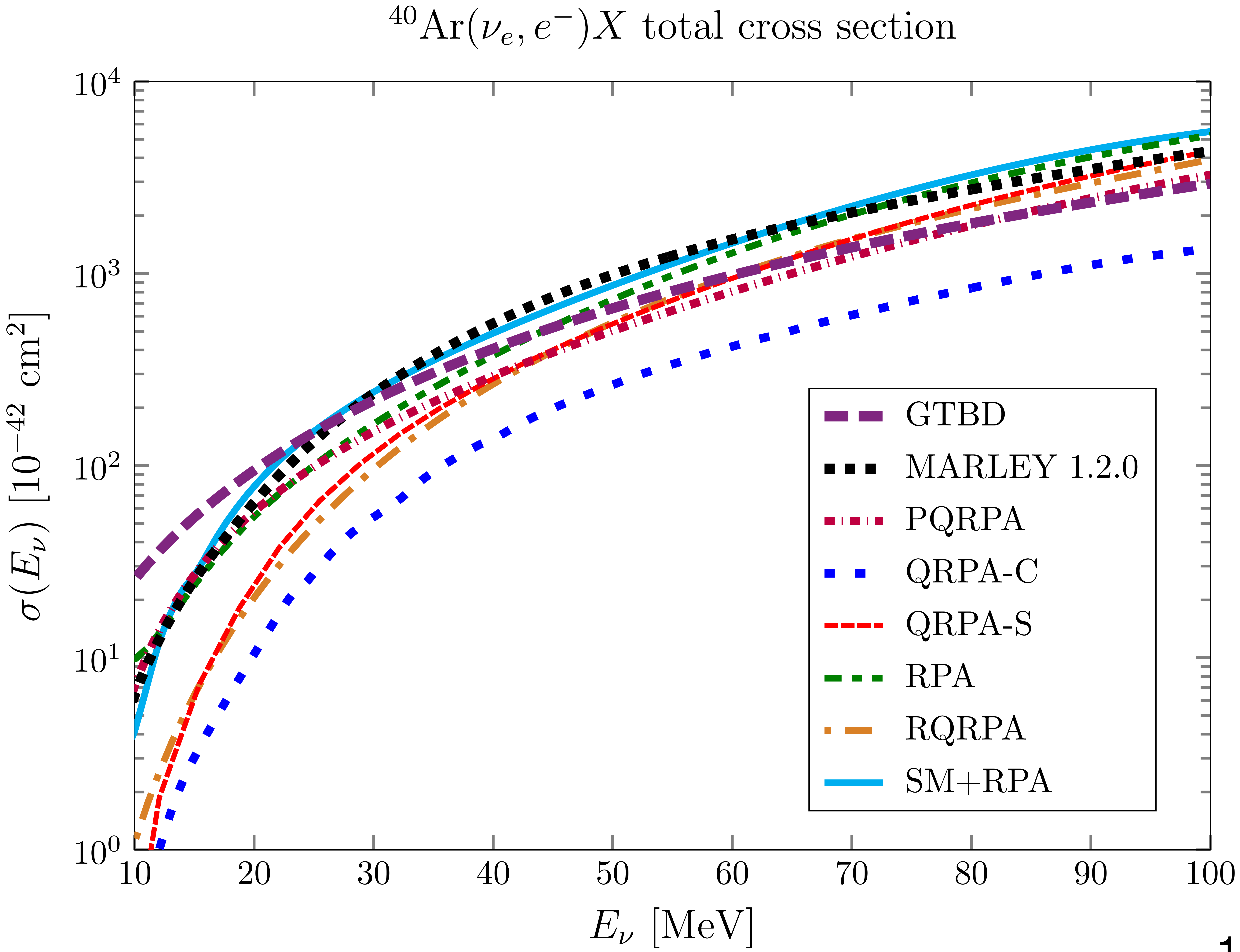
Total cross section (1)

- No direct data, calculations benchmarked with other nuclei, beta decay, etc.
- “Spread of models” approach used in first **DUNE toy study**
- Reweightable except below MARLEY threshold



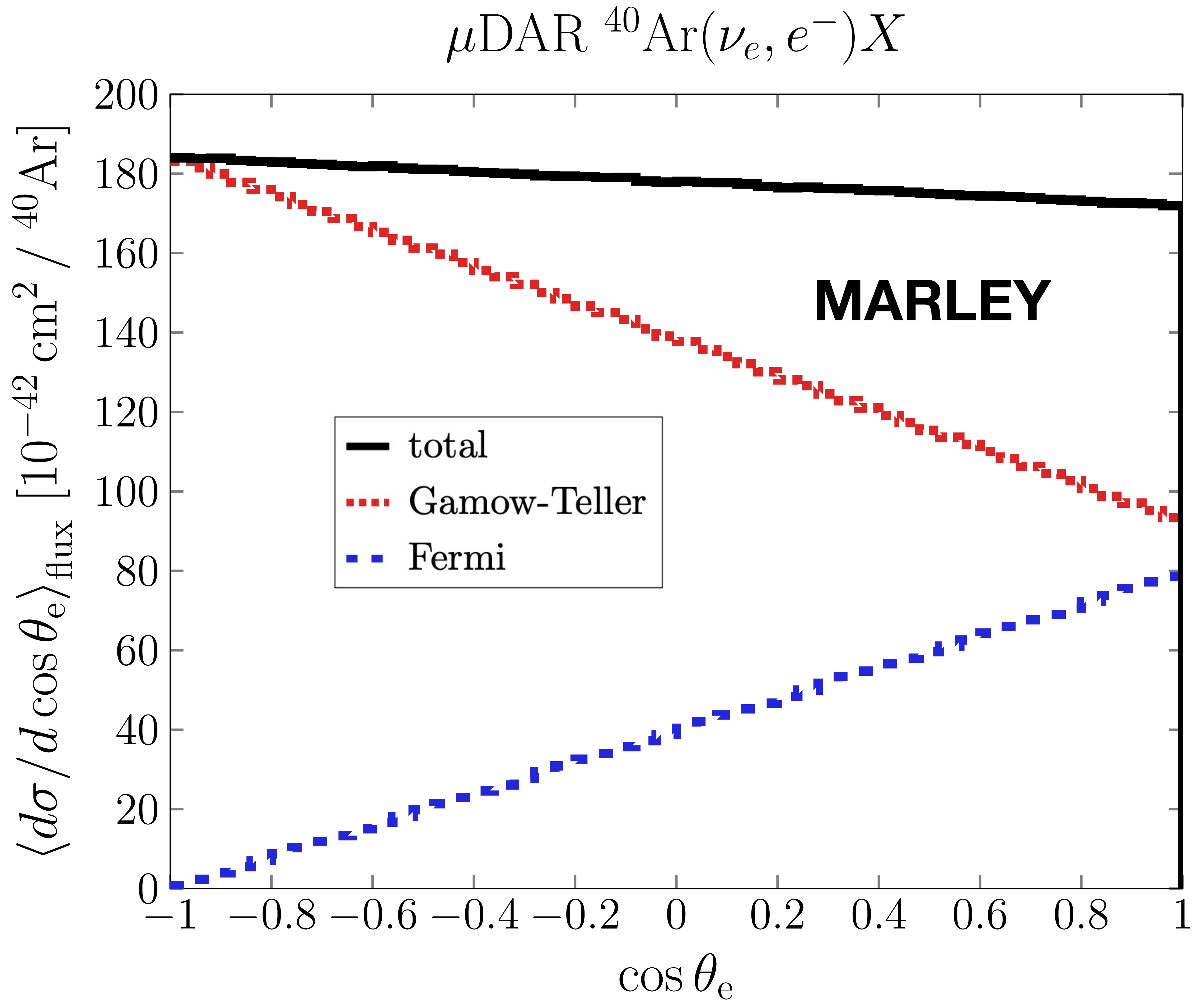
Total cross section (2)

- **Allowed approximation** (AA) better than it deserves to be
- $j_L(|\mathbf{q}|r)$ dependence in matrix element
  - L = 0 survives in AA
- Neglects forbidden but overestimates allowed for $|\mathbf{q}| \neq 0$

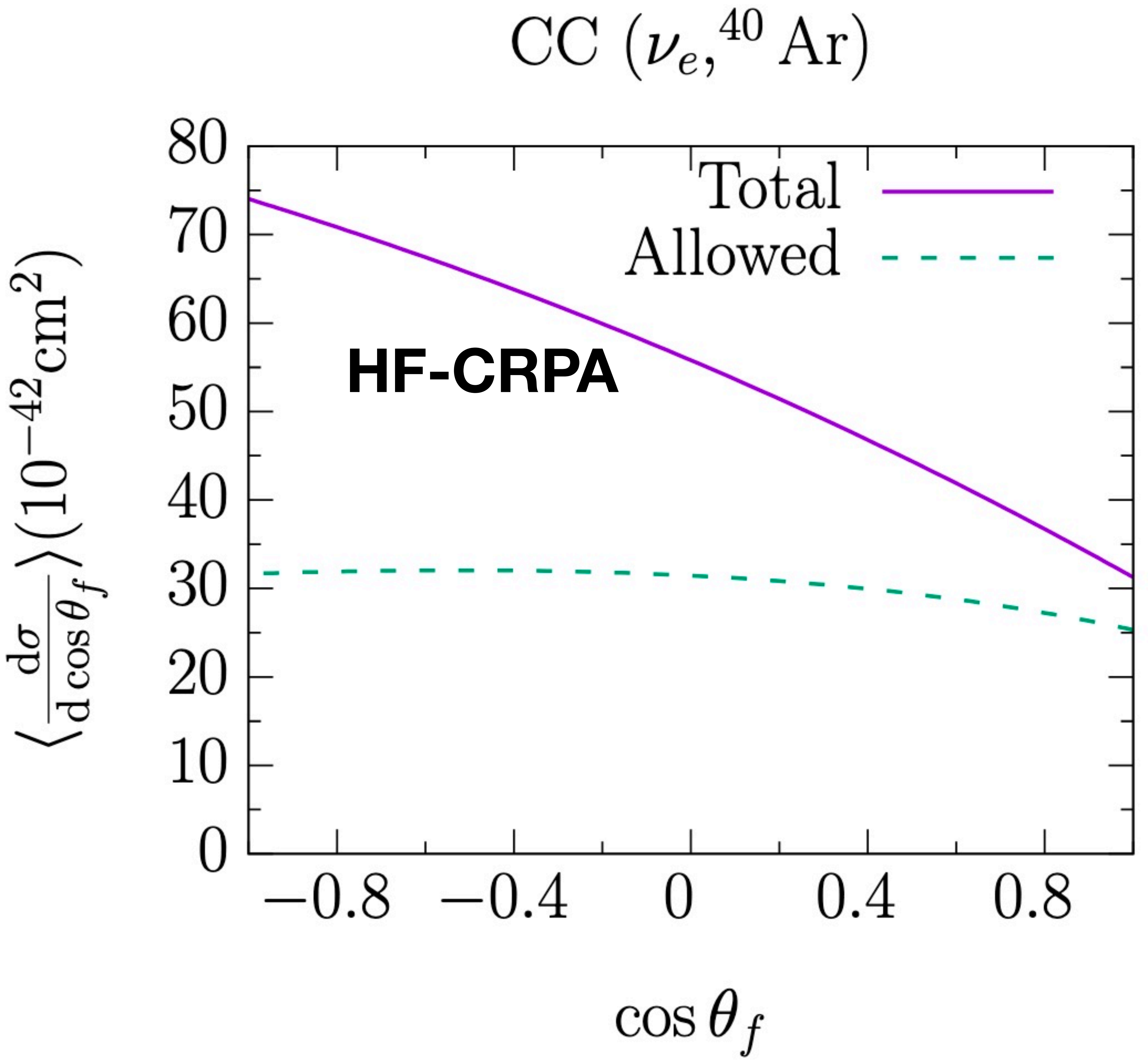


Inclusive angular distribution

- AA under-predicts backwards strength (interesting for supernova pointing)
- Reweightable, should be done in 2D together with T_f

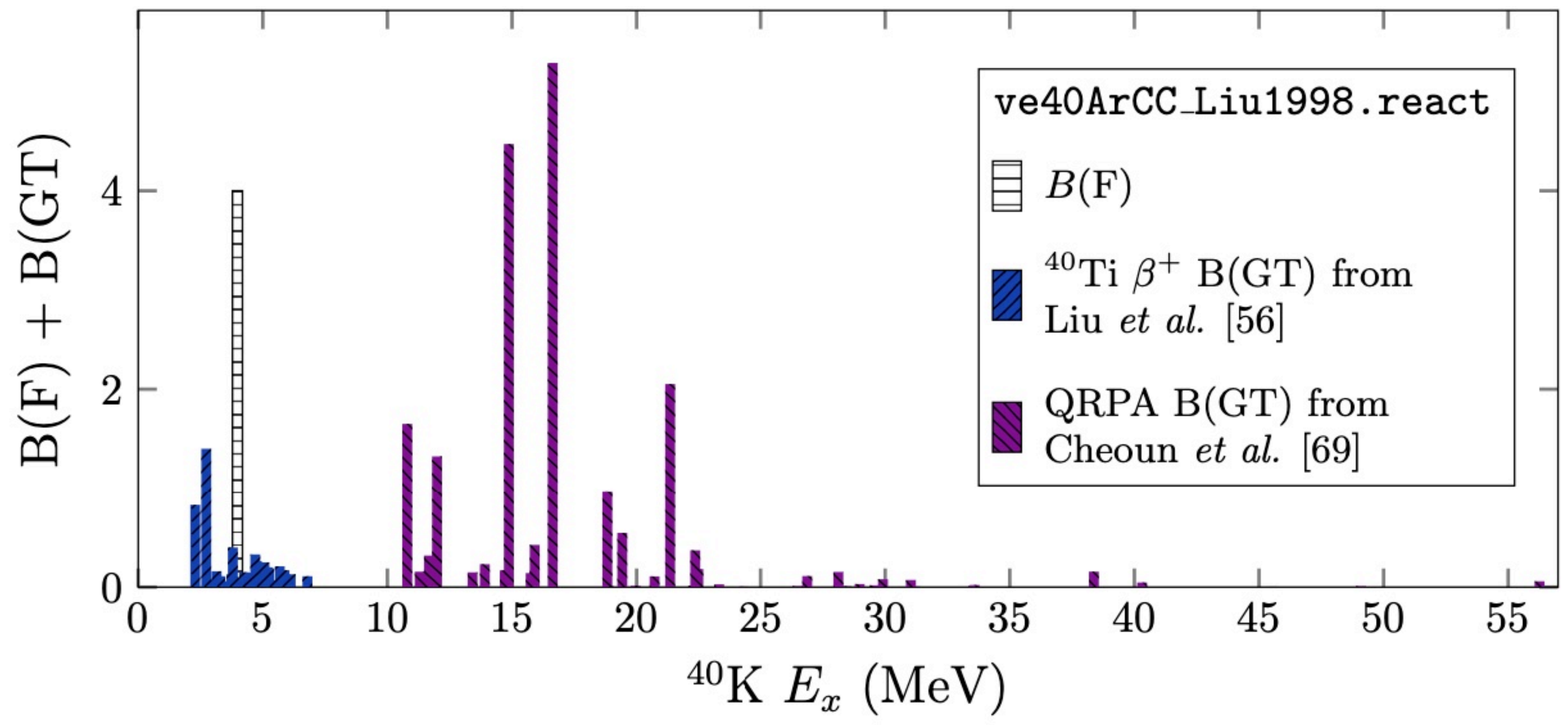


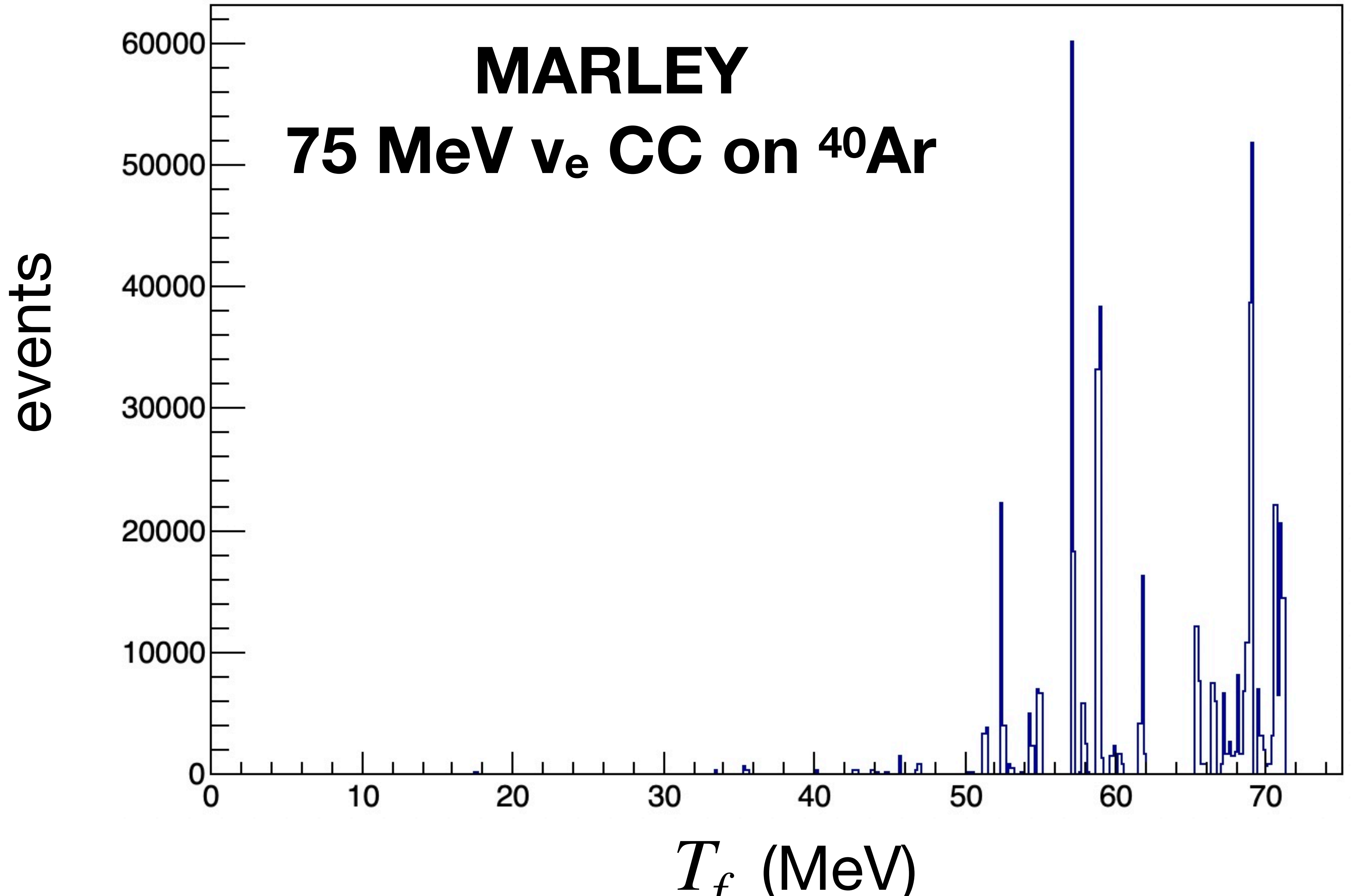
Phys. Rev. C 101, 045502 (2020)



Final-state lepton energy distribution

- MARLEY currently takes tabulated matrix elements at face value
  - Discrete E_x values even in the continuum
  - Leads to **lines** in T_f for monoenergetic ν, some not real
- Matched to measured levels in discrete region, no correction in continuum
- Only fully reweightable between models if the nuclear level placement is the same





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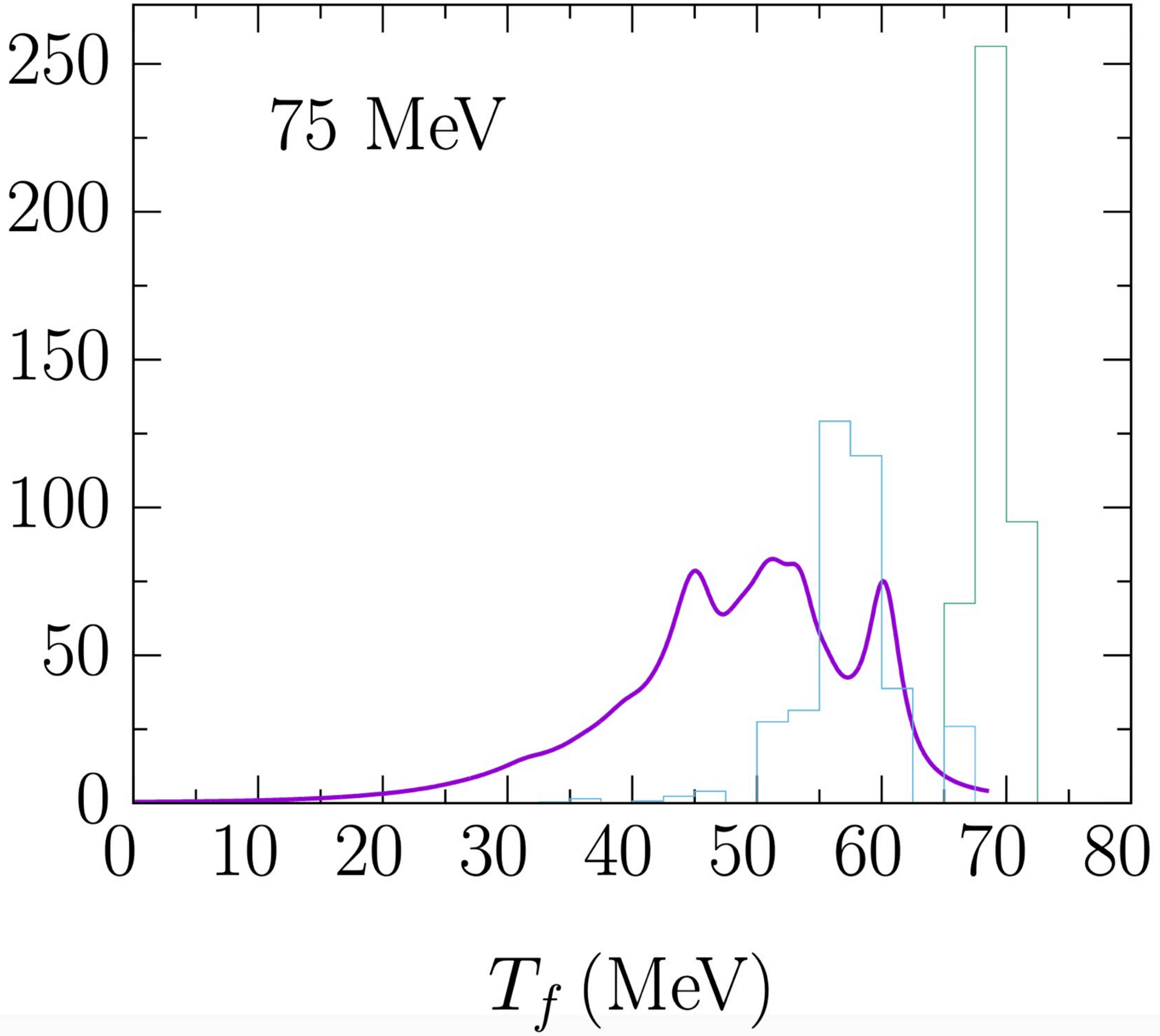
- Only fully reweightable between models if the nuclear level placement is the same

Phys. Rev. C 101, 045502 (2020)



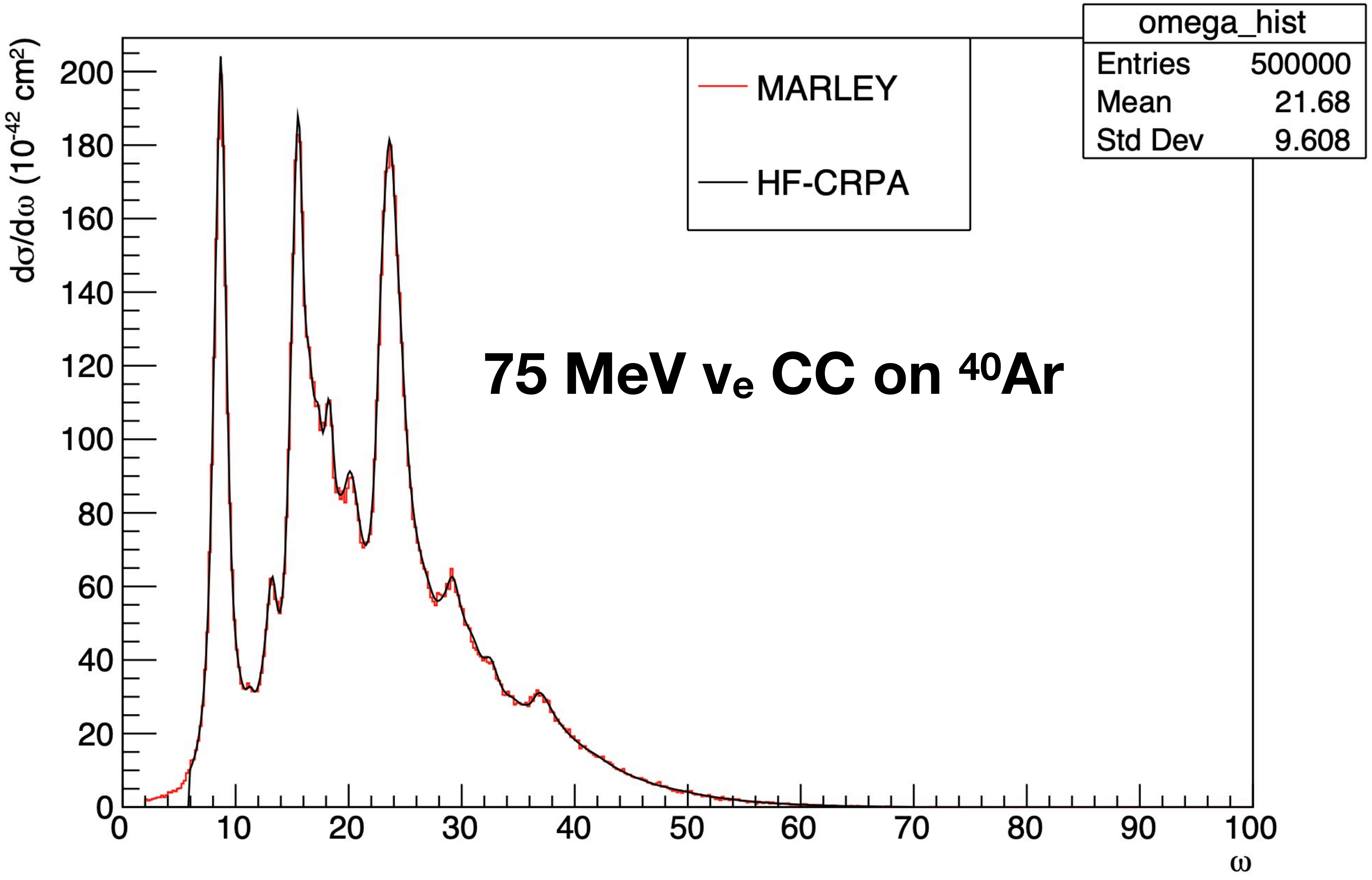
HF-CRPA prediction compared to **MARLEY** (discrete piece in **green**)

HF-CRPA as an improvement

- **New code** reproduces HF-CRPA inclusive cross section
  - Continuum treated as such
  - Includes forbidden transitions

- Will be reweightable to other predictions with proper continuum and discrete level treatments

- Work in progress. Still need
  - Strength to discrete levels
  - Handling of HF-CRPA cross section below measured nucleon separation threshold

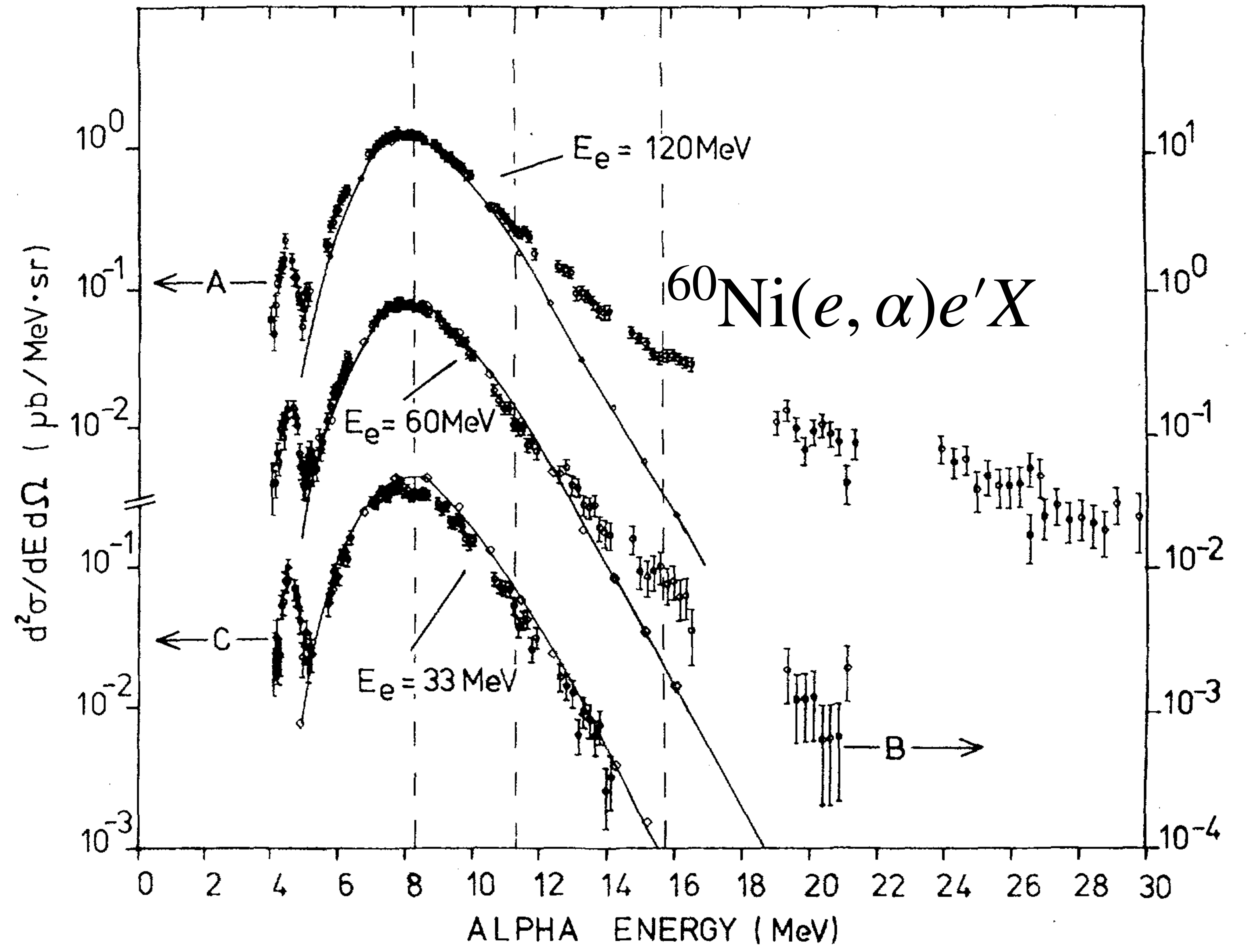


Many thanks to Alexis for providing the nuclear responses and helpful guidance

De-excitation uncertainties

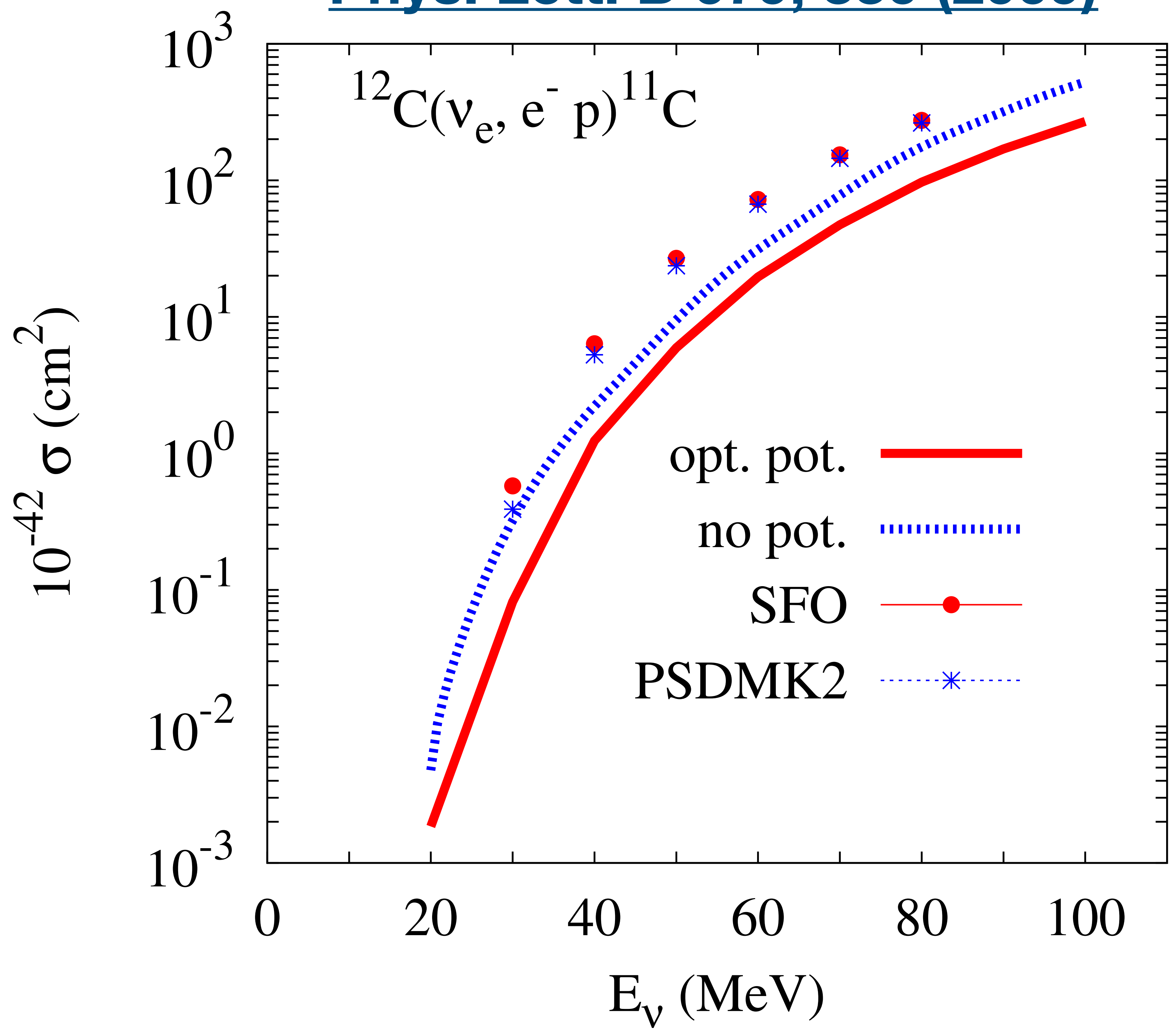
- **Big picture:** compound nucleus assumption is basically universal in O(10 MeV) literature
  - How severe is it as an approximation?
  - This matters: **neutron emission** limits neutrino energy resolution, needs to be well-modeled

Phys. Rev. Lett. 40, 709 (1978)



Compound nucleus calculation shows excellent agreement at E_e = 33 MeV, which worsens as the electron energy increases

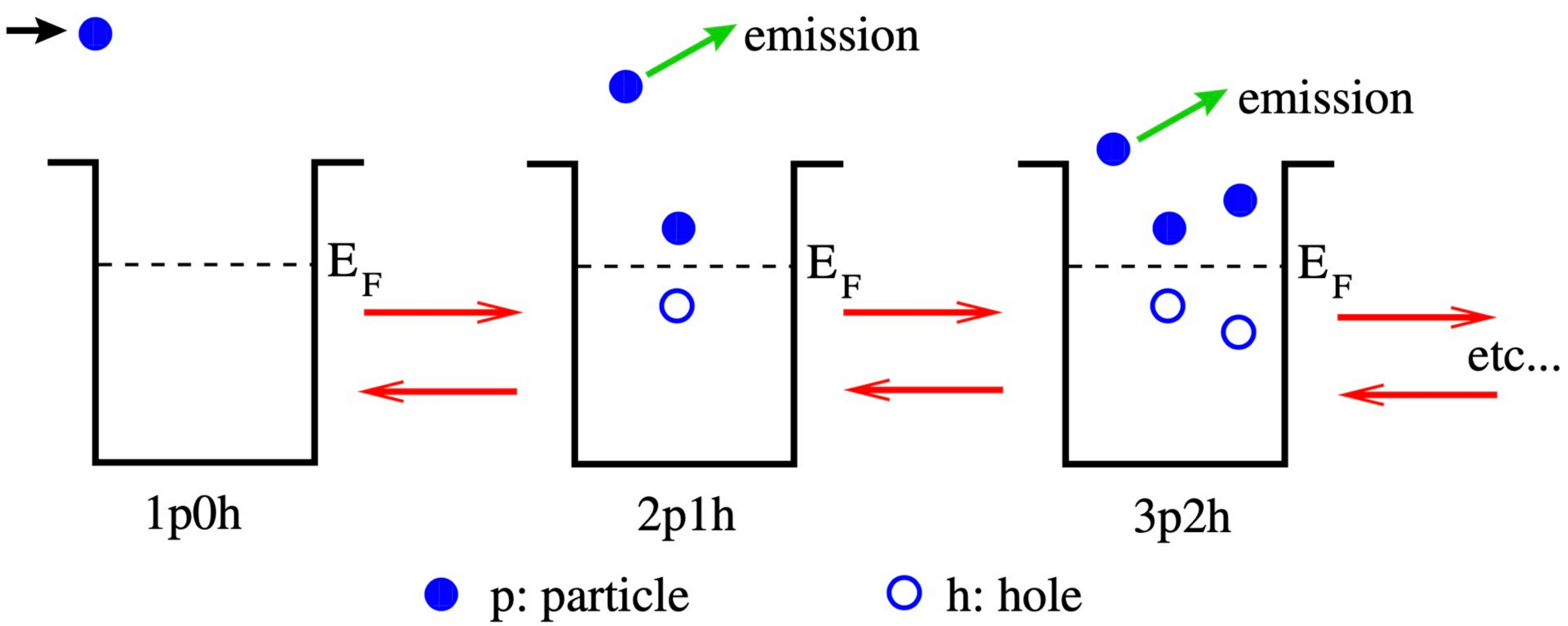
Phys. Lett. B 679, 330 (2009)



Two-step cross section (points, shell model + compound nucleus) dominates over direct knockout (solid red line). Turning off FSIs gets closer (dashed blue line).

What other components might be needed?

- **Pre-equilibrium** particle emission
  - Often treated with an **exciton model**
  - Appears unexplored for low-energy ν-A
  - Some work on muon capture, e.g., [Phys. Rev. C 107, 054314 (2023)]
  - MARLEY treatment in early development



- **Direct knockout** contribution
  - Coupled to a de-excitation model in multiple high-energy codes:
    GiBUU + SMM
    NuWro/GENIE + INCL + ABLA
    FLUKA (PEANUT)
  - Implementation could perhaps be added in a similar style

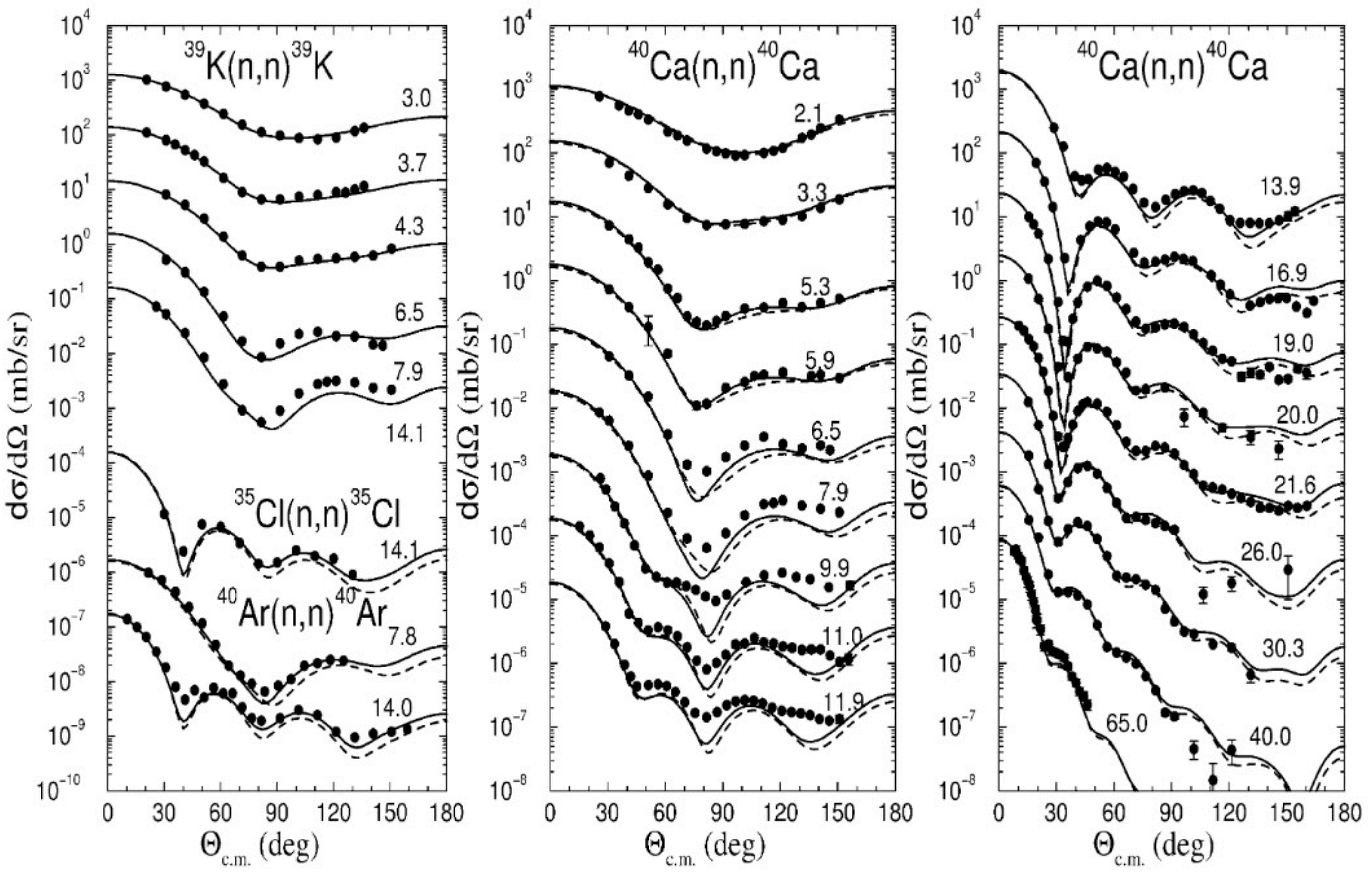
Some exciton model ingredients are shared with compound nucleus (e.g., optical potential)

See recent paper using NuWro + INCL + ABLA
arXiv:2309.05410 (accepted by PRD)

Compound nucleus model ingredients

- MARLEY's nuclear level densities, **optical model**, and γ-ray strength functions are all based on semi-empirical models
  - Global parameter fits across chart of nuclides
  - **No detailed fit uncertainties**
- Alternative parameterizations exist, could be implemented in code framework with some effort
- Redoing fits (just near A = 40?) would be very labor-intensive
- **Reweighting mostly straightforward** for relevant parameters

Nucl. Phys. A 713, 231–310 (2003)



Dashed line is the global fit that MARLEY currently uses.
Solid lines are local fits to specific nuclei.

NuHepMC as an “enabling technology”

- Proposed universal event format for neutrino generators
- Lower barriers to entry in experimental production, generator/data comparisons
- Please throw tomatoes so we can improve the standard
- Full de-excitation history now recorded in MARLEY, step towards reweighting

NuHepMC: A standardized event record format for neutrino event generators

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Abstract

Simulations of neutrino interactions are playing an increasingly important role in the pursuit of high-priority measurements for the field of particle physics. A significant technical barrier for efficient development of these simulations is the lack of a standard data format for representing individual neutrino scattering events. We propose and define such a universal format, named NuHepMC, as a common standard for the output of neutrino event generators. The NuHepMC format uses data structures and concepts from the HepMC3 event record library adopted by other subfields of high-energy physics. These are supplemented with an original set of conventions for generically representing neutrino interaction physics within the HepMC3 infrastructure.

NuHepMC as an “enabling technology”

- Proposed universal event format for neutrino generators
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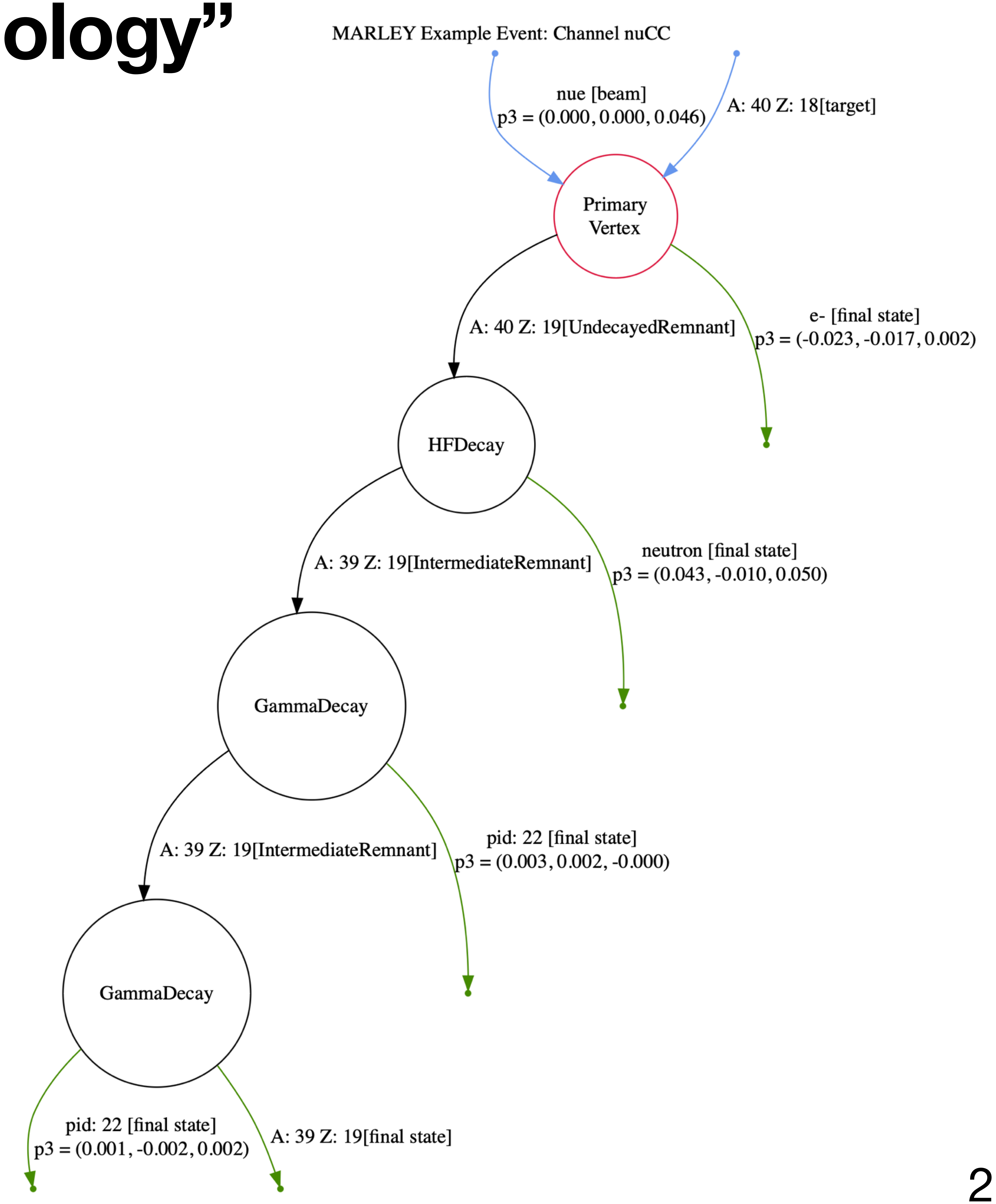
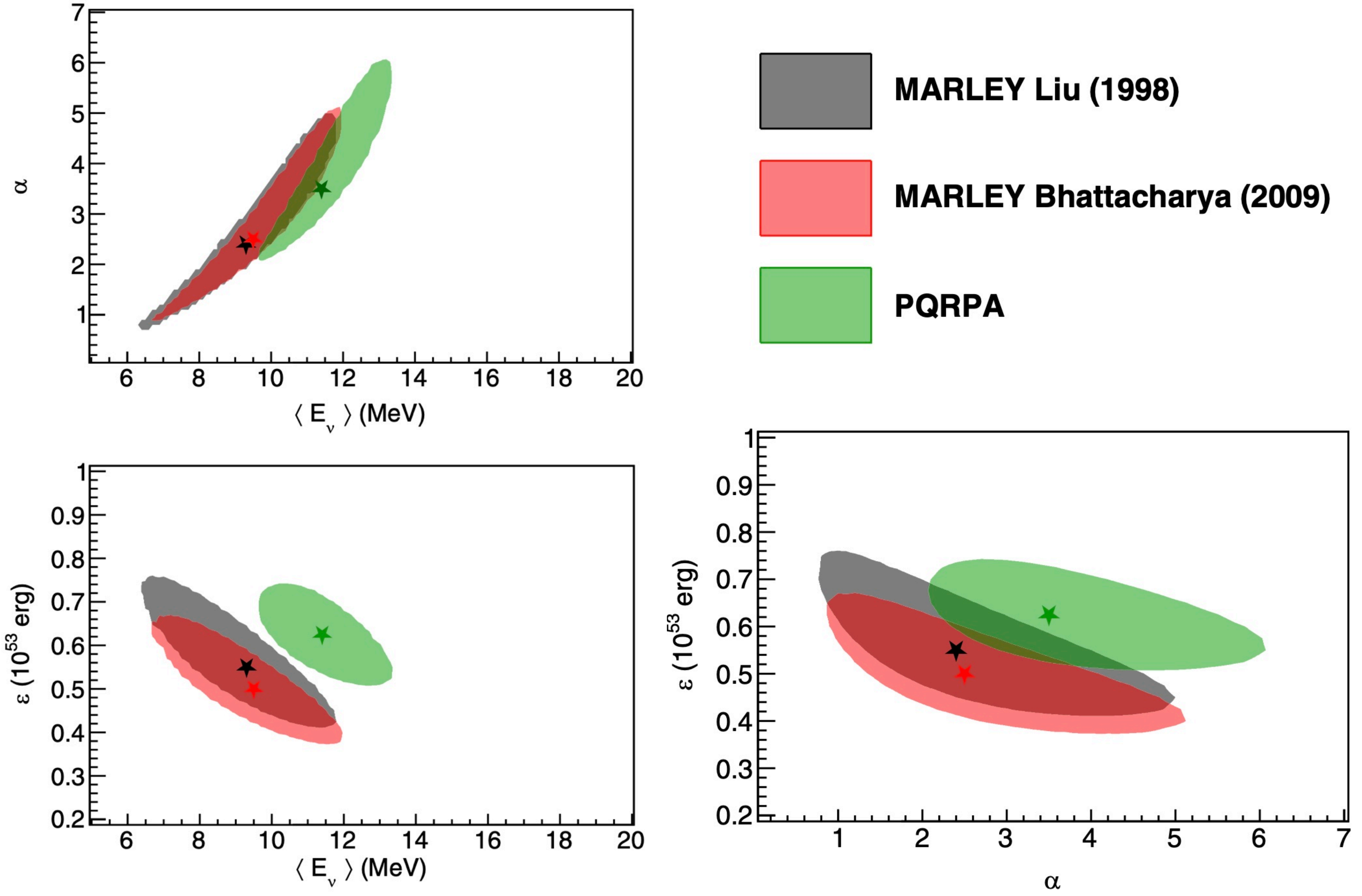
- Please throw tomatoes so we can improve the standard 🍅🍅
- **Full de-excitation history** now recorded in MARLEY, step towards reweighting



Recent study for DUNE: $\sigma(\mathbf{E}_\nu)$ uncertainty only

Phys. Rev. D 107, 112012 (2023)

- **Toy analysis** seeks to extract flux parameters from simulated DUNE supernova neutrino data
- ε = energy release (erg)
- $\langle E_\nu \rangle$ = mean neutrino energy (MeV)
- α = shape parameter (dimensionless)



Current understanding of $\sigma(E_\nu)$ is **inadequate.**

Measuring ε (other parameters) to 10% requires 5% (20%) knowledge of the cross section!

Conclusion

- Interaction simulations are critical for supernova neutrino measurements, especially ν_e in DUNE
- More work needed to fully quantify uncertainties, this talk suggests some first steps
- Low-energy neutrino cross-section data and theory work to interpret it both needed