

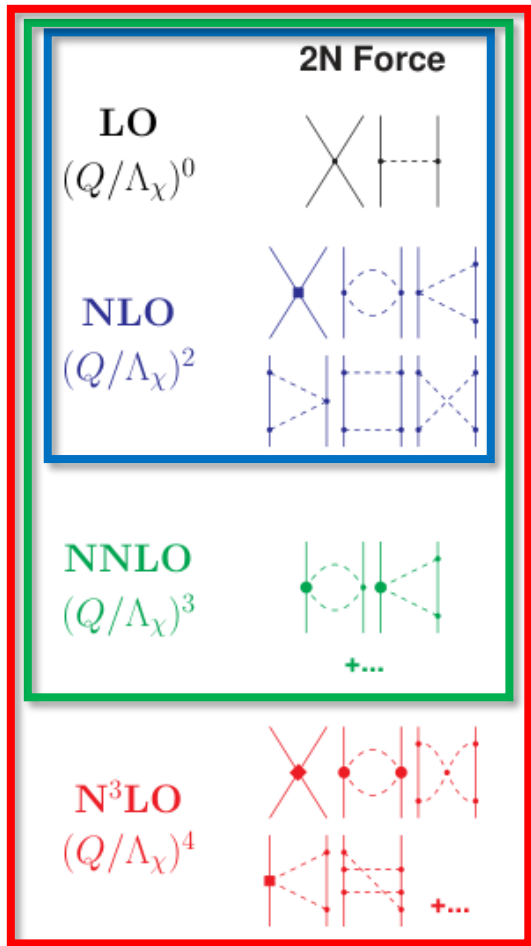
- Question: what is the best strategy to infer **the most probable values of low-energy constants in chiral EFT** from data?
 - Not only the most probable values
 - ***But also LEC distributions***
- Question: Can new computational paradigms such as ***machine learning*** (ML) and quantum computing (QC) change the game in low-energy nuclear physics?
 - ML is very promising

Estimating Uncertainties in Chiral Interactions with Normalizing Flows

Pengsheng Wen

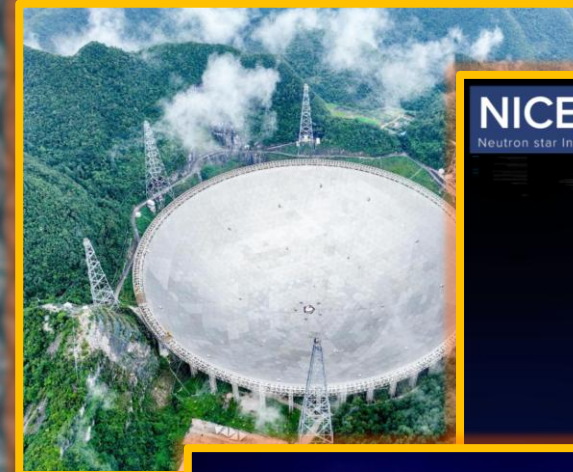
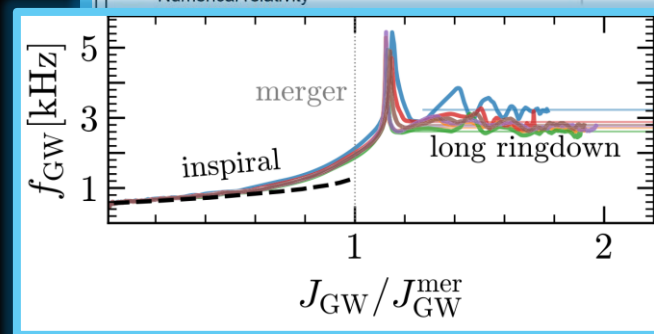
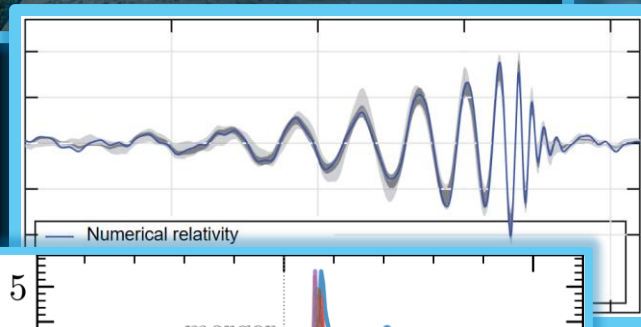
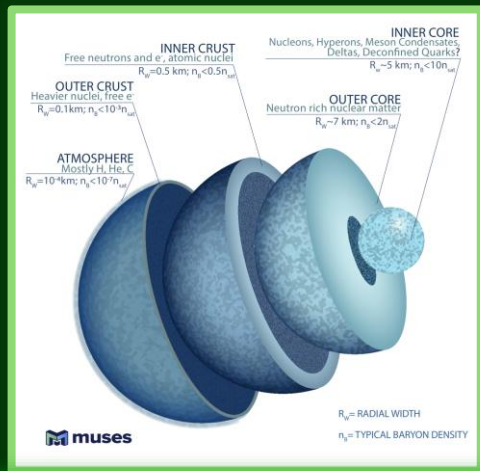
Jeremy W. Holt

Texas A&M University



Uncertainties in nuclear force from chiral effective field theory

Astrophysics motivation: Neutron stars and multiple messengers



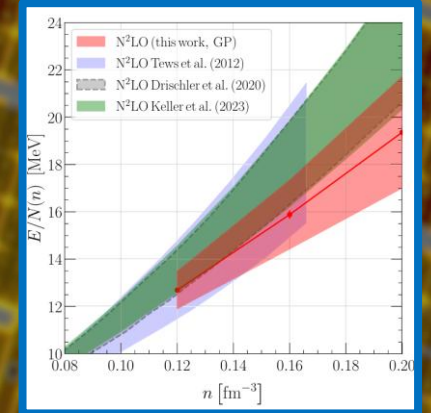
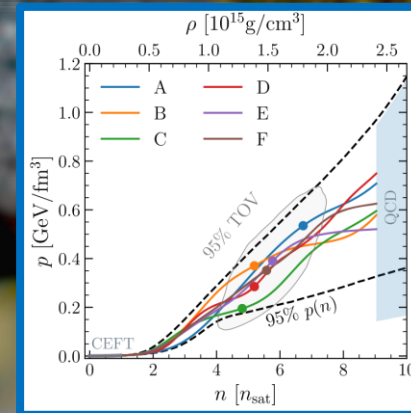
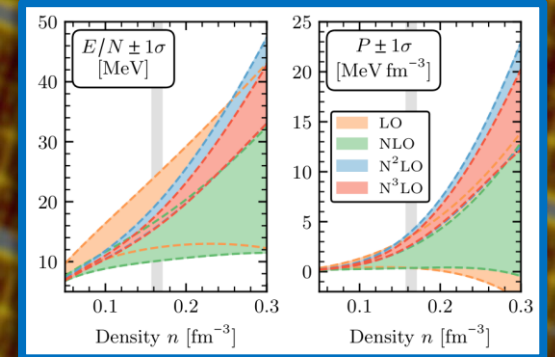
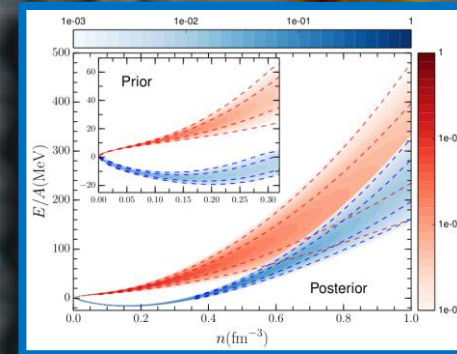
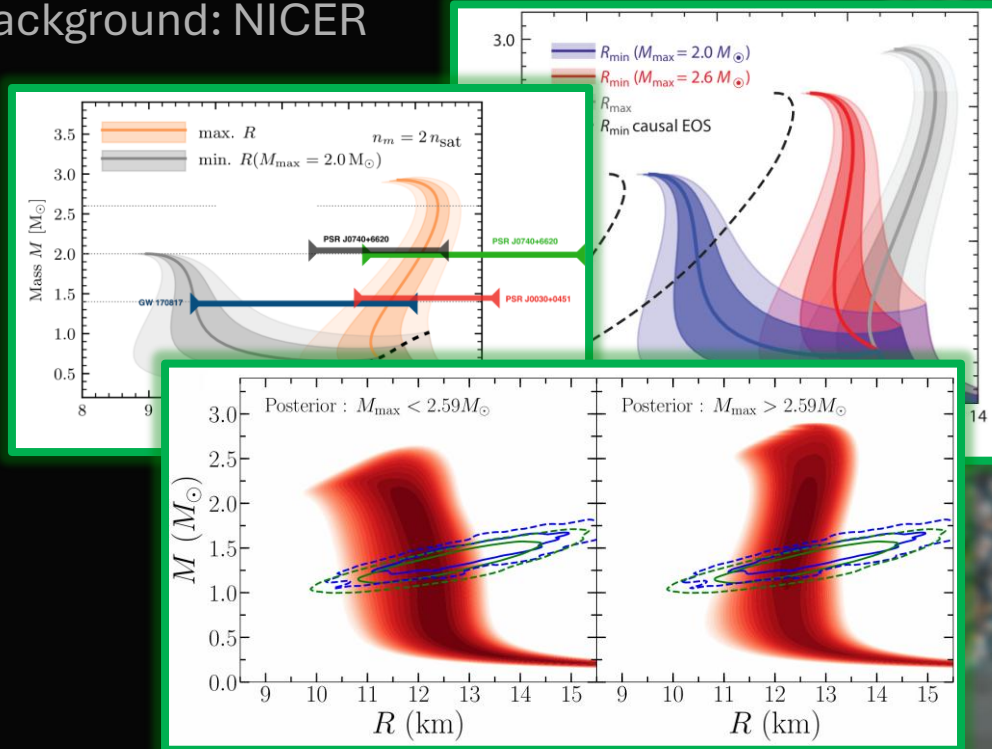
Neutron star

Gravitational wave

Electromagnetic signal

Nuclear equation of state uncertainties

Background: NICER



Uncertainty: Neutron star mass-radius relation

Uncertainty: nuclear equation of state

Lattimer, J. M., *Annu. Rev. Nucl. Part. Sci.* **71**, 433–464 (2021)
 NASA NICER Team
 Lim, Y. eta, *Phys. Rev. C* **104**, (2021)

Lim, Y., Holt, J., *Phys. Rev. Lett.* **121**, 062701
 Drischler, C., Holt, J. W. & Wellenhofer, C. *Annu. Rev. Nucl. Part. Sci.* **71**, 403–432
 Lattimer, J. M. *Annu. Rev. Nucl. Part. Sci.* **71**, 433–464
 Ecker, C., Gorda, T., Kurkela, A. & Rezzolla, L. *Nat Commun* **16**, 1320

Sources of uncertainty in chiral nuclear forces

order truncation n

+

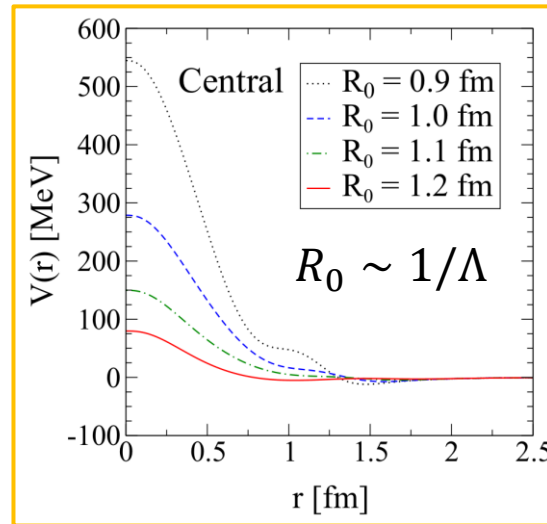
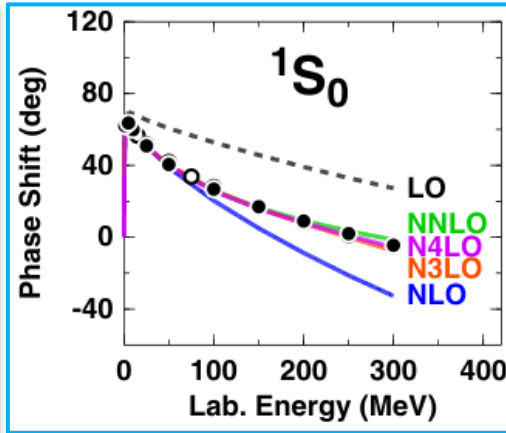
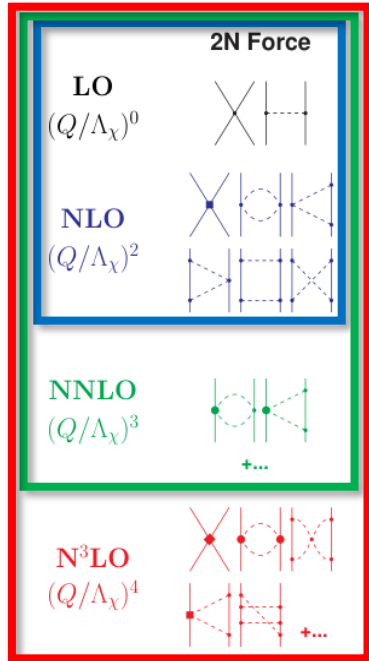
resolution scale Λ

+

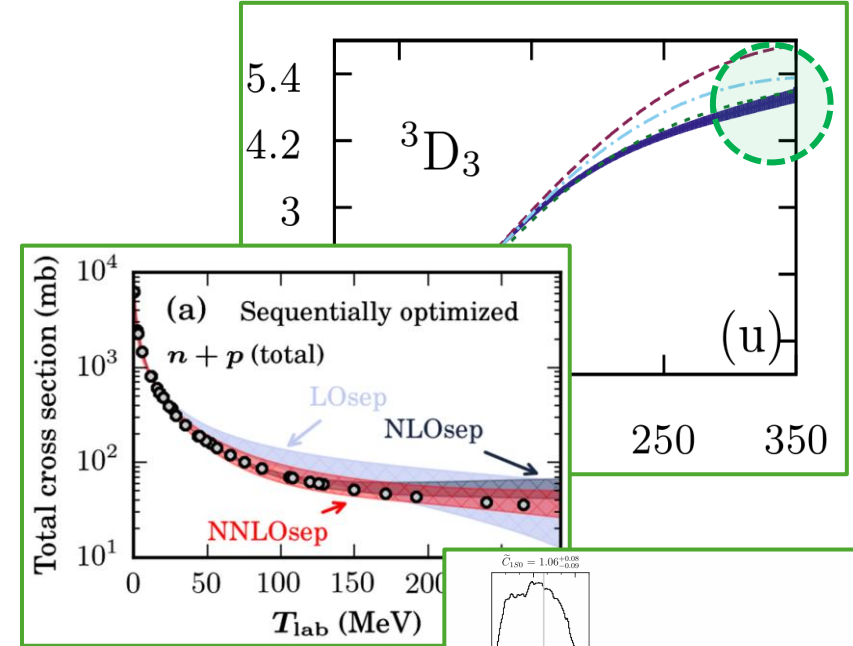
fitting LECs to experiment

Dynamic complexity
Long range
short range (LECs)

how the short distance physics is resolved



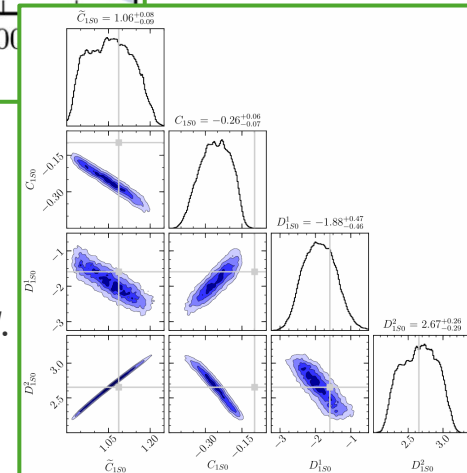
Gezerlis, A. et al. *Phys. Rev. C* **90**, 054323



Navarro et al.
Phys. Rev. C **89**, 064006

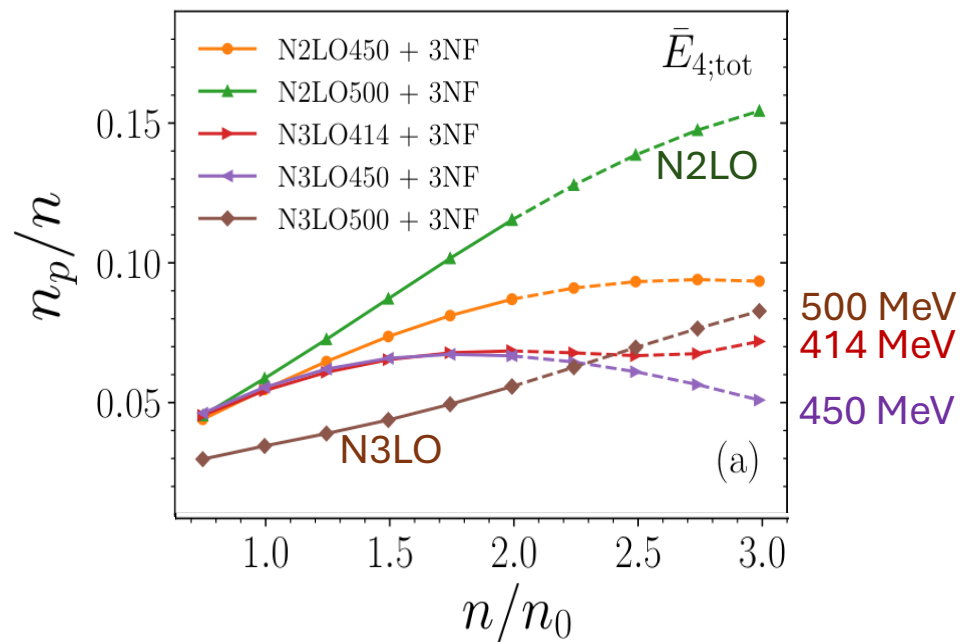
Carlsson et al.
Phys. Rev. X **6**, 011019

S Wesolowski et al 2019 *J. Phys. G: Nucl. Part. Phys.* **46** 045102

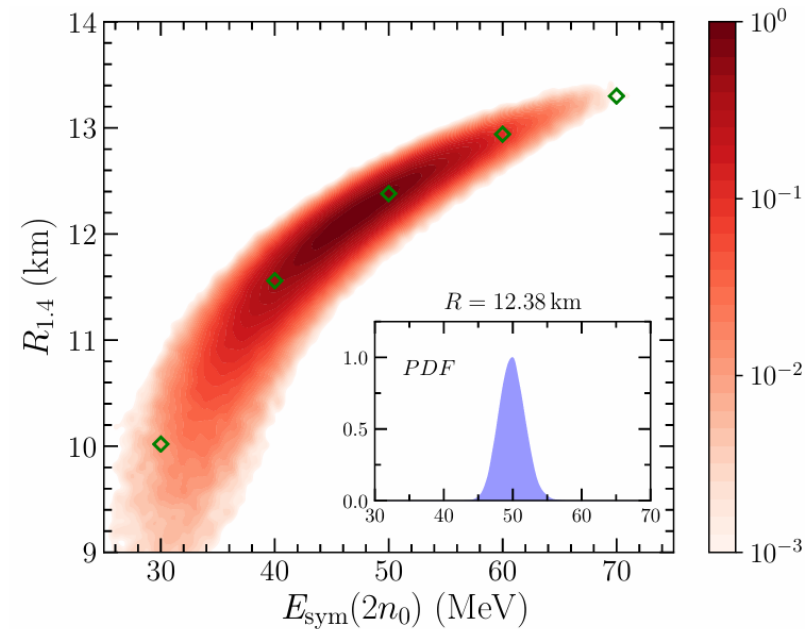


Propagated uncertainties to the nuclear equation of state

- Uncertainty shown in EOS and beyond
 - Source: **order truncation n + resolution scale Λ**
 - Propagated uncertainties to proton fractions, EOS and neutron stars



P. Wen, J. W. Holt, Phys. Rev. C 103 (2021) 6, 064002



Drischler, C., Holt, J. W. & Wellenhofer, C.
Annu. Rev. Nucl. Part. Sci. **71**, 403–432 (2021)

ChEFT uncertainties: recent progress

- (2003) Entem & Machleidt: 4th-order NN force, *PRC*
- (2013) Ekström, Baardsen, Forssén,...: optimized NN force at 3rd-order, *PRL*
- (2014) Gezerlis, Tews, Epelbaum, ...: Local NN force at 3rd-order for QMC, *PRC*
- (2015) Epelbaum, Krebs, and Meissner: improved NN force at 4th-order, *EPJA*
- (2015) Epelbaum, Krebs, and Meissner: NN forces at 5th-order, *PRL*
- (2015) Ekström, Jansen, Wendt,...: NN force at 3rd-order fitted to medium-mass nuclei, *PRC*
- (2015) Piarulli, Girlanda,...: Minimally nonlocal NN force at 4th-order with Δ isobars, *PRC*
- (2017) Entem, Machleidt, Nosyk: NN force at 5th-order, *PRC*
- (2018) Reinert, Krebs, Epelbaum: Semi-local NN force at 5th-order, *EPJA*
- (2018) Ekström, Hagen, Morris,...: NN force at 3rd-order with Δ isobars, *PRC*
- (2018) A. Baroni, ...: Local NN force with Δ , *PRC*
- (2020) Maria, Ingo: Local NN force
- (2025) B. S. Hu, ...: N3LO_{texas}
- ...

Developing & refinement

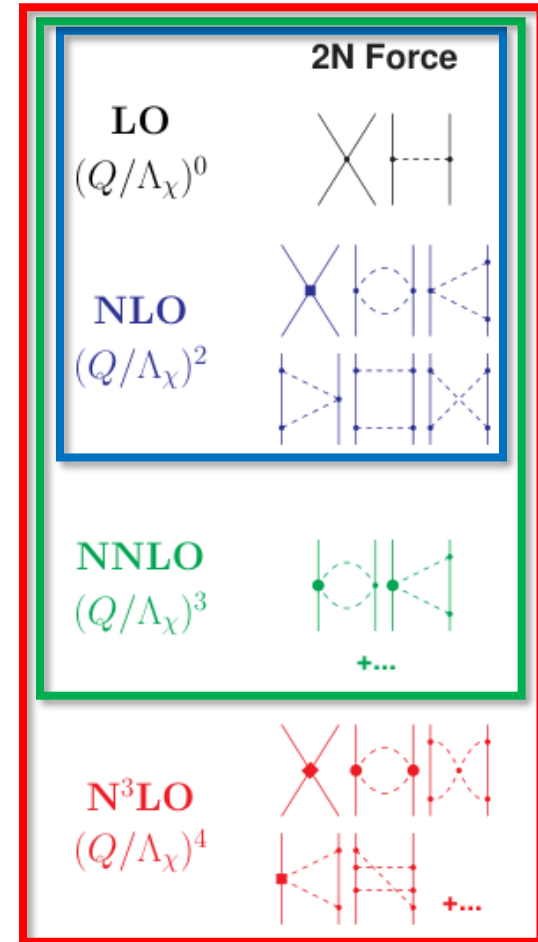
- (2018) P. Reinert et al., *EPJA* (2018)
- (2019) S. Wesolowski et al., *JPG* (2019)
- (2020) C. Drischler et al., *PRL* (2020)
- (2020) Volkotrub et al., *JPG* (2020)
- (2022) Isak et al., *PRC* (2022)
- (2023) Oliver et al., *PRC* (2023)
- (2023) Isak et al., *PRC* (2023)
- (2024) Isak et al., *PRC* (2024)
- ...

Uncertainty estimation attempts

Bayesian analysis for LECs

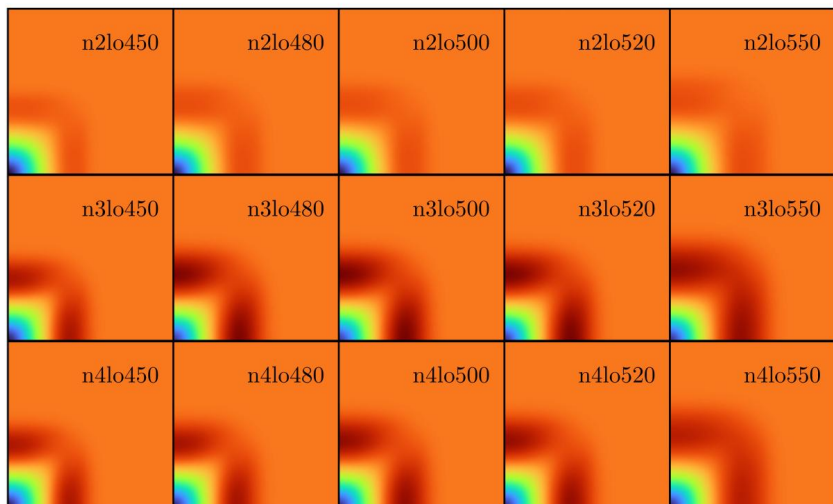
truncation error LO \rightarrow NLO \rightarrow N2LO...

Resolution: $\Lambda = 450, 500, 550$



Comprehensive statistical analysis of ChEFT uncertainties

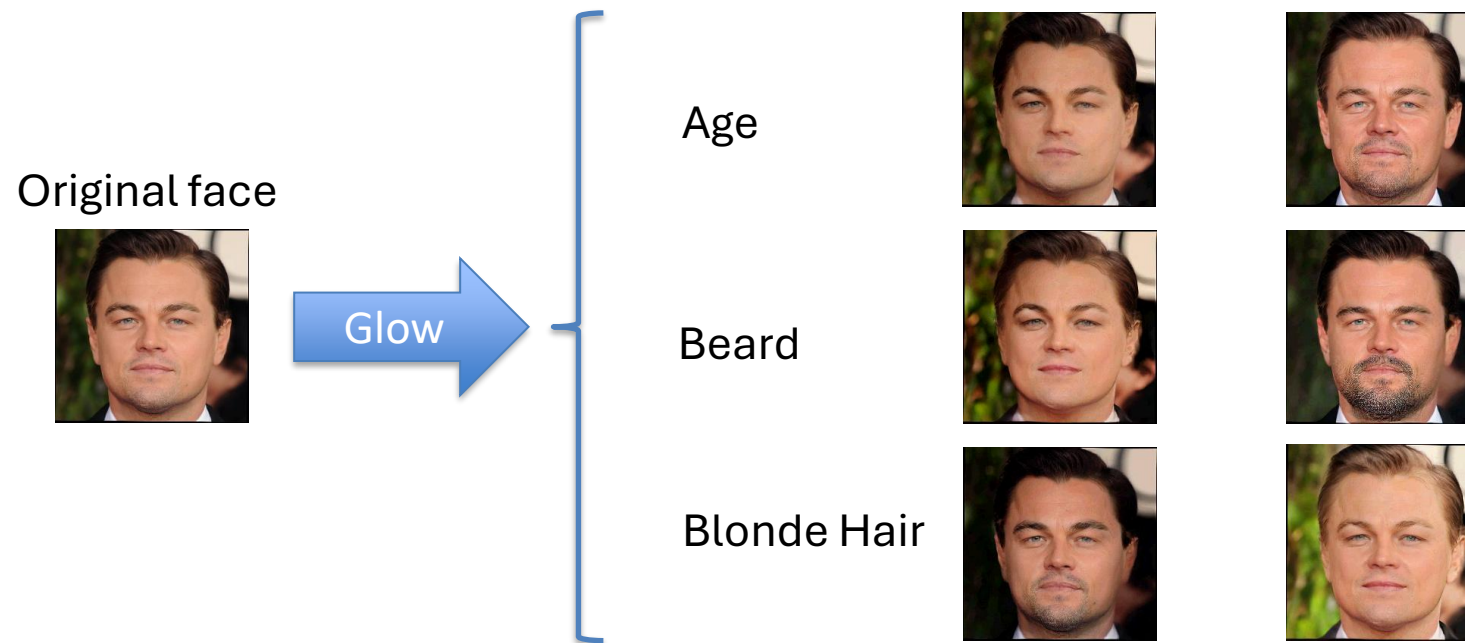
- ❖ How nuclear interactions evolve with chiral order and continuum of Λ ?
- ❖ From experimental scattering data to multi-variate LEC distributions as a function of Λ
- ❖ Efficient calculation frameworks for 3NF LEC fitting over continuum of Λ



**Generative modeling for nuclear interactions:
learning from high-quality chiral interactions**

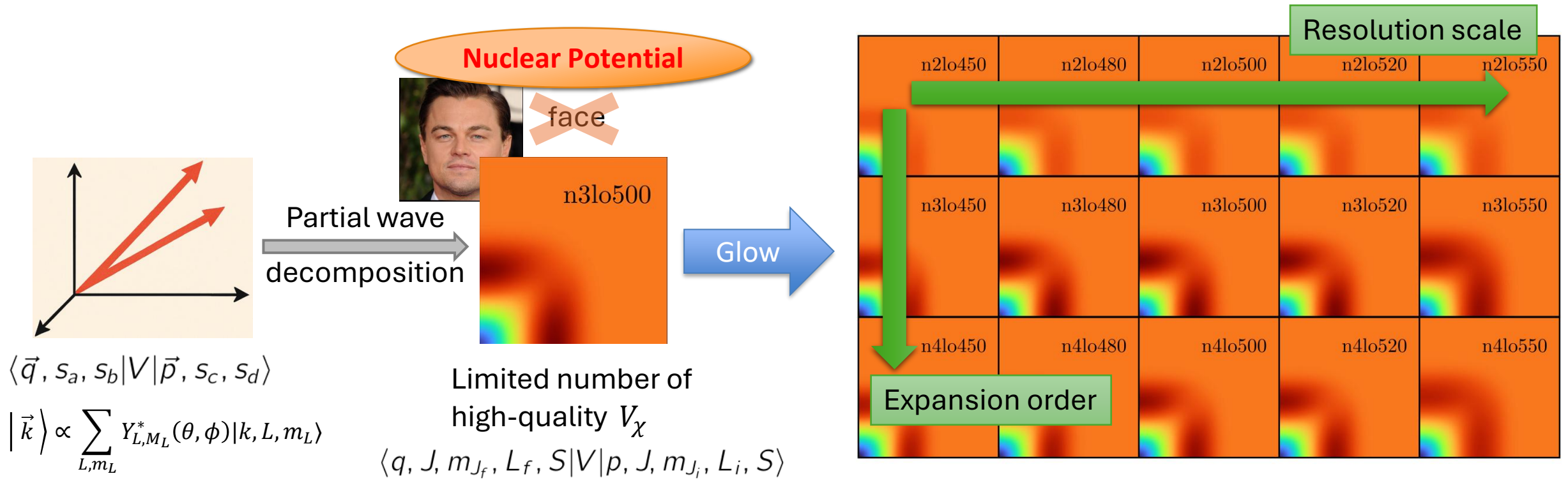
Generative flow model for image generation and manipulation

Glow: Generative normalizing flow



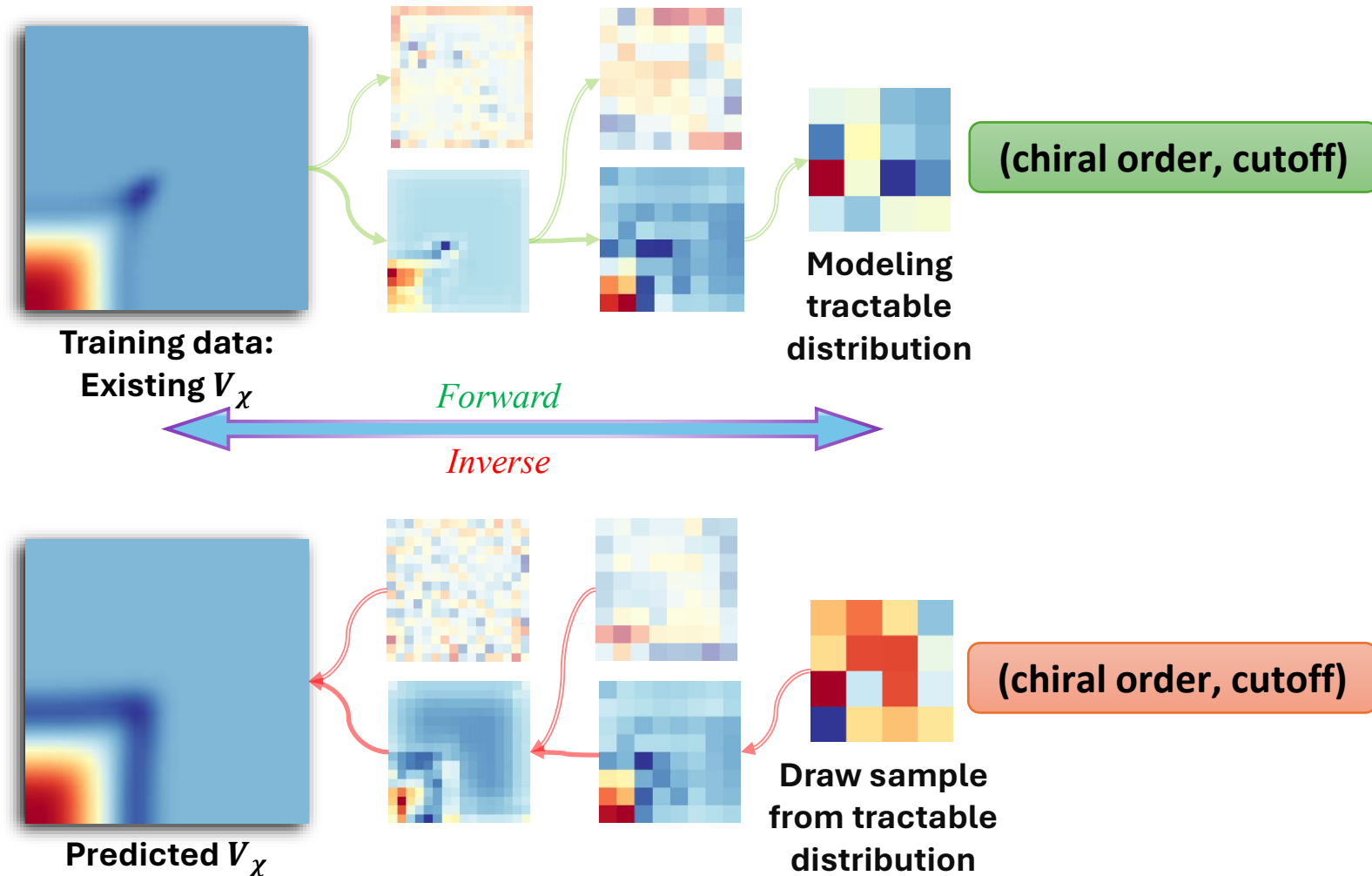
Glow model for image generation and manipulation

Glow: Generative normalizing flow

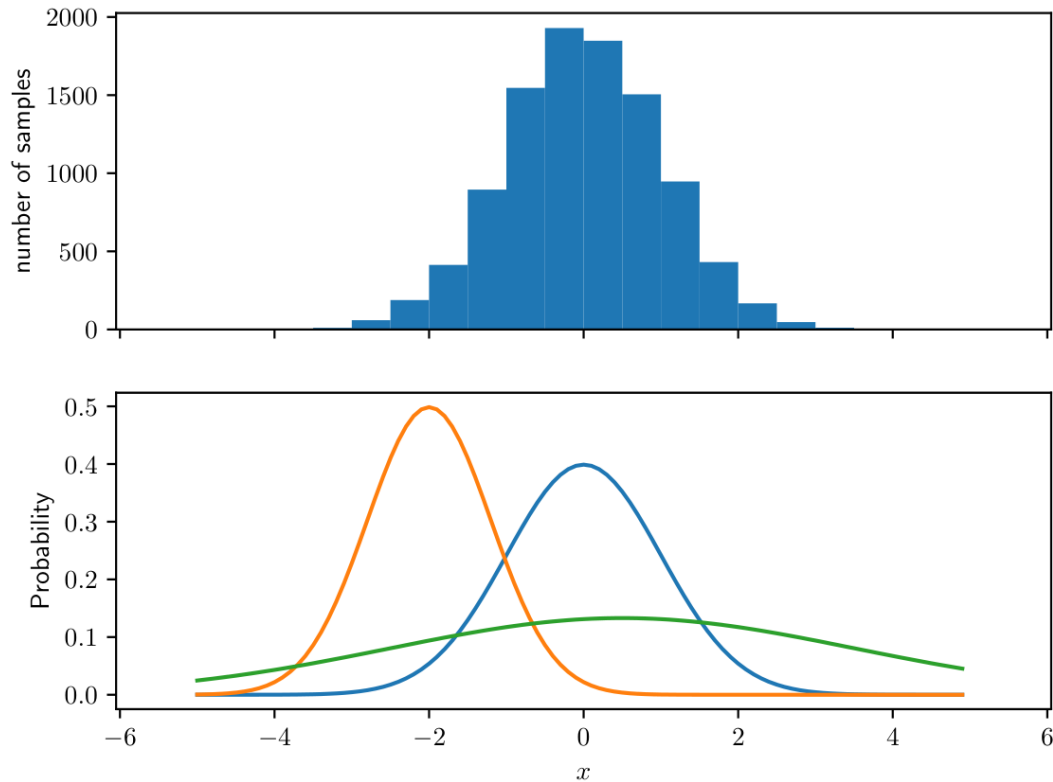


Modeling and generating partial-wave matrix elements

Partial wave decomposition:
 V as an “image”



Generating images using normalizing flows



Maximize likelihood: capture the properties of a given set of samples

Example: $x \sim \mathcal{N}(\mu = 0, \sigma = 0.1)$

$$\mathcal{L}_1 = \prod_i \mathcal{N}(X_i; \mu = 0, \sigma = 0.1)$$

$$\mathcal{L}_2 = \prod_i \mathcal{N}(X_i; \mu = -2, \sigma = 0.8)$$

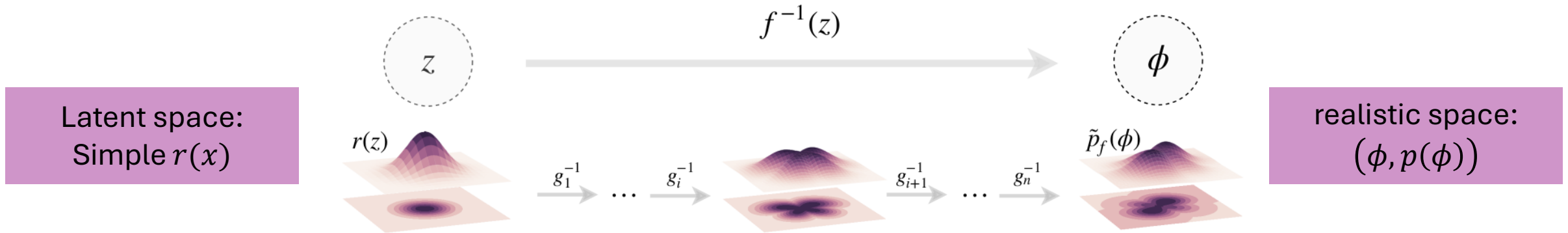
$$\mathcal{L}_3 = \prod_i \mathcal{N}(X_i; \mu = 0.5, \sigma = 3)$$

$$\rightarrow \max(\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3) = \mathcal{L}_2$$

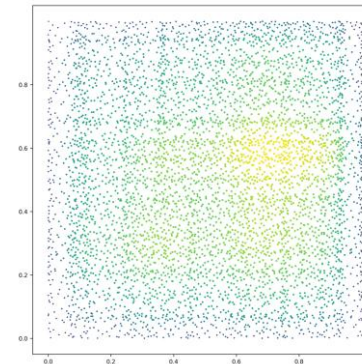
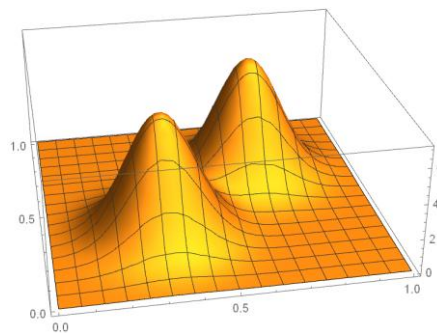
A proper probability distribution model $\mathcal{N}(\mu, \sigma) \rightarrow$ the maximum likelihood \mathcal{L}

Basic idea of normalizing flows

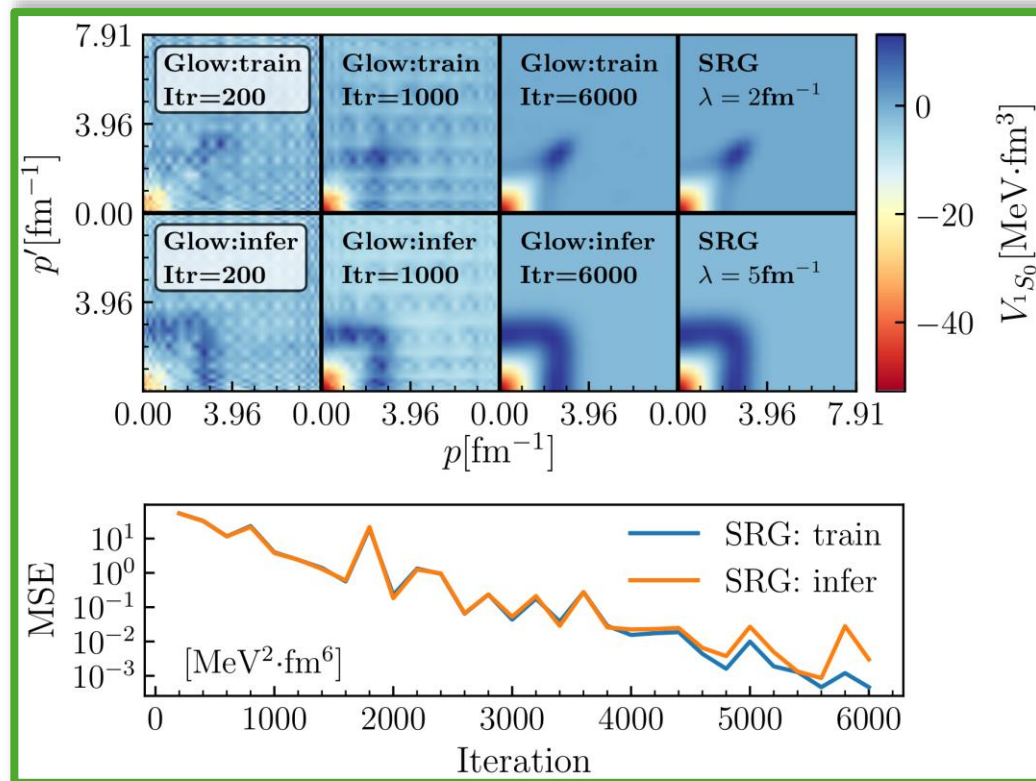
Normalizing flow: utilizing expressive transformation function



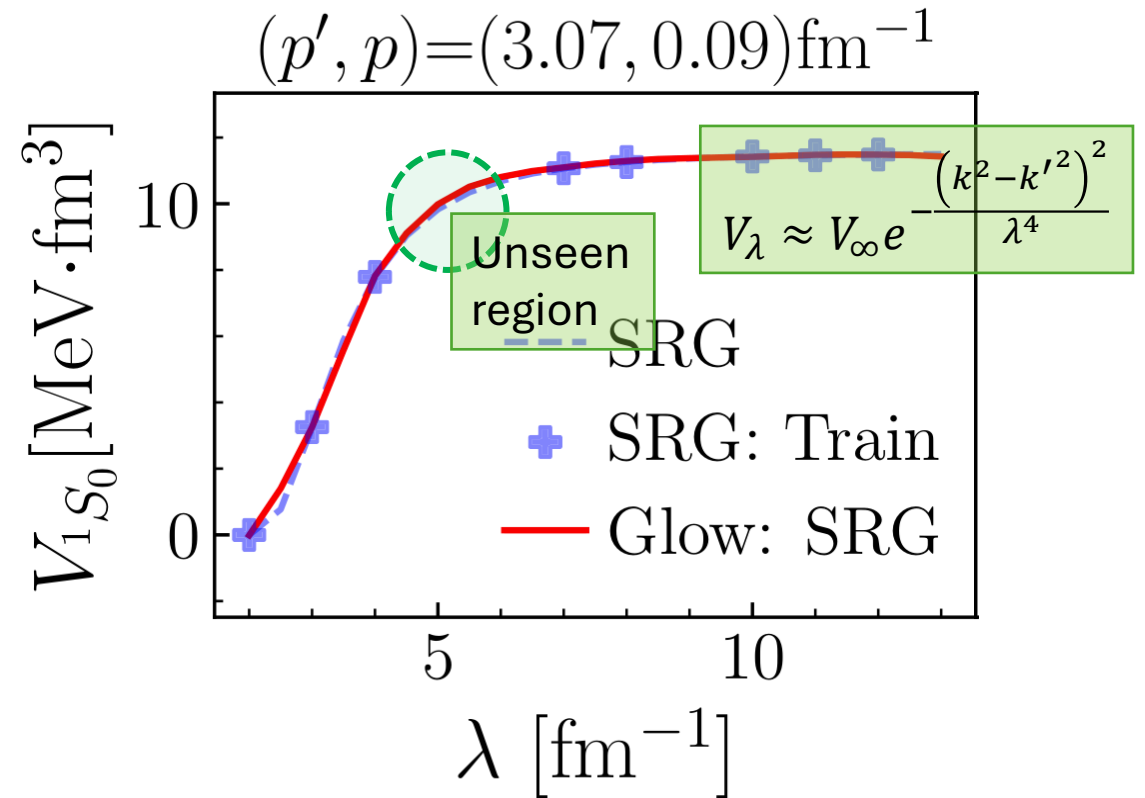
Example: 2D camel function



Test: Glow for similarity renormalization group potentials



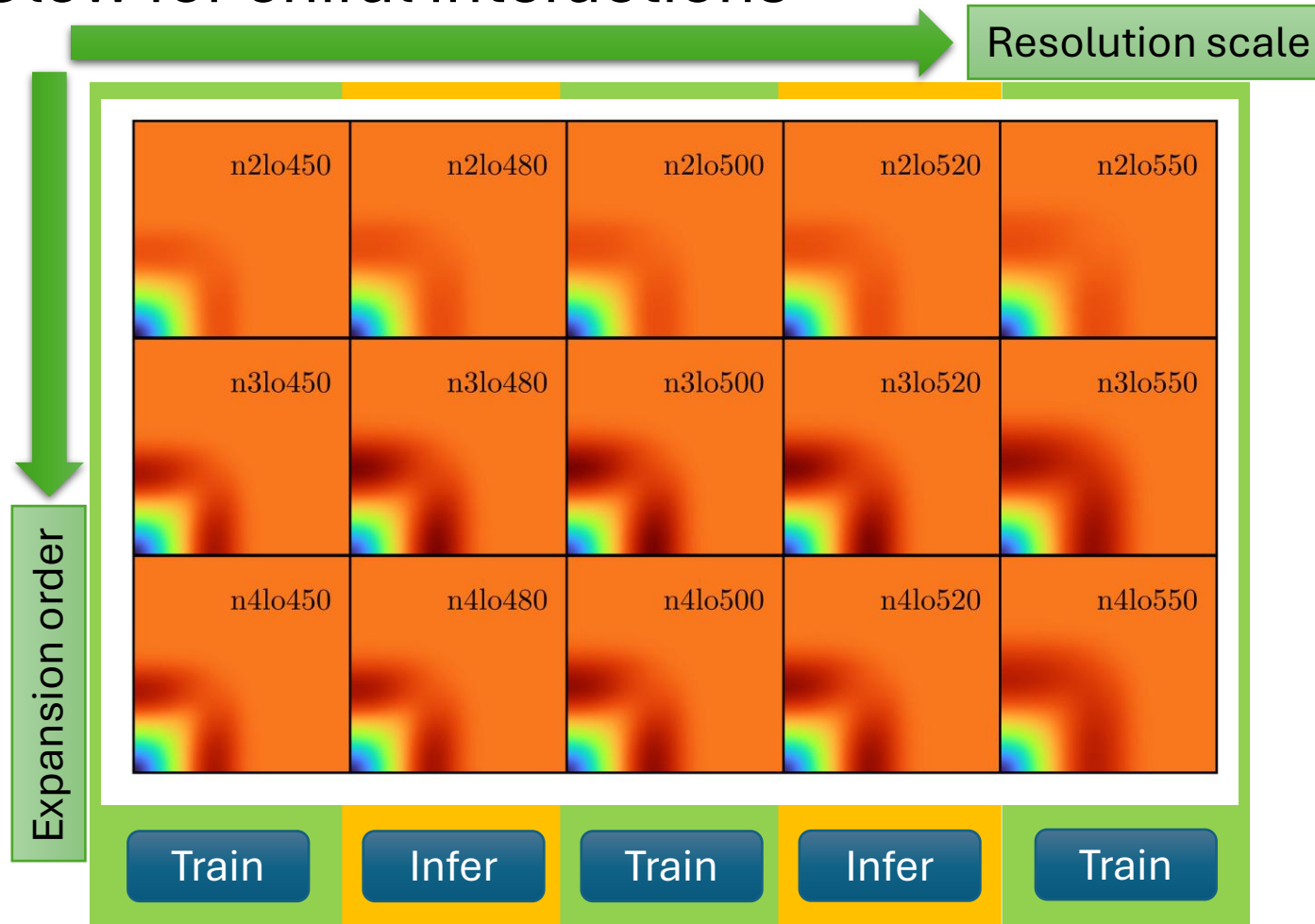
Glow for similarity renormalization group potentials



Rebuild the SRG potentials precisely.
Predict SRG potentials at arbitrary λ values precisely.

Generating new chiral interactions

Glow for chiral interactions

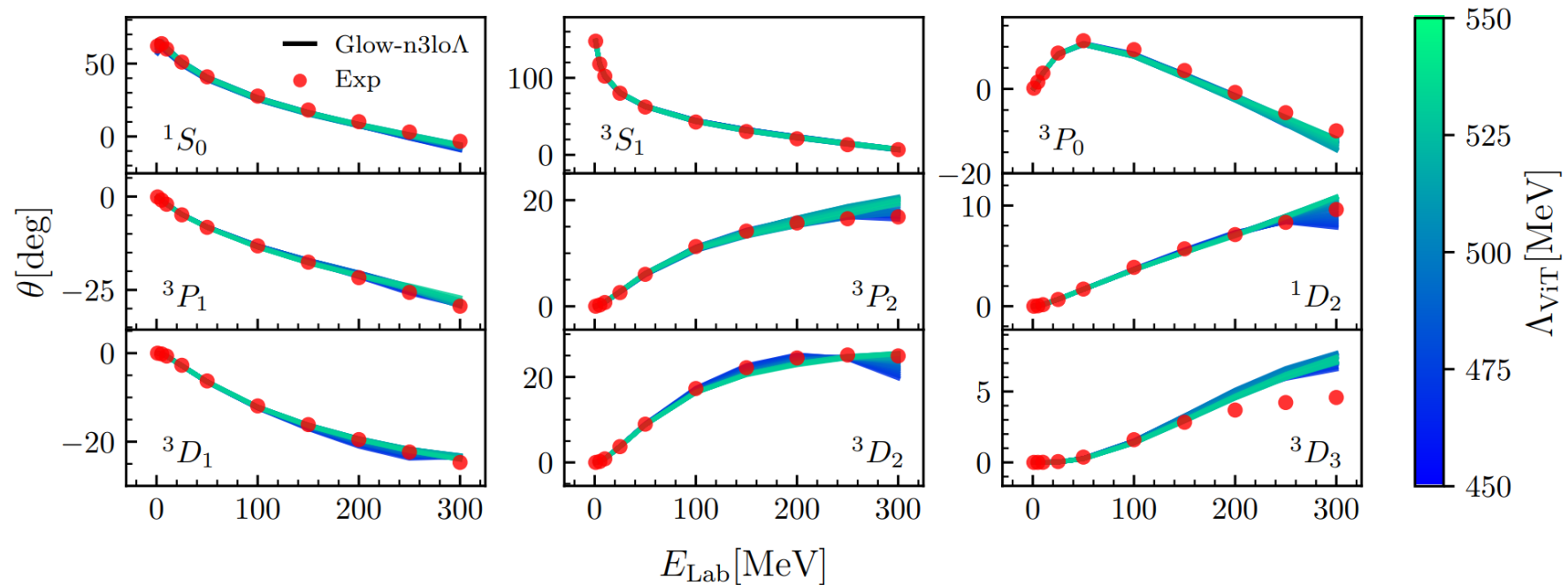


Distinguish **truncation orders** in ChEFT

Predict how the chiral potentials **evolve with cutoff**

Benchmarking Glow-generated nuclear forces

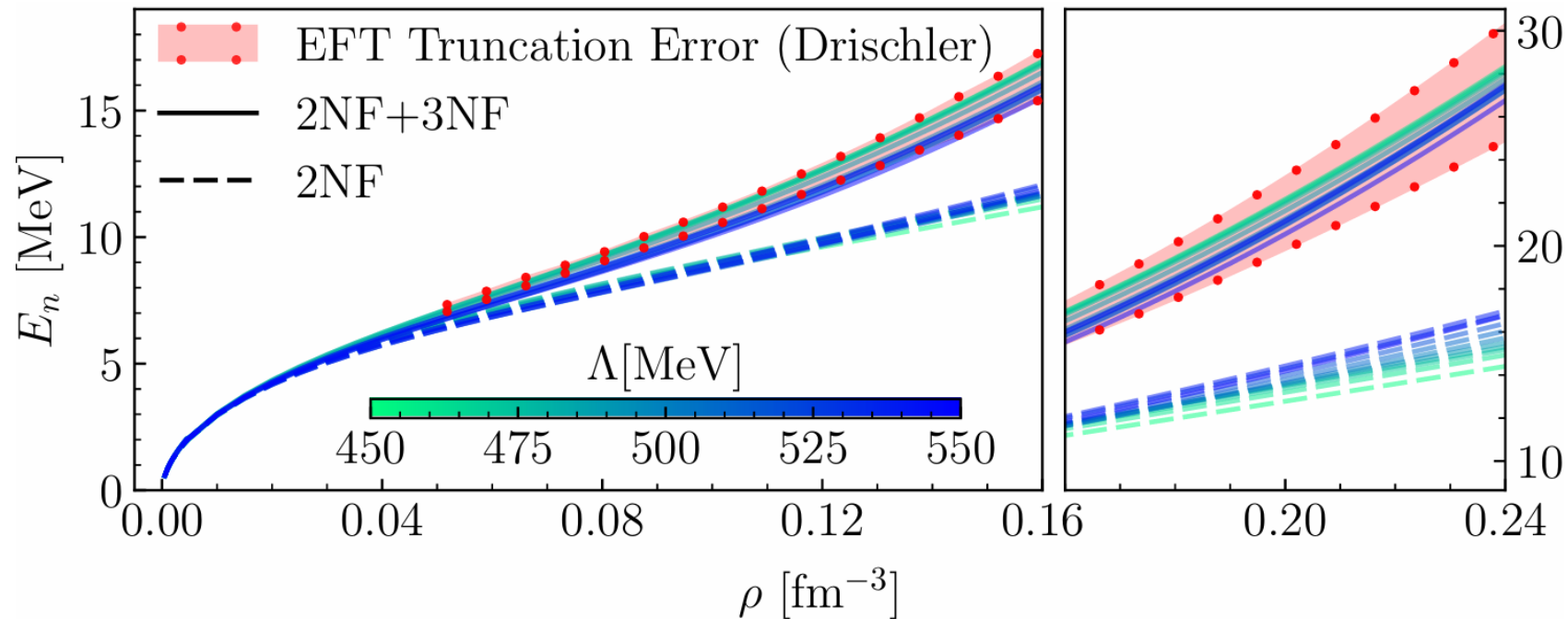
- Glow for chiral interactions: check reasonability by phase shifts



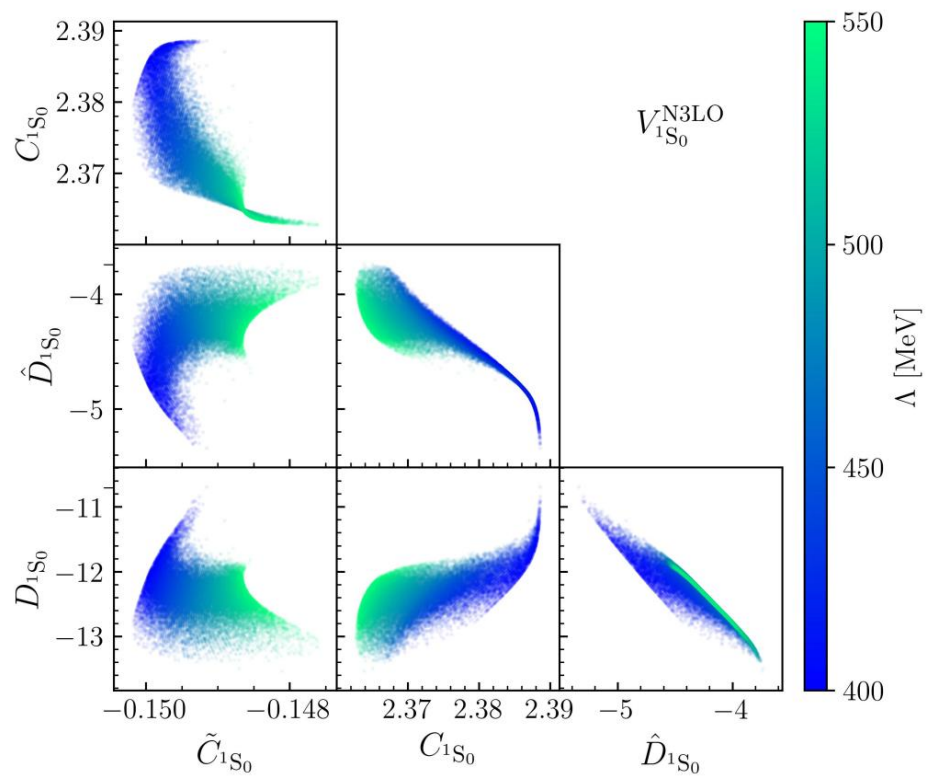
Good phase shift result \rightarrow The Glow-generated potentials are **physically reasonable**
Reveal the **uncertainty** from Λ

Propagated uncertainties in EOS

- Glow for chiral interactions: predicted EOS



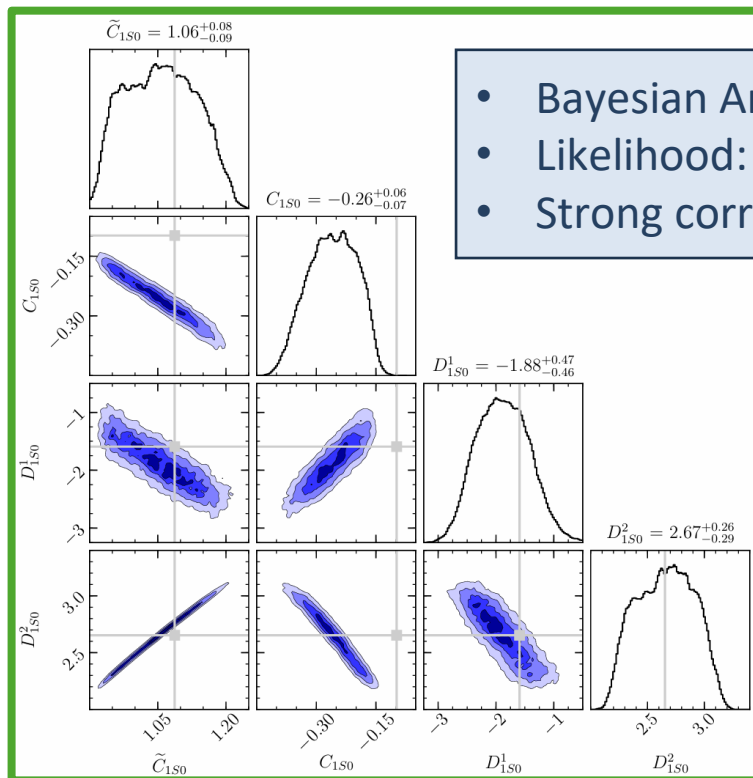
Low-density region: Uncertainty from cutoff Λ
High-density region: Uncertainty from Truncation Error



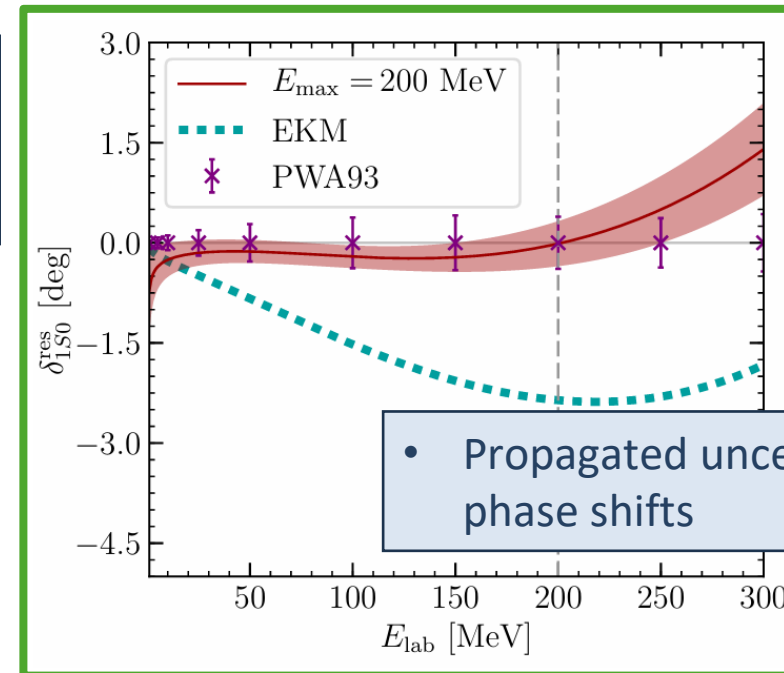
**Fitting LEC Distributions
Over a Continuum of Resolution Scales**

Challenges in Constraining LEC Distributions

- High-precision constraints from partial-wave analysis
 - Relative uncertainty for 1S0 phase shift at 1MeV: $0.018/62.074 \approx \mathbf{0.0003}$
 - Narrow allowed region \rightarrow unstable sampling from MCMC
 - Include truncation errors \rightarrow broaden the allowed region \rightarrow make MCMC feasible



- Bayesian Analysis \times MCMC
- Likelihood: + truncation error
- Strong correlation



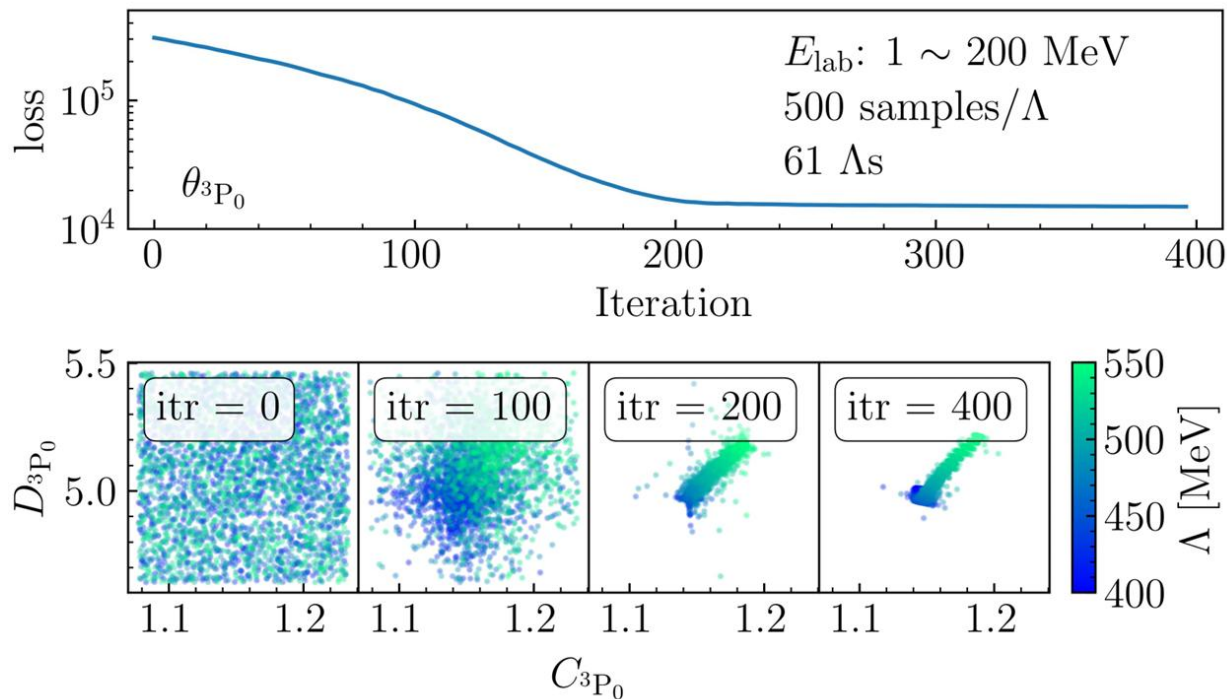
- Propagated uncertainties in phase shifts

Challenges in Constraining LEC Distributions

- Precise experiment analysis from partial wave decomposition
 - Relative uncertainty for $1S_0$ phase shift at 1MeV: $0.018/62.074 \approx \mathbf{0.0003}$
 - Narrow allowed region \rightarrow nightmare for MCMC
 - Include truncation errors \rightarrow broaden the allowed region \rightarrow make MCMC feasible
- High dimensional parameter space
 - Number of LECs: 20+ @ N3LO chiral interactions
- Possible strong and complicated correlations
 - Difficult to model a distribution

Constraining LEC Distributions with Normalizing Flows

- Careful Treatment of LEC Uncertainties from experiment
 - Fitted to lab observables with uncertainties (phase shifts from PWA)
 - Modeling the LEC distributions using normalizing flow



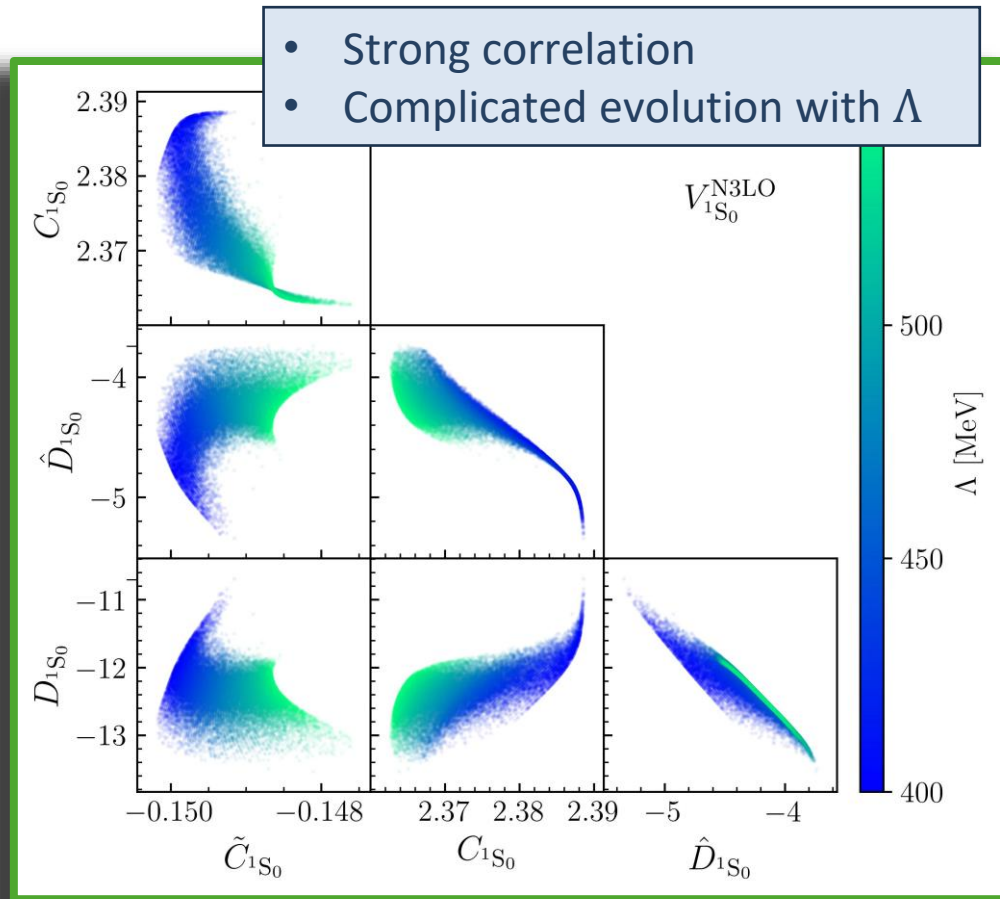
- **Conditional normalizing flow:**

- generate samples of LECs
 $\text{nflow}(\Lambda) \rightarrow \text{LECs}$

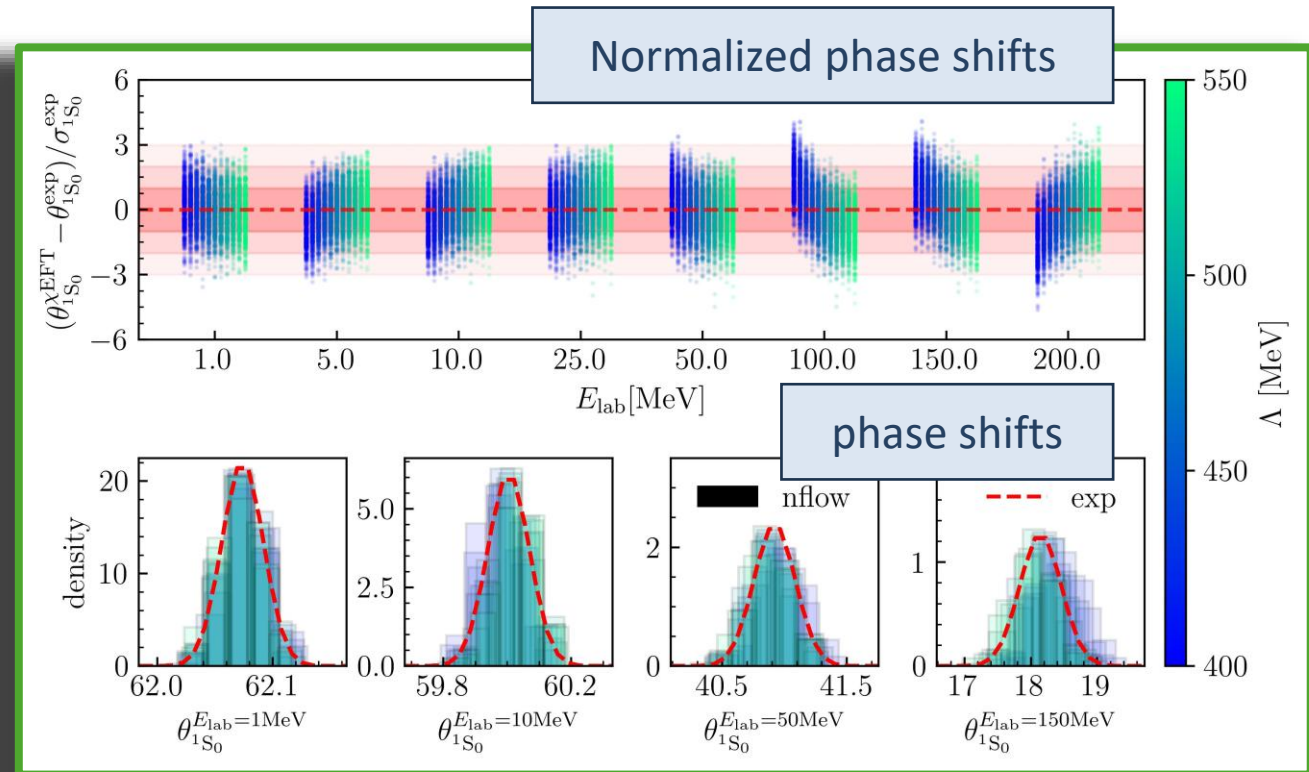
- **Loss function:**

- Measures the difference between $p_{\text{nflow}}(\theta(\text{LECs}))$ and $p_{\text{expr}}(\theta(\text{LECs}))$
- **Prior free**

Constraining LEC Distributions with Normalizing Flows



LEC samples generated by normalizing flow over a wide range of Λ

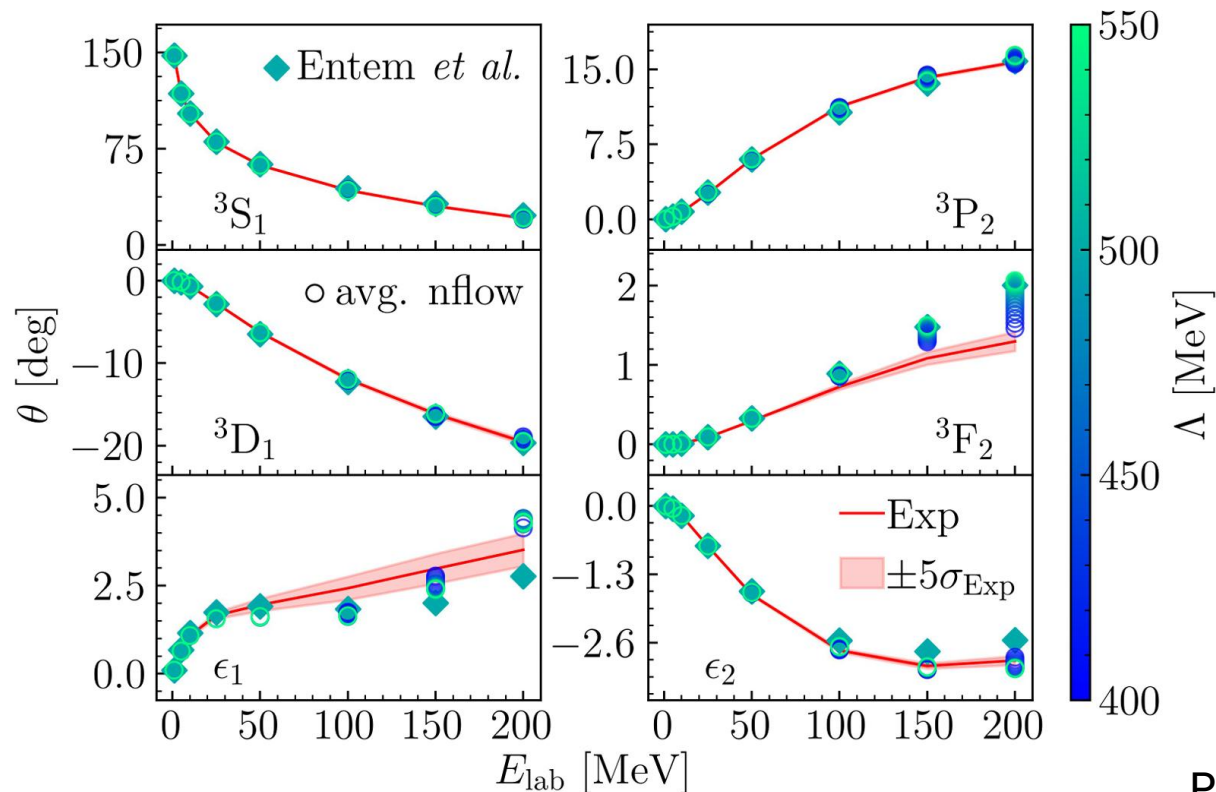


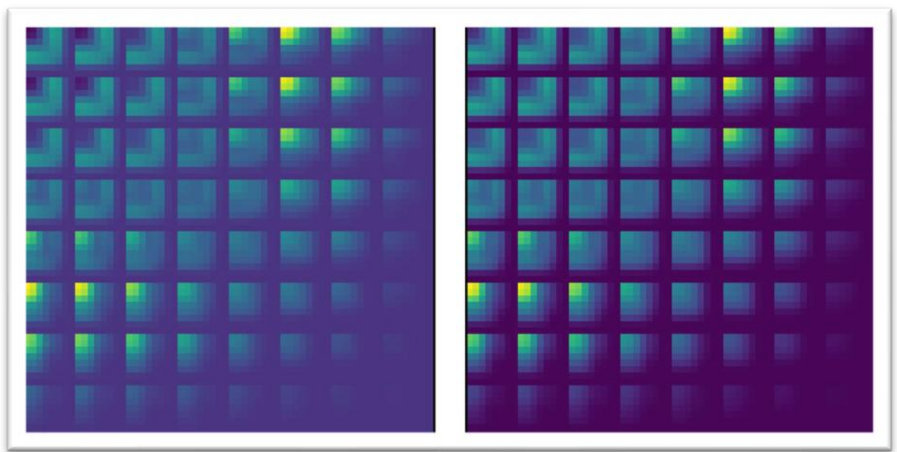
P. Wen, J. W. Holt, in preparation

Propagated phase shift distributions

Expected phase shifts from flow-generated LECs

- Mean value of phase shifts
 - \approx expected value of phase shifts over learned LEC distributions
 - \rightarrow High-quality LECs found by normalizing flow across a wide region of Λ .

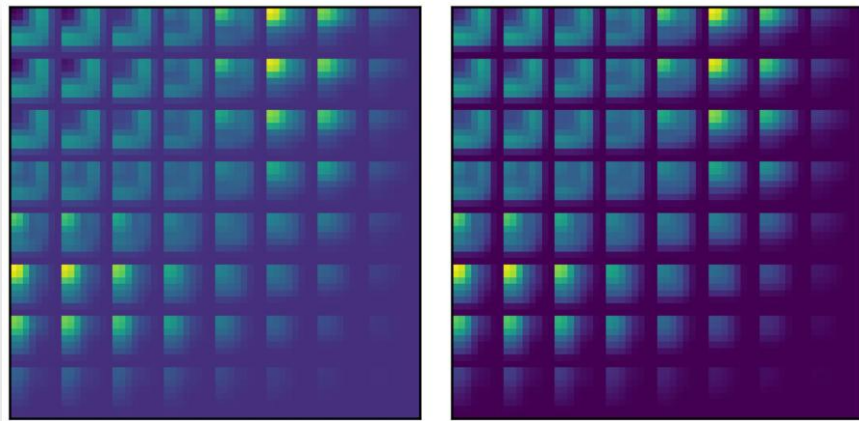




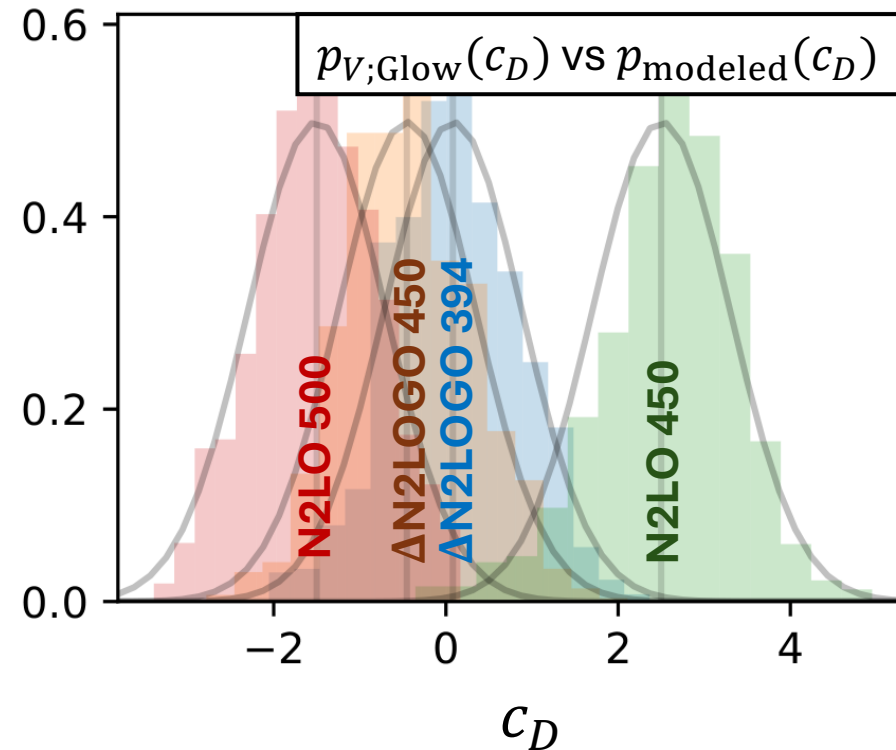
Normalizing flow for 3NF

Glow for 3NF (preliminary)

- V_{3NF} viewed as “image”
 - Partial wave decomposition $\rightarrow V(p, q, p', q')$
 - Rearrange momentum mesh points $\rightarrow V([p, q], [p', q'])$
 - Friendly for Glow model



V_{3NF} from Glow



Neural quantum state for few-body system

- Neural Quantum State

- $u_{ij}^{(\mathbf{x})}, f_{ij}^{(c)}$: correlation functions dependent on r
- $\hat{O}_{ij}^{(\mathbf{x})}$: spin-isospin operators ($\mathbf{x} = \vec{\sigma}_i \cdot \vec{\sigma}_j, S_{ij}, \dots$)
- $|\Phi\rangle$: anti-symmetrized state for **fermion** system

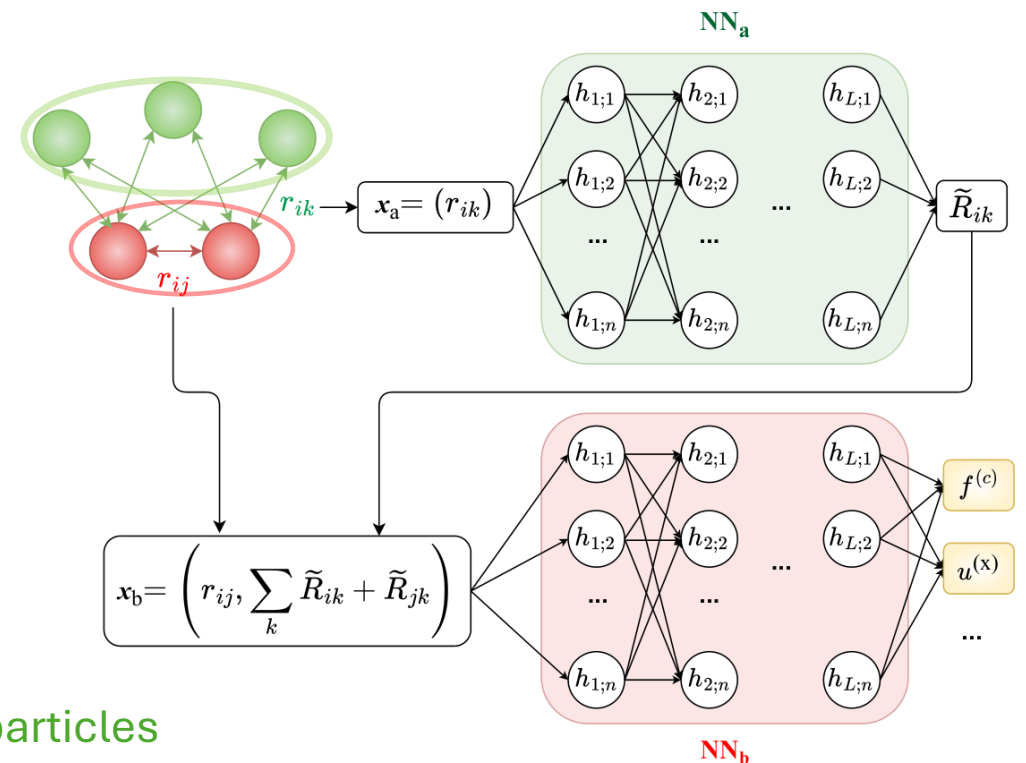
- Two-independent Neural Networks NN_a and NN_b

$$\tilde{R}_{\alpha\beta} = \text{NN}_a(r_{\alpha\beta}), \quad \alpha \neq \beta \leq A$$

$$\text{Spatial parts in wave function} = \text{NN}_b\left(r_{ij}, \sum_{k \neq i,j} \tilde{R}_{ik} + \tilde{R}_{jk}\right)$$

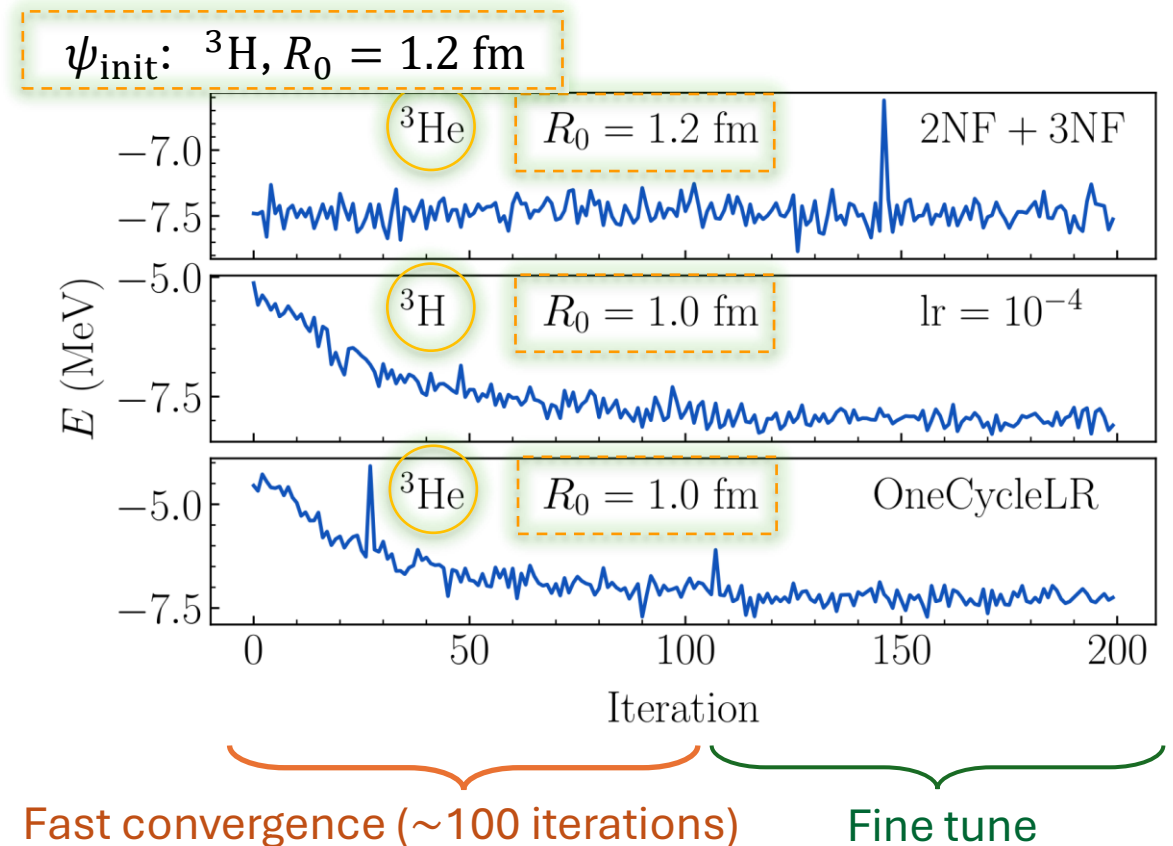
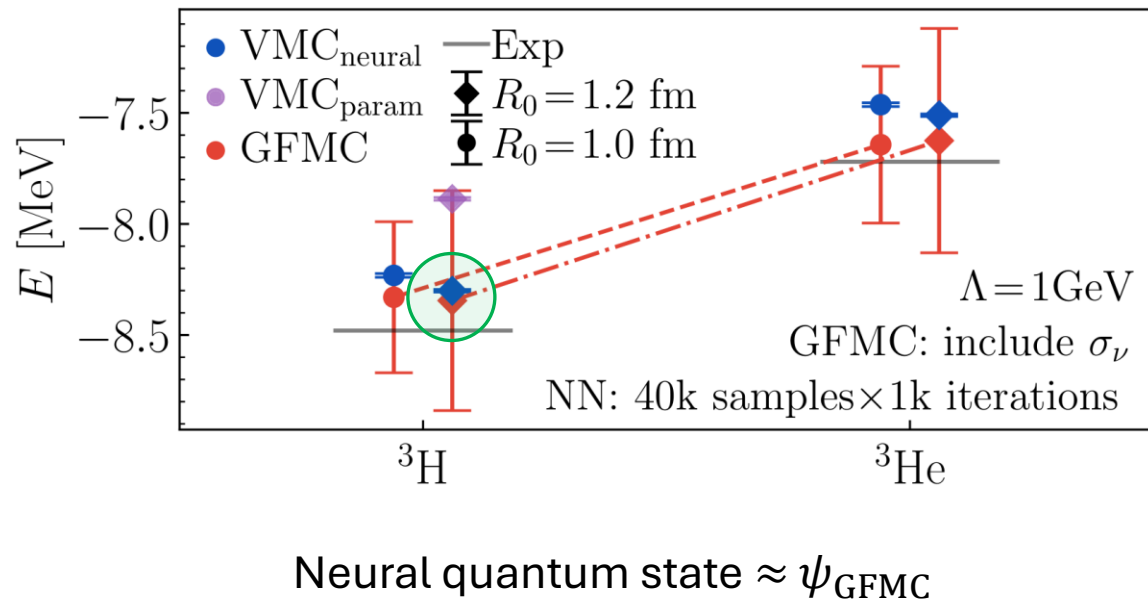
Influence from third particles

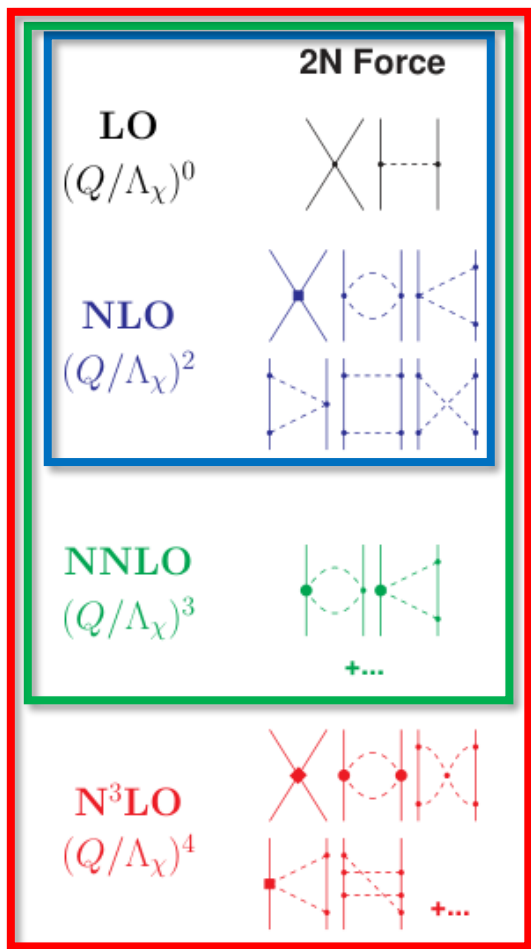
$$|\psi\rangle = \mathcal{S} \prod_{i < j} \left(1 + \sum_{\mathbf{x}} u_{ij}^{(\mathbf{x})} \hat{O}_{ij}^{(\mathbf{x})} \right) f_{ij}^{(c)} |\Phi\rangle$$



Efficient fitting framework for 3NF distributions

- VMC training of neural quantum states
 - Good approximation to the ground states from GFMC
 - Fast adaptation to other nuclear interactions and nuclei
 - → **Efficient method to fit LECs for 3NF**





Summary

Summary

- Normalizing flow:
 - Glow:
 - Learn high-quality nuclear interactions
 - Build physically reasonable nuclear interactions
 - Systematically analyze uncertainties from resolution scale
 - Conditional normalizing flow
 - Fit LEC distributions over a Continuum of Resolution Scales with experiments
- Neural quantum state
 - Precise description of light nuclei
 - Fast adaptation to different nuclear forces and nuclei
 - Efficient method for 3NF fitting



Thank you!