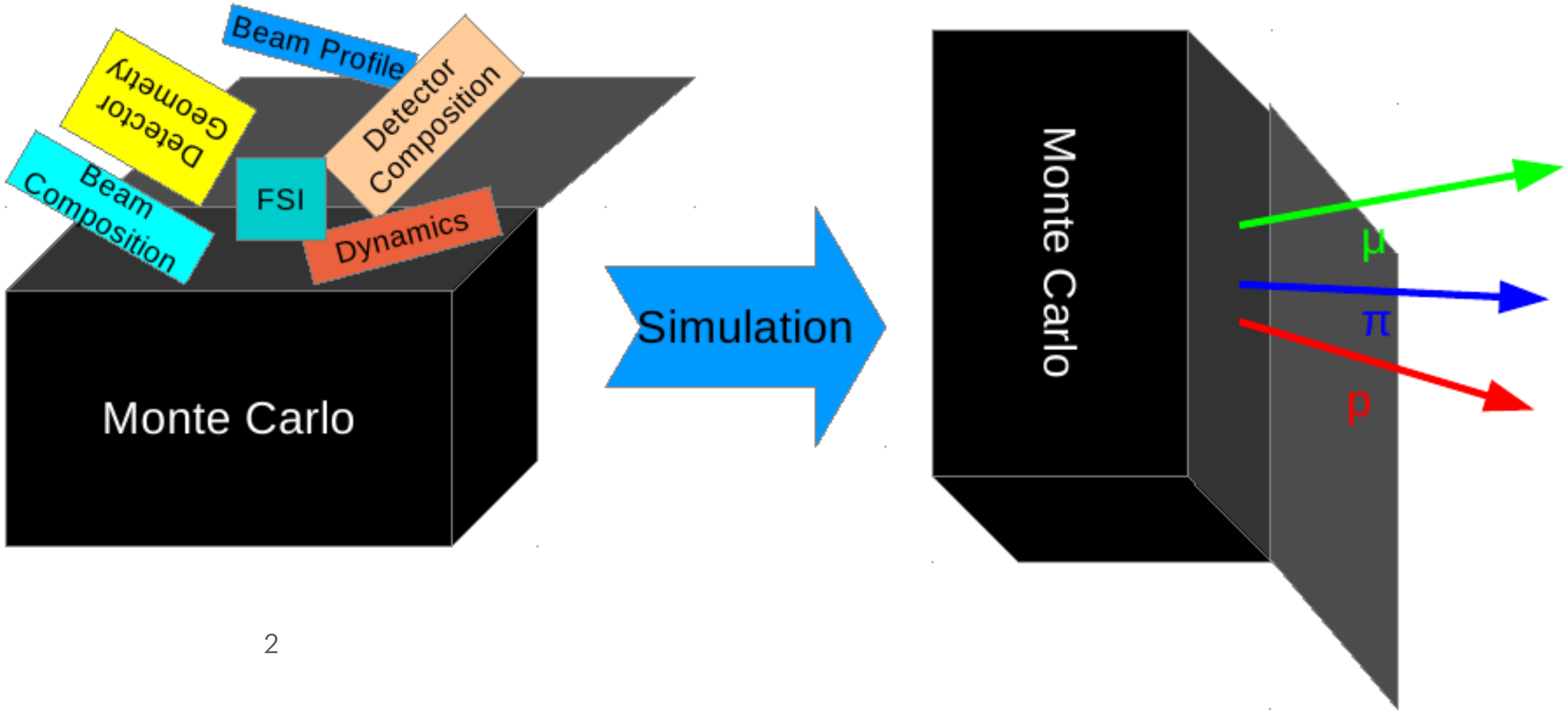
Overview of Monte Carlo generators- challenges and prospects

Jan Sobczyk
Wrocław University

Outline

- Motivation
- What is there in Monte Carlo (MC) event generators?
- A market of MC generators.
- Electron scattering.
- Final state interactions.
- Systematic uncertainties.
- Outlook.



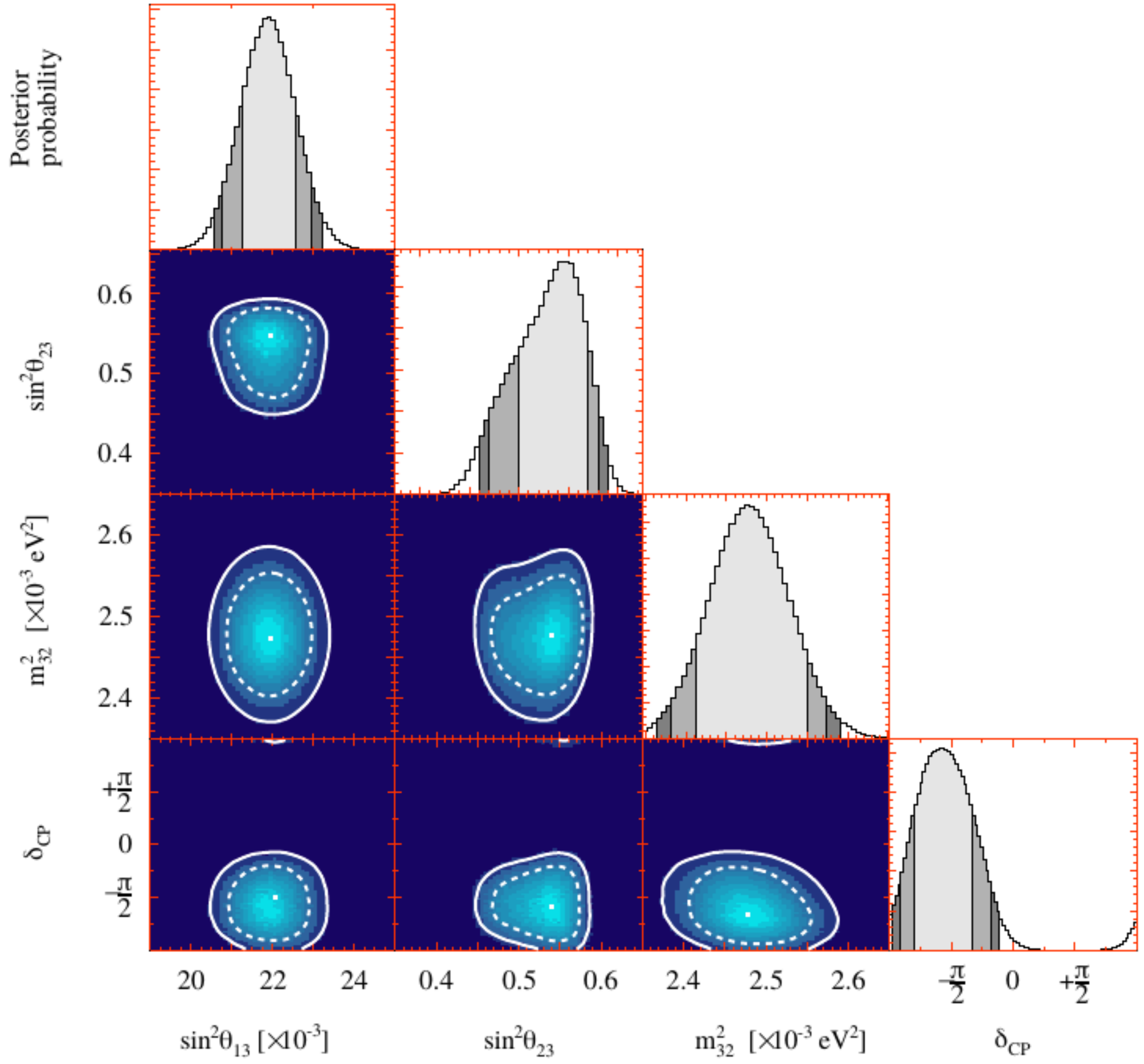
-> Vishvas Pandey

Motivation: oscillation experiments

- MCs - basic tools in short and long baseline oscillation experiments.
- MCs used at all stages of experimental analysis:
    - ➡ flux,
    - ➡ detector response,
    - ➡ interactions.

In this talk - neutrino interactions only.

The quality of MC simulation tools will be of critical importance in the future.



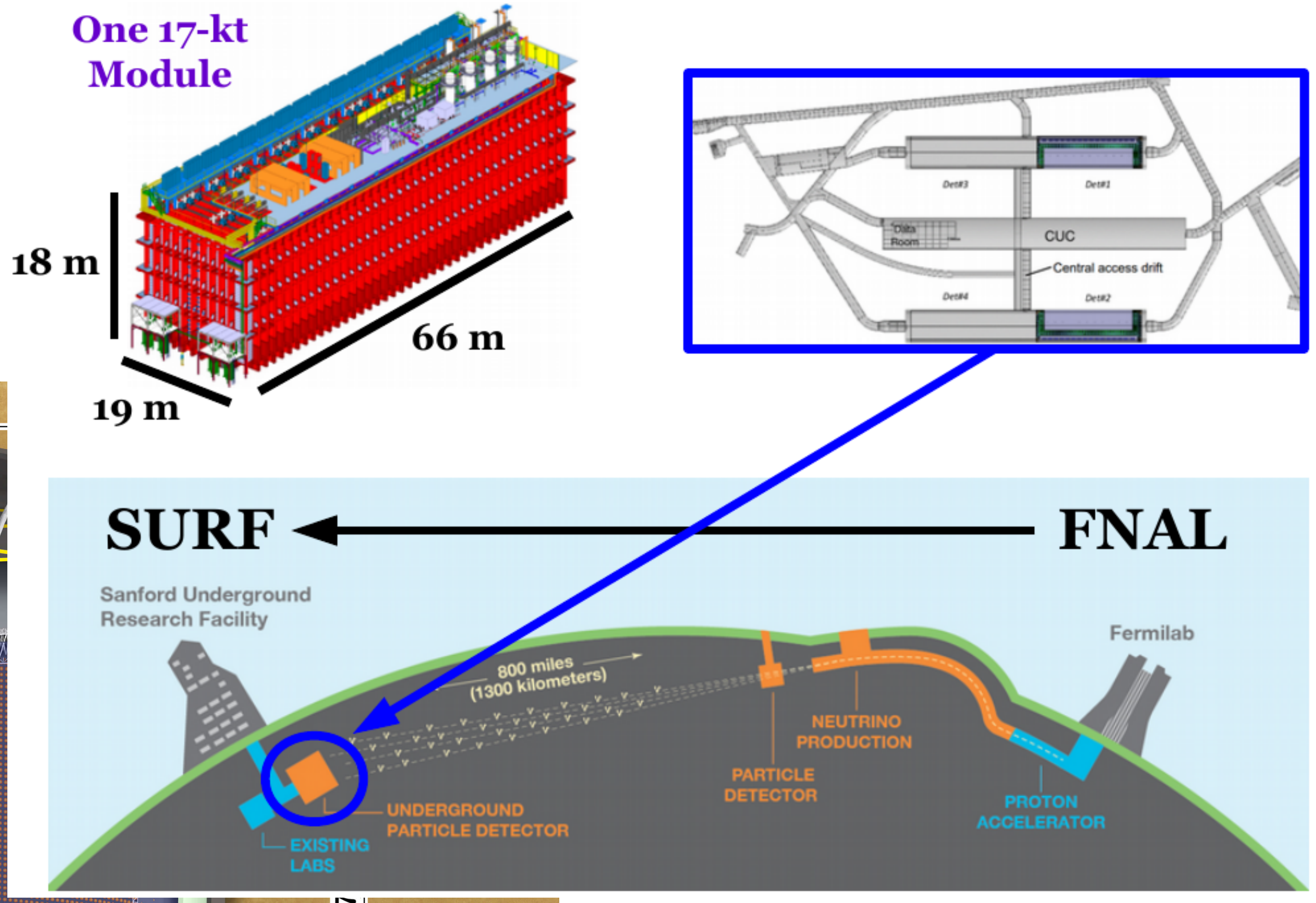
(T2K recent oscillation results)

Neutrino cross sections are known up to ~ 10 – 20% (?).

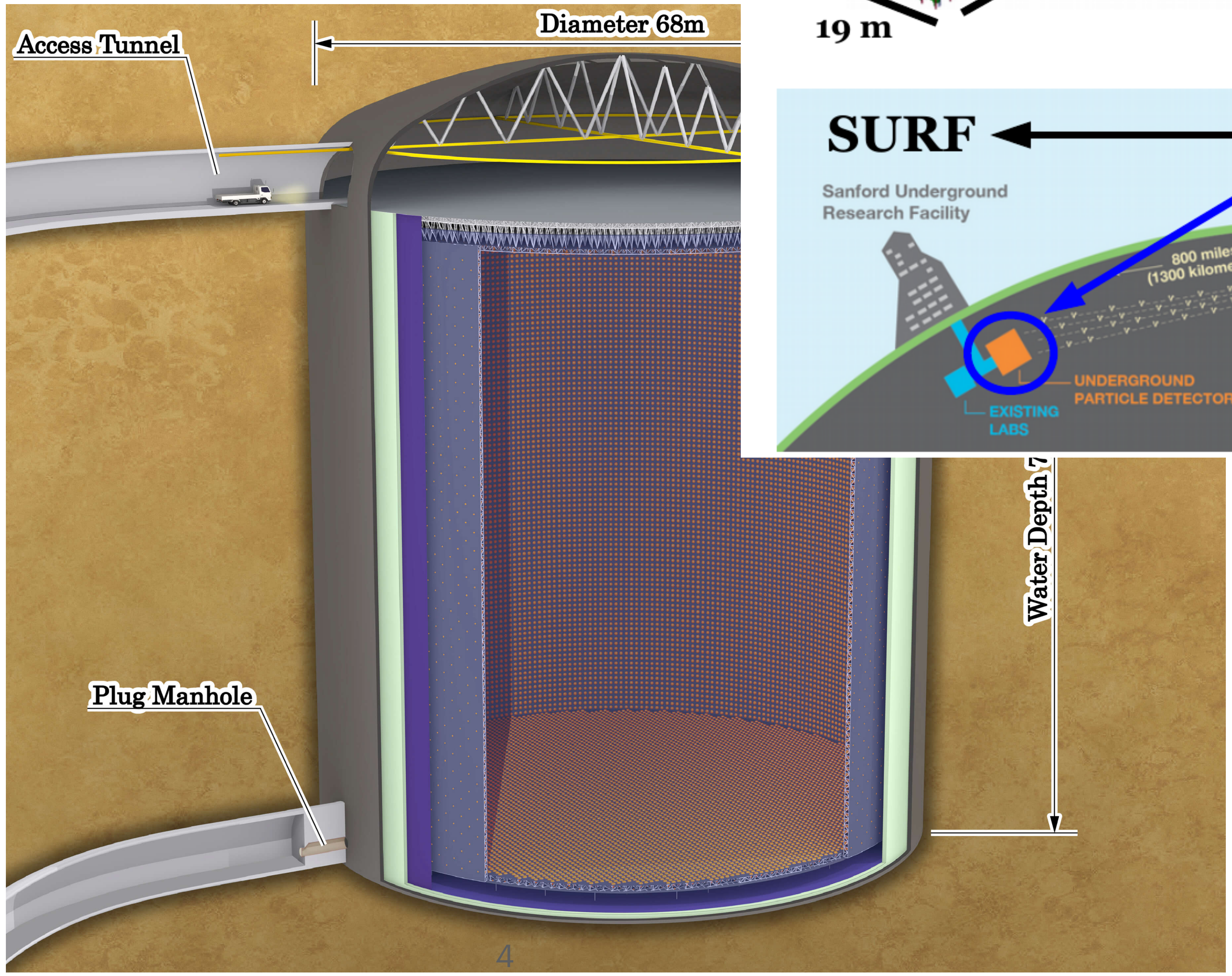
Precision of MC predictions cannot be better than knowledge of cross sections.

Motivation: oscillation experiments

- New generation of experiments -> small statistical errors.
- Future long-baseline programe (DUNE, HK) - systematic uncertainties should be reduced to be commensurate with the statistical uncertainties



DUNE experiment



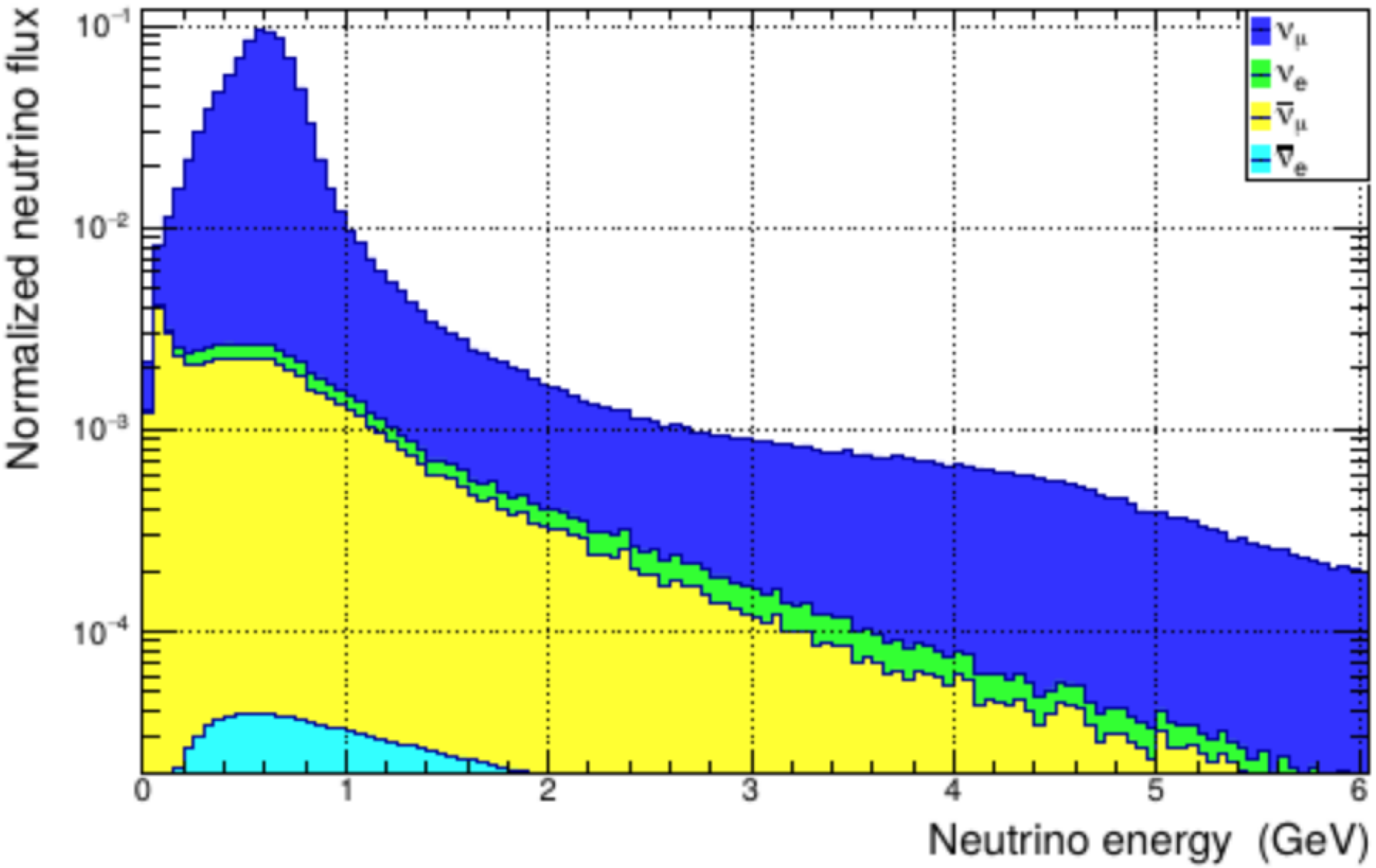
HyperKamiokande experiment

Motivation: cross section measurements

->Afroditi Papadopoulou

-> Federico Sanchez

- MCs - a tool in cross section measurements.
- Neutrino experiments - always inclusive because beams are far from monoenergetic.
- Need to identify individual components of experimental signal.
- Analysis much harder compared to electron scattering.



T2K off-axis flux.

Motivation — other applications

High precision is needed in search for BSM

Examples of potential applications

(from Nina Coyle presentation at Fermilab workshop in March 2023).

✓ Light (eV-scale) sterile neutrinos (arXiv:1710.06488)

✓ Neutrinophilic scalars (arXiv:1901.01259)

✓ Trident production (arXiv:1807.10973)

✓ Light dark matter (arXiv:1107.4580)

Signal of physics BSM must be isolated above uncertainties of implemented models.

- In practice models have parameters tuned to the data; realistic studies need MC generators.
- Example of analysis: Coyle, Li, Machado, arXiv:2210.03753

Basic idea of Monte Carlo generator

Monte Carlo generator of neutrino interactions is basically a code which calculates total cross section with the Monte Carlo algorithm.

Neutrino events are treated as random variables and differential cross sections define probability distribution functions (PDF).

Typically, we need equal weight events.

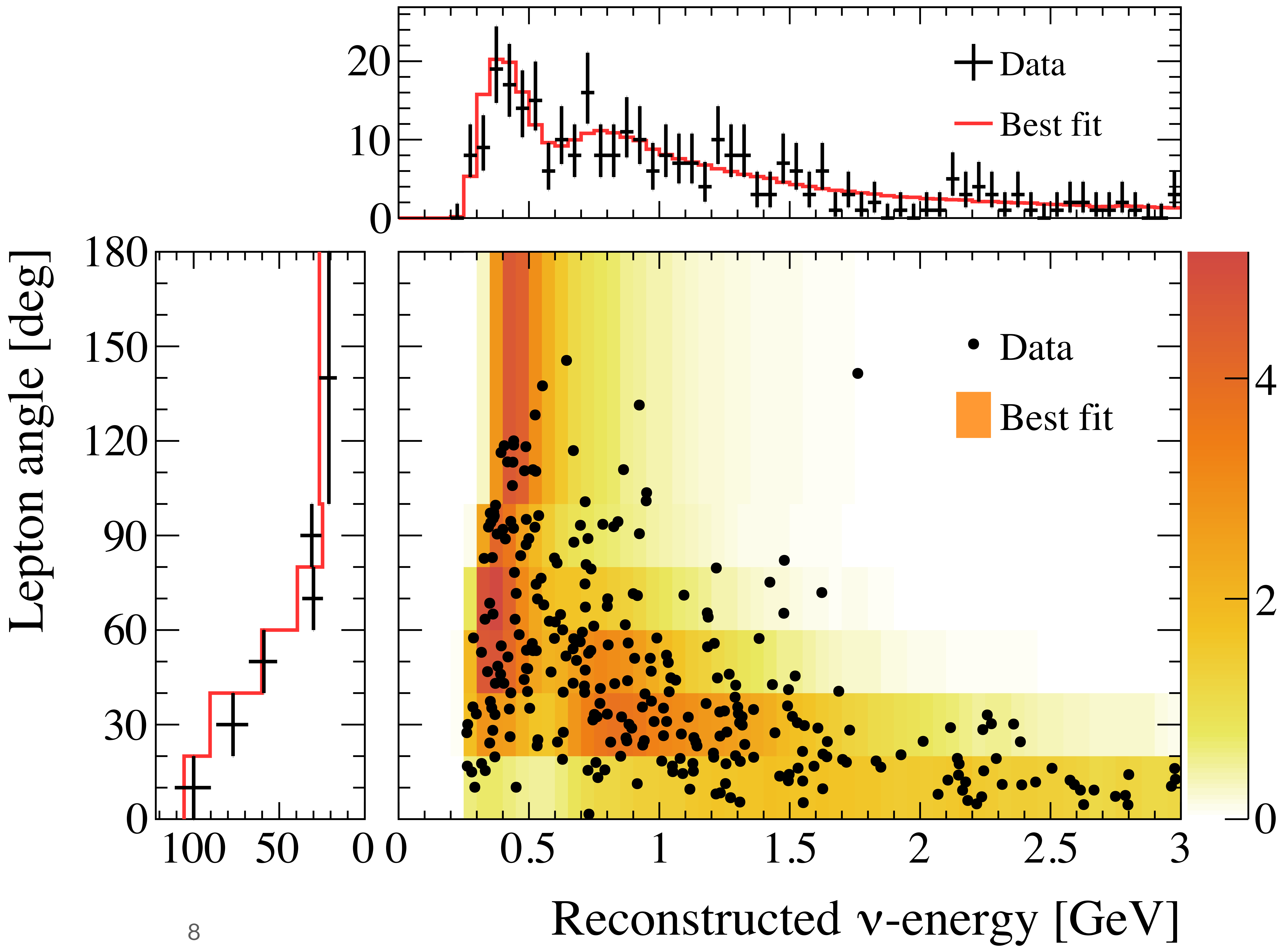
Various tricks are invented in order to make rejection/acceptance more efficient, but the basic idea remains the same.

In the real world there are equal weight events (up to efficiency corrections)

In ν oscillation experiments one compares what is seen in the detector with MC predictions.

Basic idea of Monte Carlo generator

- Experimental signal - a set of events.
- Oscillation parameters measured with maximal likelihood estimator.
- MCs provide PDF for events as random variable; PDF is parameterized by unknown oscillation parameters.



Neutrino events in T2K experiment

Bridge between theory and experiment

MC generators need expressions for all the differential cross sections for all degrees of freedom.

- In practice impossible to achieve.

Moreover...

- Not all models are implementable.
- Often theoretical models provide cross sections in a form of multidimensional nested integrations making the computations very slow so that production of sucient amount of events becomes problematic.

Stanisław Ulam, an inventor of the MC method

Basic interaction modes (NuWro example)

-> Juan Nieves

- Quasi-elastic (QEL)

$$\nu_l\, n \to l^-\, p, \quad \bar{\nu}_l\, p \to l^+\, n$$

and its neutral current counterpart:

$$\nu_l\, n \to l^-\, p, \quad \bar{\nu}_l\, p \to l^+\, n$$

- Resonance excitation (RES) defined (specific for NuWro!) by $W \leq 1.6$ GeV; for example

$$\nu_\mu\, p \to \mu^-\, \Delta^{++} \to \mu^-\, p\, \pi^+$$

- Deep inelastic scattering" (DIS) defined by $W > 1.6$ GeV
- Quasi-elastic hyperon production (HYP)

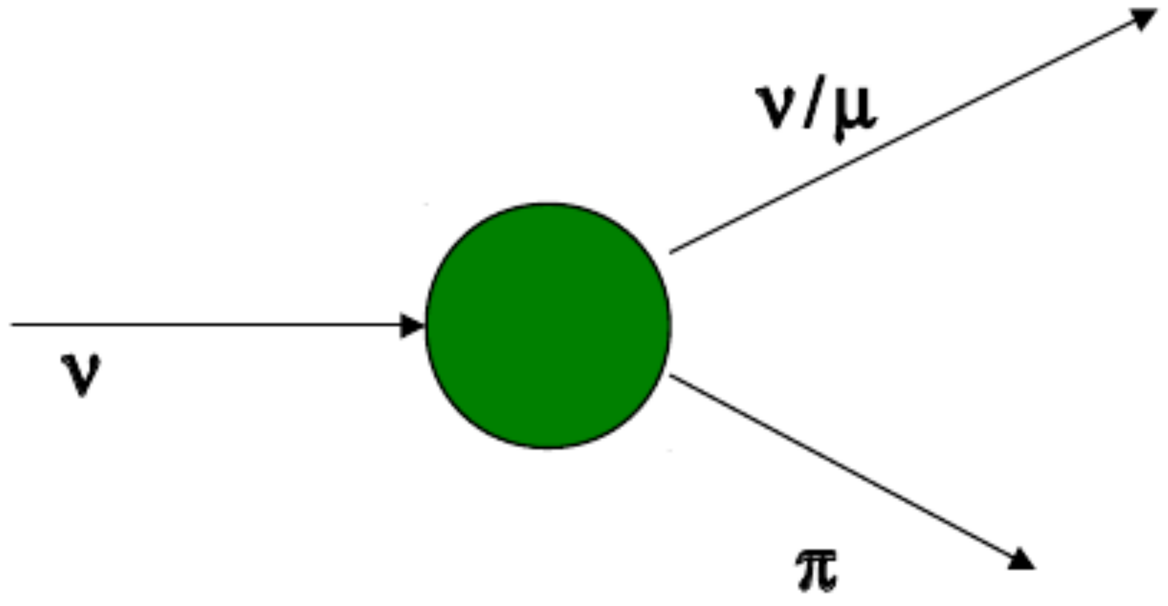
$$\bar{\nu}_l + p \to l^+ + \Lambda, \quad \bar{\nu}_l + p \to l^+ + \Sigma^0, \quad \bar{\nu}_l + n \to l^+ + \Sigma^-$$

- Neutrino-electron scattering (LEP) $\bar{\nu}_l\, e \to \bar{\nu}_l\, e, \quad \bar{\nu}_l\, e \to \bar{\nu}_l\, e, \quad \bar{\nu}_e\, e \to \bar{\nu}_l\, l$

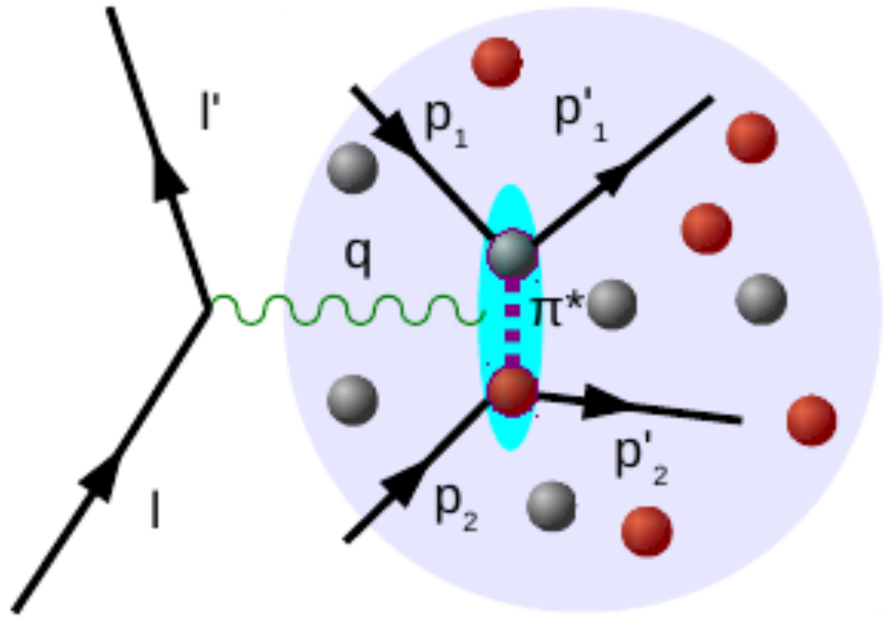
Basic interaction modes (NuWro example)

In the case of nucleus target there are two other basic dynamics:

- (COH) coherent pion production

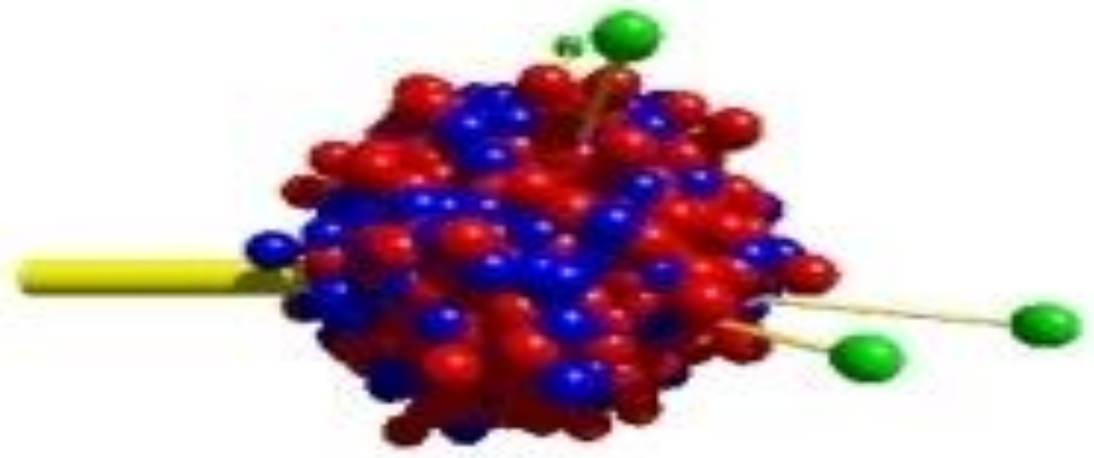


- (MEC/2p2h/two body current)



MC generators differ significantly in their treatment of the above interaction mechanisms…

… and still are able to agree with most of the data!



Market of MC generators

There are several available and actively developed MC generators applicable for ~ 1 GeV neutrinos.

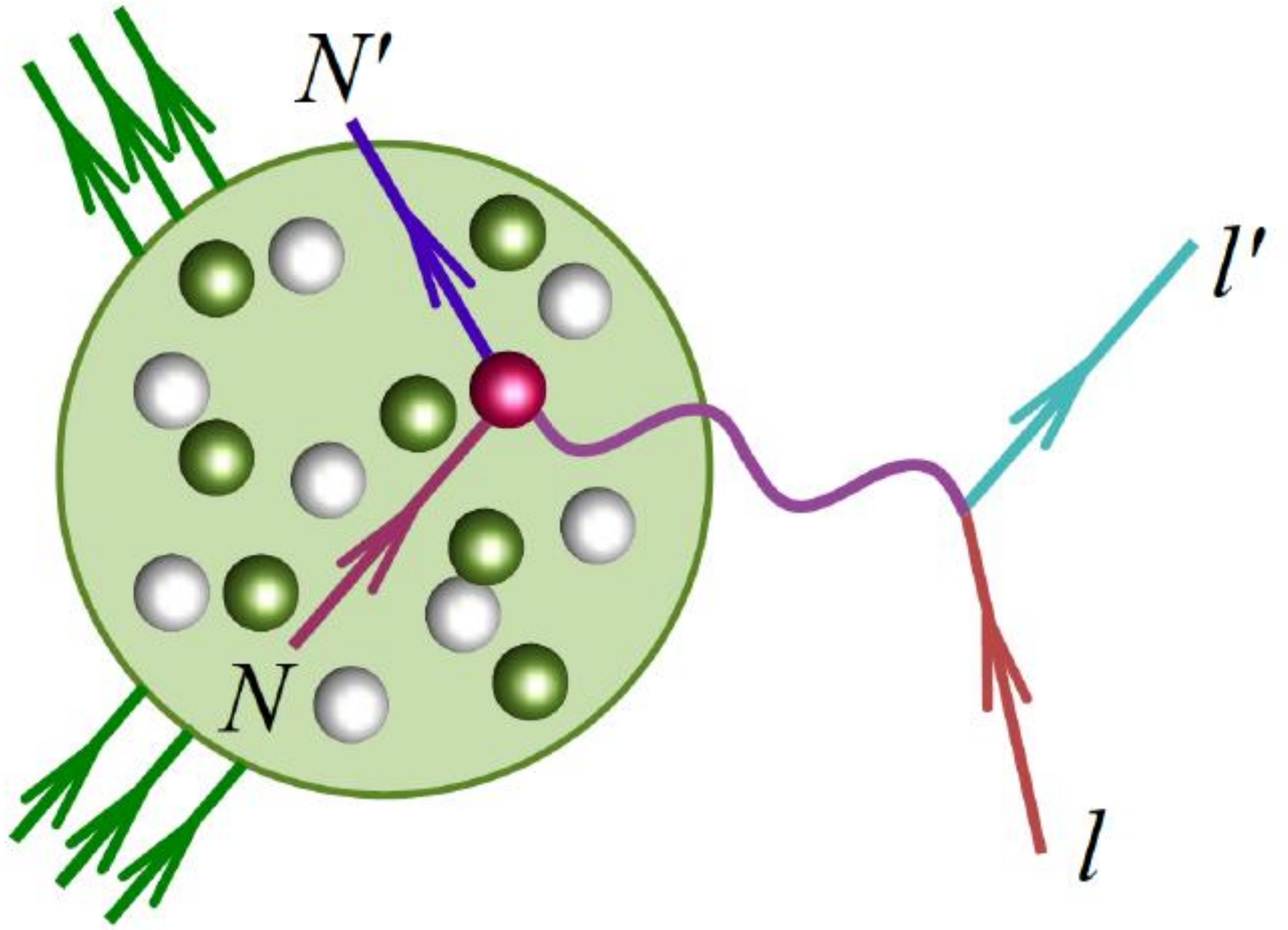
- **NEUT** - the main MC in Japanese experiments T2K, HK.
- **GENIE** - the main MC in US experiments NOvA, MicroBooNE, MINERvA, DUNE.
- **GiBUU** - developed by theoristis in Giessen with the most sophisticated FSI model; used in many comparisons and studies.
- **NuWro** - developed by theorists in Wrocław; used in many comparisons and studies.
- **Achilles** - a new project under development.

There are also MCs for lower energies - **MARLEY** -> Steven Gardiner.

-> Artur Ankowski

Nuclear effects (big picture)

In the 1 GeV region nuclear effects are typically treated in the impulse approximation (IA) scheme: neutrinos interact with individual bound nucleons or correlated pairs of nucleons.



- Within IA one needs a joint probability distribution of momenta and binding energies of target nucleons.
- Any neutrino—nucleus interaction is viewed as a two-step process: a primary interaction is followed by nal state interactions (FSI): before leaving nucleus hadrons undergo reinteractions.

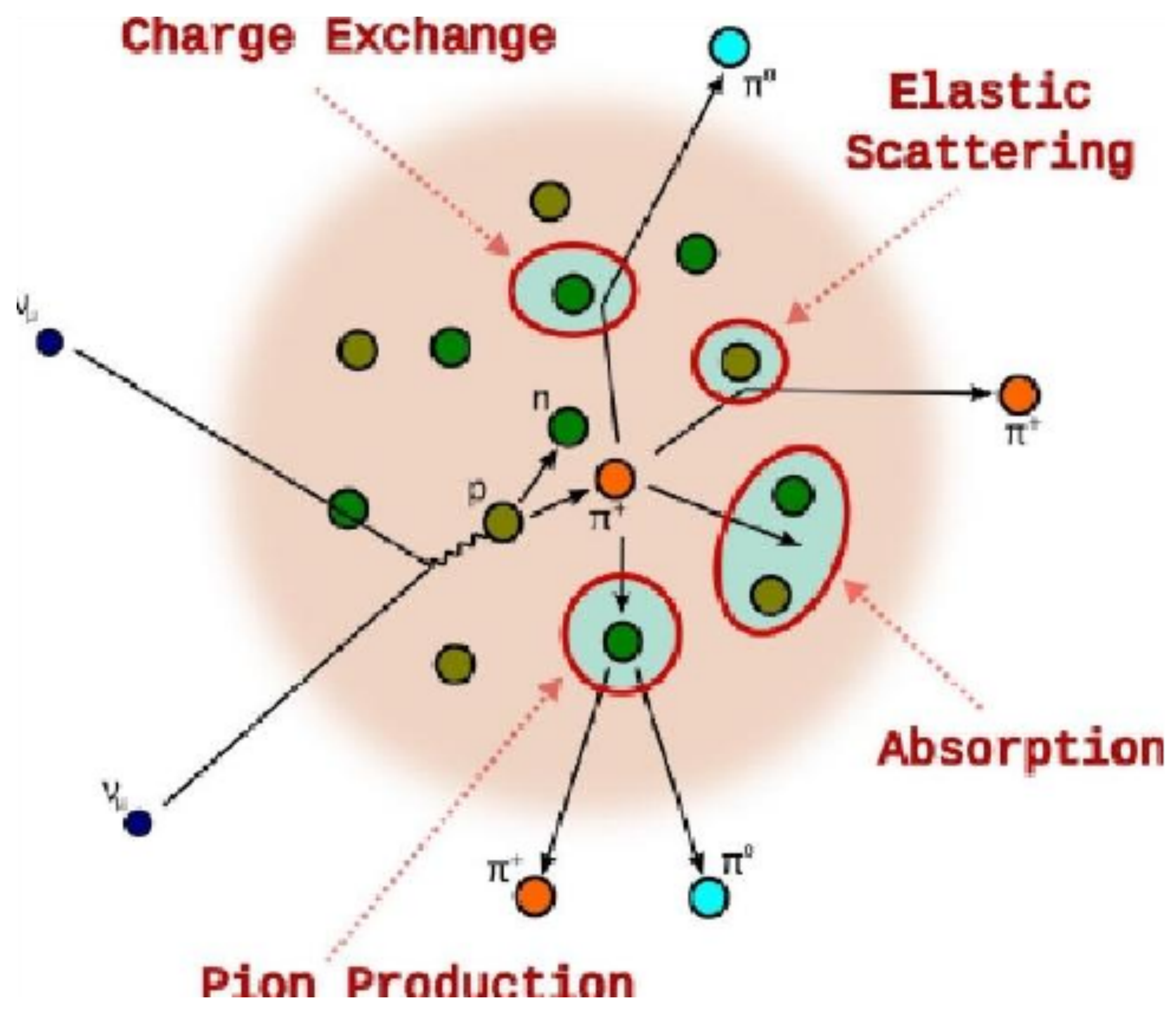
In some models de Forest prescription for off-shell matrix elements is applied

The most important differences between MCs is in the treatment of nuclear effects

-> Alexis Nikolakopoulos

Final state interactions

- In the MC jargon FSI is a unitary transformation connecting hadronic state right after primary interaction and final configuration of hadrons which may be detected experimentally.



Probability to go through nucleus without reinteractions is called hadron transparency.

Pions...

- can be absorbed
- can be scattered elastically
- (if energetically enough) can produce new pions
- can exchange electic charge with nucleons

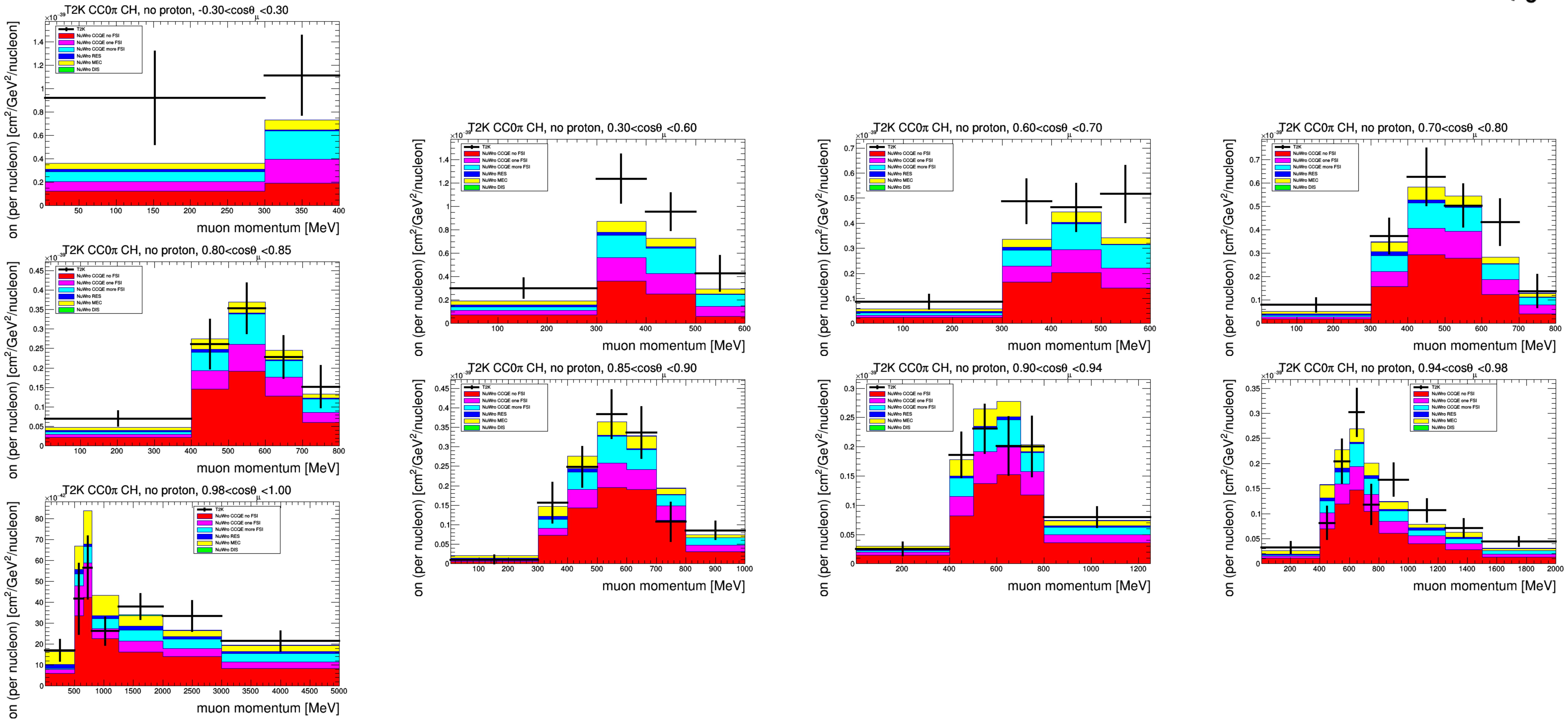
A similar picture can be drawn for other hadrons.

Some MCs include models of nucleus de-excitation.

Monte Carlo performance

MC is a tool to analyze experimental cross section results

Example 1: T2K CC0π with no detected proton Phys.Rev. D98 (2018) 032003



Individual contributions from particular interaction modes are shown, as modeled by NuWro: CCQE with no FSI, CCQE with one FSI, CCQE with more FSI, RES, MEC, DIS.

- A lot of sensitivity to proton FSI.

Monte Carlo performance

Example 2.

Proton inferred kinematics

Phys.Rev. D98 (2018) 032003

MC is a tool to analyze experimental cross section results

- Assumption that interaction was CCQE and occured on a bound neutron at rest.
- FSI are neglected.

From energy and momentum conservation one can derive expected momentum of knocked-out proton $\vec{p}_{inferred}$. Proton is detected with momentum $\vec{p}_{observed}$. A useful observable (one of many) is

$|\vec{p}_{observed}| - |\vec{p}_{inferred}|$

It is an alternative to better known approach of transverse kinematics imbalance proposed by Xianguo Lu.

Monte Carlo performance

MC is a tool to analyze experimental cross section results

Example 2.

Proton inferred kinematics

Phys.Rev. D98 (2018) 032003

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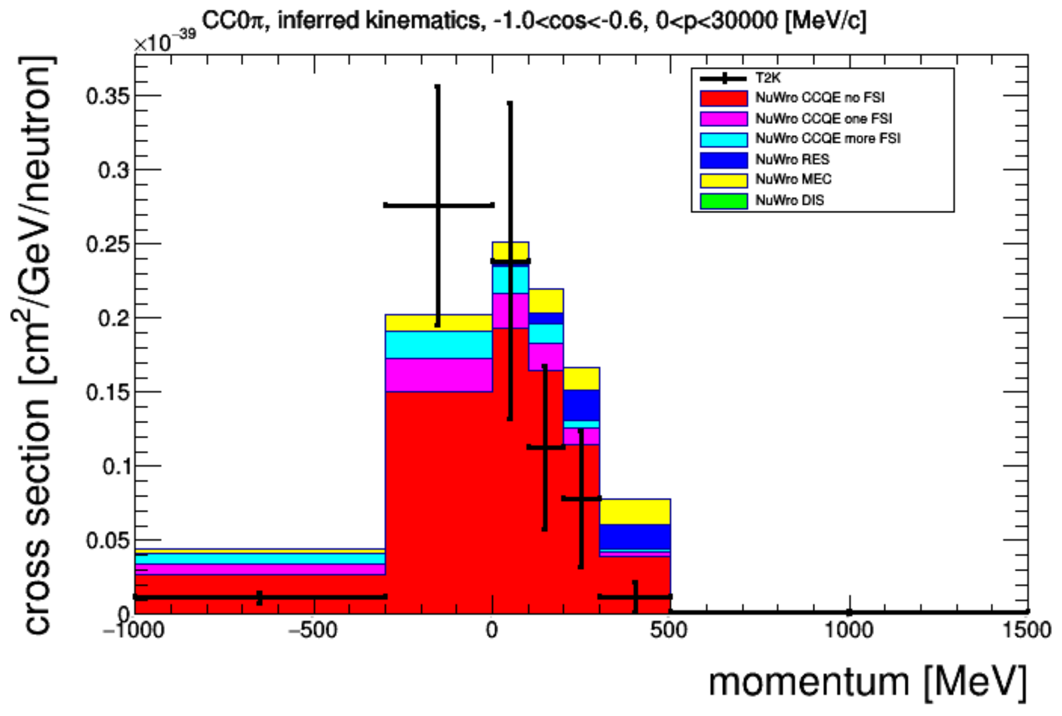
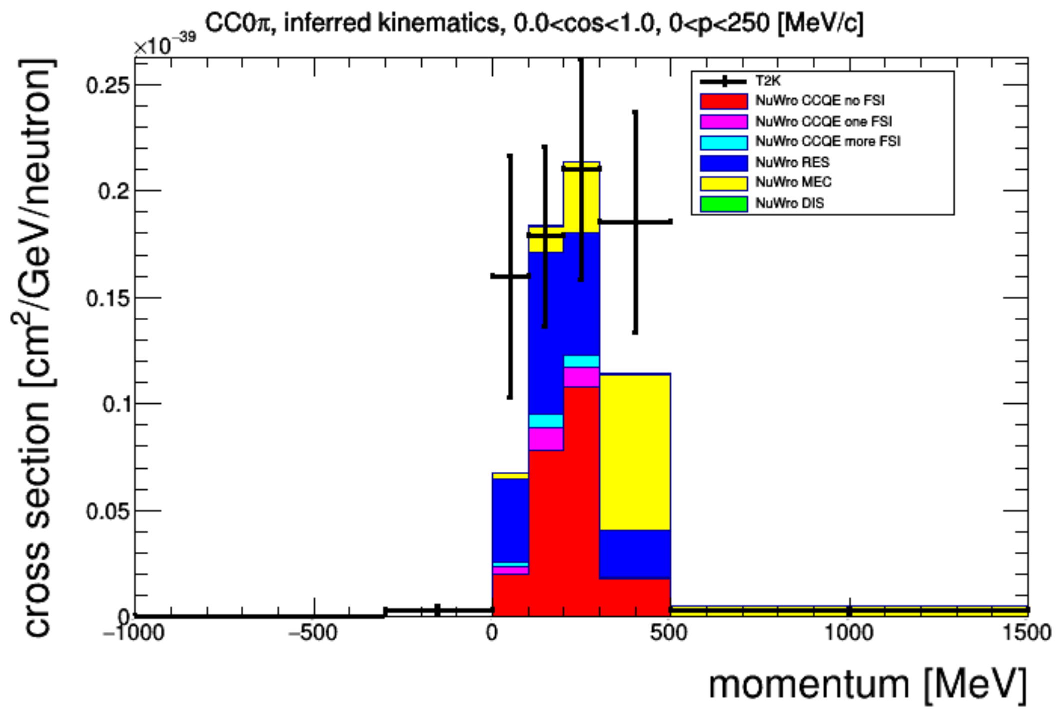
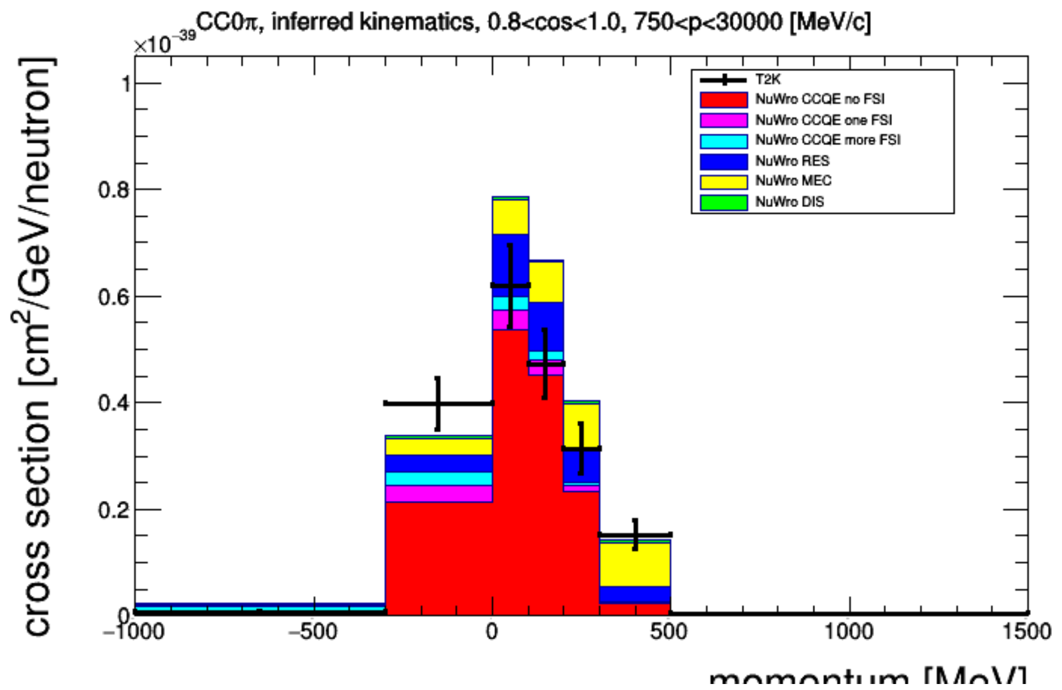
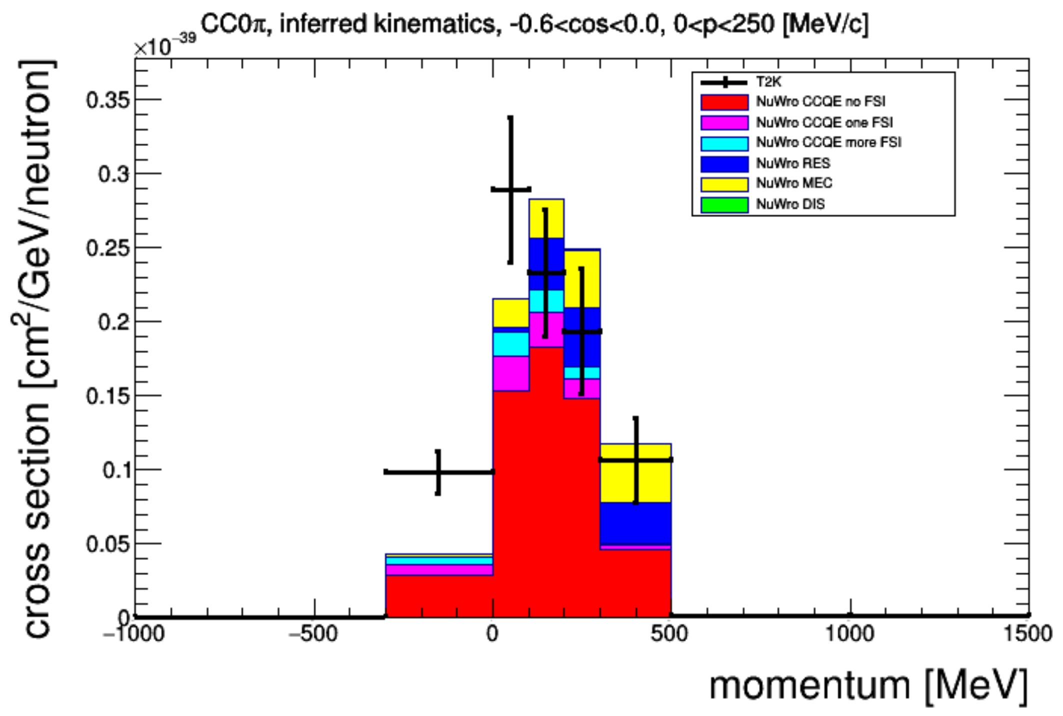
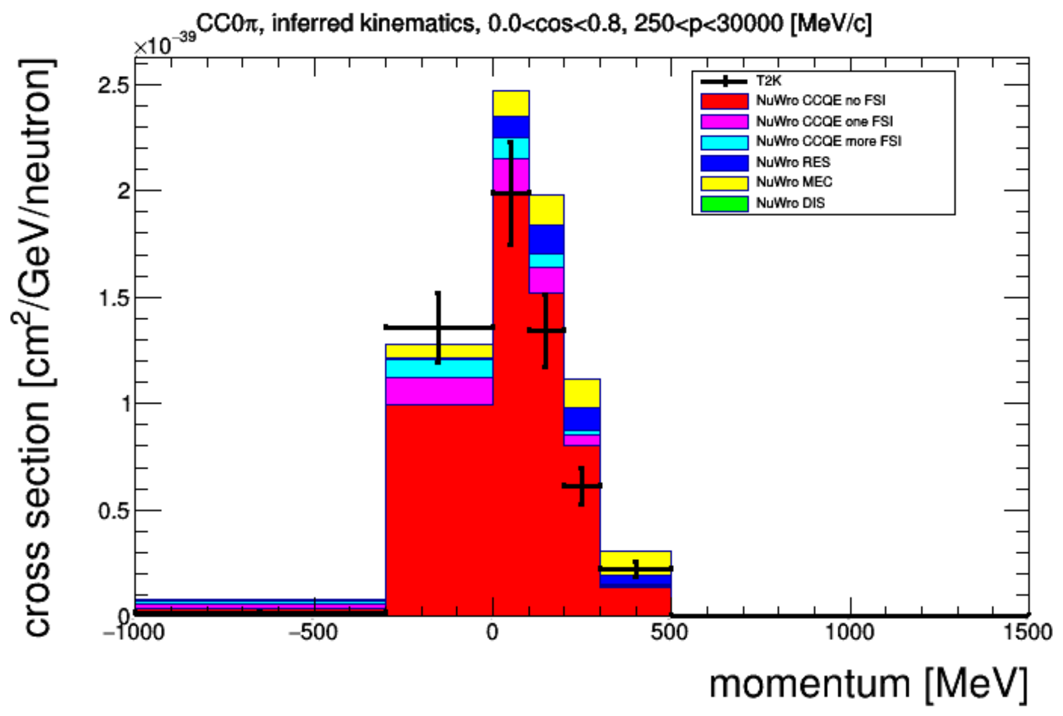
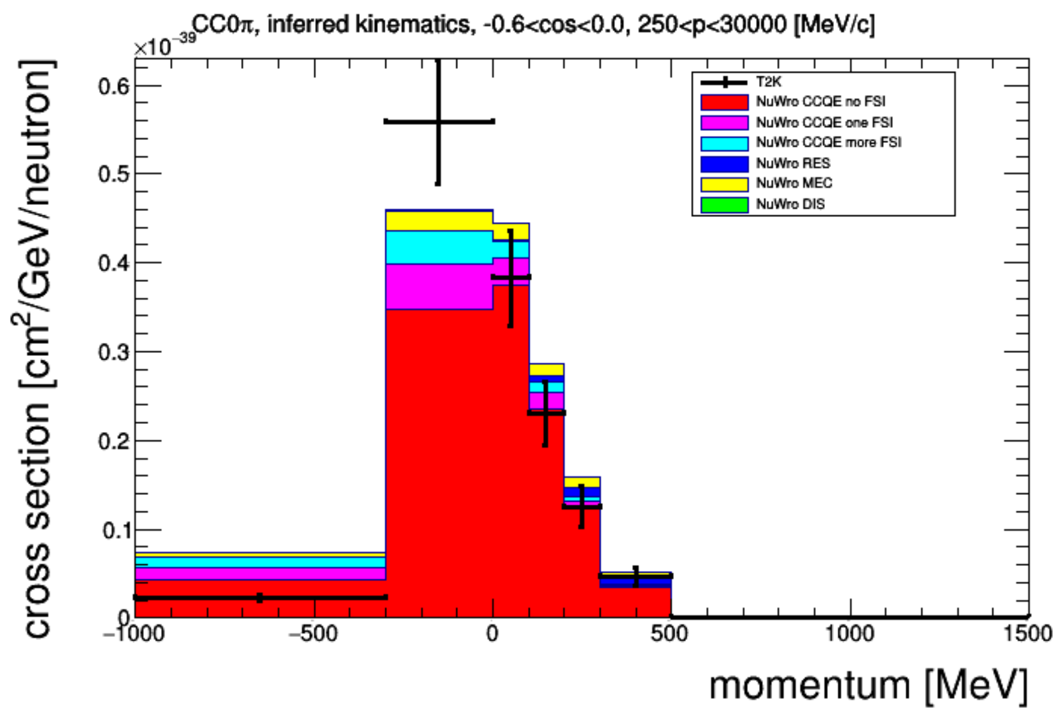


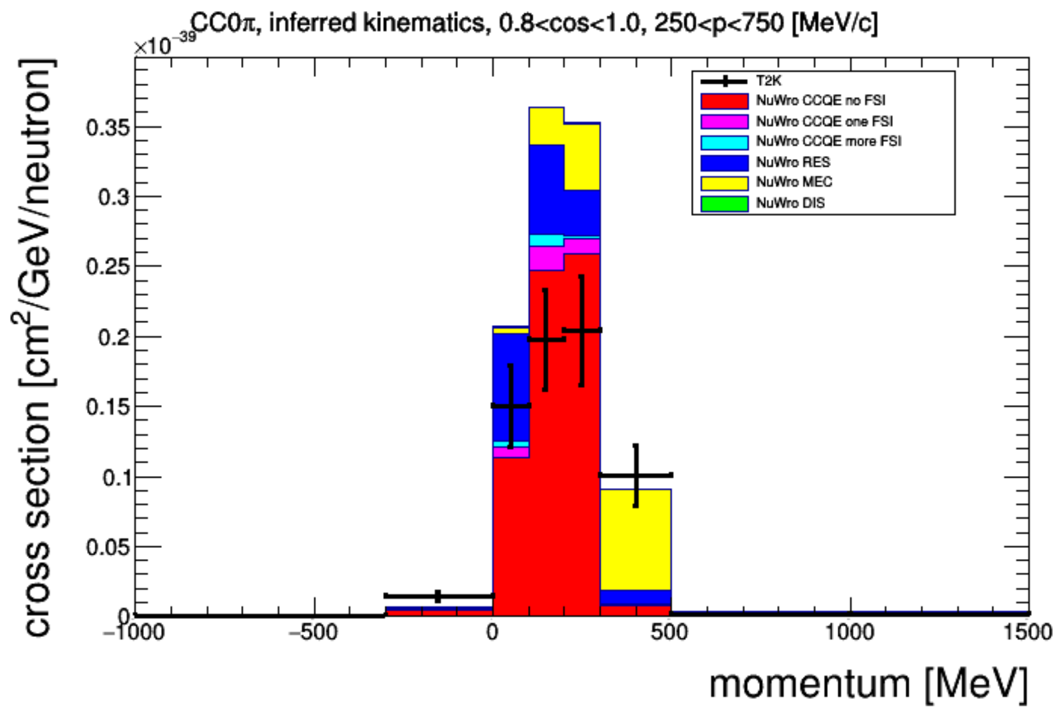












MC development strategies

- ✓ Implementation of better (more realistic, wider applicability) theoretical models.
- ✓ Thinking of MCs more like of effective *black box* by performing extensive fits to experimental data.
  - ➡ By selecting particular subsets of data one obtains GENIE tunes.
- ✓ Neural network methods to find effective accurate description (model) of the data.
  - ➡ Inclusive electron-nucleus data
    O. Al Hammal, M. Martini, et al, Phys. Rev. C 107 (2023) 065501.

-> Julia Tena Vidal

GENIE

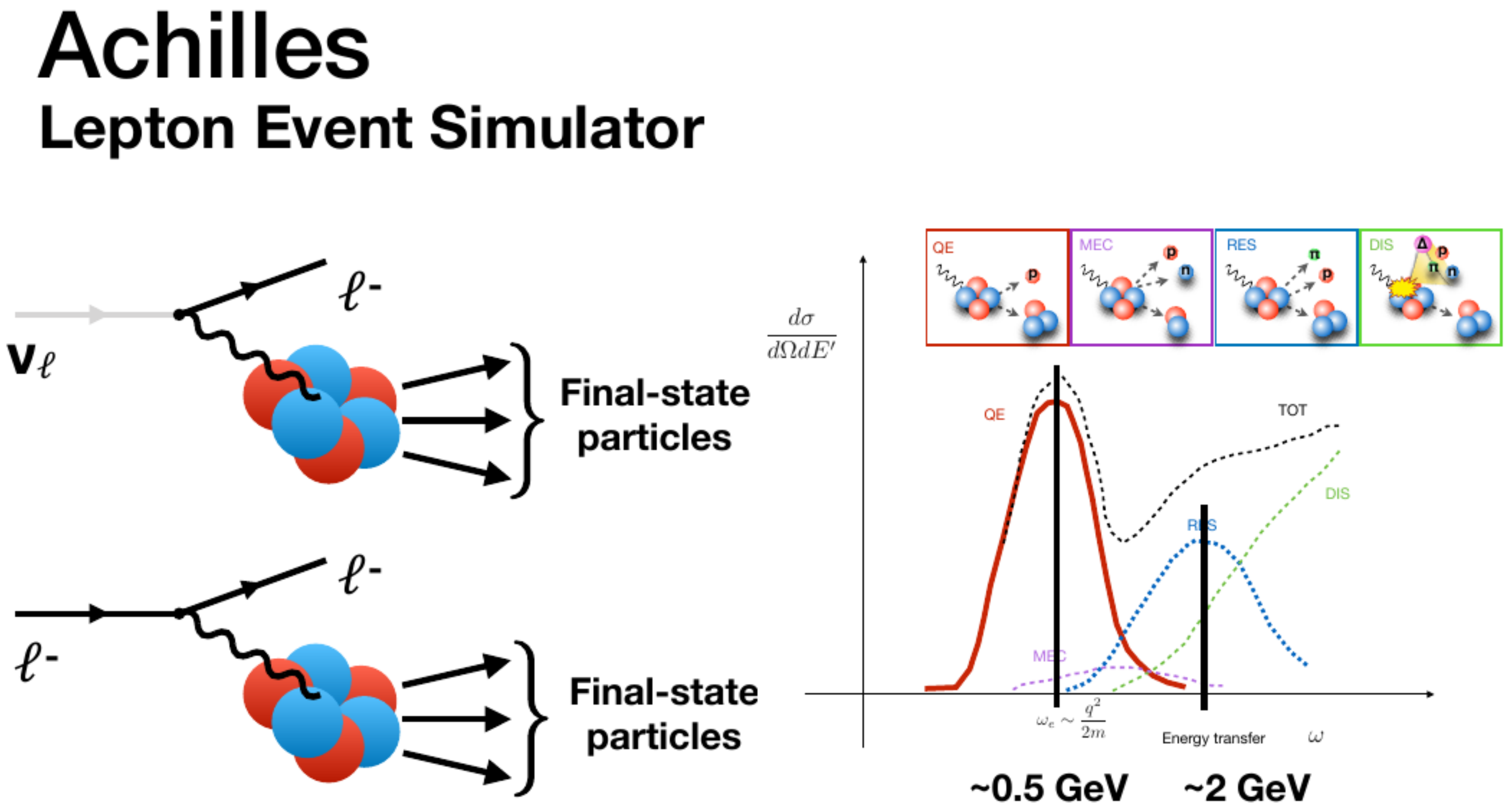
- A successor of NEUGEN
- A large collaboration of both experimentalists and theorists.
- Can be used for very low and very large energies.
- GENIE is a leader in developing tools for global analysis of cross section data.
  - ➡ Global tune improves data/MC agreement. Data-driven uncertainties are estimated as well.
  - ➡ Recent emphasis on using Professor (known in the collider community)

https://professor.hepforge.org

NEUT

- Simulation library developed for SK and T2K.
- Energy range from 100 MeV to 10 TeV.
- Mainly light targets: C, O, but also Ar, Fe and heavier.
- Secondary hadron interactions: nucleon, pion, kaon, eta, omega.
- Pion cascade based on Oset et al model in the Delta region, experimental pion-nucleon for larger energies.
- CCQE: Fermi gas, local Fermi gas with RPA corrections (Juan Nieves), spectral function (Omar Benhar).
- Three models of axial FF (including z-expansion).
- Two alternative single pion production models (Rein Sehgal, DCC - Sato, Lee).

Achilles



Currently supports quasielastic scattering.

New developments:

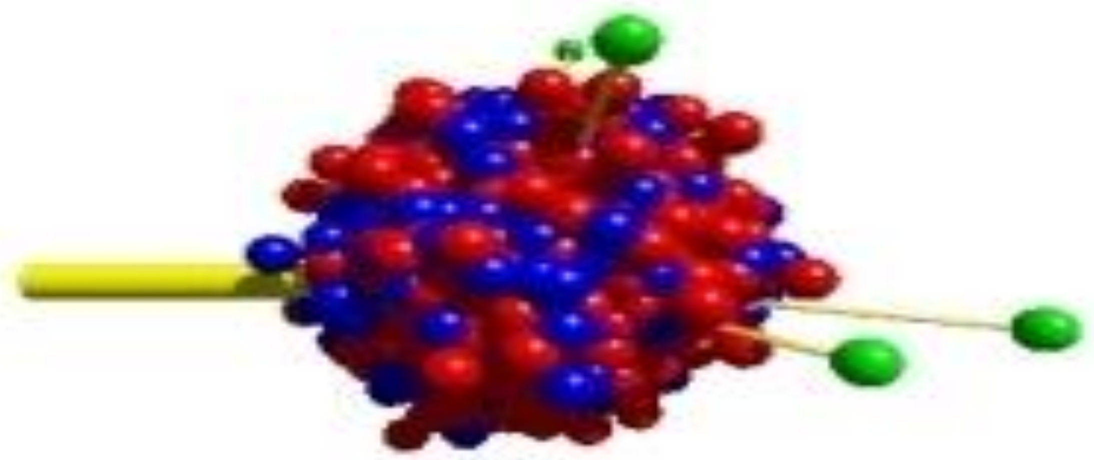
- general factorization of leptonic and hadronic tensors API for nuclear models.
- important motivation is a search for BSN (beyond Standard Model) physics.

A new project: https://arxiv.org/abs/2205.06378

It evolved from a new approach to intranuclear cascade:

J. Isaacson, W.I. Jay, A. Lovato, P. A. N. Machado, N. Rocco, Phys. Rev. C 103, 015502 (2021).

GiBUU



In the last year various applications of GiBUU to other types of reactions.

- Color transparency: https://www.mdpi.com/2624-8174/4/2/29
- Dilepton production in pion-induced reactions: https://journals.aps.org/prc/abstract/10.1103/PhysRevC.106.064910
- Close collaboration with an electron-experiment at JLAB that looked for Lambda production in nuclei, see: https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.130.142301

A new version of GiBUU is coming soon.

NuWro

General information

- Basic motivation: investigation of an impact of alternative choices of nuclear models on observables.
- Optimized for ~ 1 GeV neutrinos.
- Used by many experimental groups (T2K, MINERvA, MicroBooNE, ...).
- Written in C++.
- Output files in ROOT format.
- PYTHIA is used for hadronization in DIS.
- Open source code, repository: https://github.com/NuWro/nuwro .

The most recent release is 21.09.

NuWro - current activities and plans

New single pion production model

R. Gonzalez-Jimenez, K. Niewczas, N. Jachowicz, Phys.Rev.D 97 (2018) 1, 013004; K. Niewczas, A. Nikolakopoulos, J.T. Sobczyk, N. Jachowicz, R. Gonzalez-Jimenez, Phys.Rev.D 103 (2021) 5, 053003

MEC Ghent model

K. Niewczas, PhD thesis

Nuclear de-excitation model

KamLAND Collaboration, S. Abe, et al., e-Print: 2211.13911 [hep-ex].

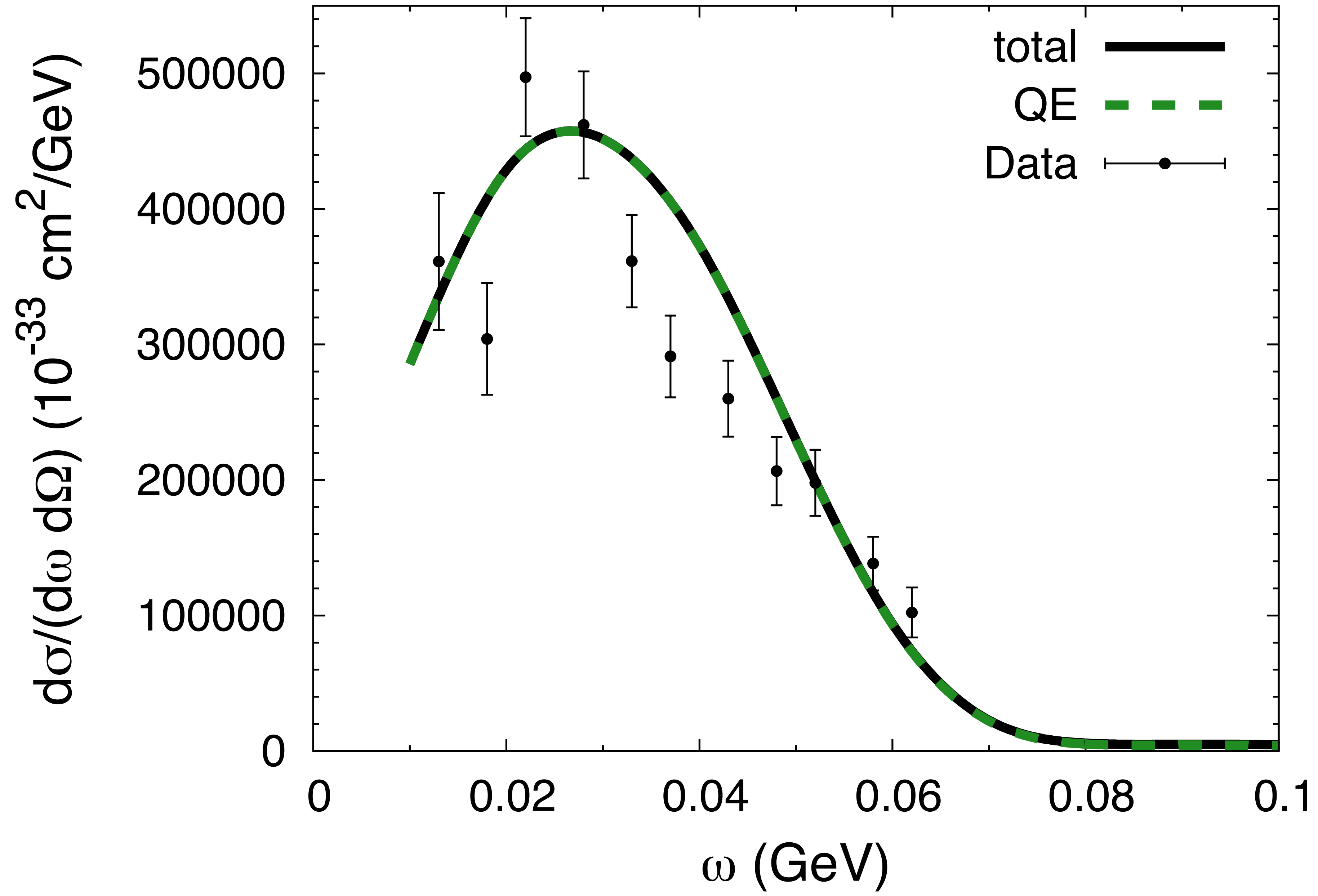
A. Ershova, S. Bolognesi, et al., Phys.Rev.D 106 (2022) 3, 032009

-> Natalie Jachowicz

MC - treatment of low energy neutrinos

MC generators - developed for atmospheric neutrinos and long baseline experiments.

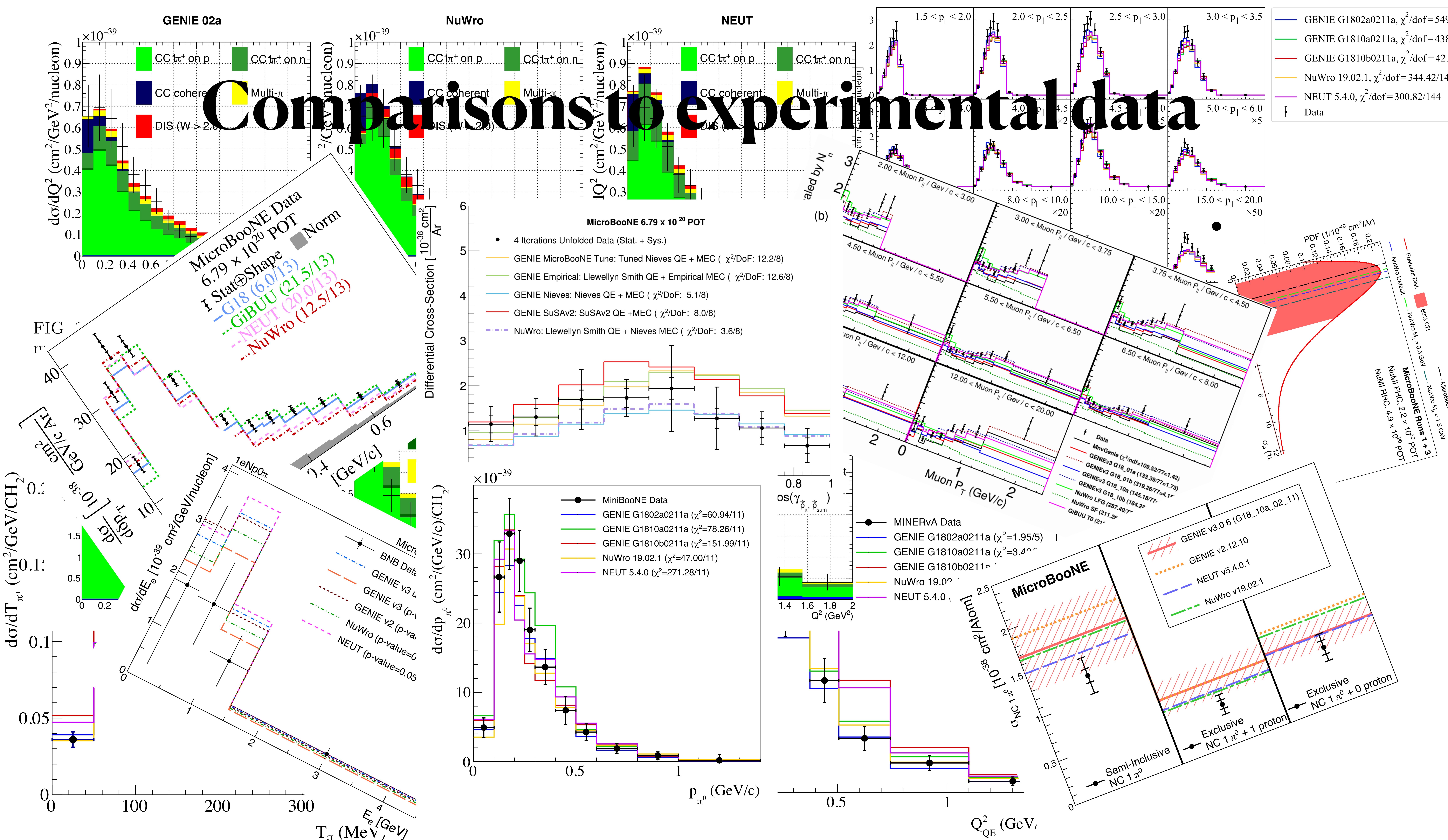
- The range of applicability is usually described as starting from ~100/200 MeV.
- Region of lower energy transfer needs e.g. CRPA model of Natalie Jachowicz.
  - GENIE has a model of CEvNS.
    - ➡ GENIE also has a model of CRPA but not fully incorporated.
  - NEUT sometimes need to be runned in 10-100 MeV region for estimation of BKGR from atmospheric neutrinos.



GIBUU performance
E=240 MeV, 36 Deg

- GiBUU:
  - ➡ Nuclear excitations described in average;
  - ➡ A limit of applicability is energy transfer < 50MeV

Comparisons to experimental data



-> Artur Ankowski

-> Adi Ashkenazi

Electron scattering

A powerful method of benchmarking neutrino MCs.

- A lot of precise electron scattering data (mostly inclusive, though).
- Initial electron energy, energy and momentum transfers are known and it is possible to study individual dynamical mechanisms.

- Neutrino and electron scatterings share the same nuclear effects.
  - ➡ initial state,
  - ➡ final state interactions.

Electron scattering => vector part of the weak current operator.

Important new data from JLAb e4ν Collaboration. In the future data from Mainz.

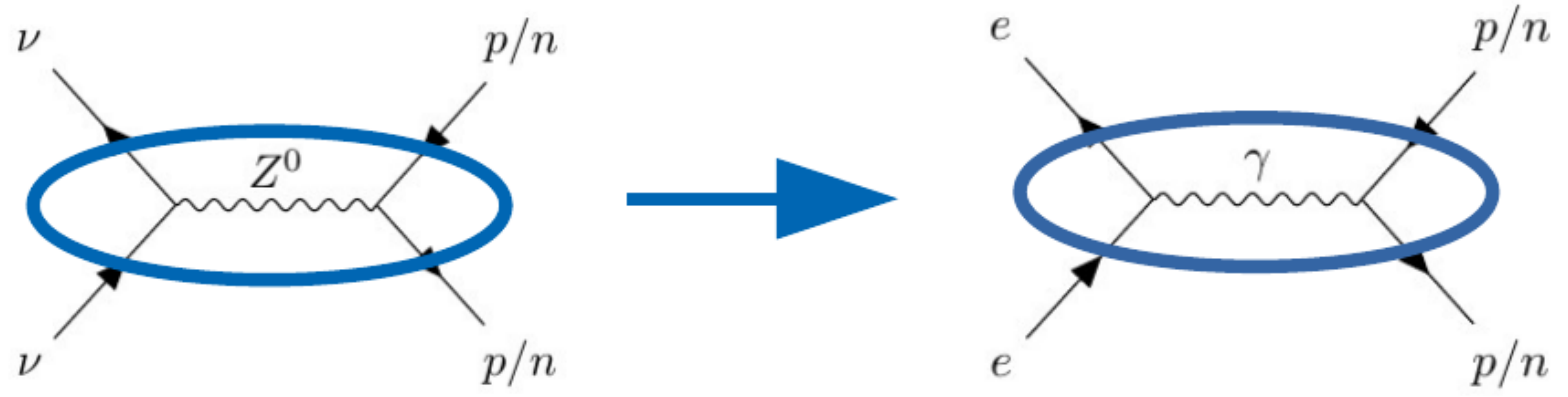
Electron scattering in MCs - practical issues

As much as possible should be left untouched,

➡ procedures to select initial nucleon, generate events, assign kinematics

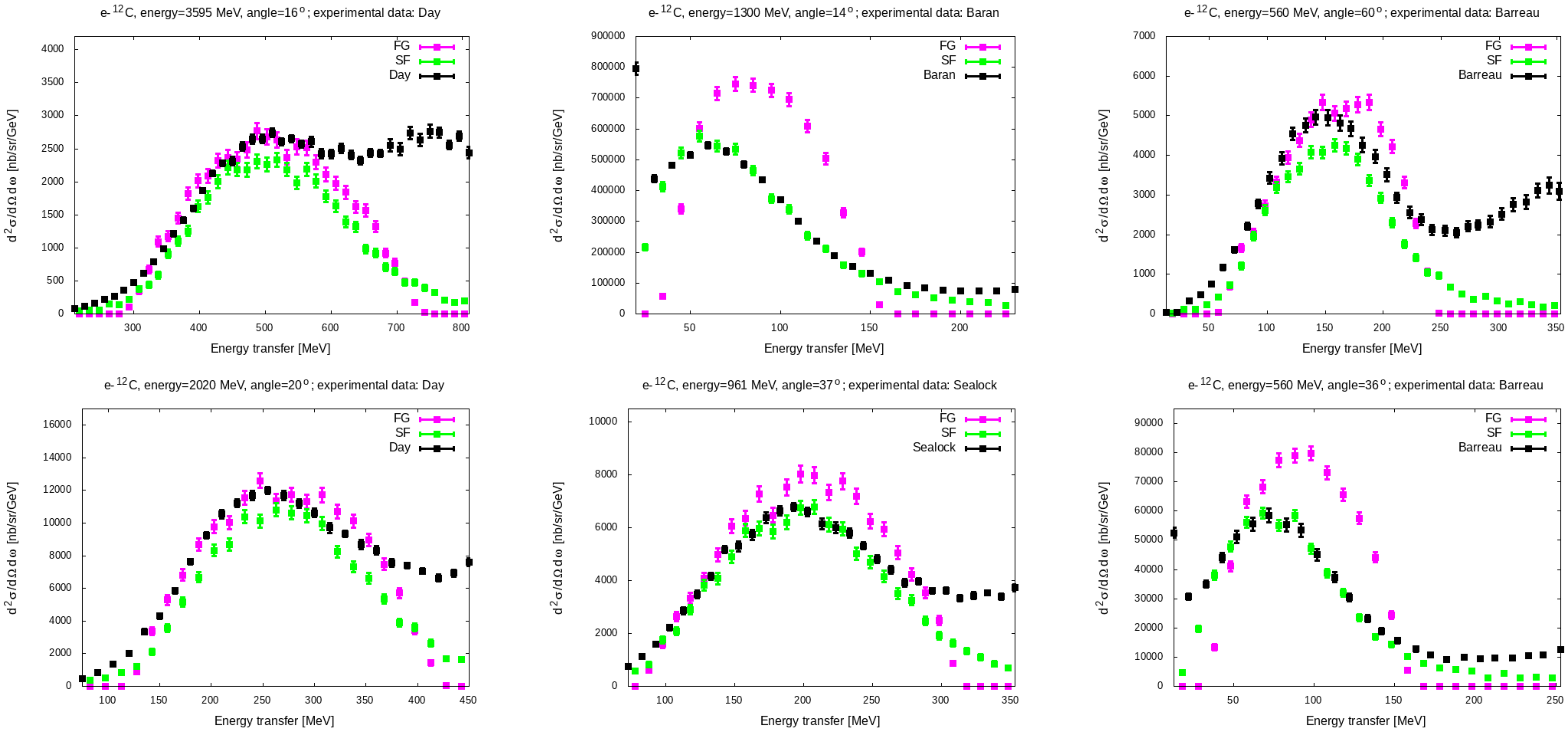
➡ FSI.

Vertices, boson propagator, vector form-factors are modified accordingly; axial contribution is removed.



Instead of collecting all events, one must specify a spherical cone (following an experimental acceptance!) to collect final state electrons.

Electron scattering - examples



Comparison of eWro (NuWro) implementations of spectral function and Fermi gas models with a sample of data.

-> Alexis Nikolakopoulos

Final state interactions

Several approaches to model FSI.

- GENIE hA model - one effective interaction only; easy in handling but cannot be accurate'
- Intranuclear cascade (NEUT, NuWro, GENIE hN model) - extensively studied for decades.
- Hadronic transport model (GiBUU) - better theoretical justification; time consuming in practise.
- INCL, Achilles - alternative way of modelling hadron-hadron interactions.

Key ingredient are microscopic nucleon-nucleon cross sections for bound off-shell hadrons.

Cascade model

Basic theoretical assumptions (Y. Yariv et al):

- Energies transferred in collisions are large compared to binding energy.
- Hadrons wave-packages have good enough definitions of position and momentum.
- De Broglie wave length is much smaller than mean-free-paths between collisions.
- Scattering from different nucleons can be considered independent.
- With many scatterings interference terms between scattered waves cancel out.

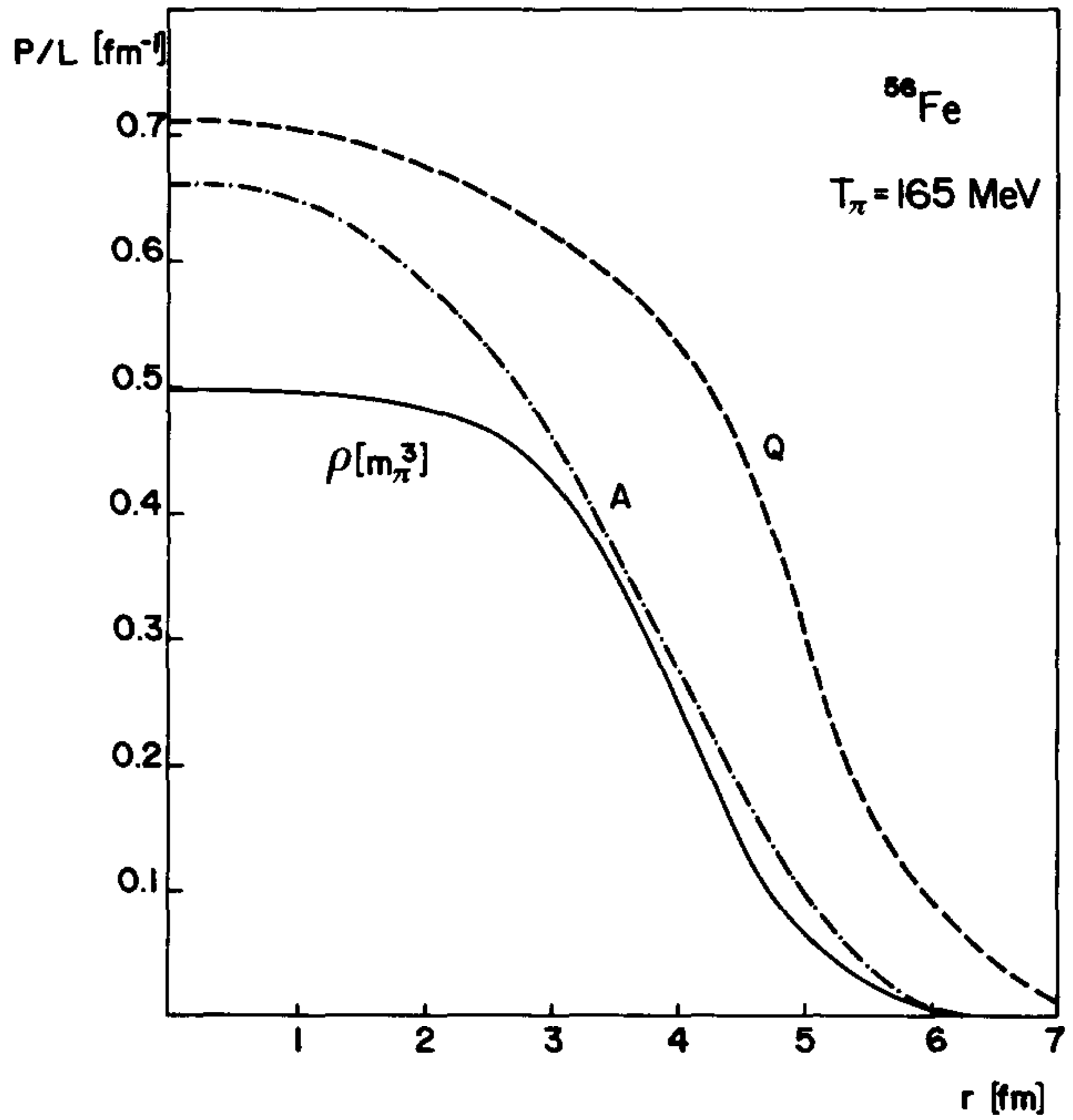
Assumptions are satisfied if nucleon kinetic energy is large enough (>200 MeV).

Final state interactions

Microscopic approaches:

Pions:

LL.Salcedo, E. Oset et al, Nuclear Physics A484 (1988) 557-592



. Probability per fm for quasielastic scattering (dashed line) and absorption (dashed dotted line) and nuclear density (in pion masses) as a function of the radius.

Nucleons:

V. R. Pandharipande and S. C. Pieper, Phys. Rev. C45 (1992)791.

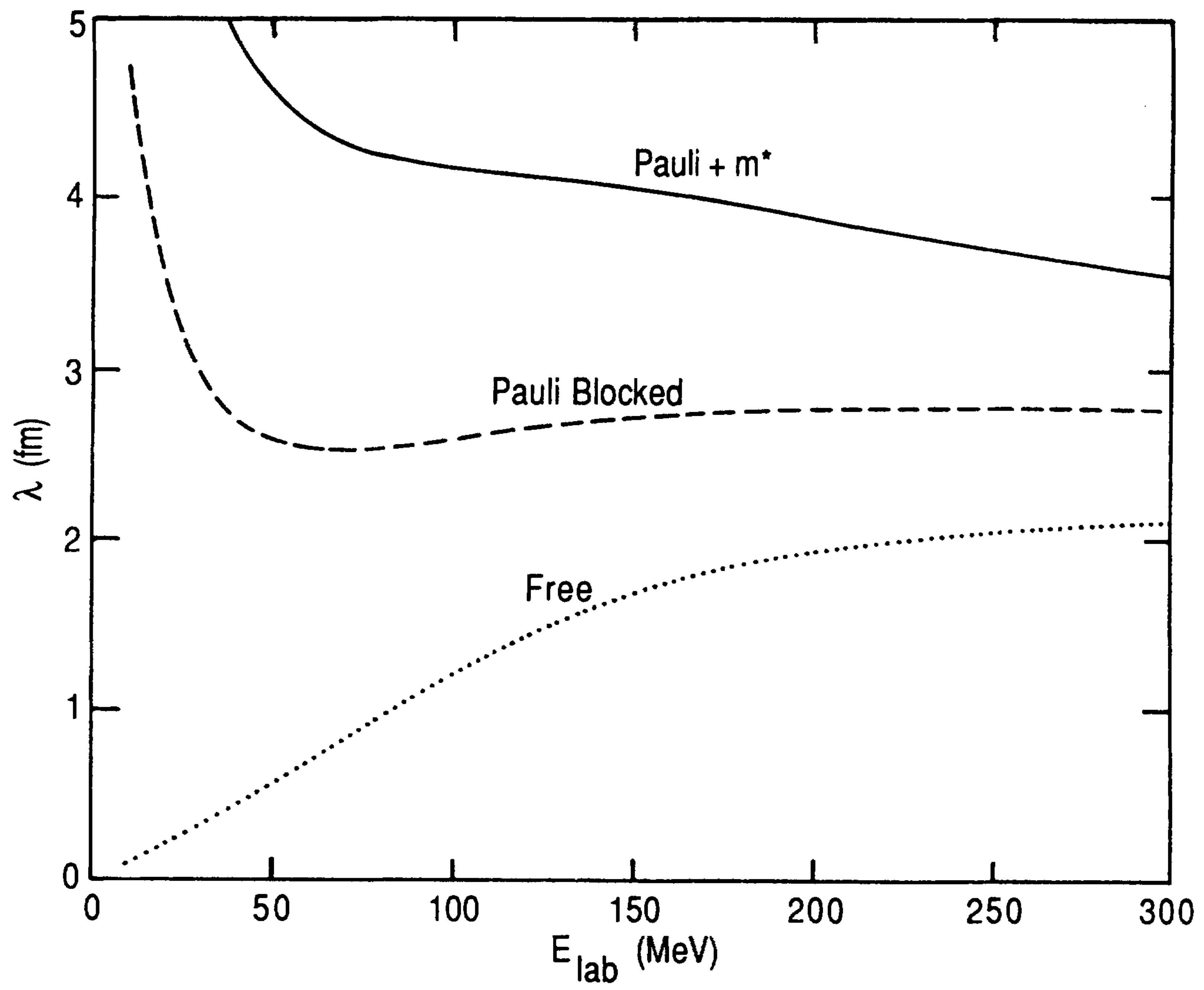
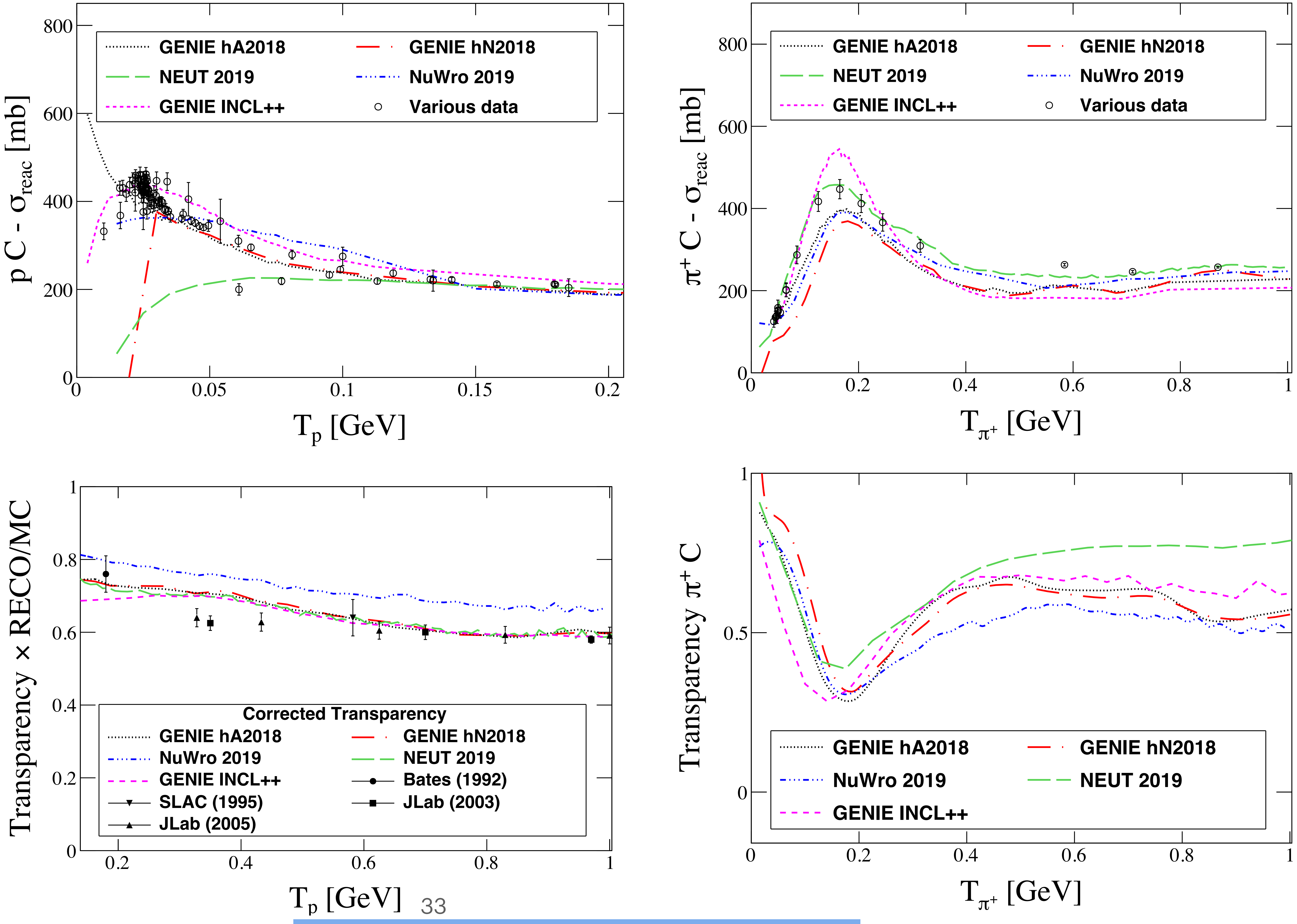


FIG. 3. The mean free path of protons in symmetric nuclear matter at saturation density as a function of the proton energy.

Final state interactions

Monte Carlo FSI models are tested against hadron-nucleus cross section and hadron transparency data.

Correction factor is necessary because „MC transparency" is not the same as experimentally measured transparency (soft scatterings are not seen).



S. Dytman et al, *Phys.Rev.D* 104 (2021) 5, 053006

-> Alessandro Lovato (?)

Final state interactions

Transparency versus reaction cross section

Alternative approaches to cascade lead to distinct relations between transparency and reaction cross section.

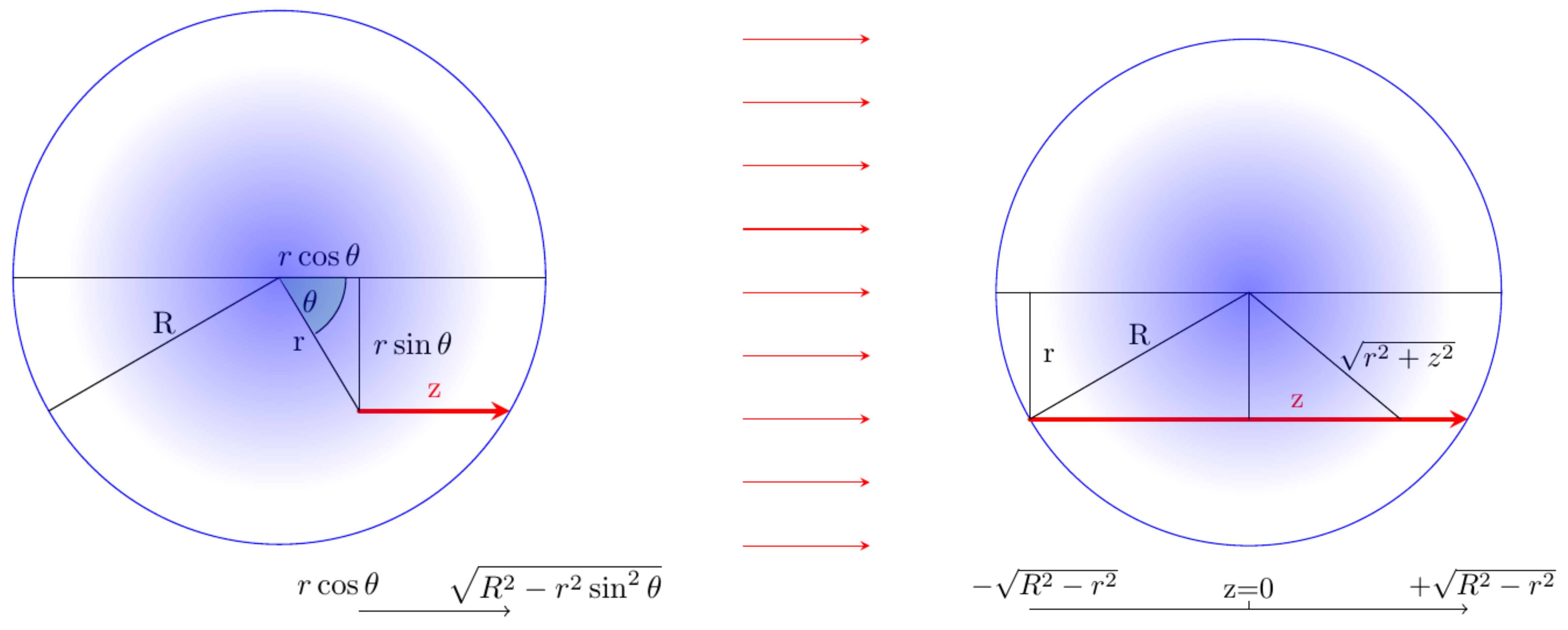
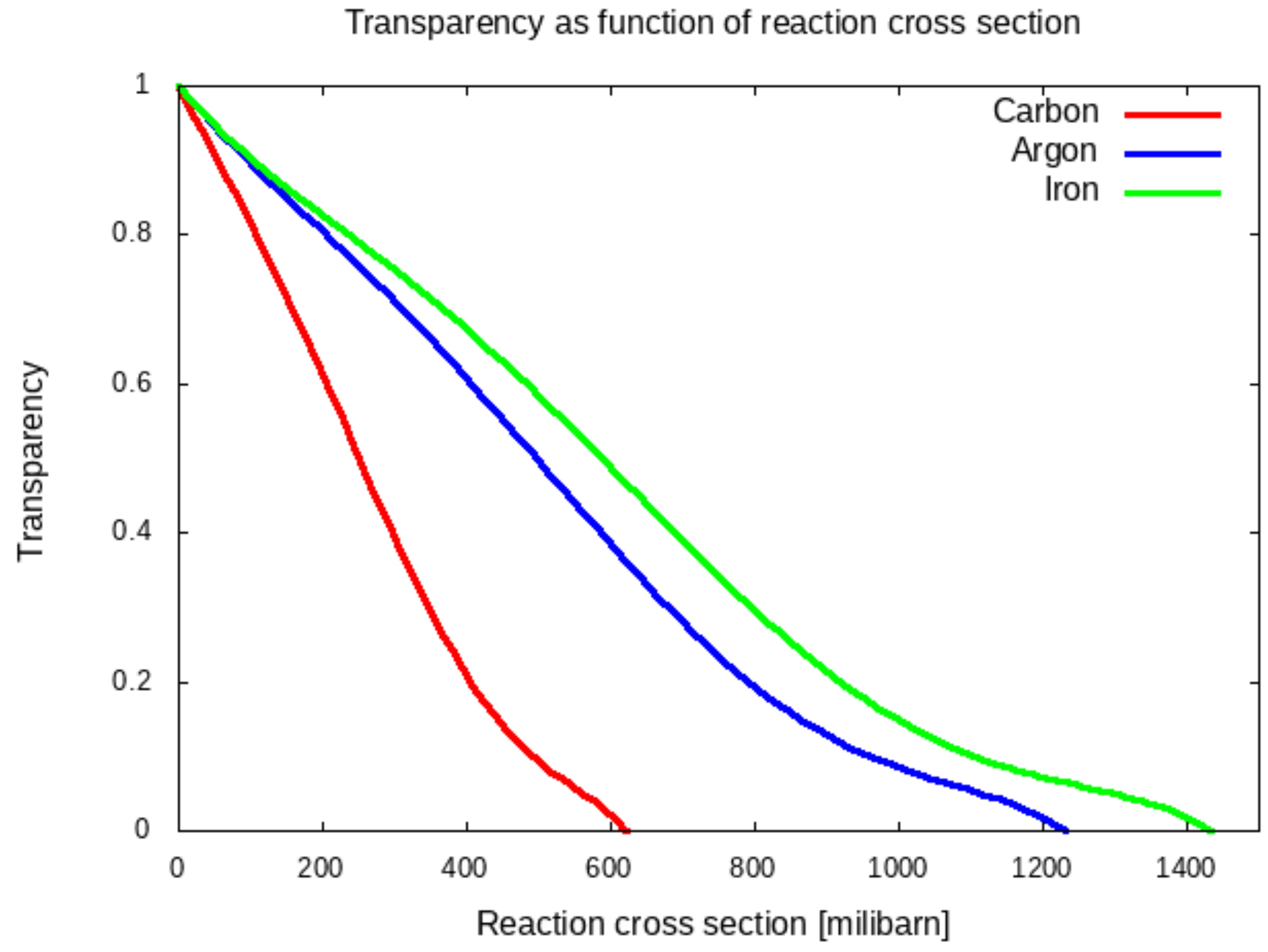


FIG. 1. Computation of transparency (left) and reaction cross section (right) in the toy model.

$$T = \frac{2\pi}{A}\int_{-1}^{+1} d(\cos\theta)\int_0^R dr\ r^2\rho(r) \cdot \exp\left\{-\int_{r\cos\theta}^{\sqrt{R^2-r^2\sin^2\theta}} dz\sigma\tilde{\rho}\left(\sqrt{z^2+r^2\sin^2\theta}\right)\right\}$$

$$\sigma_{reac} = \pi R^2 - 2\pi\int_0^R dr\ r \cdot \exp\left\{-\int_{-\sqrt{R^2-r^2}}^{\sqrt{R^2-r^2}} \sigma\rho\left(\sqrt{z^2+r^2}\right) dz\right\}$$



Points on the curves correspond to values of microscopic cross section

S. Dytman et al, *Phys.Rev.D* 104 (2021) 5, 053006

-> Noemi Rocco (?)

Systematic uncertainties

Not only central predictions but also estimate of theoretical uncertainties

Sources of theoretical uncertainties

- Incomplete knowledge of parameters inside theoretical models

   ➡ e.g. value of axial mass M_A in dipole axial FF

- Approximations used in theoretical computations.
- Limitations of assumptions defining a theoretical approach.

Full detector MC simulations are time consuming => effort to translate theoretical uncertainties into *reweighting factors*.

Events are unchanged but they get multiplicative factors - weights.

Difficult if uncertainty applies to the phase space.

NuWro event reweighting tools

NuWro like other MCs developed event reweighing tool

- `reweight-to` reads events from the output root file and re-calculates the cross sections for the new values of parameters, keeping the kinematics and the event topology unchanged.
- Two options for storing the effect od reweighting: either a new root file with modified weights, or a file containing array with new weights
- A list of available reweighting includes: C_5^A, M_A^{RES} and non-resonant background for pion production, M_A^{CCQE} for CCQE and NC elastic, z-expansion parameters, overall normalization of individual dynamics.
- NEUT and GENIE are more advanced.

Outlook

- Good quality of Monte Carlo event generators is essential for a success of long baseline neutrino program.
- In the last ~10 years physics models implemented in MCs improved significantly compared to the era of Fermi gas.
- There is a lot of activity, several independent codes are developed.

  ➡ Advantage: possibility to check correctness of implementations.

  ➡ Disadvantage: often duplication of work.

  ➡ Hard to find young people to work on MCs: need a knowledge theory, coding skills and understanding of experimental demands.