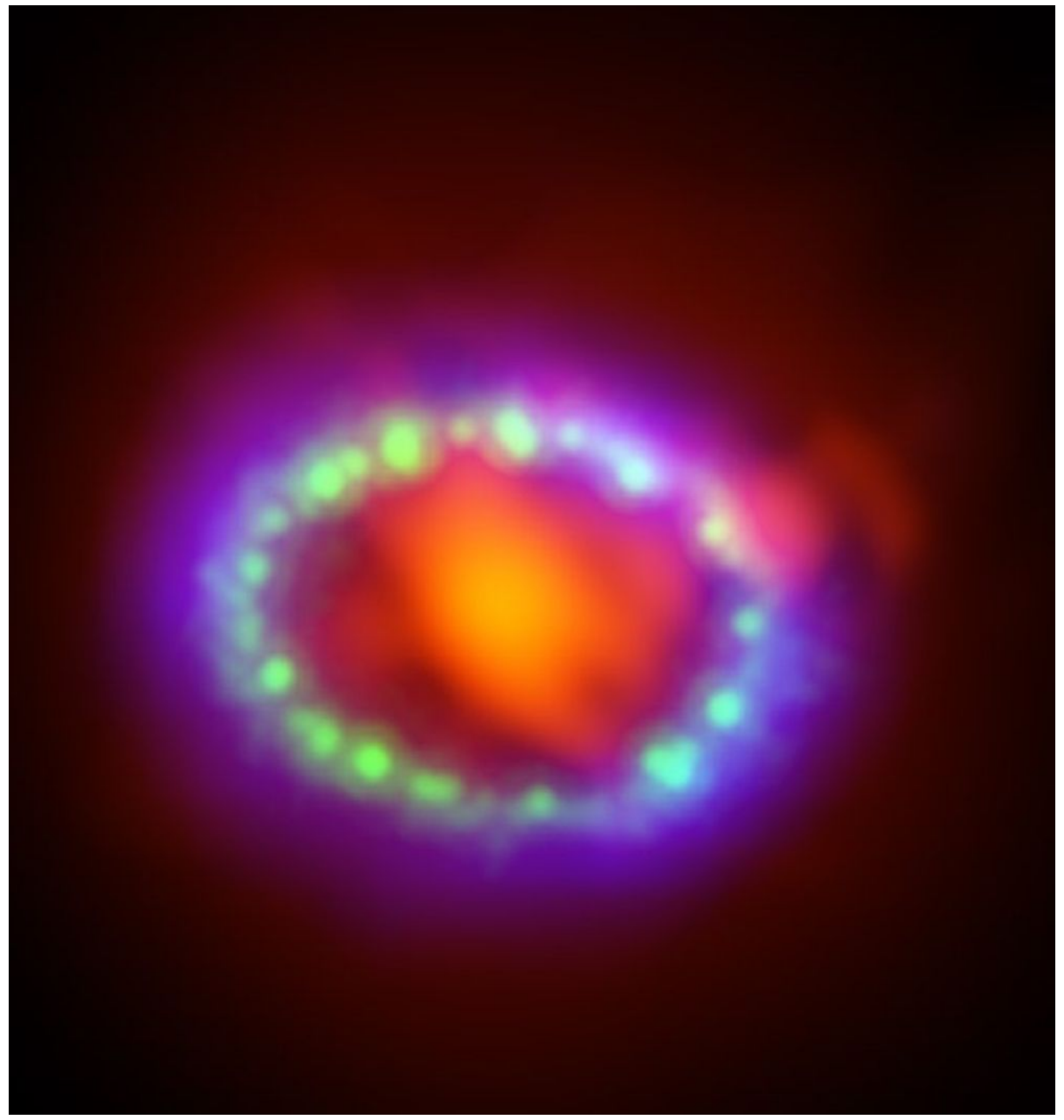
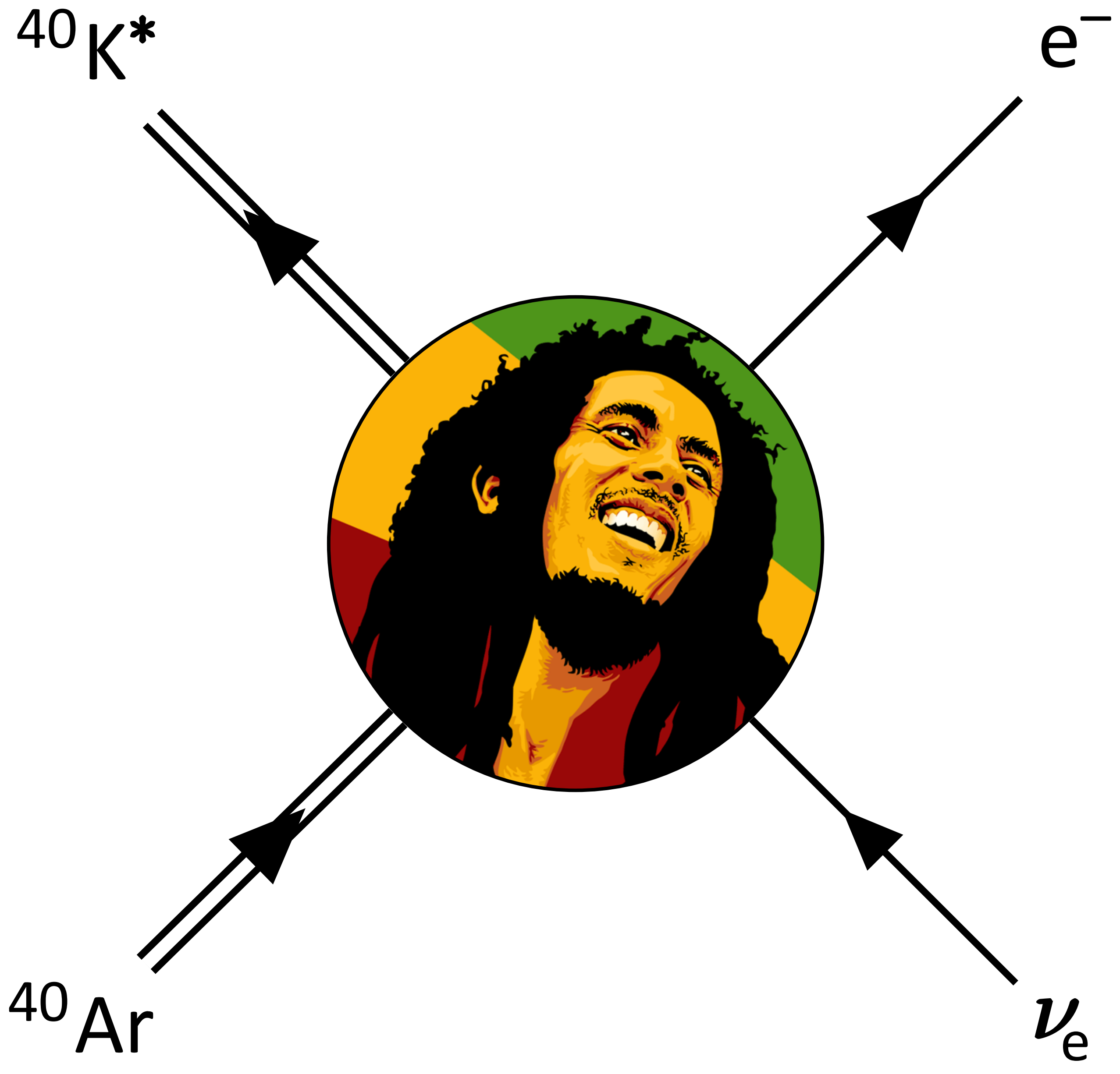
The MARLEY neutrino event generator





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

Astrophysical neutrinos and the origin of the elements (INT 23-2)

7 August 2023

Neutrino event generators

- **"Bridge" between theory and experiment:** model predictions are made easily usable
  - Full final-state predictions needed!

- Essential for a variety of tasks needed for experimental analyses:
  - Efficiency and background estimates
  - Neutrino energy reconstruction
  - Quantifying systematic uncertainties

- Cross section data informs further theory improvements

Neutrino event generator landscape

Four major packages at accelerator energies (~100 MeV to ~20 GeV)

Experiment-focused generators

Meet the needs of current oscillation experiments

[Eur. Phys. J. Spec. Top. 230, 4449 (2021)]

C++. Primary generator for Fermilab experiments. Largest group (still just a handful of active developers). Ambitions to be the universal platform.

NEUT (no official logo)

[Eur. Phys. J. Spec. Top. 230, 4469 (2021)]

C++/Fortran. Primary generator for J-PARC experiments (T2K, Super-K, Hyper-K). Not yet fully open source.

Theory-focused generators

Aid theoretical investigations of neutrino scattering

[J. Phys. G: Nucl. Part. Phys. 46 113001 (2019)]

Fortran. Supports neutrino projectiles as part of larger framework. Most sophisticated FSI model. Limited infrastructure (no geometry handling, unweighting, etc.)

NuWro

[Nucl. Phys. Proc. Suppl. 229-232, 499 (2012)]

C++. Many model options, often the first adopter of new theory developments from the literature.

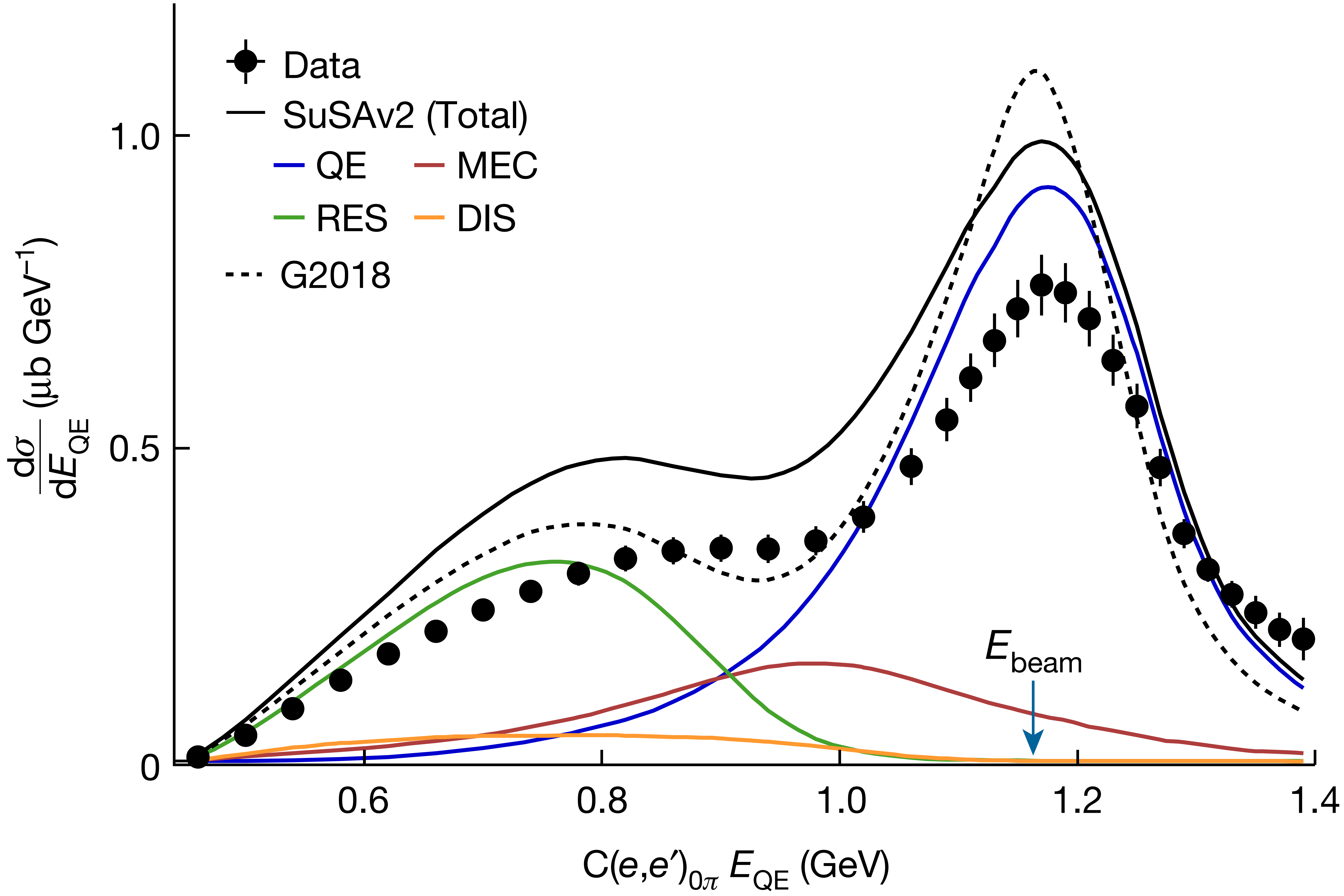
Checking neutrino energy reconstruction with electrons

- Apply neutrino energy estimation methods to electron-nucleus data
  - Monoenergetic beam
  - “Simple” 0π case

- Large fraction of events are misreconstructed

- Current generator-based models describe the bias poorly
  - Clear need (and path) for improvements!

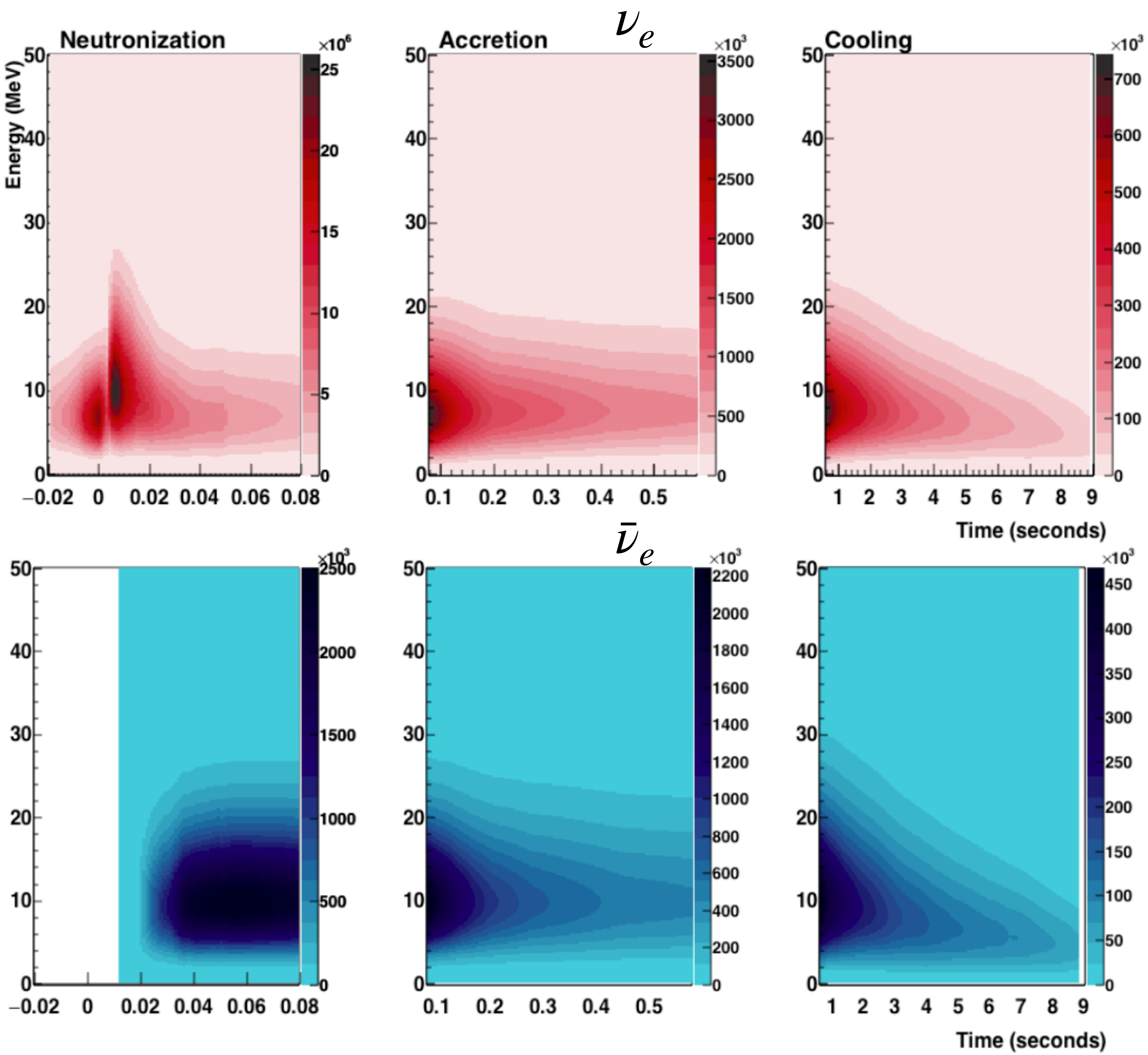
[Nature 599, 565 (2021)](https://doi.org/10.1038/s41586-021-04046-5)



Supernova neutrino time profile

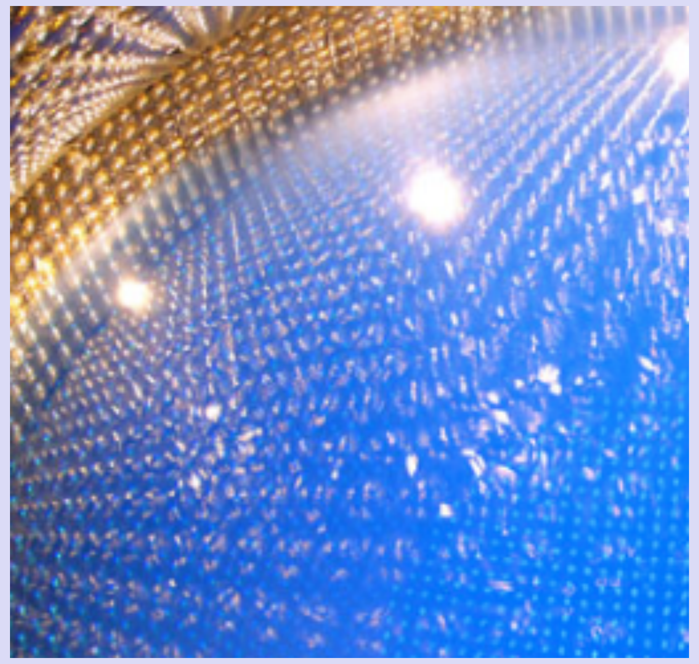
DUNE TDR (arXiv:2002.03005)

- Key observables are the **energy**, flavor, and arrival time of the neutrinos
  - 3 distinct species: $\nu_e, \bar{\nu}_e, \nu_x$
- Physics signatures imprinted on the time-dependent fluxes
- Each species provides distinct information
  - Detection of all highly desirable

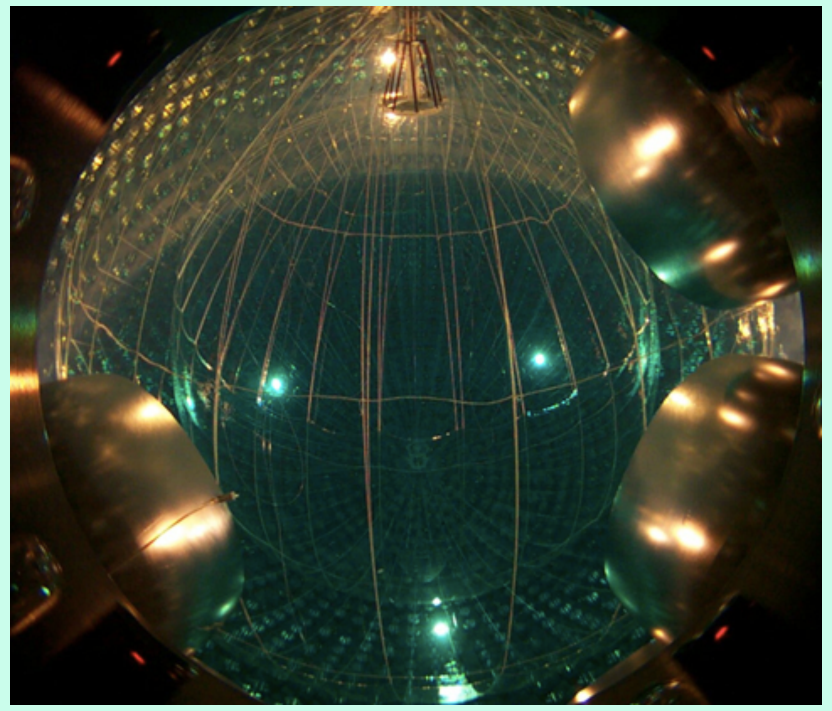


Current main supernova neutrino detector types

Water



Scintillator



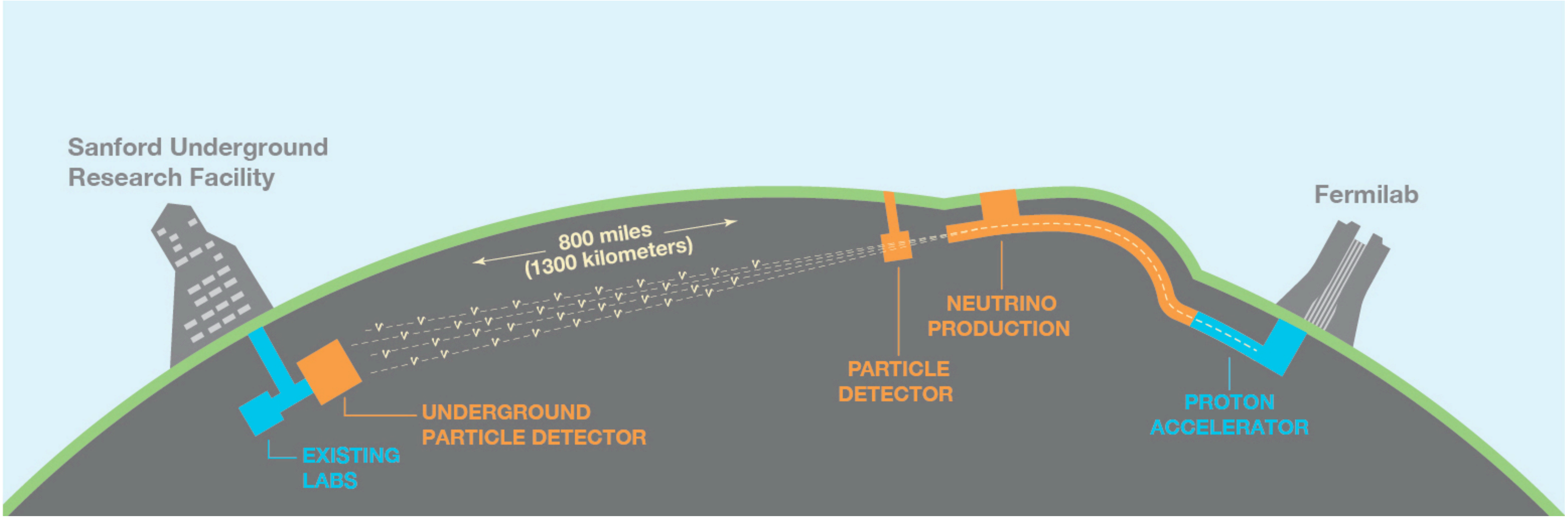
Argon

Lead

K. Scholberg

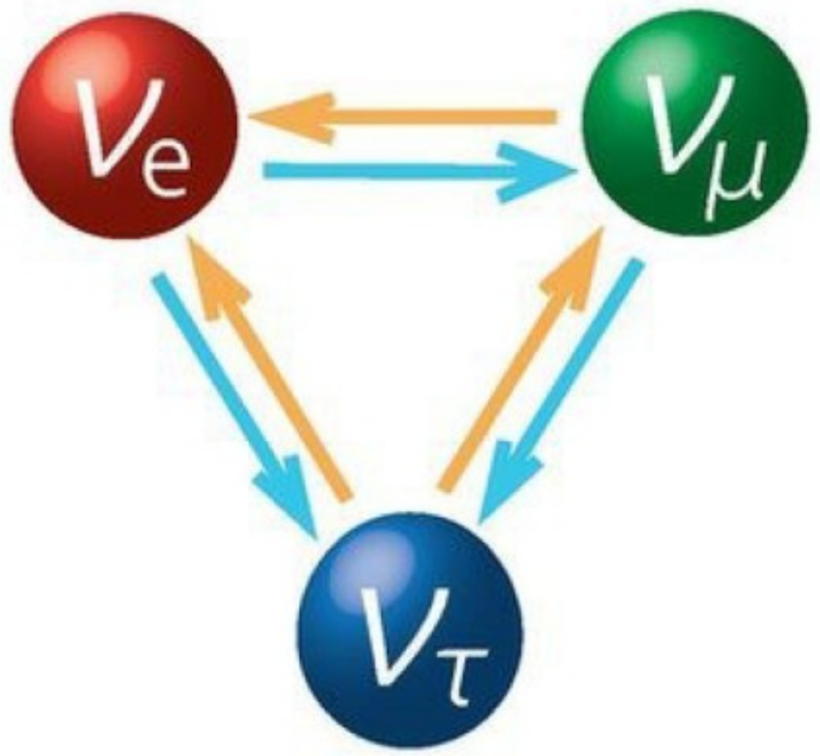
+ some others (e.g. DM detectors)

The Deep Underground Neutrino Experiment (DUNE)



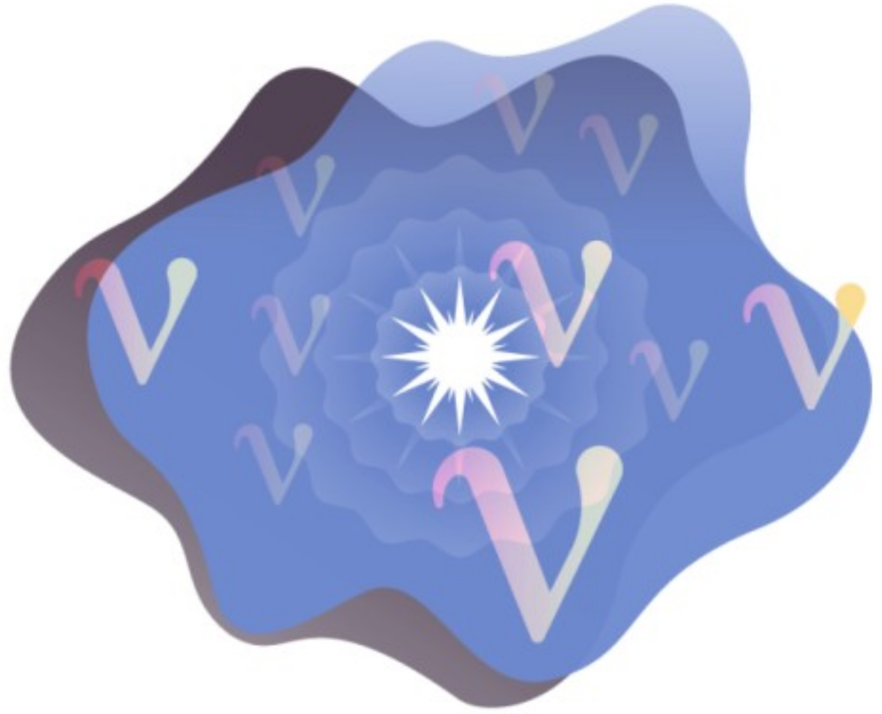
- World’s most powerful neutrino beam (1.2 MW+) and two groups of detectors
  - **Far detector**: 4 × 17 kton LArTPCs (40 kton total fiducial mass)
  - **Near detector**: Multi-component (including liquid and gaseous argon)
- Data taking to begin circa 2030

Primary science goals of DUNE



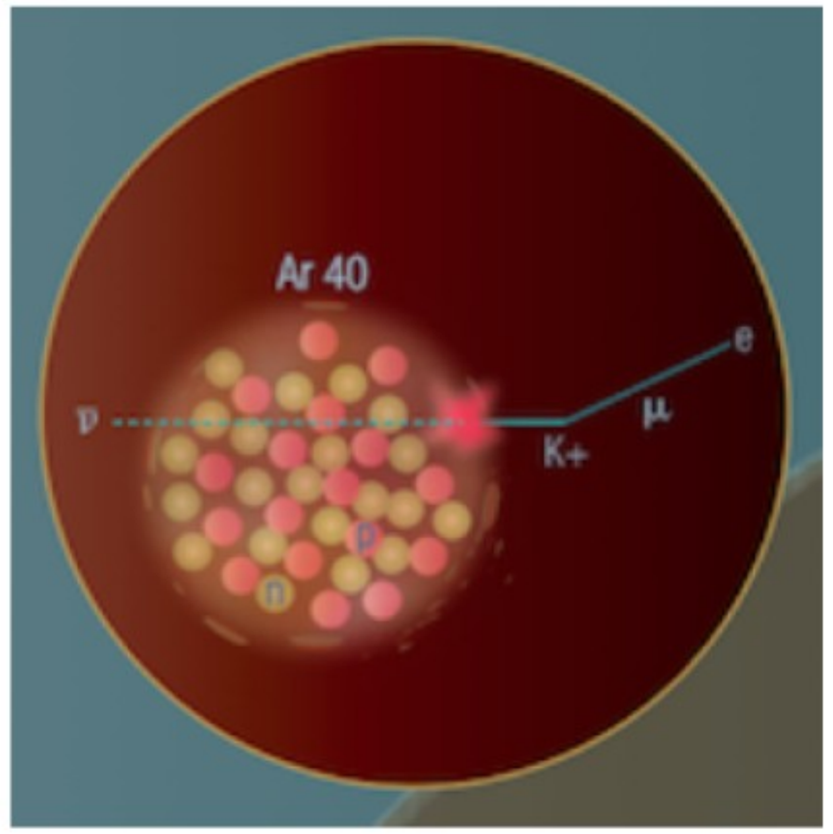
Accelerator neutrino oscillations

- 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

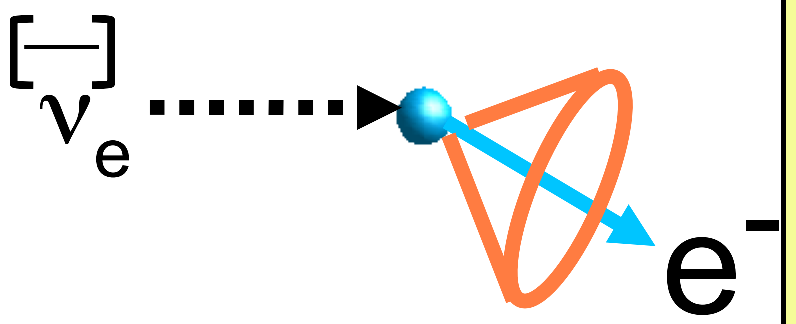
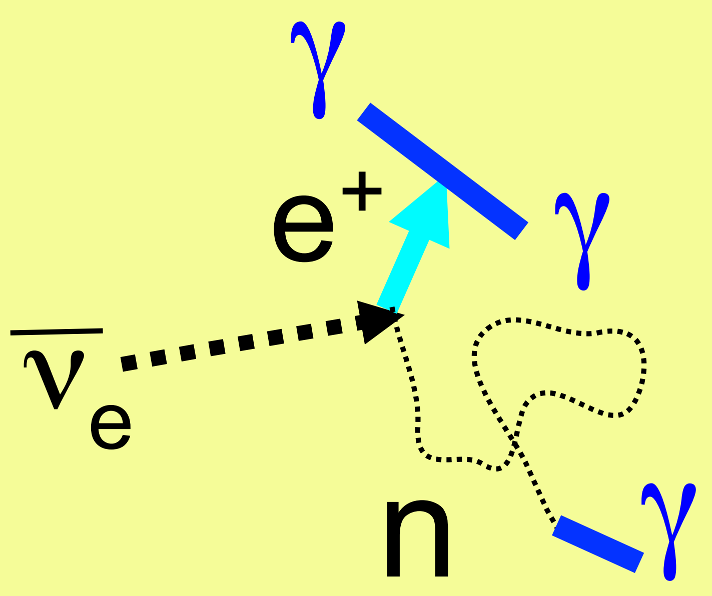
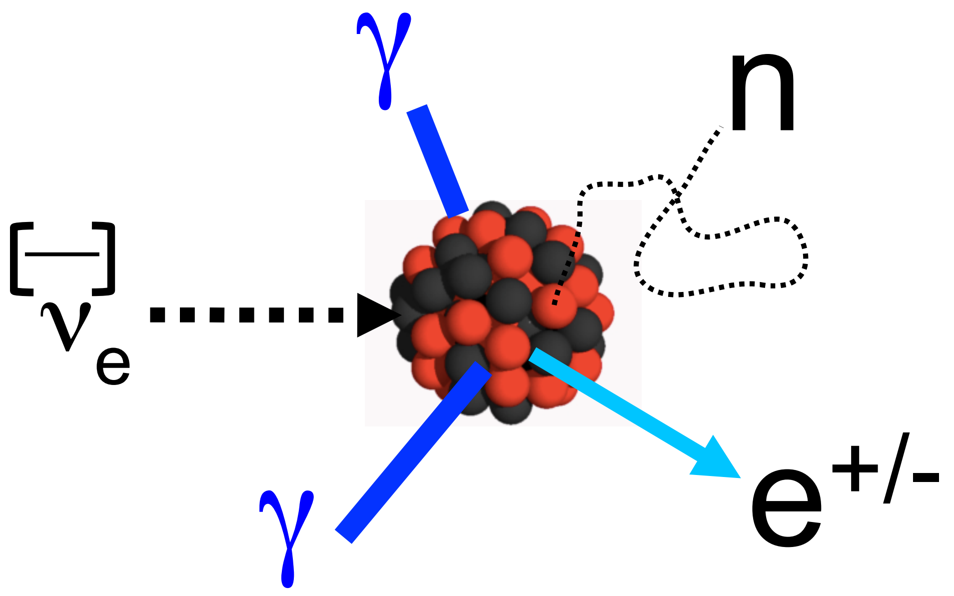
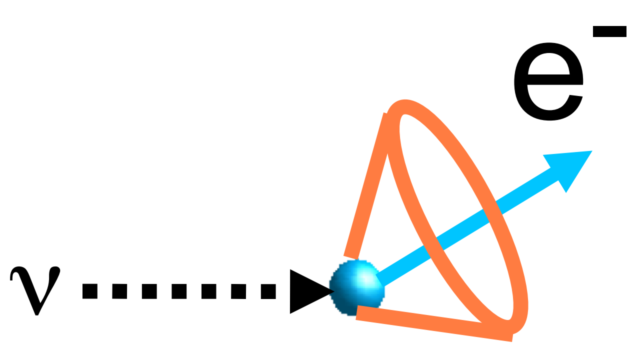
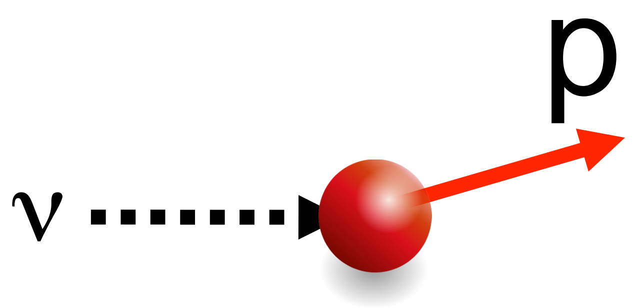
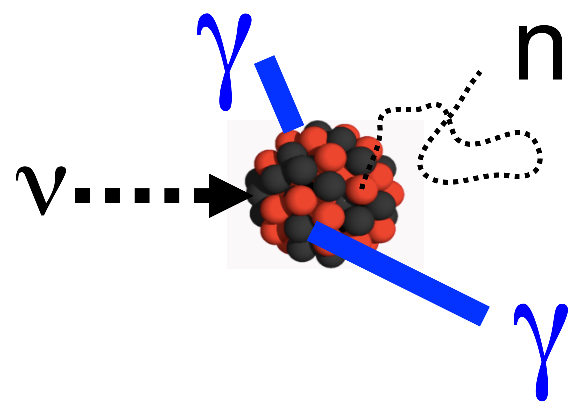
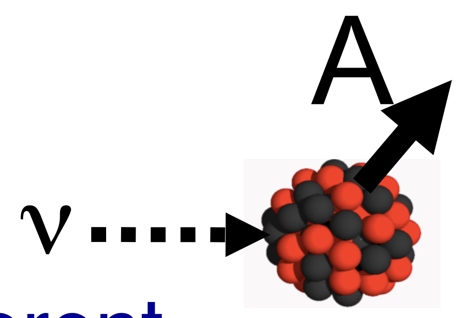


Explore physics beyond the Standard Model

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

Supernova-relevant neutrino interactions

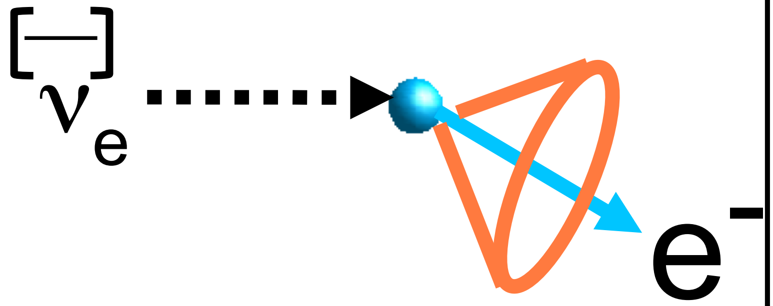
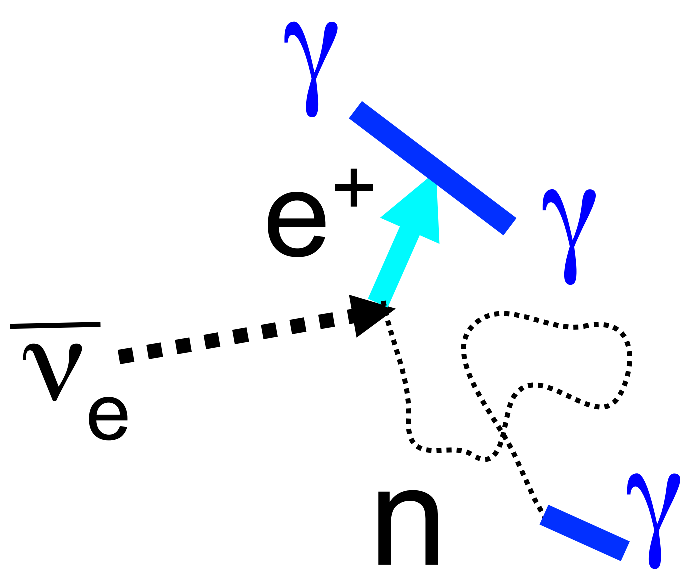
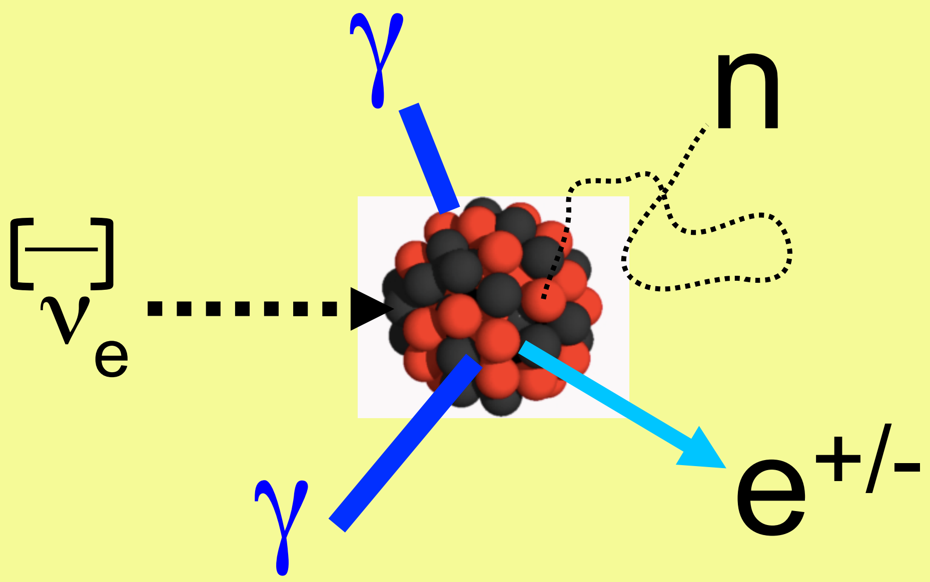
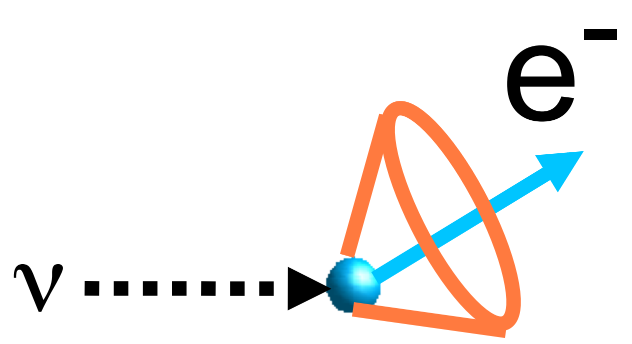
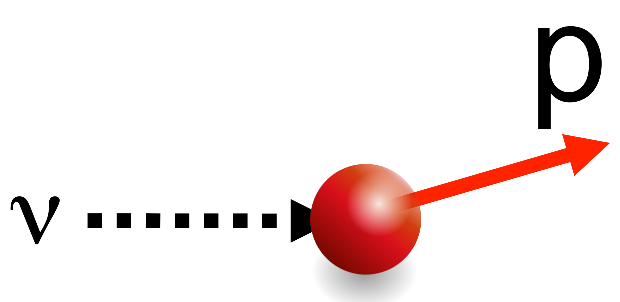
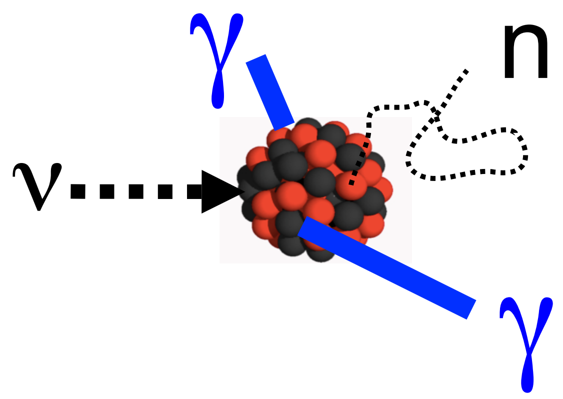
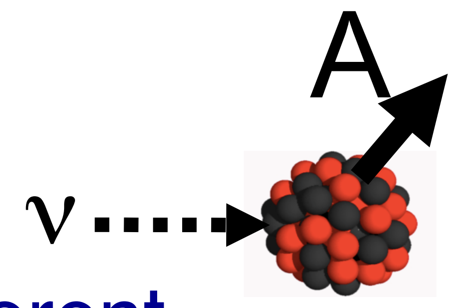
K. Scholberg

	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

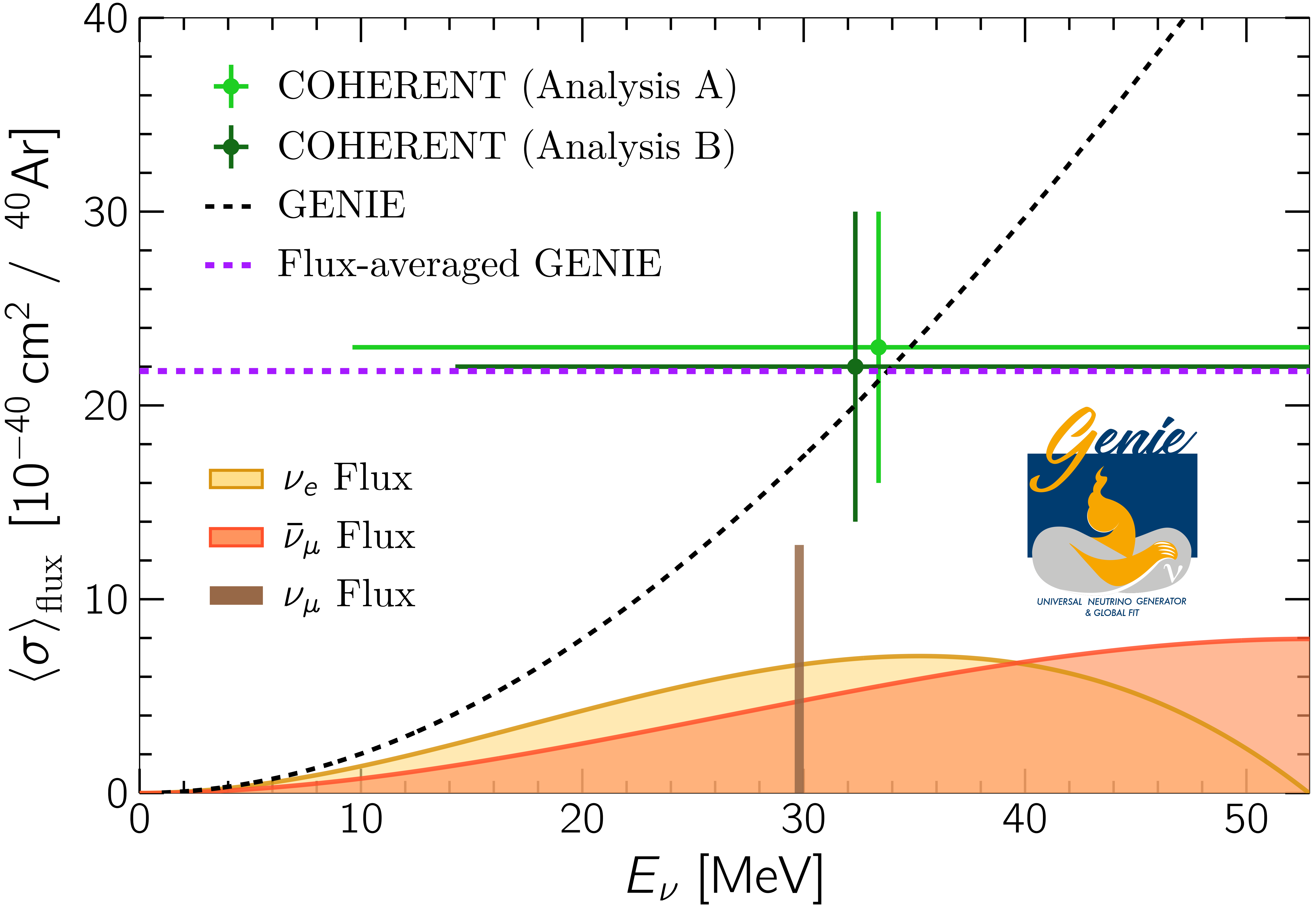
	Electrons	Protons	Nuclei
Charged current	Elastic scattering $\nu + e^- \to \nu + e^-$ 	Inverse beta decay $\bar{\nu}_e + p \to e^+ + n$ 	$\nu_e + (N,Z) \to e^- + (N-1, Z+1)$ $\bar{\nu}_e + (N,Z) \to e^+ + (N+1, Z-1)$  Various possible ejecta and deexcitation products
Neutral current	 Useful for pointing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

Why a dedicated low-energy generator?

- ν-e, ν-p, and CEvNS are “easy” (the last up to the nuclear form factor)
    - GENIE v3 provides a model for all of these
- Inelastic reactions on complex nuclei are hard
    - Physics approximations in GENIE regime (~GeV) break down

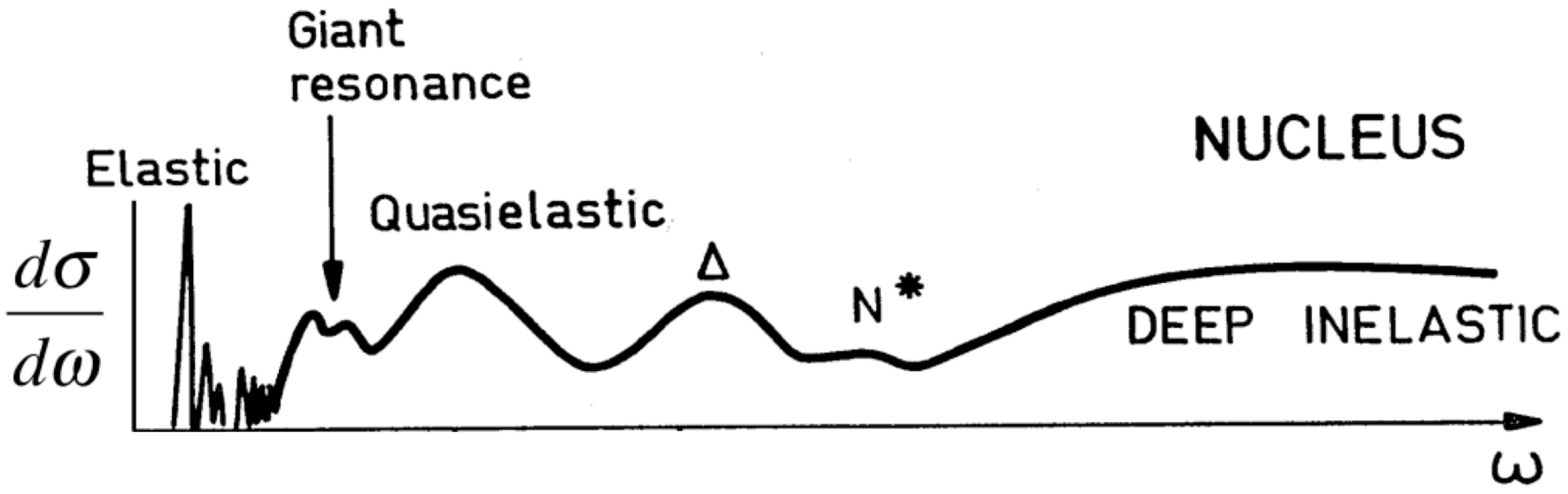
Eur. Phys. J. Spec. Top. 230, 4449 (2021)

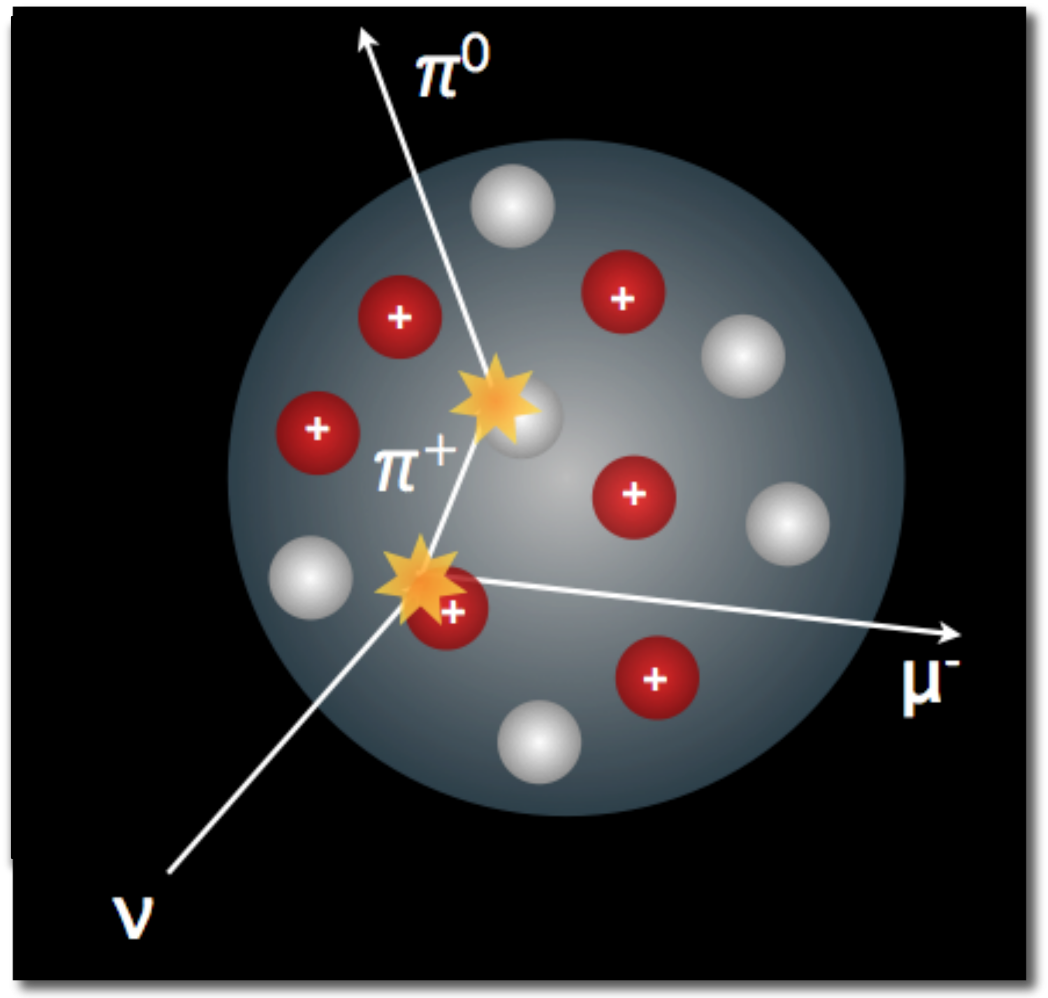


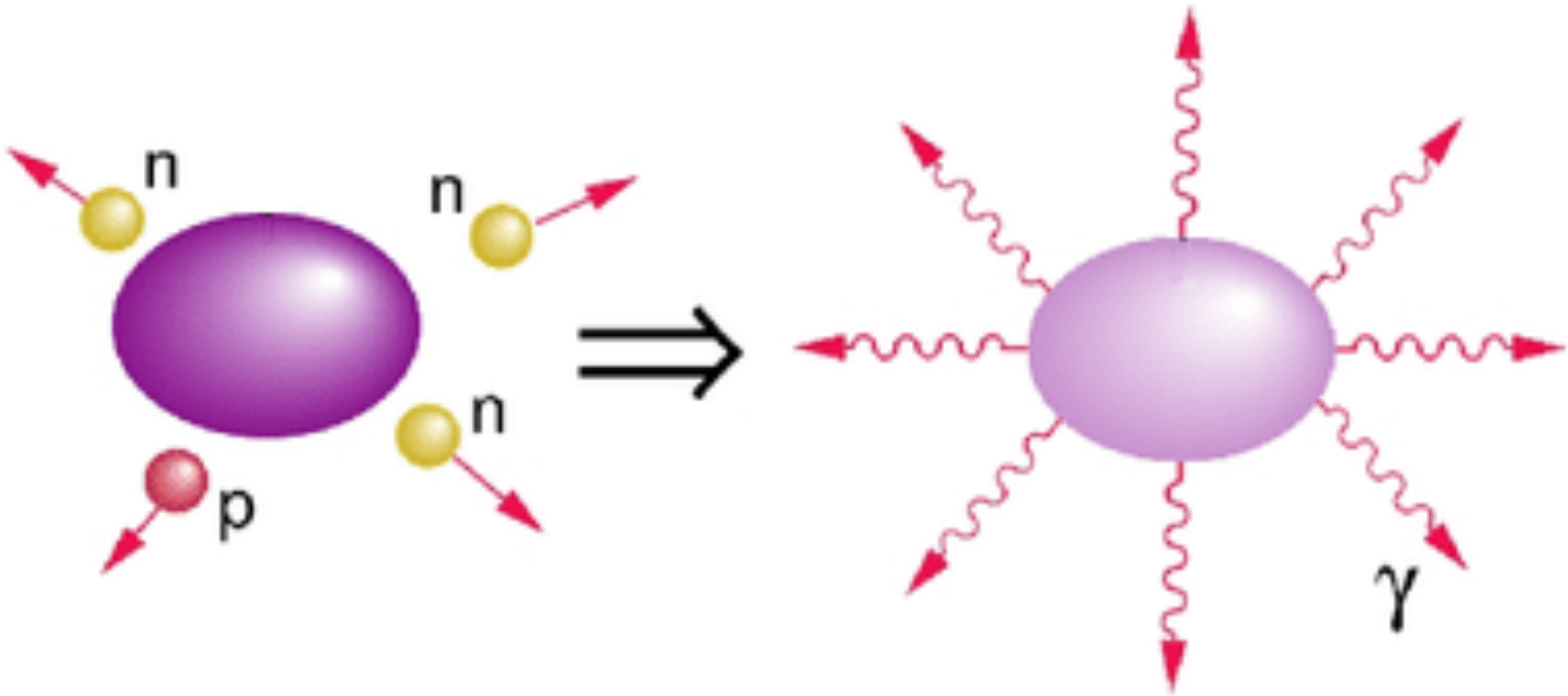
COHERENT data from Phys. Rev. Lett. 126, 012002 (2021)

Why a dedicated low-energy generator?

- Variants of a **Fermi gas** are the "traditional" nuclear model
  - Neglects discrete level structure, giant resonance excitations
  - Few-MeV transitions can't be neglected at 15 MeV like they can at 1 GeV
- **Direct knockout** picture used at high energies
- **Compound nucleus** picture used at low energies

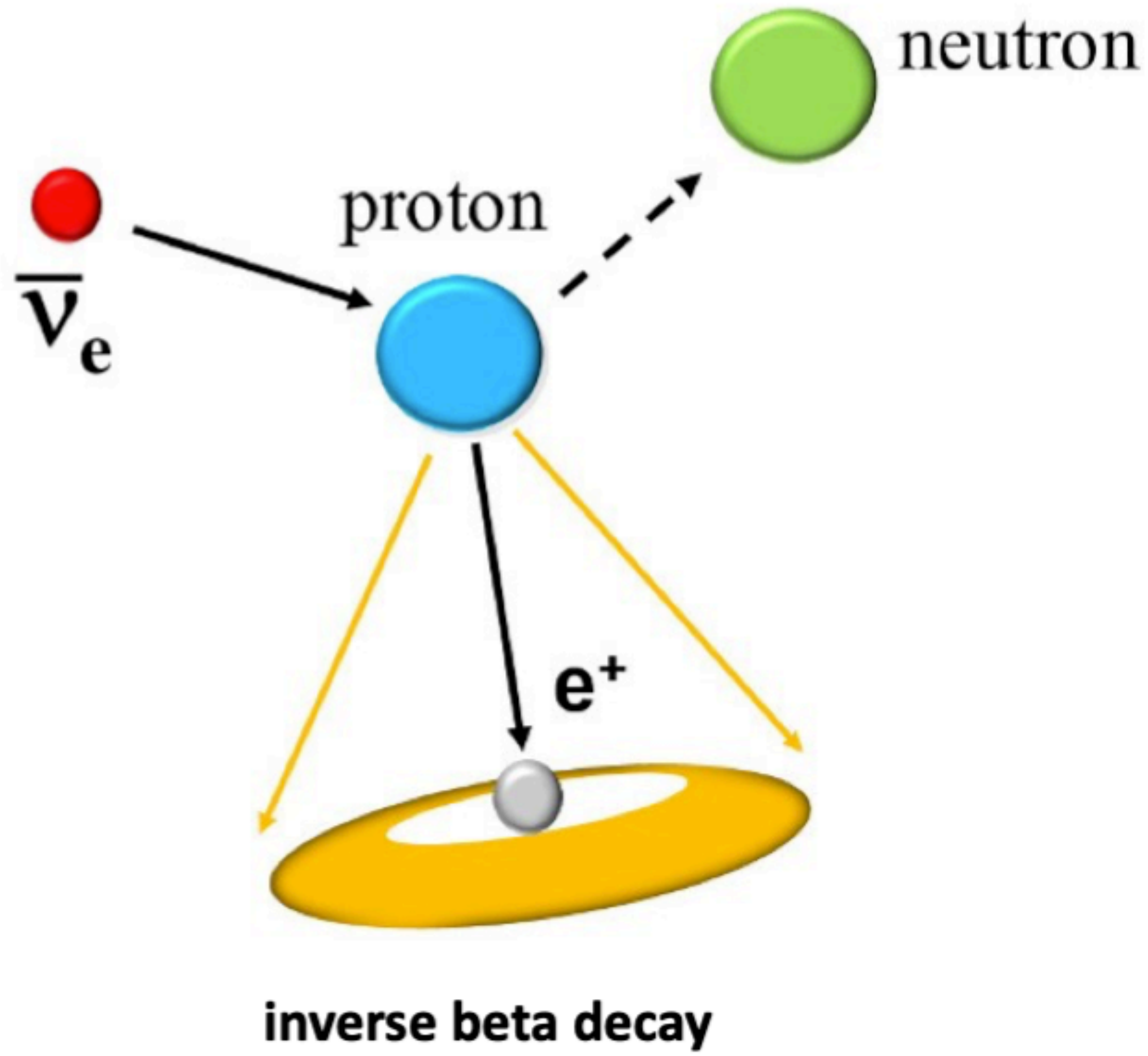






Modeling this physics is essential for neutrino calorimetry

IBD: e⁺ sufficient to infer E_ν



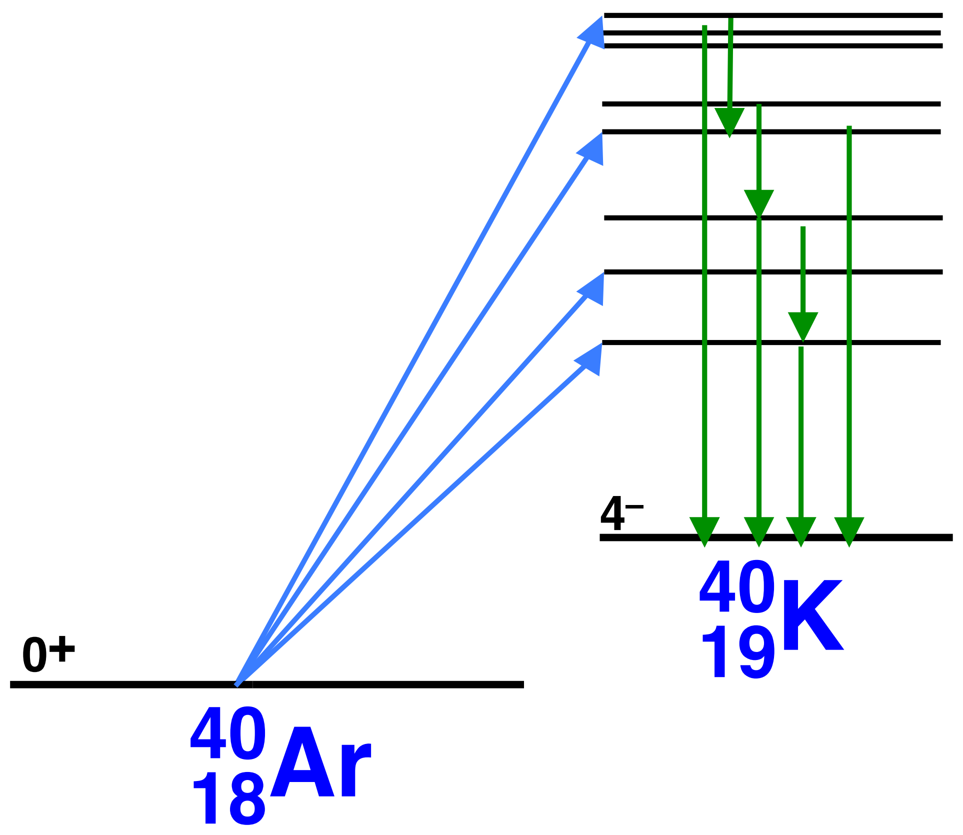
Outgoing e^+ energy

Neutron proton mass difference

Recoil energy of neutron (negligible)

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

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



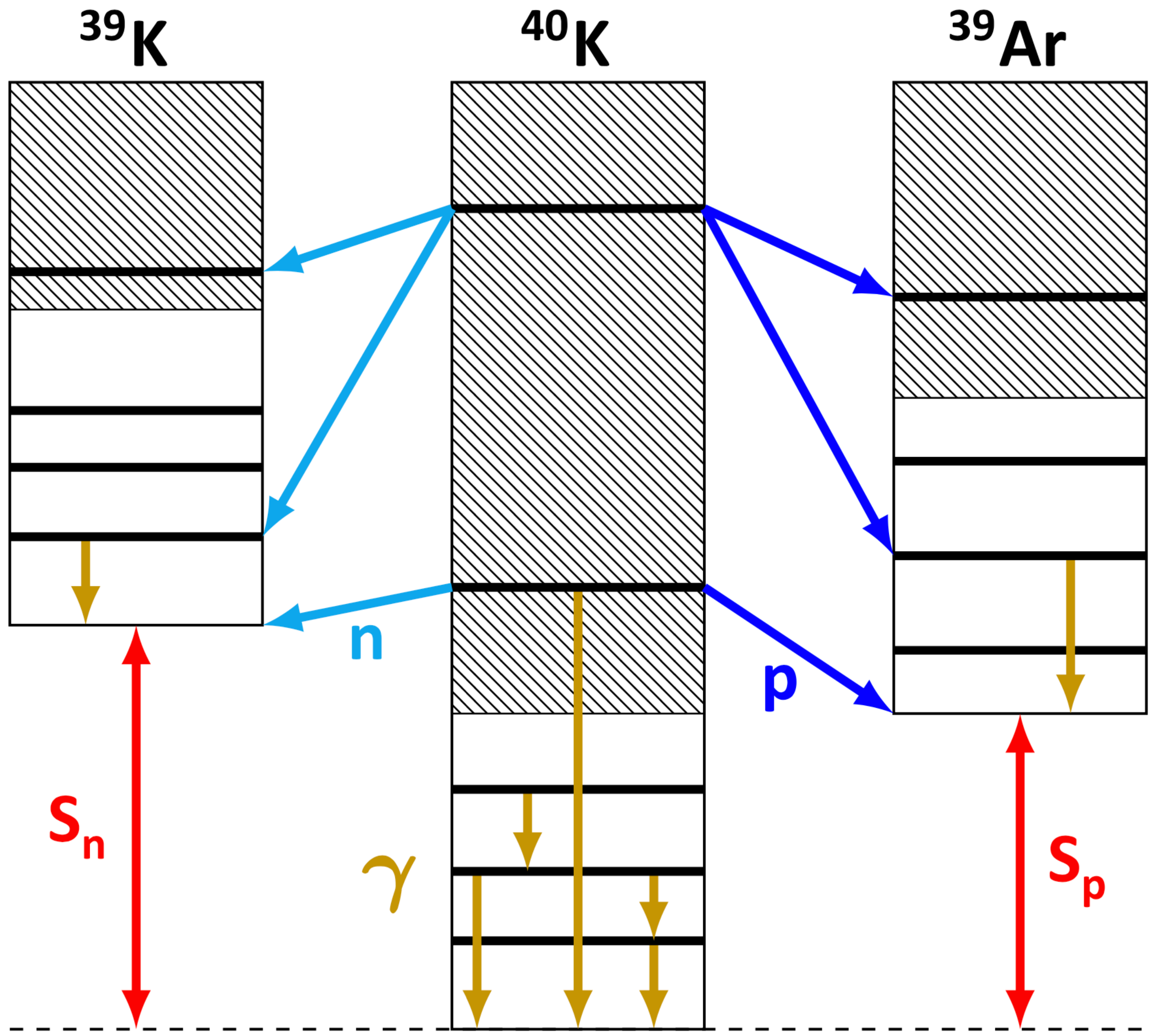
ν-A is much more complex

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

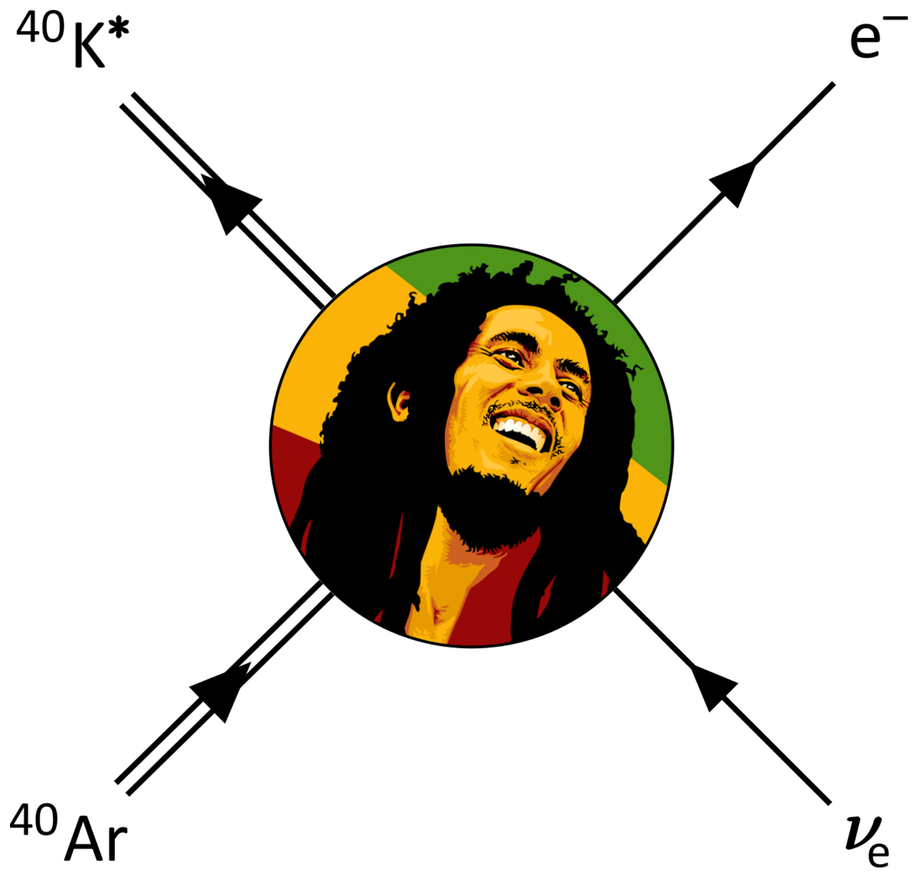
Neutrino event generator landscape

Remain crucial at tens-of-MeV, but the community is significantly smaller

sntools J. Open Source Softw. 6, 2877 (2021)

Python. Coverage of all interaction channels of interest for water and liquid scintillator SN neutrino detectors. Excellent integration with flux models, etc.

MARLEY Comput. Phys. Commun. 269, 108123 (2021)



C++. Primarily simulates inelastic ν-nucleus scattering at O(10 MeV). Emphasis on de-excitation physics modeling.

SKSNSim https://github.com/SKSNSim/SKSNSim

C++. Super-K focused generator which implements IBD, ν-e, and inelastic CC+NC interactions on oxygen

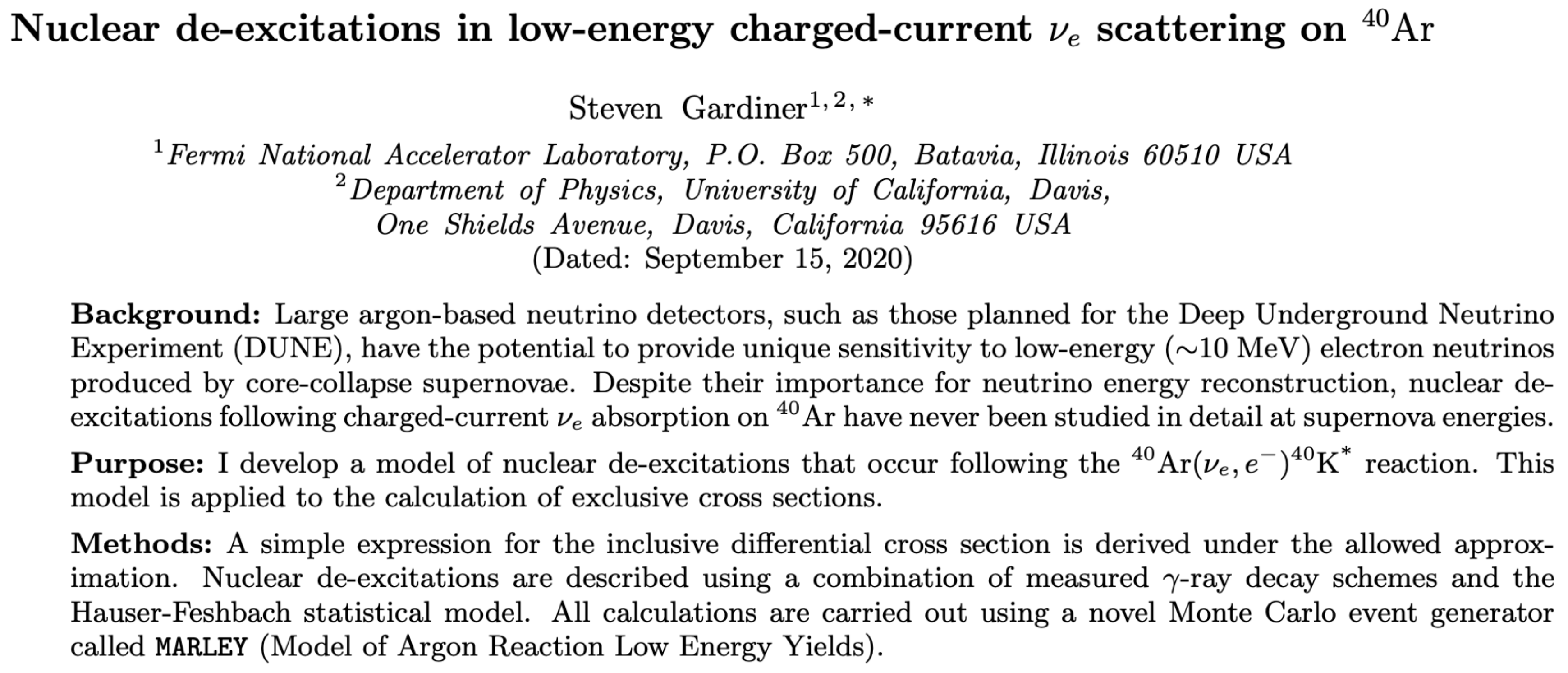
newton https://github.com/itscubist/newton

C++/Fortran. Implements IBD, ν-e, and CC on oxygen. Interfaces with TALYS de-excitation code. Appears to no longer be maintained.

And an unnamed proprietary generator from JUNO …

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

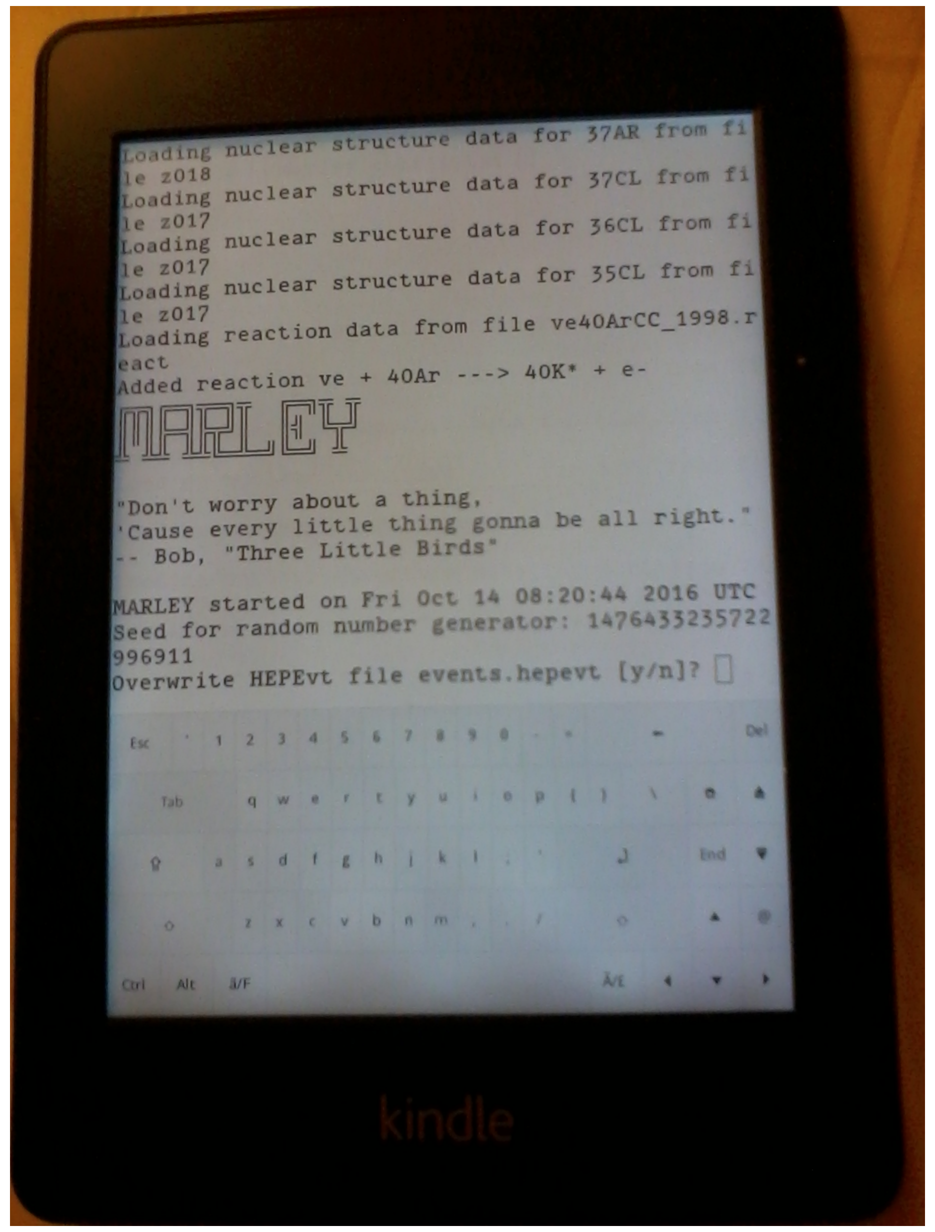
Steven Gardiner[1,2,*]

[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 $^{40}\text{Ar}(\nu_e, e^-)^{40}\text{K}^*$ reaction. This model is applied to the calculation of exclusive cross sections.

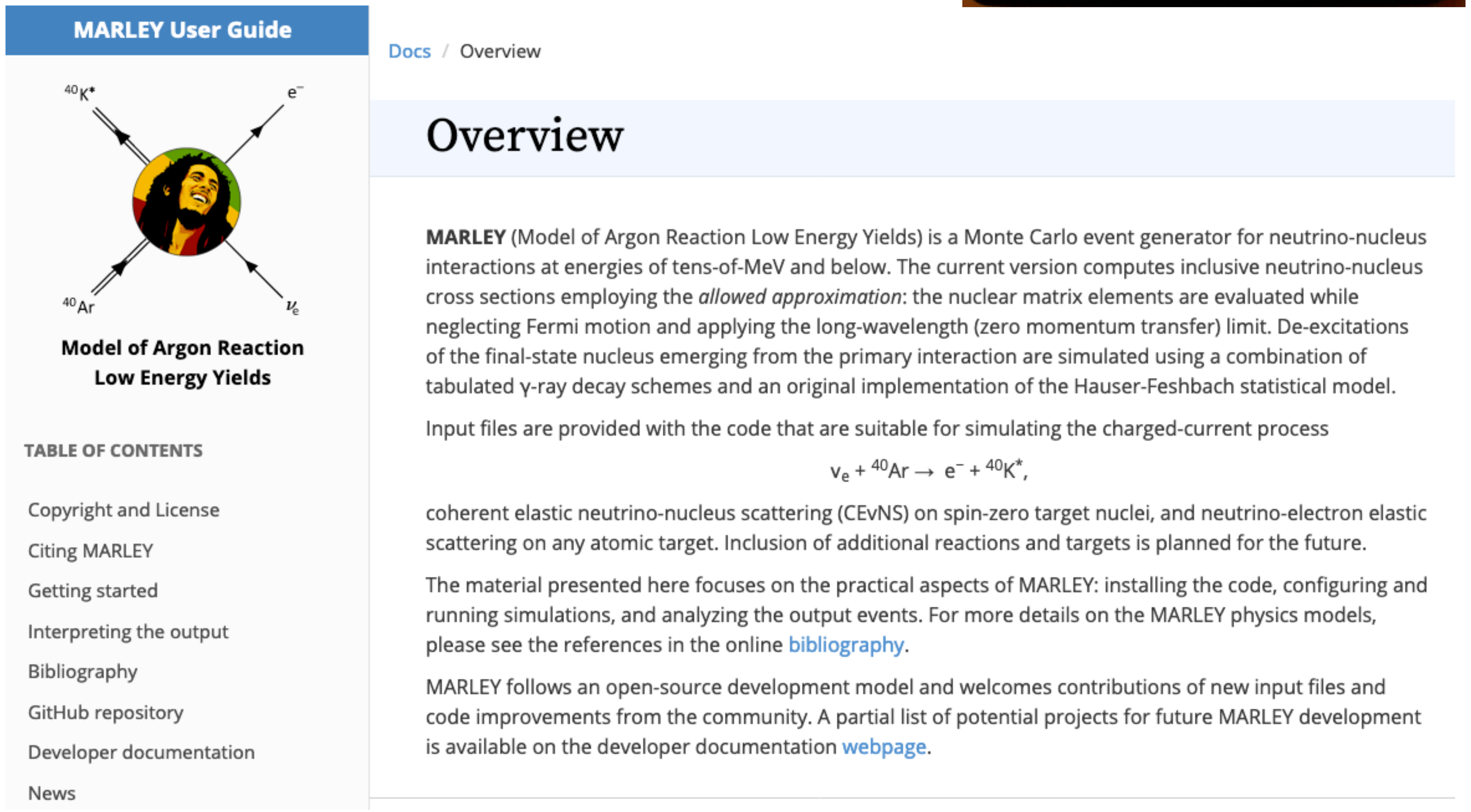
Methods: A simple expression for the inclusive differential cross section is derived under the allowed approximation. Nuclear de-excitations are described using a combination of measured γ-ray decay schemes and the Hauser-Feshbach statistical model. All calculations are carried out using a novel Monte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



```
Loading nuclear structure data for 37AR from fi
le z018
Loading nuclear structure data for 37CL from fi
le z017
Loading nuclear structure data for 36CL from fi
le z017
Loading nuclear structure data for 35CL from fi
le z017
Loading reaction data from file ve40ArCC_1998.r
eact
Added reaction ve + 40Ar ---> 40K* + e-
MARLEY

"Don't worry about a thing,
'Cause every little thing gonna be all right."
-- Bob, "Three Little Birds"

MARLEY started on Fri Oct 14 08:20:44 2016 UTC
Seed for random number generator: 1476433235722
996911
Overwrite HEPEvt file events.hepevt [y/n]? 
```



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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

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

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:

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

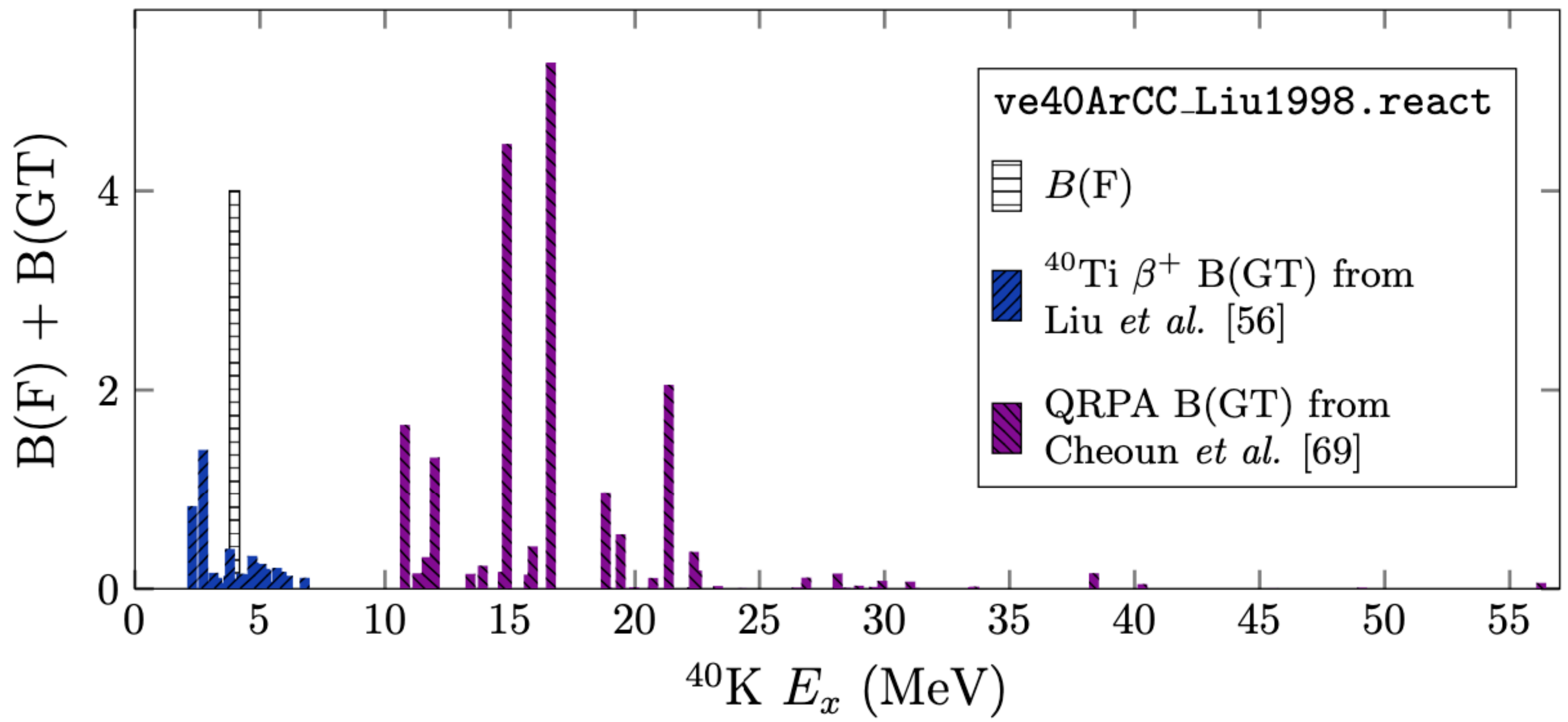
Allowed nuclear matrix elements

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

Long-wavelength limit: $q \to 0$

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

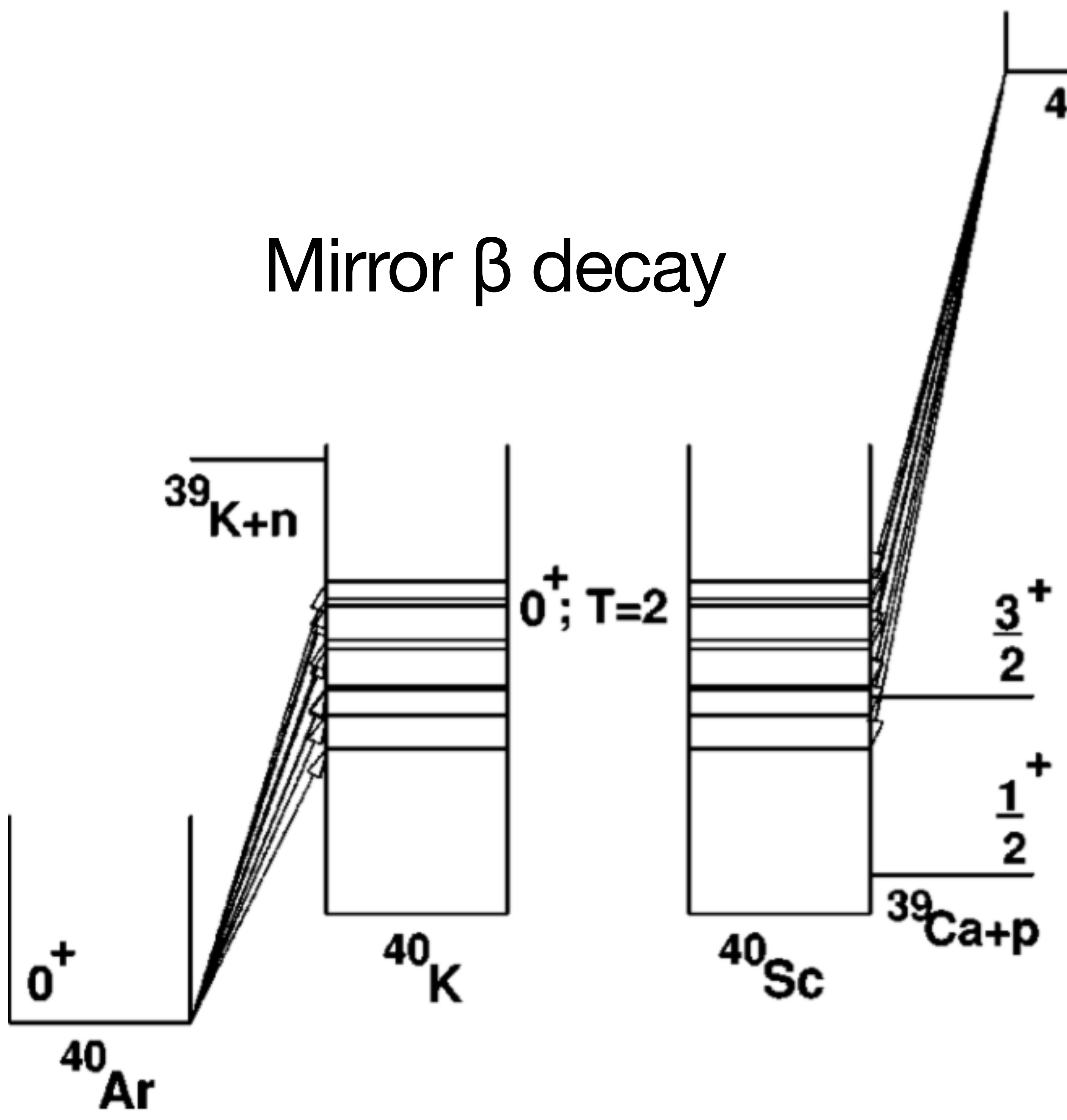
Nuclear matrix elements must be supplied as input. For ^{40}Ar, they are based on a combination of **indirect measurements** (e.g., mirror β decay) and a **QRPA calculation**



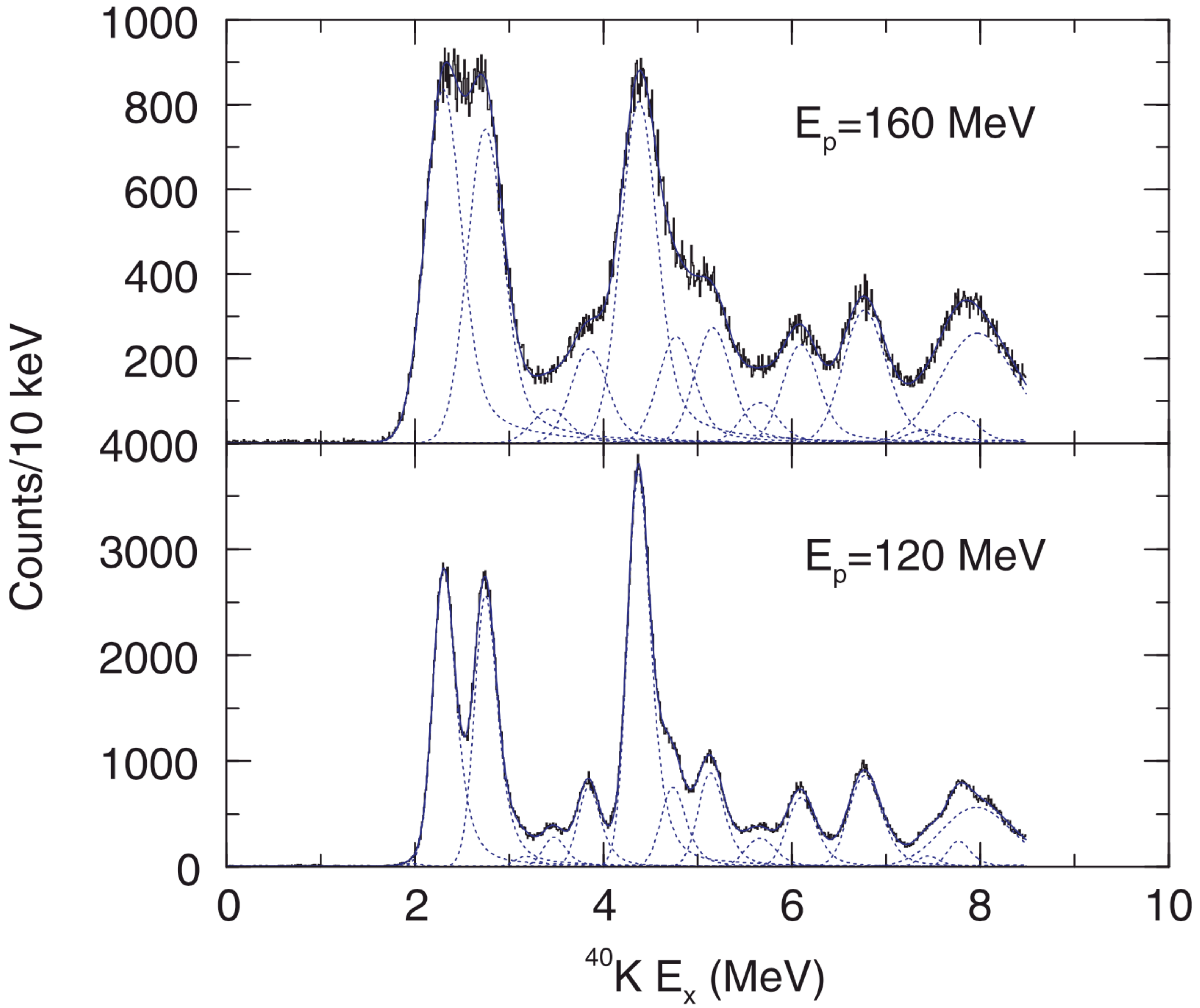
Calculating the cross section is straightforward if we can figure out the nuclear matrix elements B(F) and B(GT)

There are two relevant kinds of experiments in the literature. Both are indirect measurements.

Mirror β decay



(p,n) scattering



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"

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

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

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

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

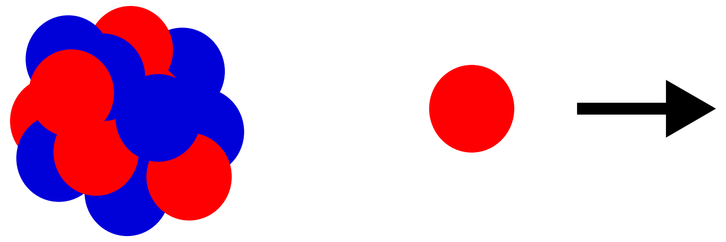
Hauser-Feshbach Model

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



$A \rightarrow \alpha + B$

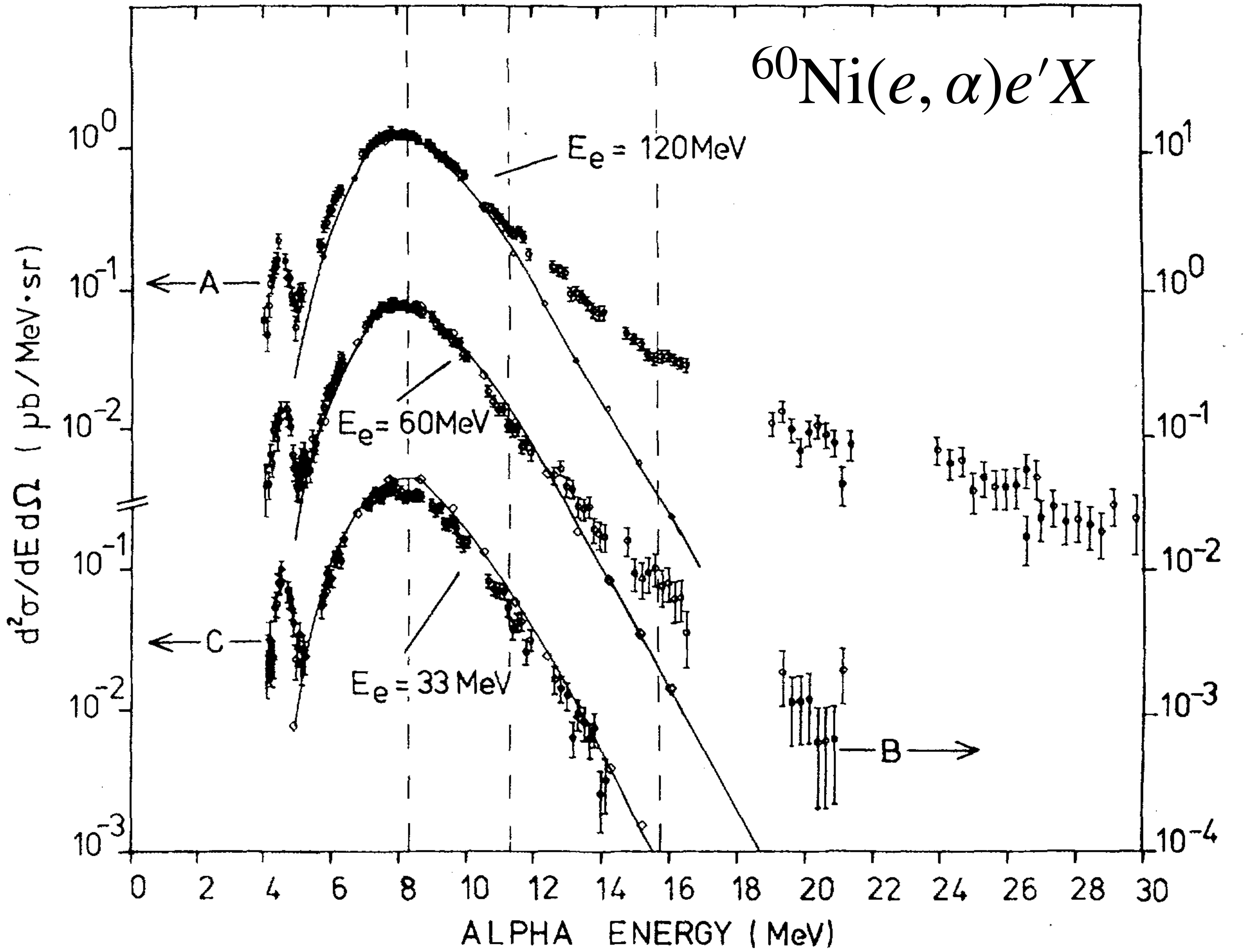
is related to its formation cross section

$\alpha + B \rightarrow A$

Is the compound nucleus assumption adequate at tens of MeV?

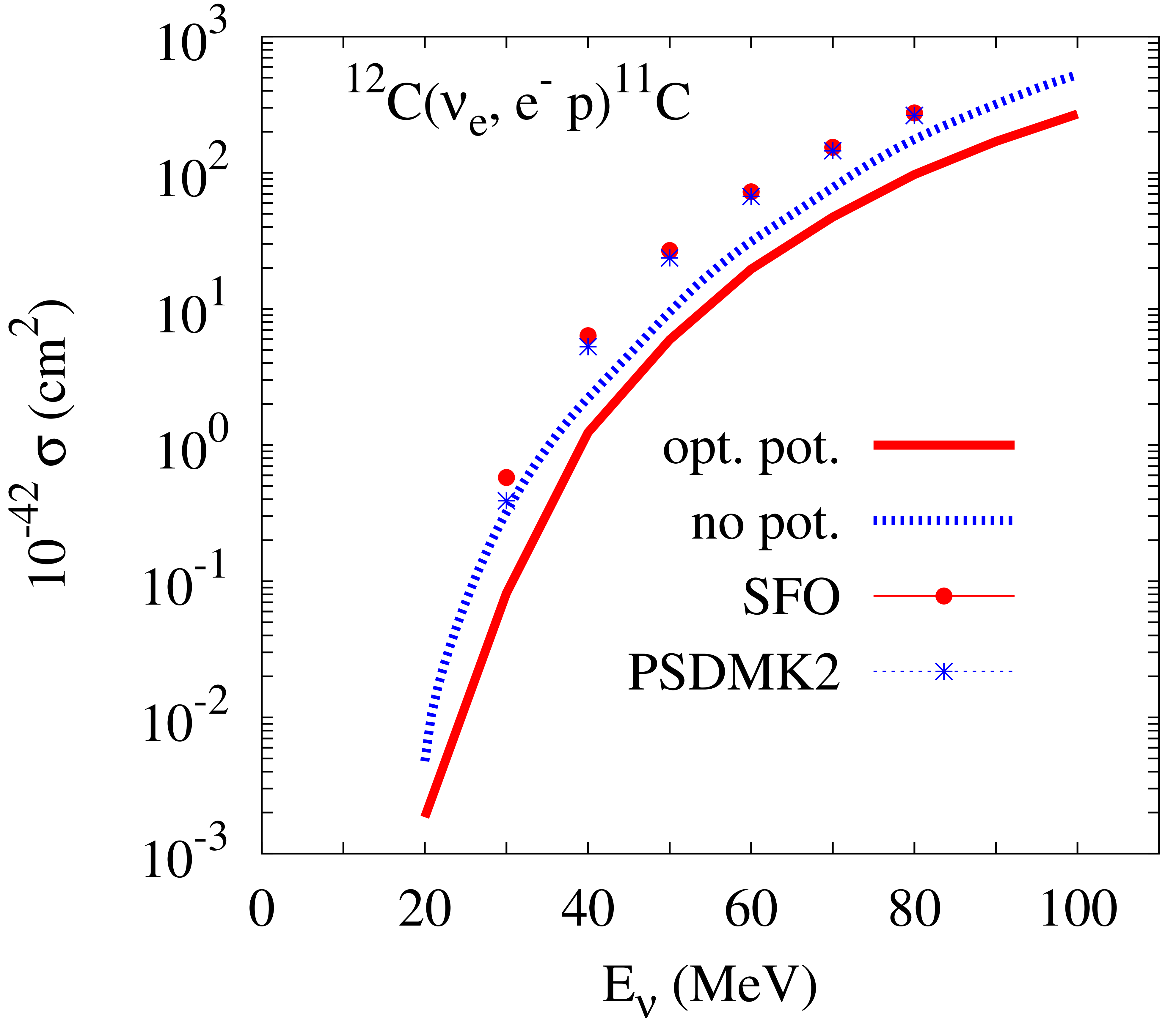
Available evidence is quite limited. Limited studies of any kind and no relevant neutrino data.

Flowers et al., **Phys. Rev. Lett. 40, 709 (1978)**



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

Kim & Cheoun, **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).

MARLEY nuclear de-excitation model

Phys. Rev. C 103, 044604 (2021)

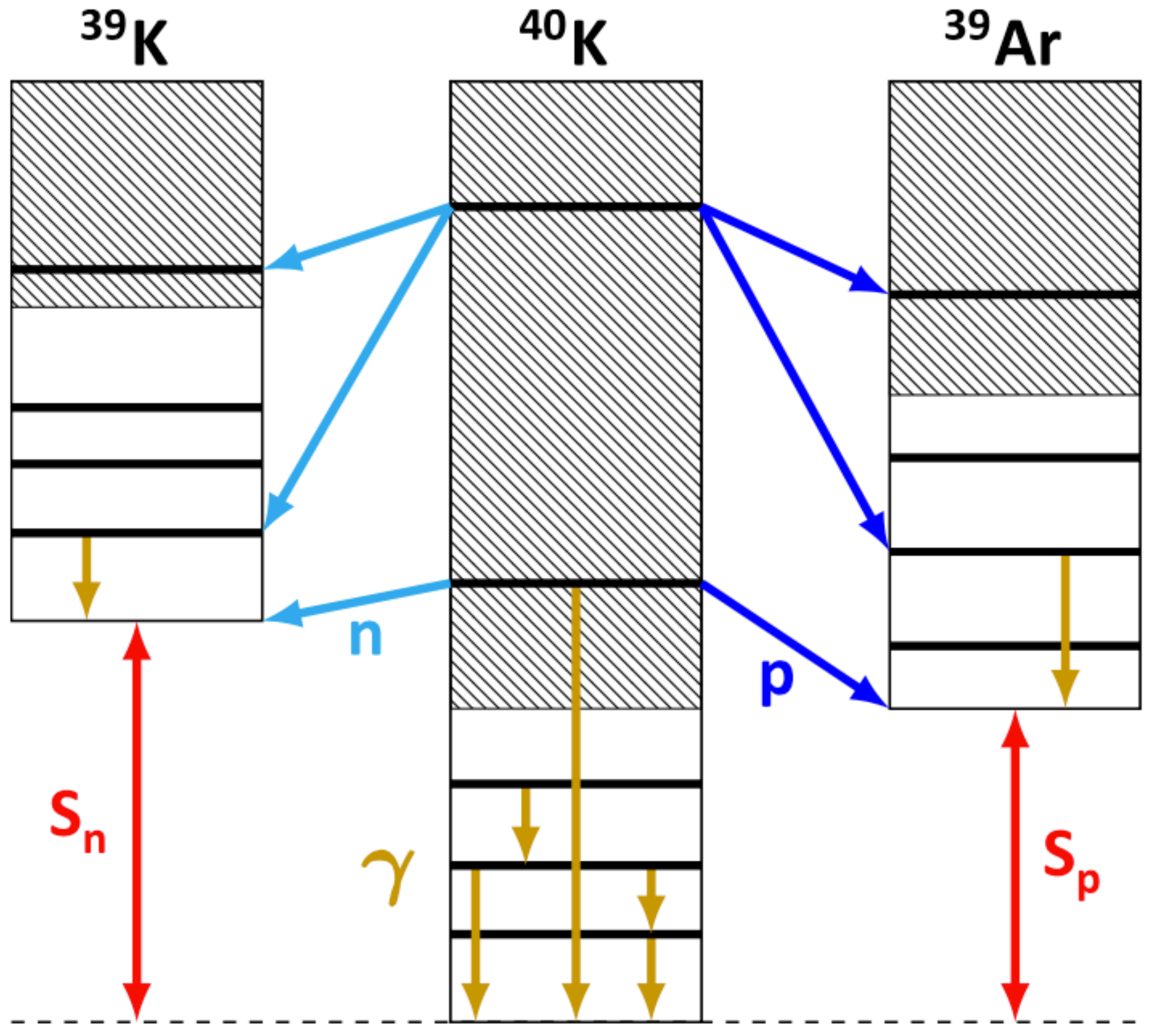
In the second step, the nucleus de-excites via a series of binary decays. Decay widths for **unbound states** are computed according to the Hauser-Feshbach formalism:

Differential decay width for emission of a nuclear fragment α ($A \leq 4$ 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

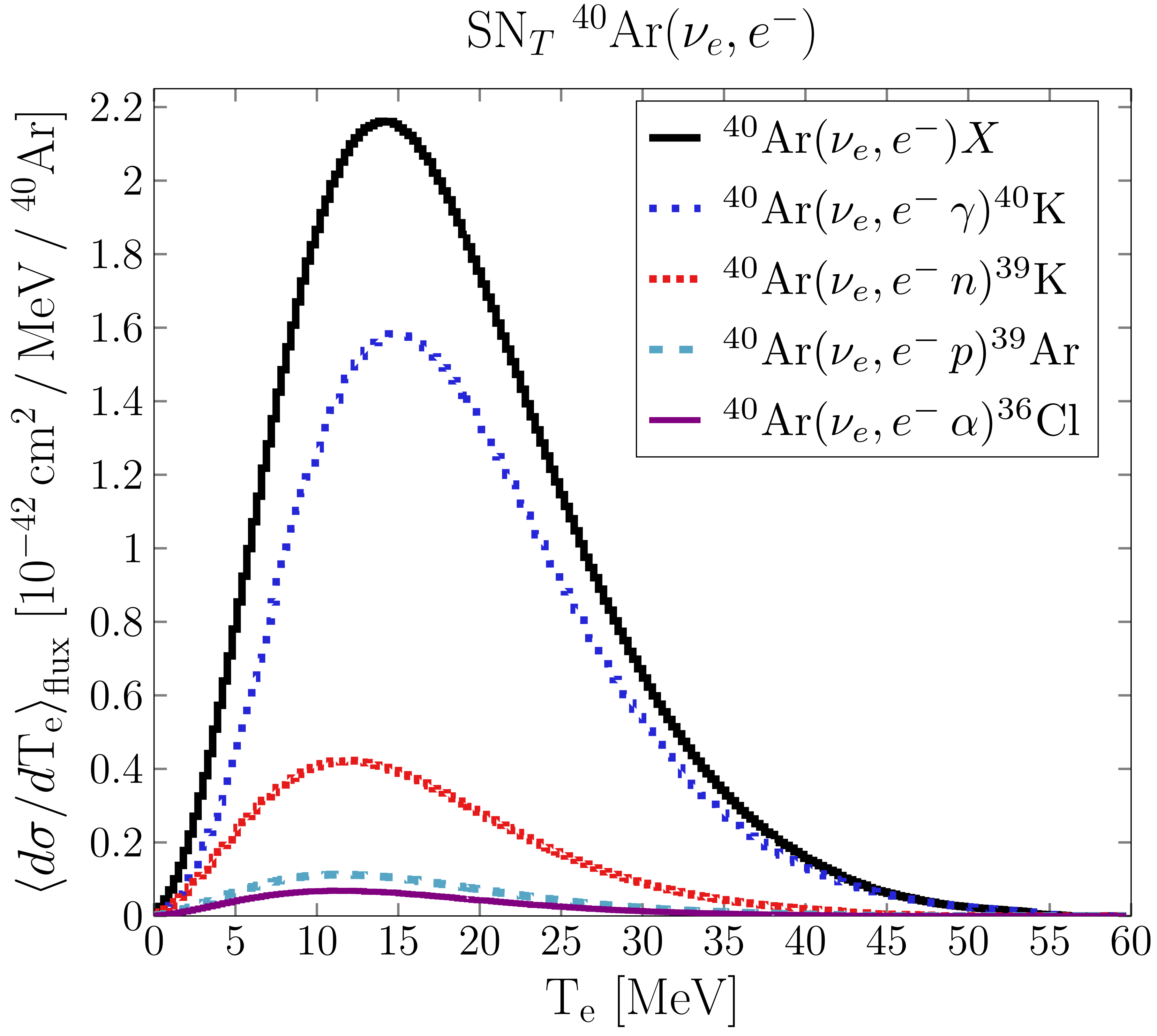
Phys. Rev. C 103, 044604 (2021)

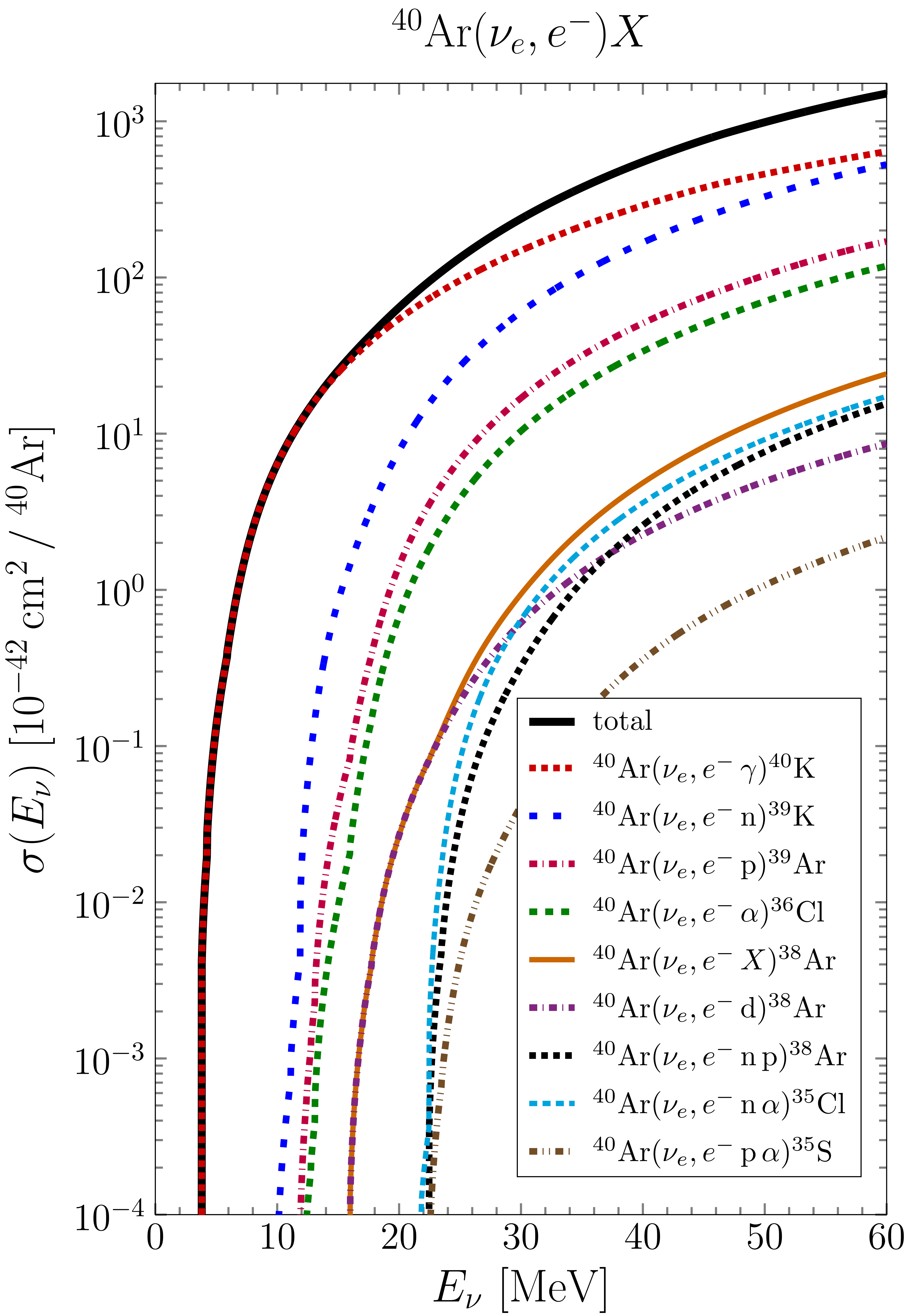
- First calculation of cross sections for **exclusive final states** of the reaction

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

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)**.



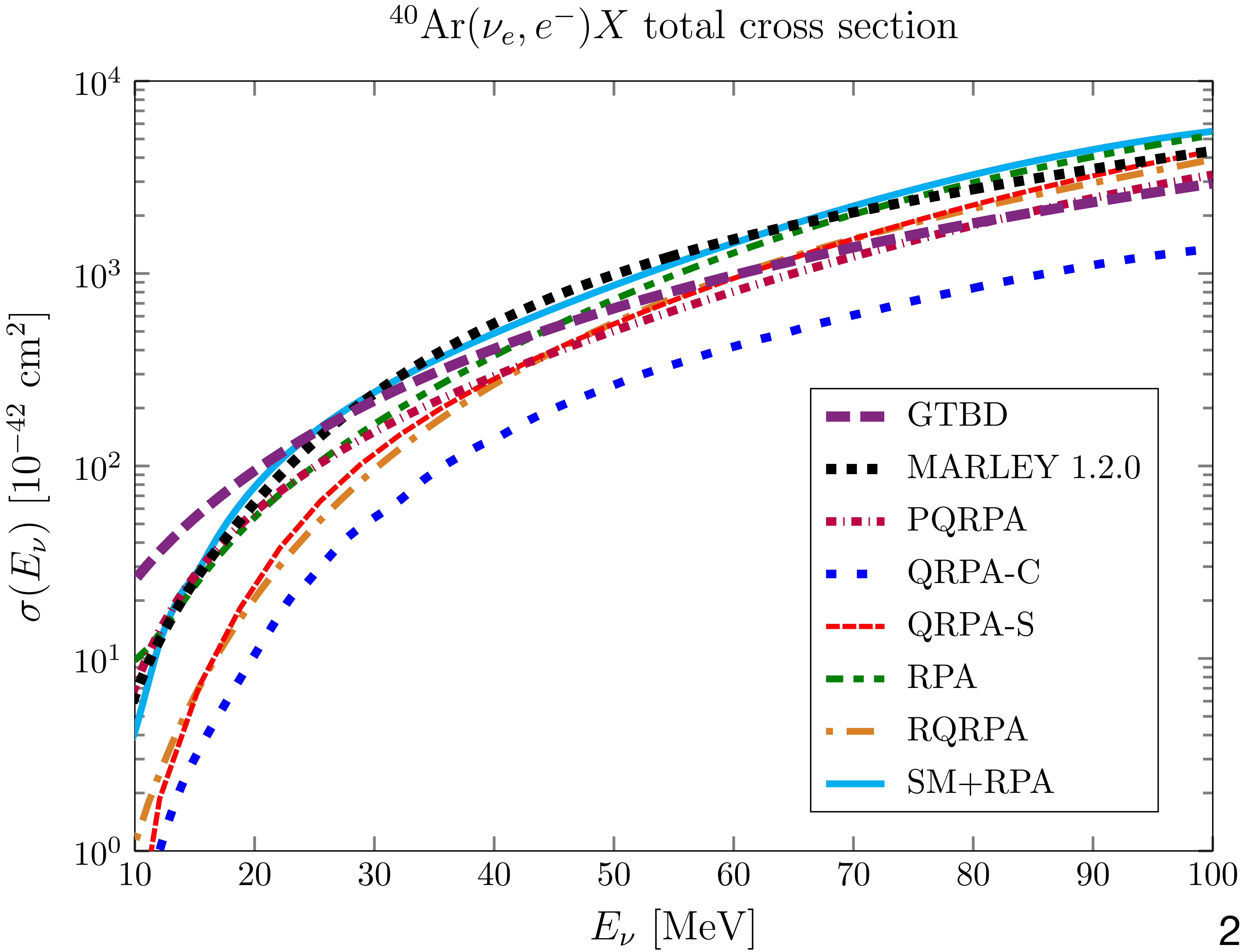


MARLEY comparison to other calculations

- Significant model disagreements

- No measurements of this important channel below 100 MeV

- Constraining theory uncertainty will be critical for DUNE



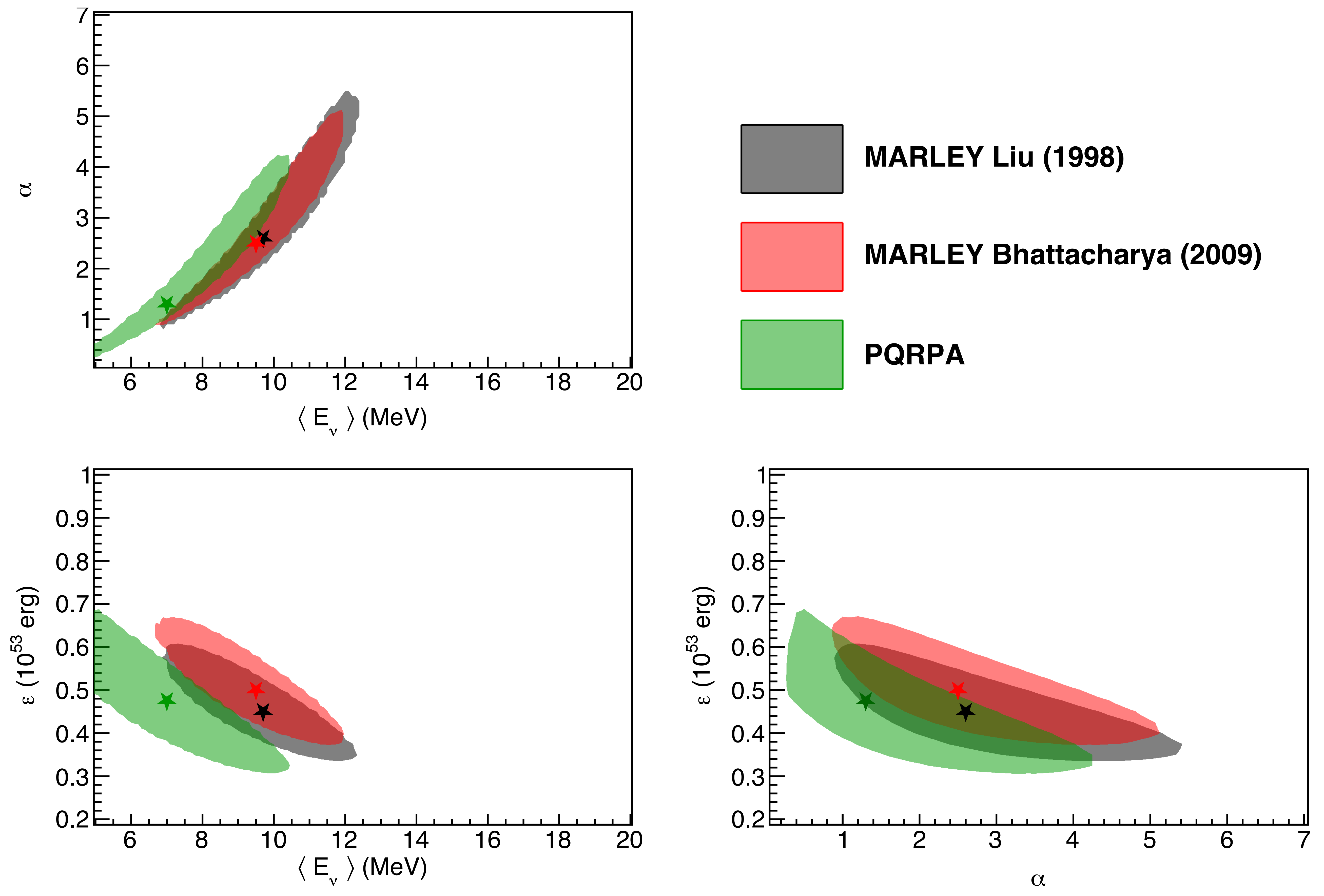
Low-energy cross-section uncertainties

- **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)

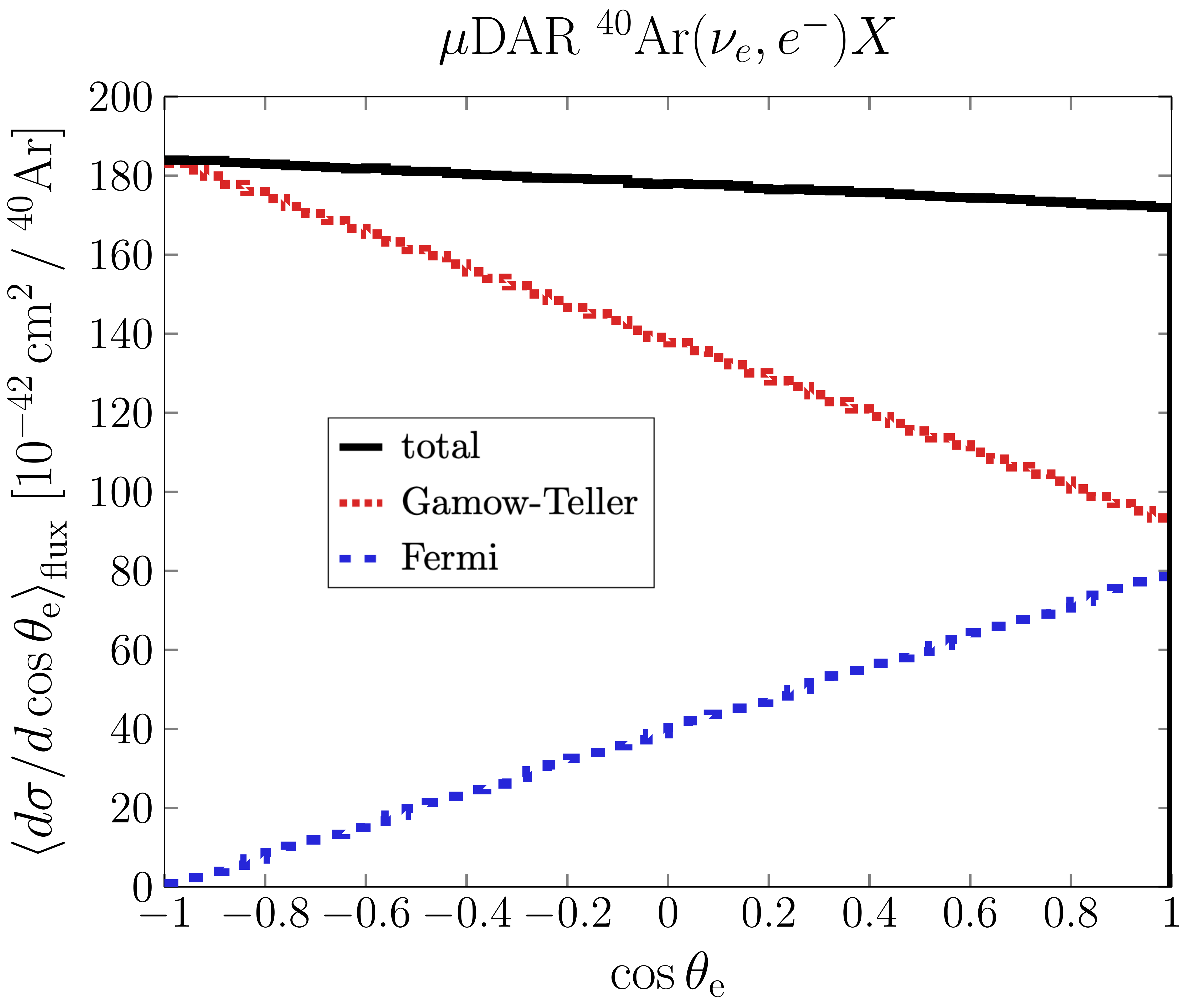


DUNE collaboration, [Phys. Rev. D 107, 112012 (2023)]()

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

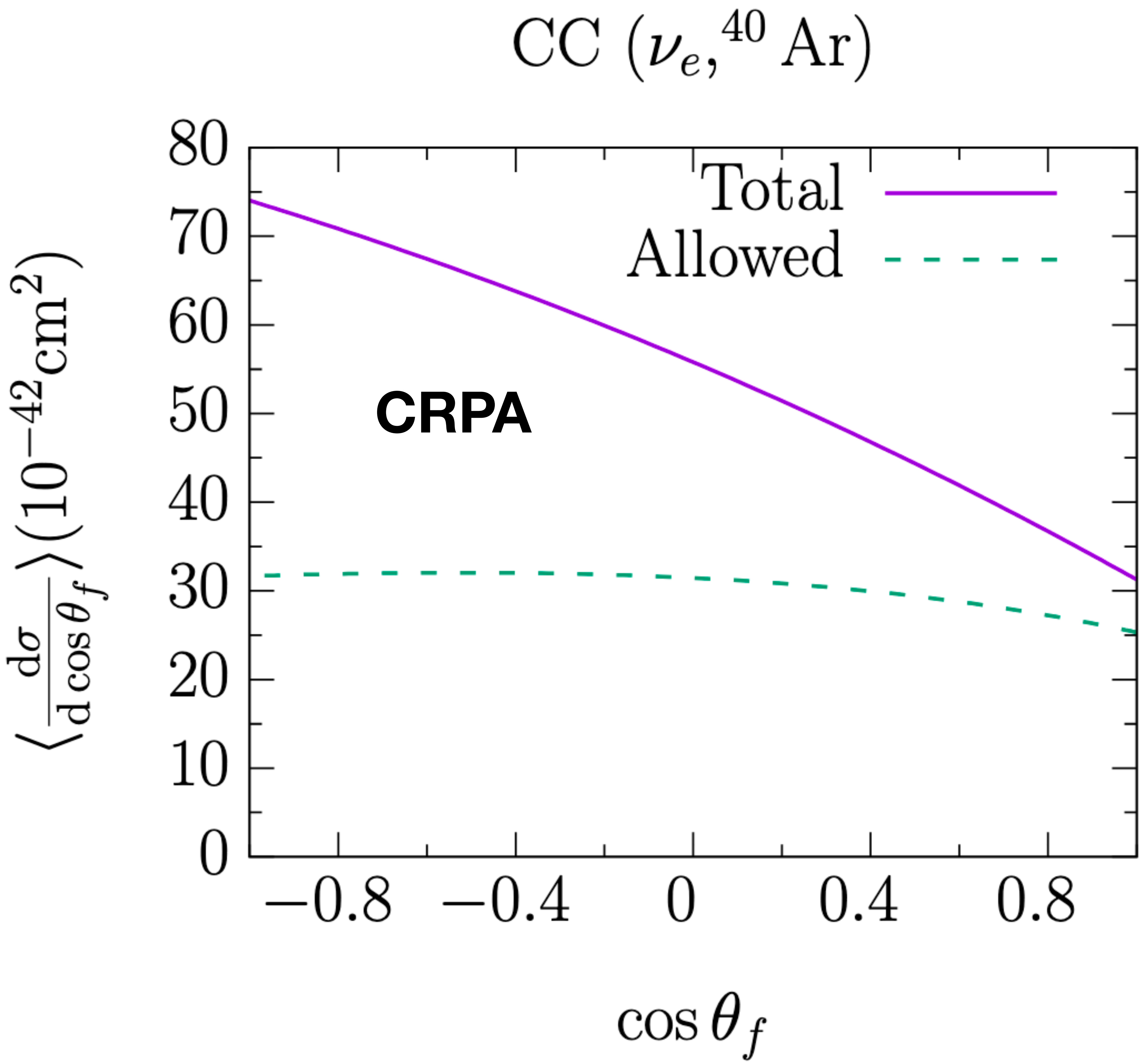
Measuring ε (other parameters) to 10% requires 5% (20%) knowledge of the cross section!

Forbidden contributions to angular distribution



For a muon decay-at-rest source, MARLEY predicts a nearly flat angular distribution, with two linear components

N. Van Dessel *et al.*, **Phys. Rev. C 101, 045502 (2020)**



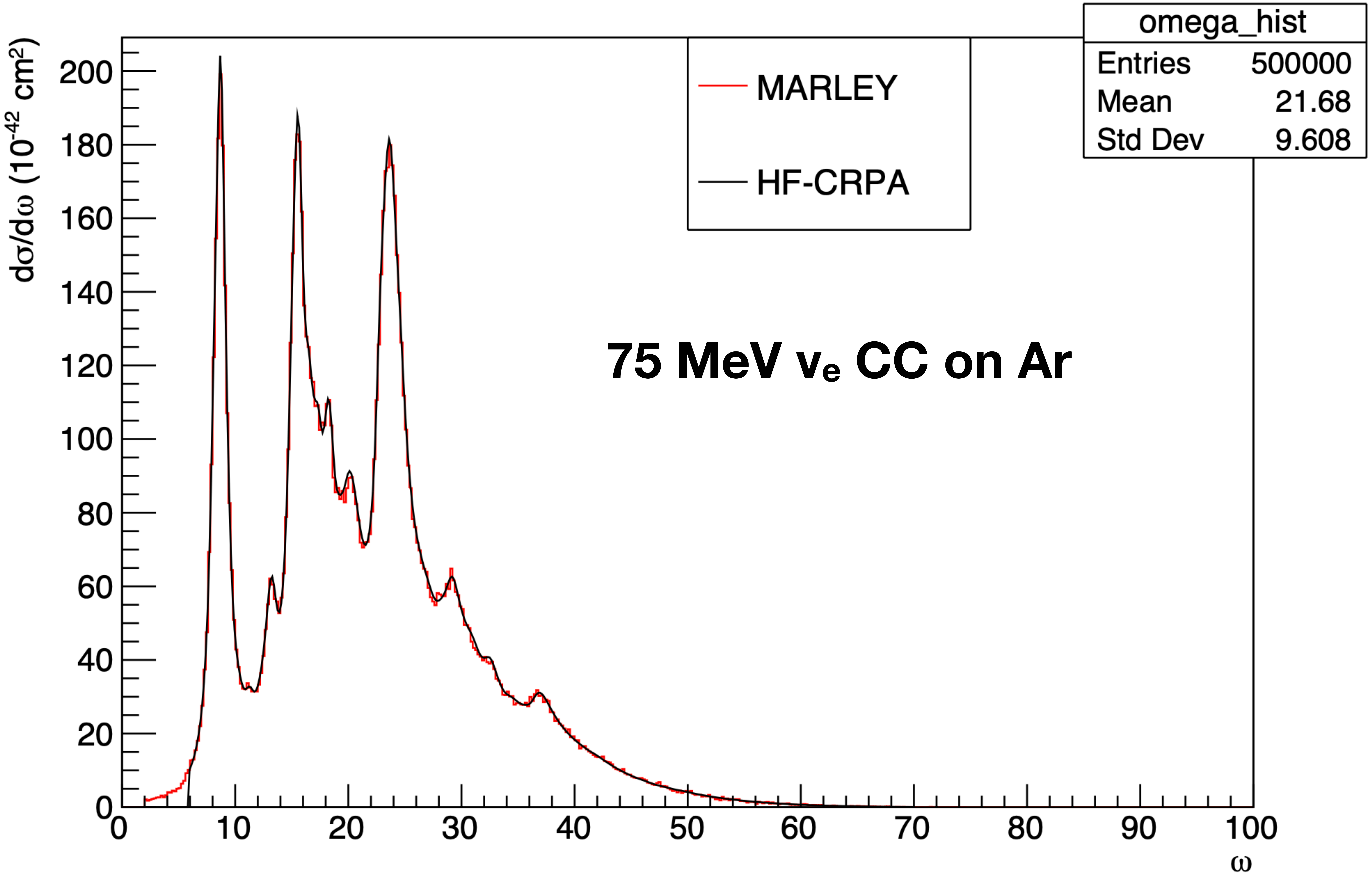
Calculations which include the forbidden transitions (HF-CRPA shown here) predict more backwards strength

Implementation of HF-CRPA model

- In progress, recently validated HF-CRPA inclusive cross section for O, Ar, Pb targets
  - See, e.g., [Phys. Rev. C 101, 045502 (2020)]() for theory details

- Testing connection to de-excitation model

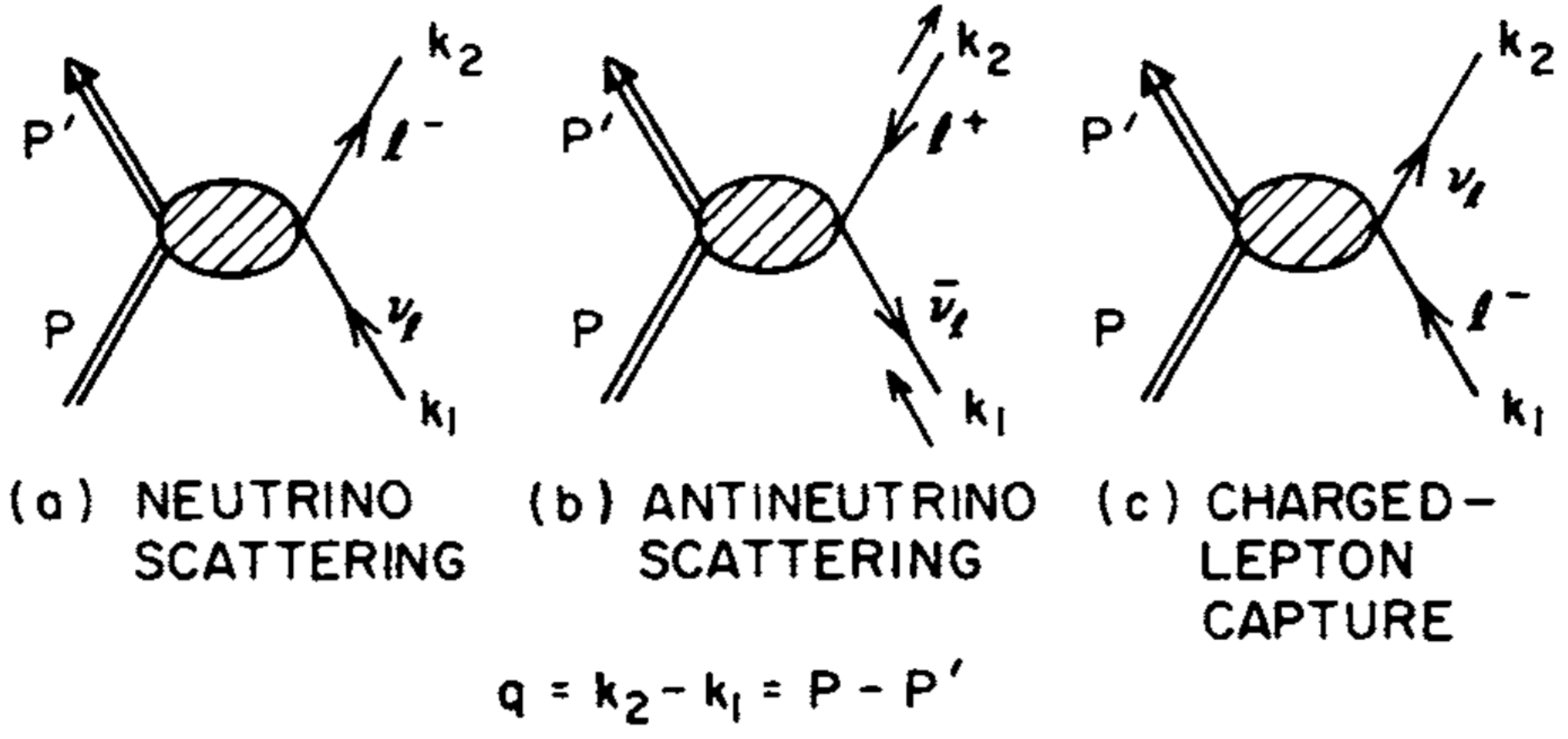
- Need to “fill in” strength in discrete level region too



Muon capture as a probe of low-energy ν scattering?

- Crossing symmetry: μ⁻ capture closely related to antineutrino CC process
    - Theoretically consistent treatment of both possible
    - No consistent simulation available (yet)

- **Data readily available**, under-utilized resource
    - Ar measurement has total rate, **exclusive final states**
    - Sensitive to inclusive calculation and de-excitation model



Bull. Russ. Acad. Sci.: Phys. 72, 735–736 (2008)

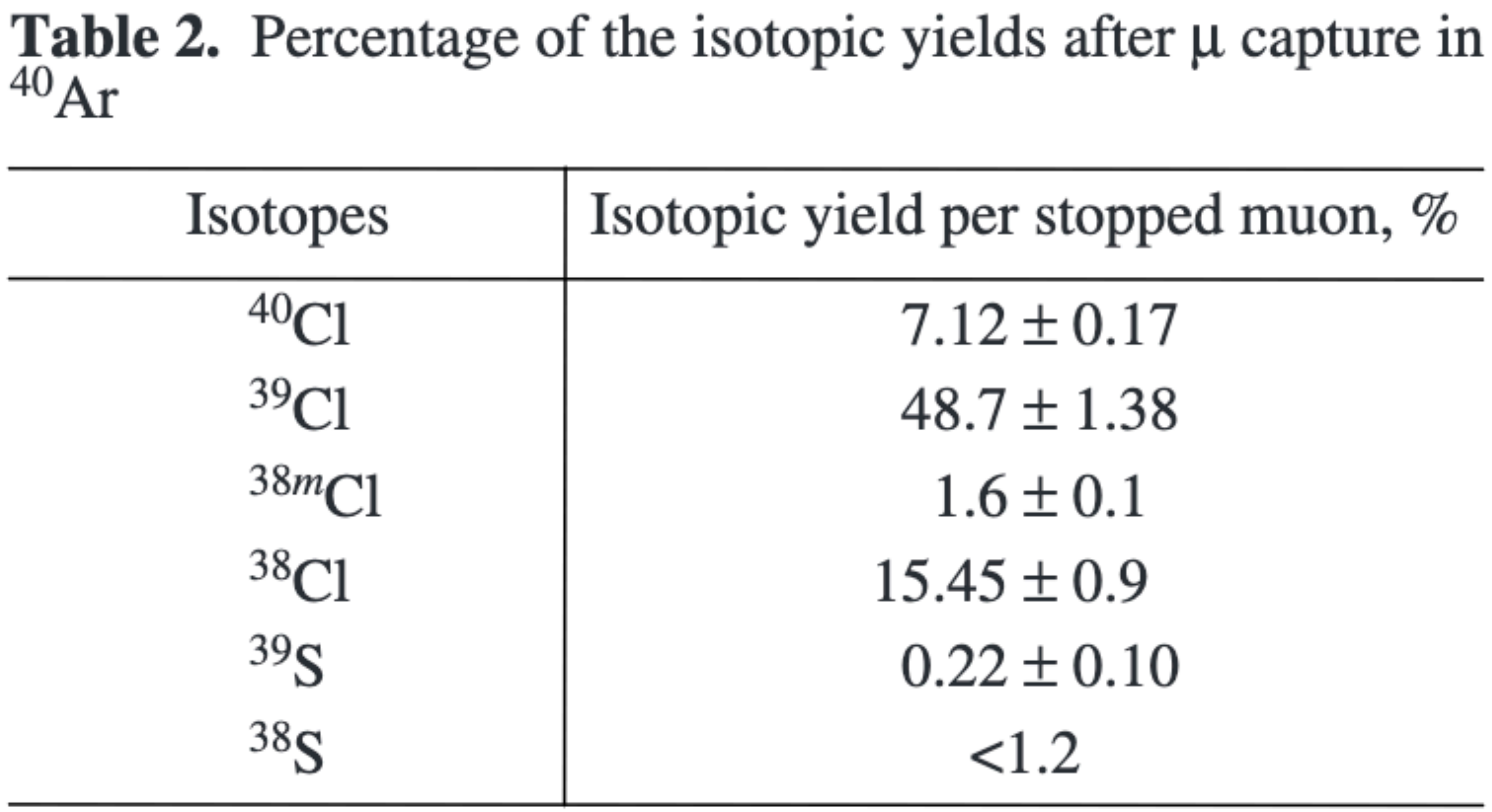


Table 2. Percentage of the isotopic yields after μ capture in ^{40}Ar

Isotopes	Isotopic yield per stopped muon, %
^{40}Cl	7.12 ± 0.17
^{39}Cl	48.7 ± 1.38
^{38m}Cl	1.6 ± 0.1
^{38}Cl	15.45 ± 0.9
^{39}S	0.22 ± 0.10
^{38}S	<1.2

Near-term plans for MARLEY development

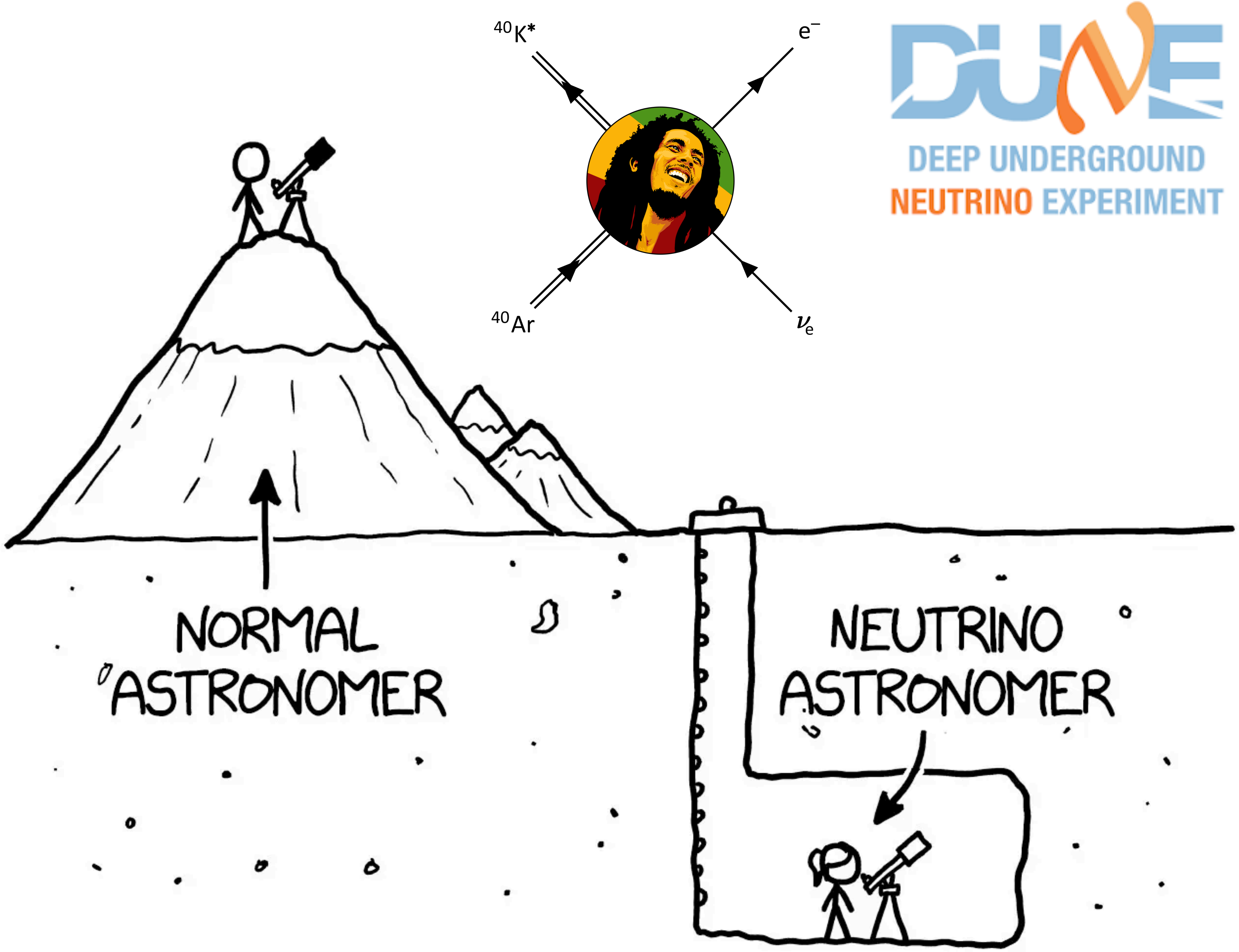
- **Pablo Barham Alzás** (CERN) awarded Neutrino Physics Center Fellowship for MARLEY development
- Will visit me at Fermilab in the coming months

- Three major goals
  - Generalize MARLEY formalism to forbidden transitions
  - Add treatment of $\bar{\nu}_e$ CC, NC for Ar
  - Begin tools for systematic uncertainty quantification
- Further collaborators welcome

Conclusion

DEEP UNDERGROUND NEUTRINO EXPERIMENT

- Interaction simulations are critical for supernova neutrino measurements, especially ν_e in DUNE
- Some initial work has been done, but the topic merits further attention
- New data will be critical for achieving the needed precision



Backup