Fermilab U.S. DEPARTMENT OF ENERGY Office of Science

Theory Systematics

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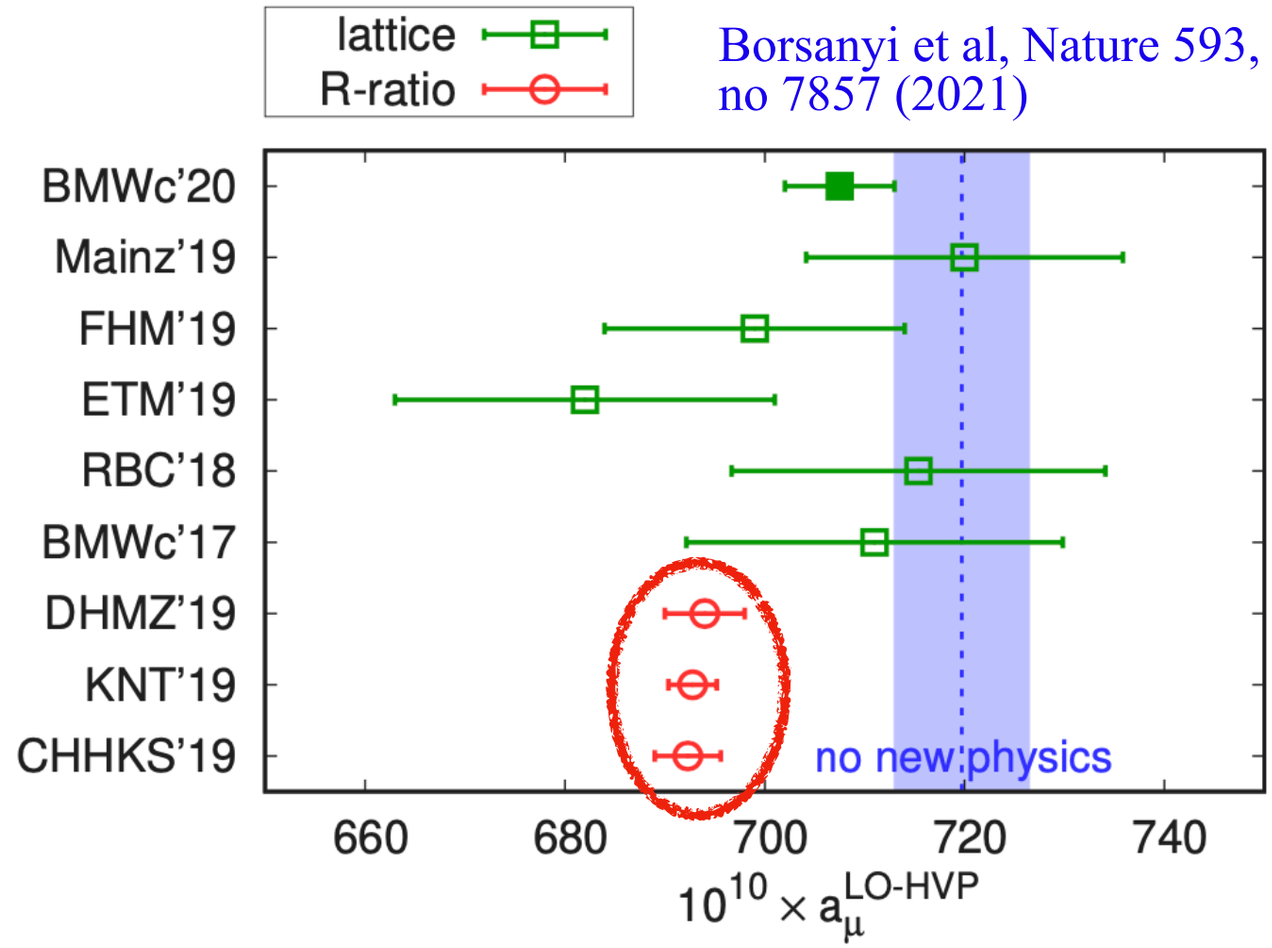
Workshop on Neutrino Event Generators

March 16, 2023

Why care about theory systematics?

Discovering new BSM physics comes from finding discrepancies between experimental results and Standard Model predictions

- Agreement between different theory calculations is necessary but not sufficient for accurate theory predictions



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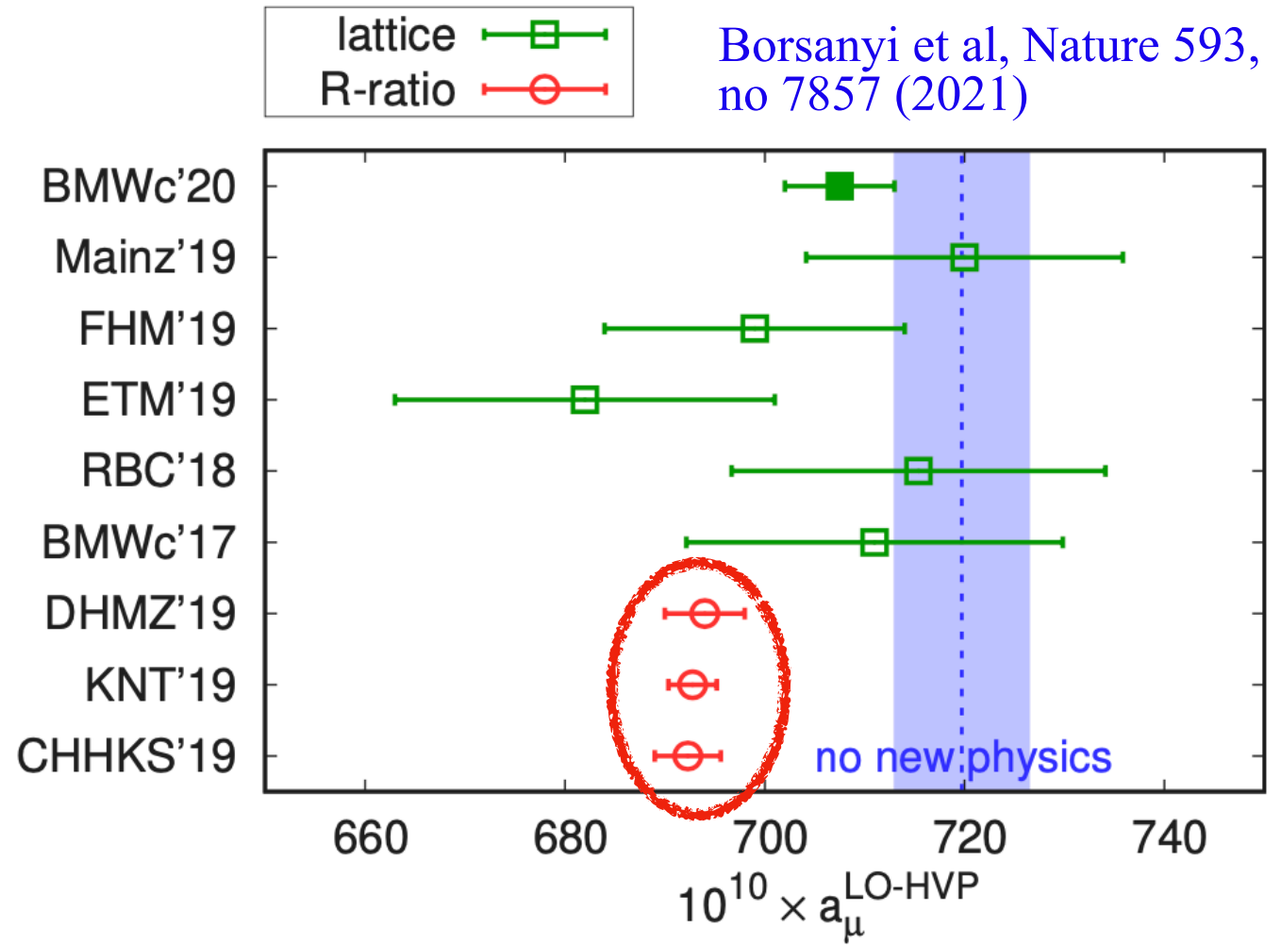


Consider a nightmare about muon g-2:

1) Suppose the true Standard Model value of g-2 signals no new physics

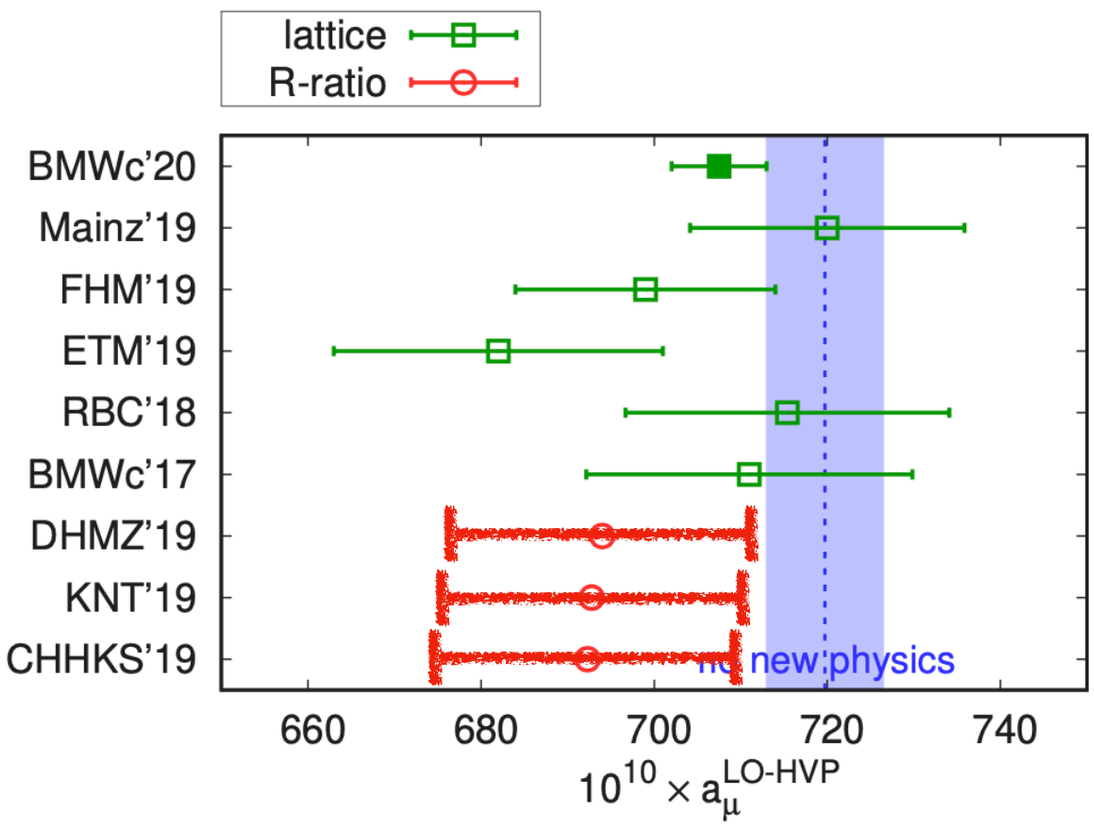
2) Suppose lattice QCD didn't reach BMWc 2020's precision until the 2030s

→ We might discover BSM physics and have to un-discover it 10+ years later…

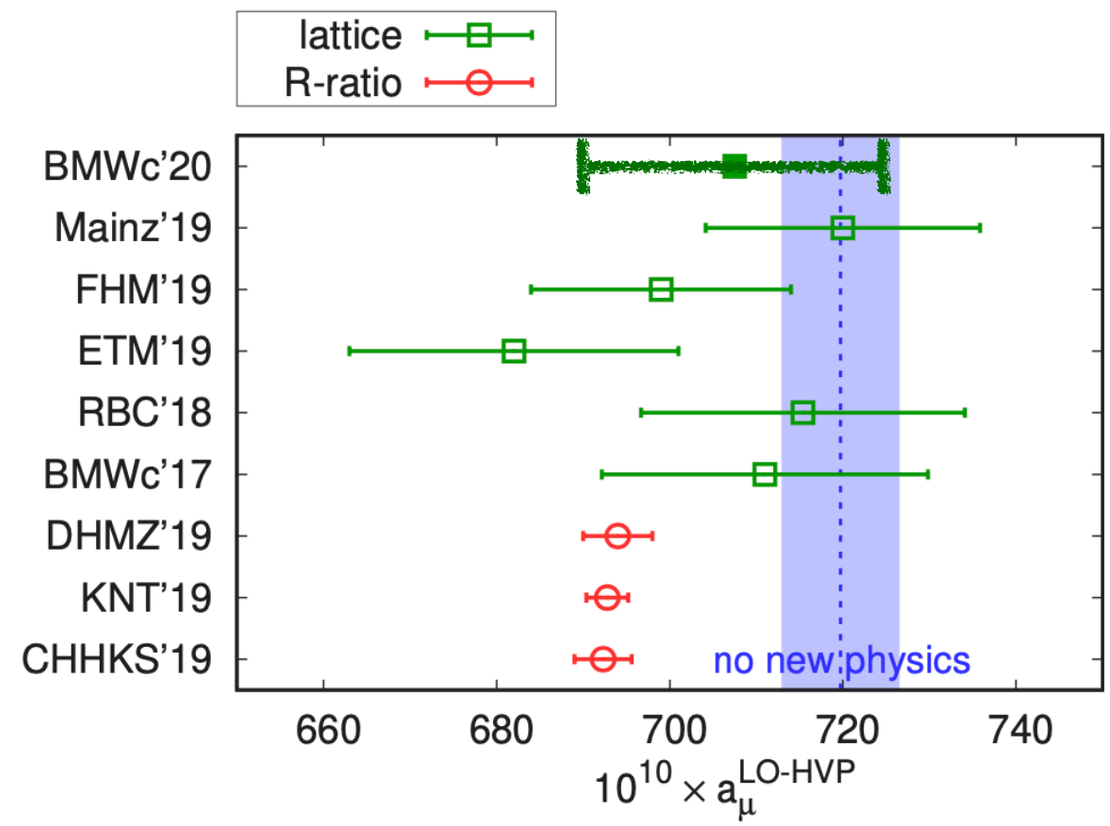
Why care about theory systematics?

Size of theory systematic uncertainties can make the difference between whether or not we think we've discovered new physics

What if R-ratio methods have underestimated theory systematics?



What if BMWc's calculation has underestimated systematics



What are theory systematics?

All the differences between theorists' calculations and the real world

- Functional form of the model (~0 for lattice QCD, significant for nuclear EFTs)
- Incomplete knowledge of input parameters
- Approximations used within calculations (non-zero lattice spacing…)

	$a_\mu^{\text{strange}}(L_{\text{ref}}, T_{\text{ref}})$		$a_\mu^{\text{light}}(L_{\text{ref}}, T_{\text{ref}})$		$a_\mu^{\text{disc}}(L_{\text{ref}}, T_{\text{ref}})$	
median	53.379		639.3		-18.61	
total error	111	(0.2%)	4.6	(0.7%)	1.56	(8.3%)
statistical error	89		2.0		1.03	
systematic error	67		1.9		1.11	
difference to NNLO improvement	–		3.7		0.36	
$M_\pi/M_K/M_{ss}$ fit	5		<0.1		<0.01	
$M_\pi/M_K/M_{ss}$ fit QED	3		0.1		<0.01	
M_Ω fit	56		0.3		0.04	
M_Ω fit QED	2		0.1		<0.01	
M_Ω experimental	5		0.1		0.01	
Continuum limit (beta cuts)	47		0.3		0.68	
$a^2\alpha_s^n$ with $n = 0$ or 3	–		1.1		0.57	
taste improvement ranges	–		0.7		0.11	
t_c in Table 11	–		0.2		0.23	

Approximations → difference to NNLO improvement

Input parameter tuning → $M_\pi/M_K/M_{ss}$ fit, $M_\pi/M_K/M_{ss}$ fit QED, M_Ω fit, M_Ω fit QED, M_Ω experimental

Approximations → Continuum limit (beta cuts), $a^2\alpha_s^n$ with $n = 0$ or 3, taste improvement ranges, t_c in Table 11

Borsanyi et al, Nature 593, no 7857 (2021)

Determining theory systematics

1) Perform additional (less precise) calculations to estimate the size of effects not included in primary calculation

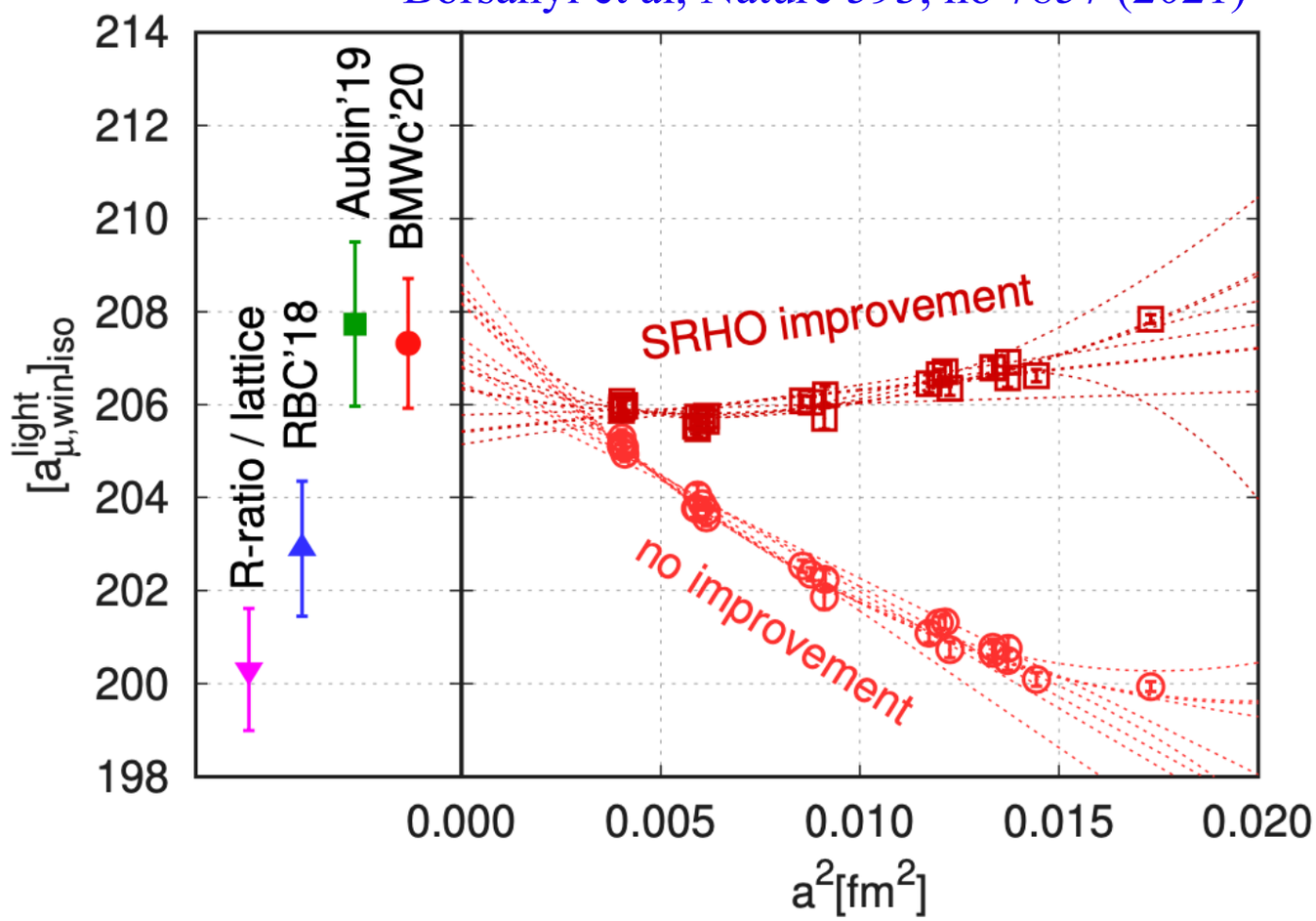
- Finite-volume effects can be approximately calculated in chiral EFT, even for quantities where we need lattice QCD for short-distance physics

2) Fit a model of systematic effect to data and subtract the best-fit

- Not choosing an overly-constrained model is essential for accurately estimating uncertainties

- Variation between results using different models provides an (incomplete!) estimate of residual systematic uncertainties

Borsanyi et al, Nature 593, no 7857 (2021)



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Defining a perturbatively renormalizable EFT for even low-energy nuclear physics remains an unsolved problem

Kaplan, Savage, and Wise, Nucl. Phys. B478 (1996);
Fleming, Stewart, Mehen, Nucl.Phys.A 677 (2000);
Nogga, Timmermans, and van Kolck, PRC 72 (2005);

Reviews: van Kolck, Front. in Phys. 8 (2020)
Epelbaum, Krebs, and Reiner, arXiv:2206.07072

tl;dr nuclear physics is hard

Even so, regularized EFTs and phenomenological nuclear models can do a very good job of describing low- and medium-energy nuclear phenomena

- It's essential to study systematic uncertainties arising from our imprecise knowledge of nucleon-level effective Hamiltonians

See Noemi's half of the talk up next!

$$H = \sum_i K_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

Nucleon kinetic energy **NN potential** **3N potential**

Model selection

Modeling systematics is an art, but model selection is math

- Polynomial expansions are just as expressive as neural nets in the limit of an infinite number of parameters — the (important!) differences are convergence rate for a given problem and generalizing from fit to prediction

Weierstrass, *Akademie der Wissenschaften zu Berlin*, (1885)

Cybenko, *Mathematics of Control, Signals, and Systems*, (1989)

- Once you have specified a family of parametric models, **information criteria** like the **AIC** provide quantity metrics for choosing the "best" number of parameters

Example: form factor z expanion

Free parameters

Known function

$$F_A(Q^2) = \sum_{k=0}^{\infty} a_k \, z(Q^2)^k$$

Infinite series must be truncated at $k = k_{\max}$ to provide a practical fit function

- How to choose $k_{\max}$? Minimize AIC (plus overfitting penalties, priors, …)

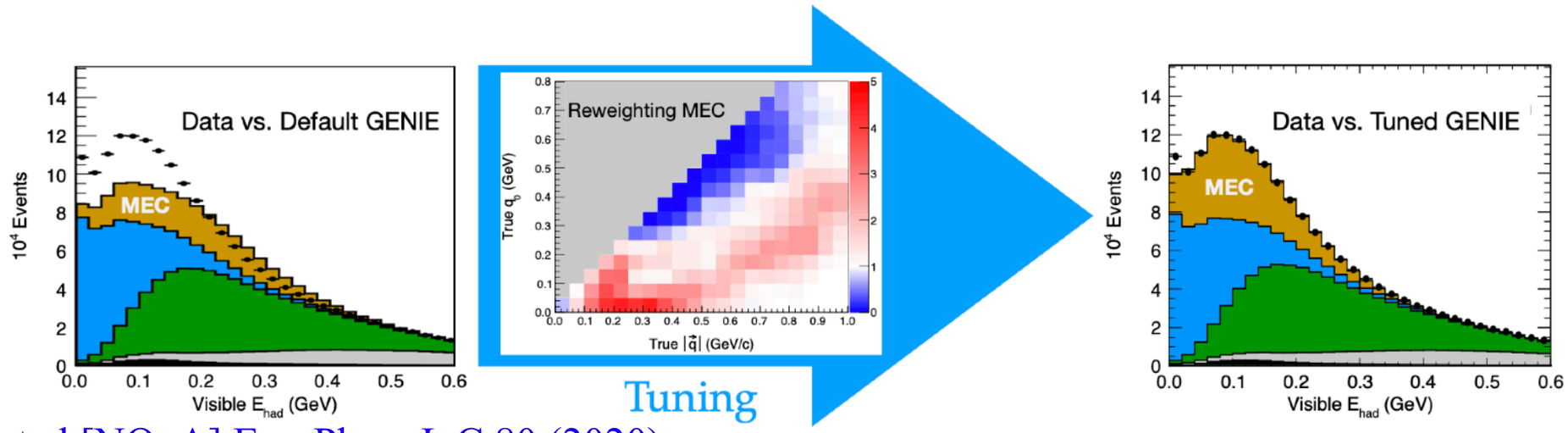
See e.g. Jay and Neill, PRD 23 (2021)

$$\mathrm{AIC}(k_{\max}) = \chi^2(k_{\max}) + 2(k_{\max} + 1)$$

Only include extra fit parameters if they provide "enough" improvement to χ^2

Tuning

Discrepancies between generators and data often corrected by tuning an empirical model of the least well known mechanism: MEC (“meson exchange”/two-body currents)



Acero et al [NOvA] Eur. Phys. J. C 80 (2020)

Coyle, Li, and Machado, JHEP 12, 166 (2022)

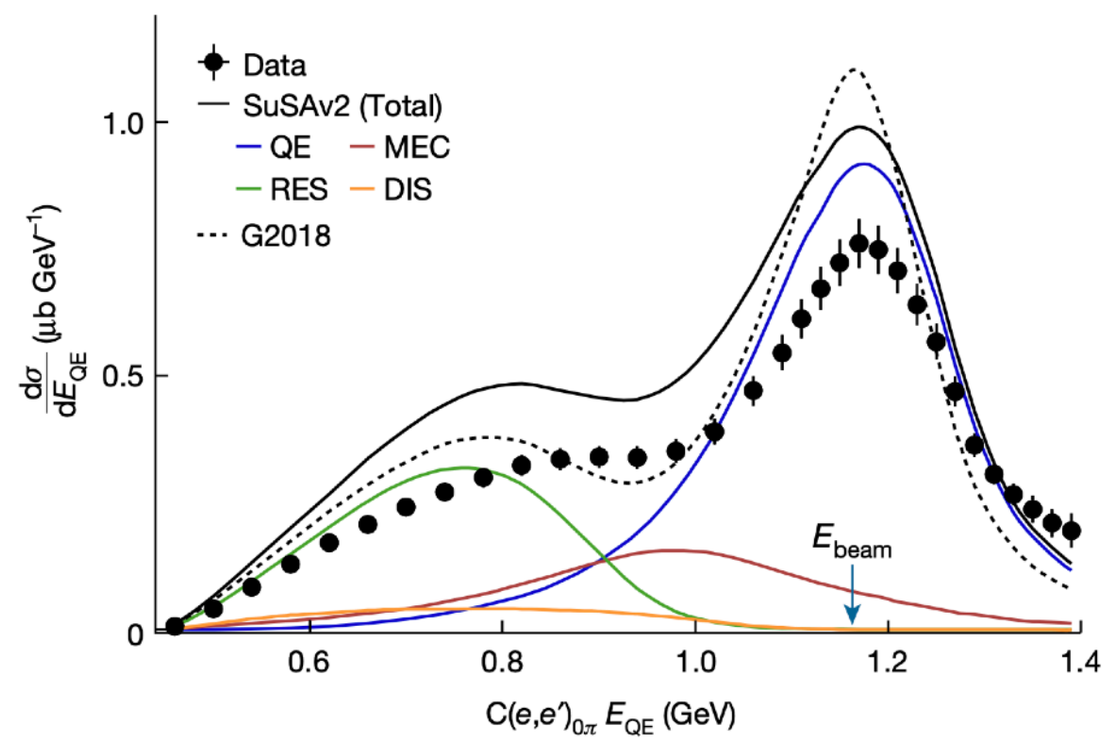
Sufficiently expressive MEC models can capture difference between theory and data for a given flux-averaged x-sec

- Tuning to reproduce one process does not mean other processes/energies will be accurately predicted, as nicely evidenced by $e4\nu$ results

Mid-modeling can distort signals of new physics, potentially biasing measurement of new physics parameters

Coyle, Li, and Machado, JHEP 12, 166 (2022)

Khachatryan et al [Clas and e4v] Nature 599 (2021)



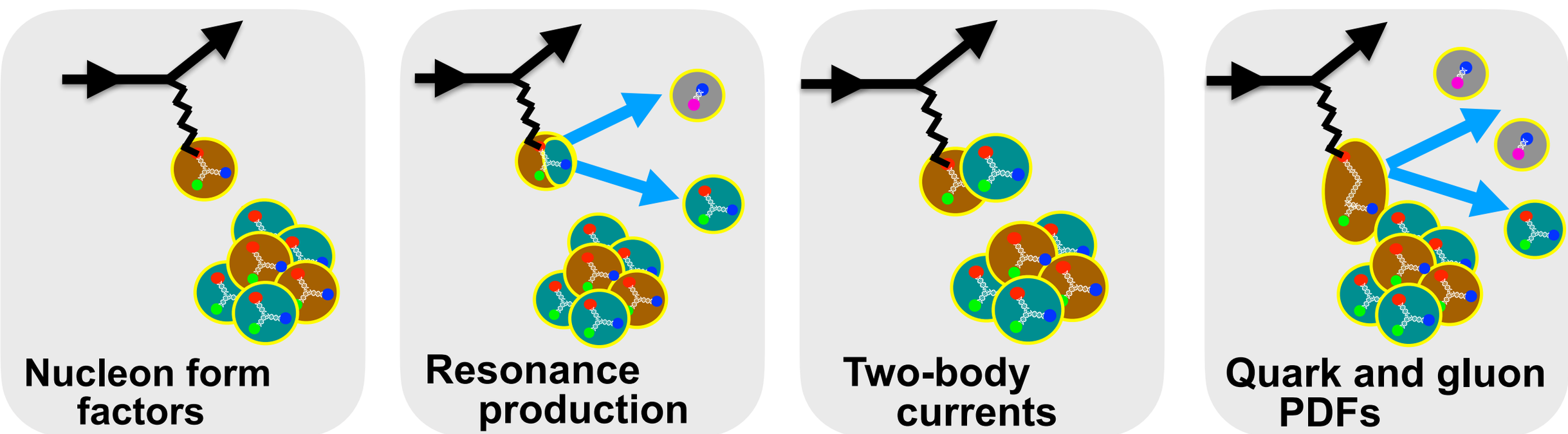
Getting to “Known Unknowns”

The first steps towards getting few-% cross-section uncertainties are understanding what input parameters we will need and what precision we will need them at.

- There is no EFT that coverages over all of DUNE kinematics

- We need data-driven nuclear models exploiting the generic hierarchy
  N-nucleon effects >> (N+1)-nucleon effects

- We need several few-nucleon observables (at …% precision) as inputs to anchor these models in experimental data + Standard Model theory



Quantifying form factor uncertainties

z expansion — model independent parameterization of axial (and other) form factors that only assumes basic field theory / QCD properties

Hill, eConf C060409, 027 (2006) Hill and Paz, PRD 82 (2010) Bhattacharya, Hill, and Paz, PRD 84 (2011)

$$F_A(Q^2) = \sum_{k=0}^{\infty} a_k \, z(Q^2)^k$$

Free parameters

Known function

$|z(Q^2)| < 1$

We should also be using this to describe resonant and non-resonant pion production form factors

Can be used to quantify relations between nucleon axial form factor uncertainties and neutrino-nucleus cross section uncertainties

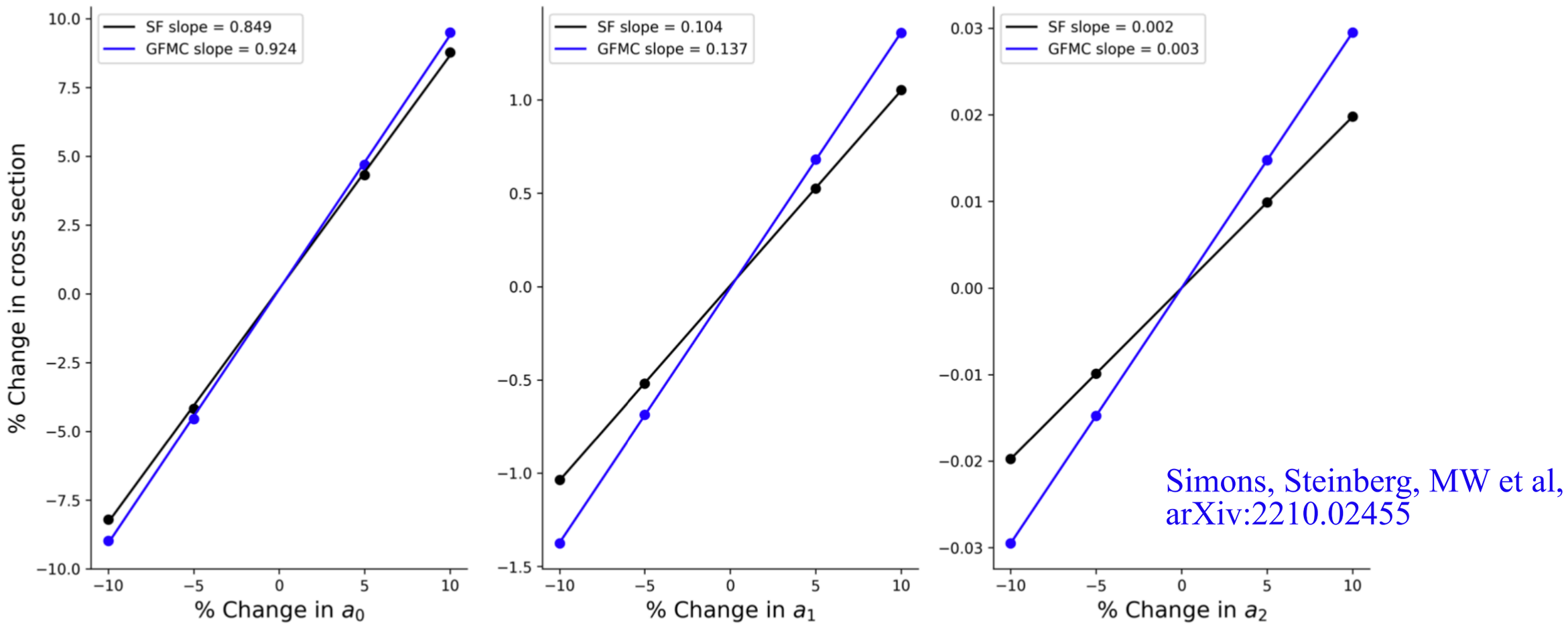
$$\delta\sigma = \sum_k \frac{\partial \sigma}{\partial a_k} \delta a_k + \ldots$$

Straightforward to determine from calculations with varying a_k

Simons, Steinberg, MW et al, arXiv:2210.02455

Axial FF uncertainty needs

Uncertainty relations calculated for MiniBooNE cross sections



Achieving 1% cross-section precision for MiniBooNE kinematics requires:

- ~ 1% precision in a_0
- ~ 10% precision in a_1
- Relatively little knowledge of $a_2, \ldots$

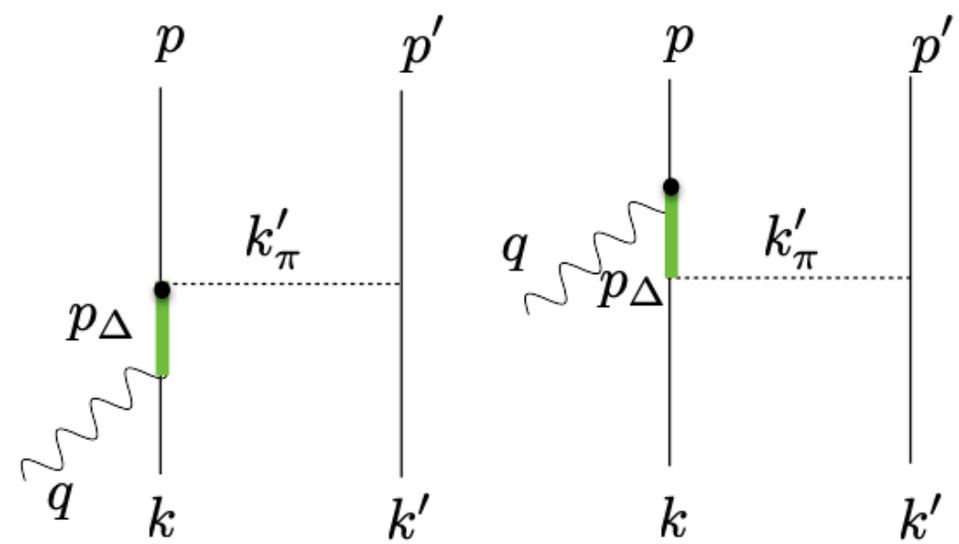
LQCD target

DUNE will be more sensitive to higher coefficients, further dedicated studies needed

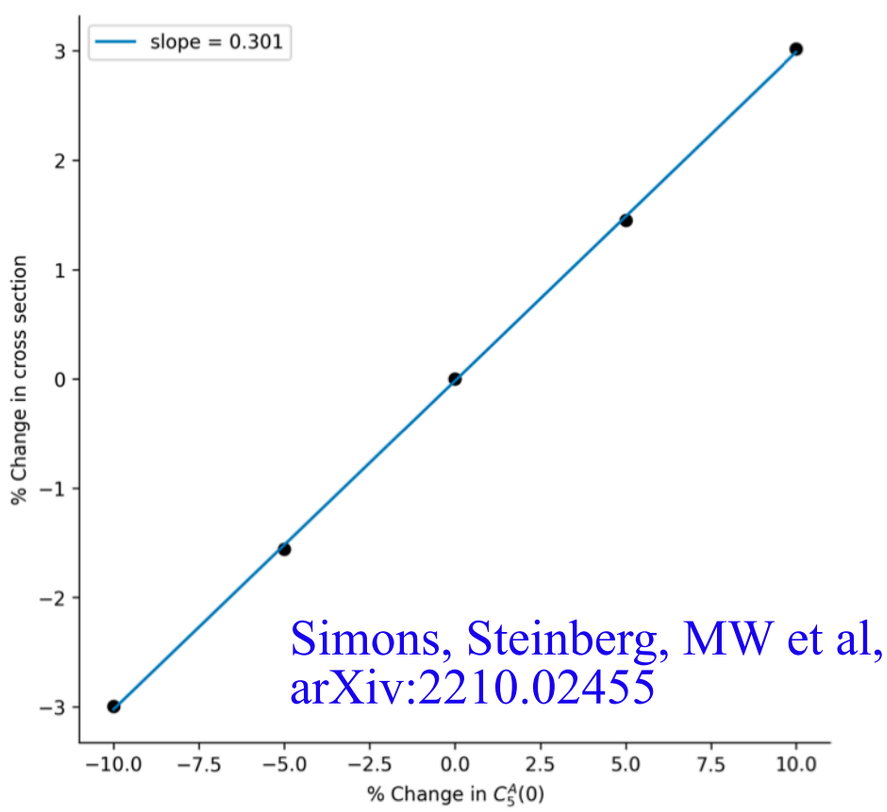
Resonance uncertainty needs

Similar uncertainties quantification can be studied for other cross-section pieces

The largest contributions to two-body currents arise from resonant $N \to \Delta$ transitions in conjunction with pion exchange



The normalization of the dominant $N \to \Delta$ transition form factor must be known to 3% precision to achieve 1% cross-section precision for MiniBooNE kinematics



Simons, Steinberg, MW et al, arXiv:2210.02455

State-of-the-art determinations of this form factor from experimental data on pion electroproduction achieve 10-15% precision (under some assumptions)

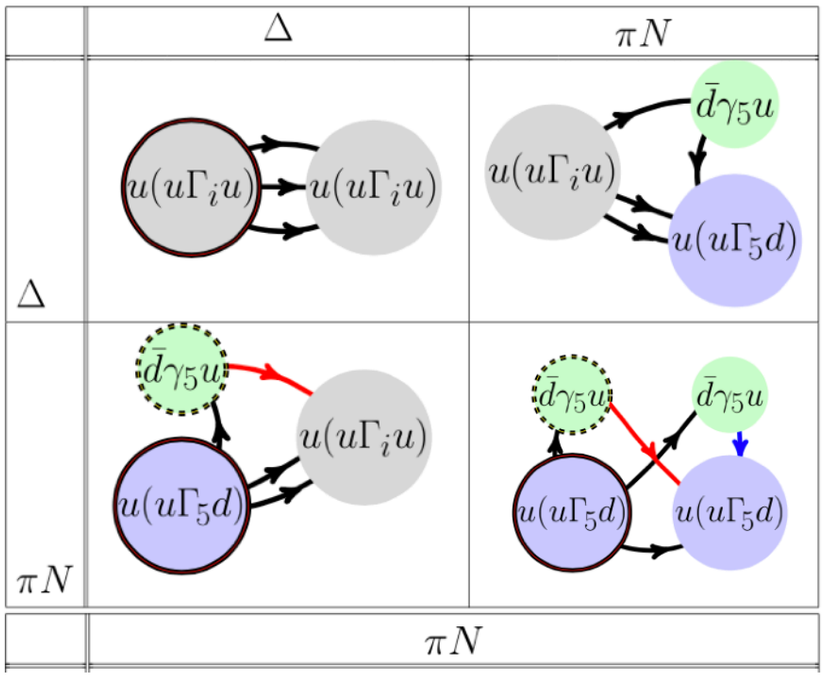
Hernandez et al, PRD 81 (2010)

Further constraints on $N \to \Delta$ transitions and two-body currents will be necessary to achieve few-percent cross-section precision

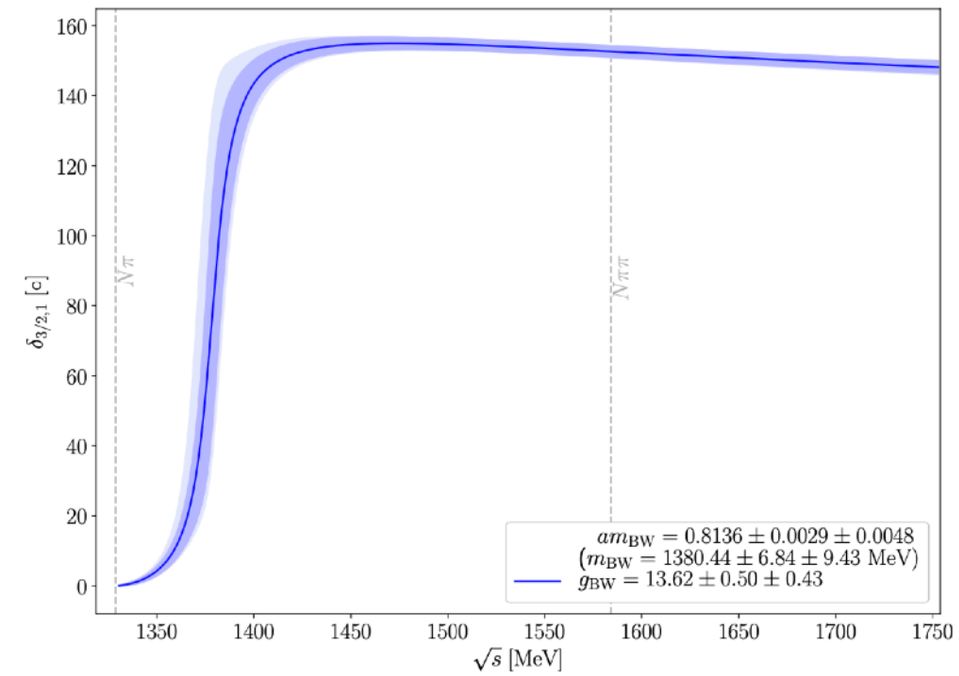
$N\pi$ systems in LQCD

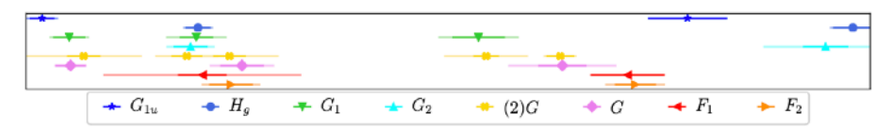
$N\pi$ and Δ systems can be explicitly studied in LQCD

Silvi et al, PRD 23 (2021)



$N\pi$ p-wave phase shift



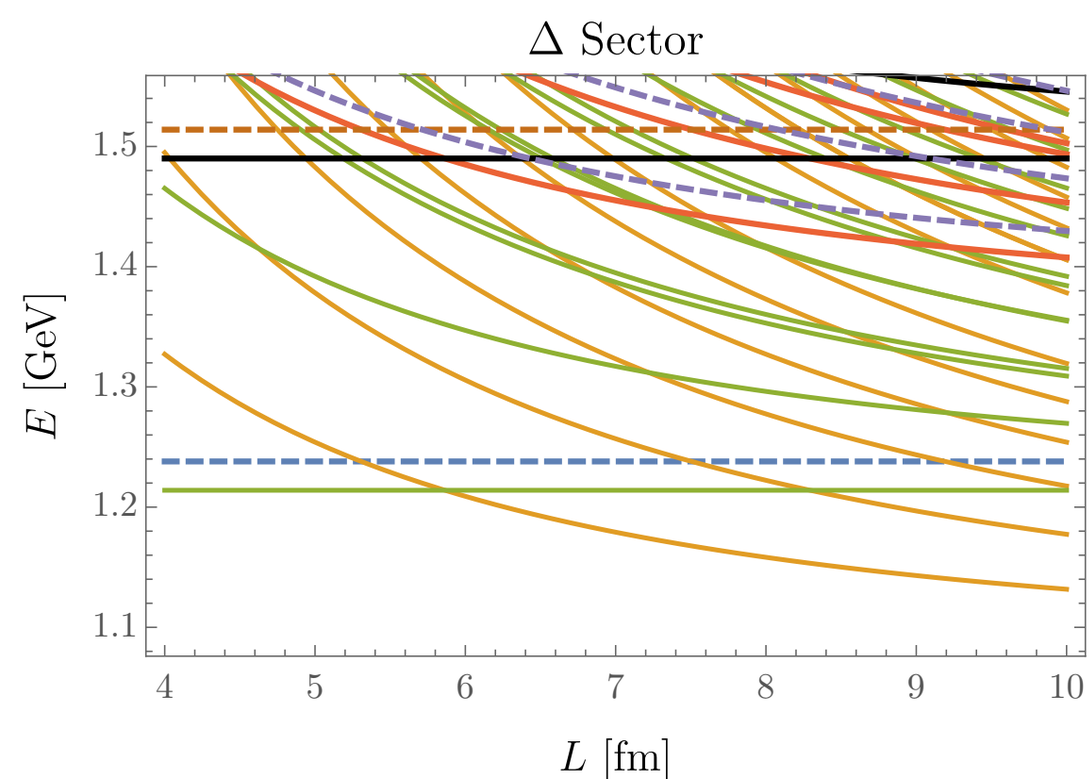


$N \to \Delta$ transition form factors can also be calculated with variational methods

Barca, Bali, and Collins, *PoS* LATTICE 2021 (2022)

Fully mapping out spectrum through the Δ resonance region will be challenging

Work in progress with Anthony Grebe



Takeaways (part 1)

Getting to few-% cross-section uncertainties will require

- Nuclear models with a limited number of parameters that can ideally be constrained using other data (e.g. few-nucleon potentials and currents, nuclear PDFs) implemented in event generators

- Relations between x-sec uncertainties and input parameter uncertainties providing precision goals for “known unknowns”

- Additional constraints on few-nucleon inputs from experiment and lattice QCD