# Bayesian methods in nuclear effective field theories

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Jefferson Lab, AI for Nuclear Physics, 2020

# The BUQEYE collaboration

**Bayesian uncertainty quantification: errors for your EFT**

| | |
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| Dick Furnstahl | Ohio State |
| Harald Griesshammer | George Washington Univerity |
| Natalie Klco | University of Washington |
| Jordan Melendez | Ohio State |
| Daniel Phillips | Ohio University |
| Matt Pratola | Ohio State (statistics) |
| Sarah Wesolowski | Salisbury University |
| Xilin Zhang | Ohio State |

**Visit us online at [buqeye.github.io]**

# BUQEYE priorities

Full uncertainty quantification for low-energy nuclear theory (structure/reactions)

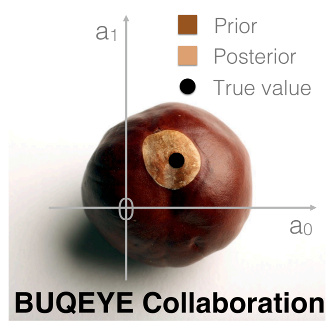
Using statistics and machine learning techniques to gain physics insight

Collaboration and coordination with experts in statistics/machine learning

Pushing through computational bottlenecks (mostly from theory calculations)

- emulation/surrogates (gaussian processes, eigenvector continuation, etc.)
- simplifications that ease computational burden

Informing experimental design from the theory side



# Uncertainty Quantification in Nuclear Physics

To produce meaningful experimental measurements and theoretical predictions, it is essential to quantify uncertainties!

$$y_{\mathrm{th}} = y_{\mathrm{exp}} + \delta y_{\mathrm{exp}} + \delta y_{\mathrm{th}}$$

Theory discrepancy:

$$\delta y_{\mathrm{th}}$$

Made up of the following:

- missing physics
- numerical/ method errors
- fitting to uncertain data

Notes

- likely to be "systematic"
- not usually fully quantified
- often assumed to be normal

Experimental discrepancy:

$$\delta y_{\mathrm{exp}}$$

Made up of the following:

- counting statistics
- background and selection effects
- systematic uncertainties

Notes

- systematic errors may not be well understood or inflated
- often assumed to be normal

# Effective field theories are special

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Also the possibility of regulator artifacts, alternate power-counting, etc.

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A healthy EFT improves systematically with order

Ignore other uncertainty sources other than EFT truncation uncertainty $\delta y_k$

$$y = \underbrace{y_{\mathrm{ref}} \sum_{n=0}^{k} c_n Q^n}_{\text{theory calculation}} + y_{\mathrm{ref}} \sum_{n=k+1}^{\infty} c_n Q^n$$

where $Q \sim \frac{p}{\Lambda_b}$ and $c_n$ s extracted from order-by-order calculations.

# Status report 1: parameter estimation

## EFTs have unconstrained parameters, the low-energy constants (LECs)

## Strategy for nuclear interactions: constrain LECs using data

For an EFT at order $k$, let LECs be given by $\vec{a}_k$

$$\text{Interaction}(\vec{a}_k) \rightarrow \text{Observable calculation} \rightarrow \text{Prediction}(\vec{a}_k)$$

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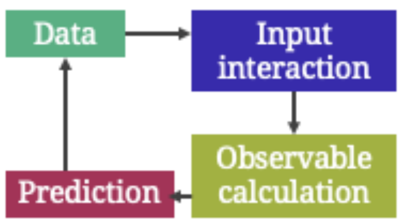
Then compare the value with data



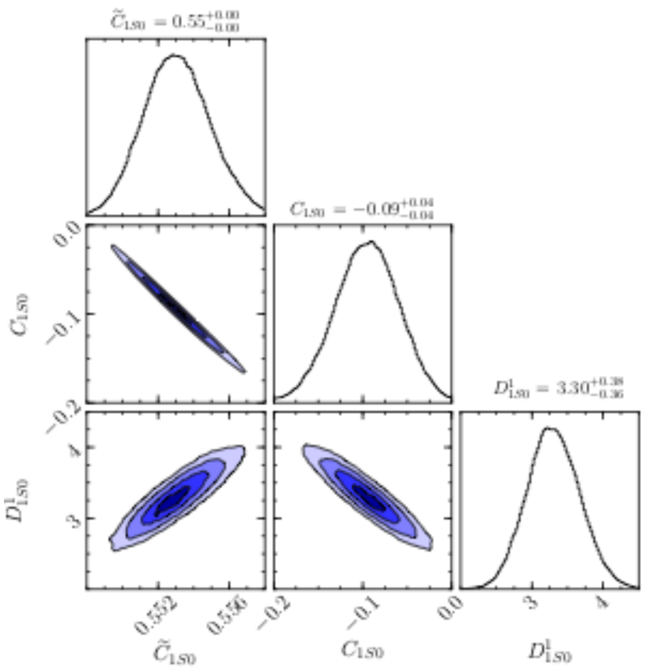

Adjust parameters $\vec{a}_k$ according to favorite optimization procedure OR

Use a Bayesian approach and compute a parameter pdf for $\vec{a}_k$

# Status report 1: parameter estimation

## nucleon-nucleon sector for chiral effective field theories

e.g. ${}^1S_0$ channel at N$^3$LO (4 parameters)



Estimate LEC probability distribution

Markov Chain Monte Carlo (MCMC)

$$\mathrm{pr}(\vec{a}_k|D, I) \propto e^{-\chi^2/2}$$

$$\chi^2(\vec{a}_k) = \sum_{i=1}^{N} \left( \frac{d_i - y_k(p_i; \vec{a}_k)}{\sigma_i} \right)^2$$

Bottleneck = theory calculation

This does not include $\delta y_{\mathrm{th}}$

SW et al., JPG 46, 045102 (2019)

# Status report 1: parameter estimation

## Including theory discrepancy in the parameter estimation procedure

SW et al., JPG 46, 045102 (2019)

Use model of EFT truncation error to include $\delta y_{\rm th}$

$$y = \underbrace{y_{\rm ref} \sum_{n=0}^{k} c_n Q^n}_{\text{theory calculation}} + y_{\rm ref} \sum_{n=k+1}^{\infty} c_n Q^n$$

Assume a prior pdf on $c_n$s and marginalize to get

$$\mathrm{pr}(\vec{a}_k | D, I) \propto e^{-\chi^2(\vec{a}_k)/2} = e^{-\frac{1}{2}(\boldsymbol{y}_{\rm exp} - \boldsymbol{y}_{\rm th}(\vec{a}_k))^T (\Sigma_{\rm exp} + \Sigma_{\rm th})^{-1} (\boldsymbol{y}_{\rm exp} - \boldsymbol{y}_{\rm th}(\vec{a}_k))}$$

Simple modified $\chi^2$ form under certain assumptions

# Status report 1: parameter estimation

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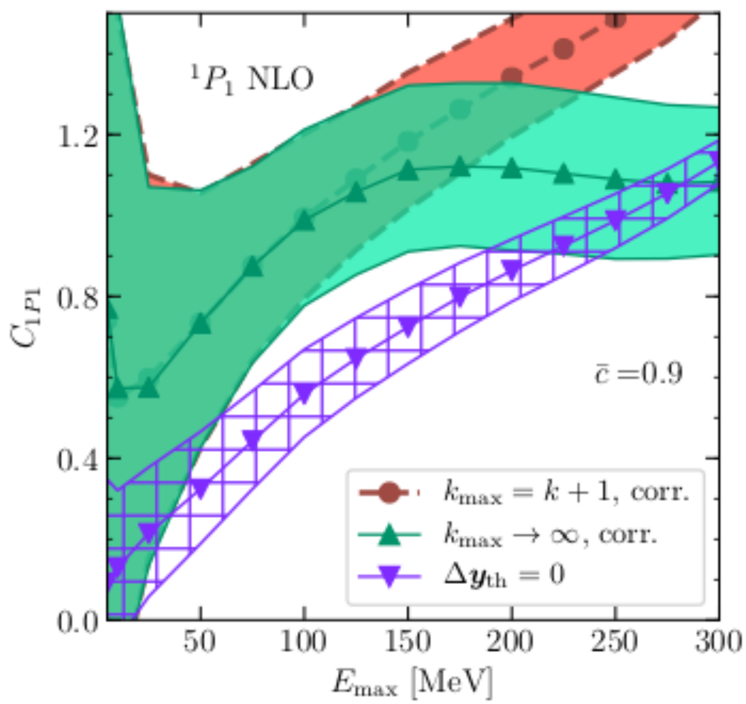
SW et al., JPG 46, 045102 (2019)

Accounting for truncation error absorbs higher-order effects



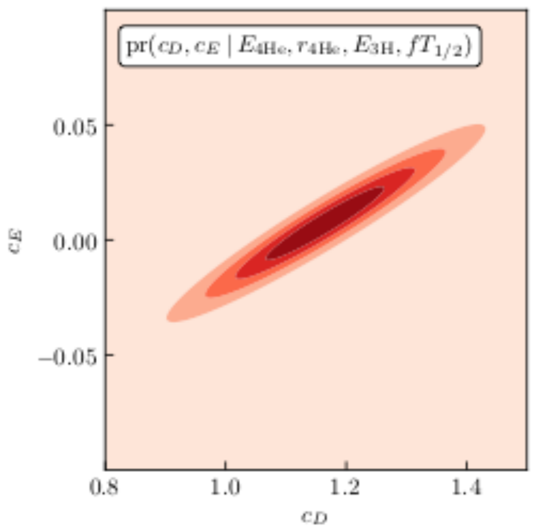

Purple: not accounting for $\delta y_{\mathrm{th}}$

Green: stabilizes when including $\delta y_{\mathrm{th}}$

# Status report 1: parameter estimation

## The three-nucleon sector (fitting $c_D$ and $c_E$) [preliminary]

SW, Andreas Ekstrom, et al. 2020 [in preparation]




Data:

- energy/radius of $^4$He
- energy of $^3$H
- $^3$H $\beta$-decay half-life

Fixed NN potential: NNLO$_{\mathrm{sat}}$

As before, including estimated $\delta y_{\mathrm{th}}$

Not including uncertainty from NN sector

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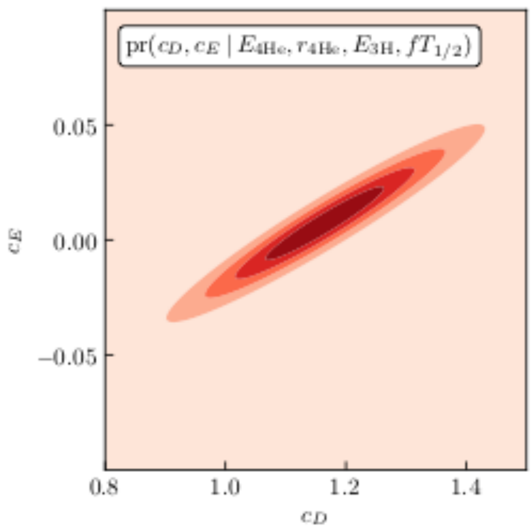


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**Made possible by eigenvector continuation** Frame et al., PRL 121 032501 (2018)

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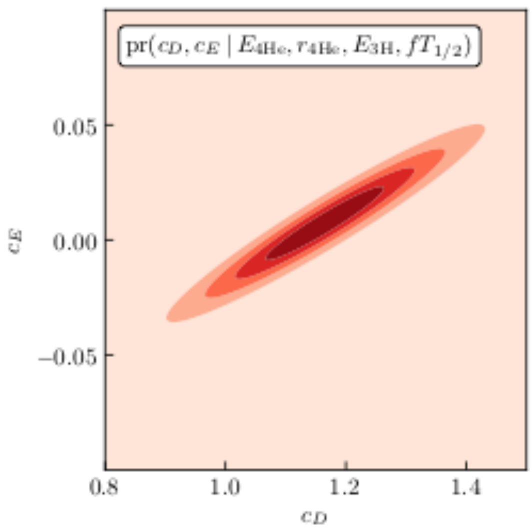
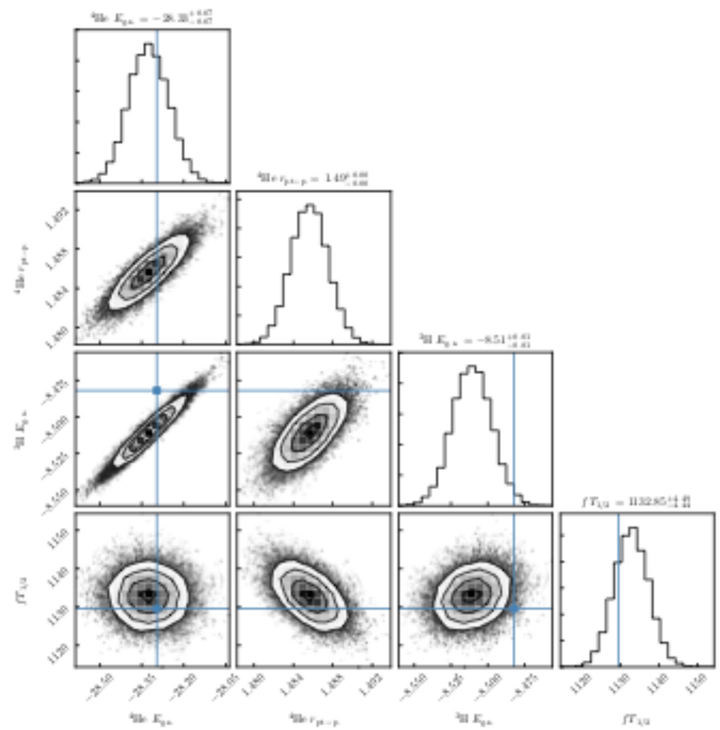


# Status report 2: Truncation error and GPs

## Further improve model of truncation error: include correlations

Jordan Melendez, SW, et al. PRC 100 044001 (2019)

### Gaussian process model to study EFT truncation errors

For observables that vary over a continuous domain $x$

E.g., NN scattering observables in energy and angle $x = \{E_{\rm lab}, \theta\}$

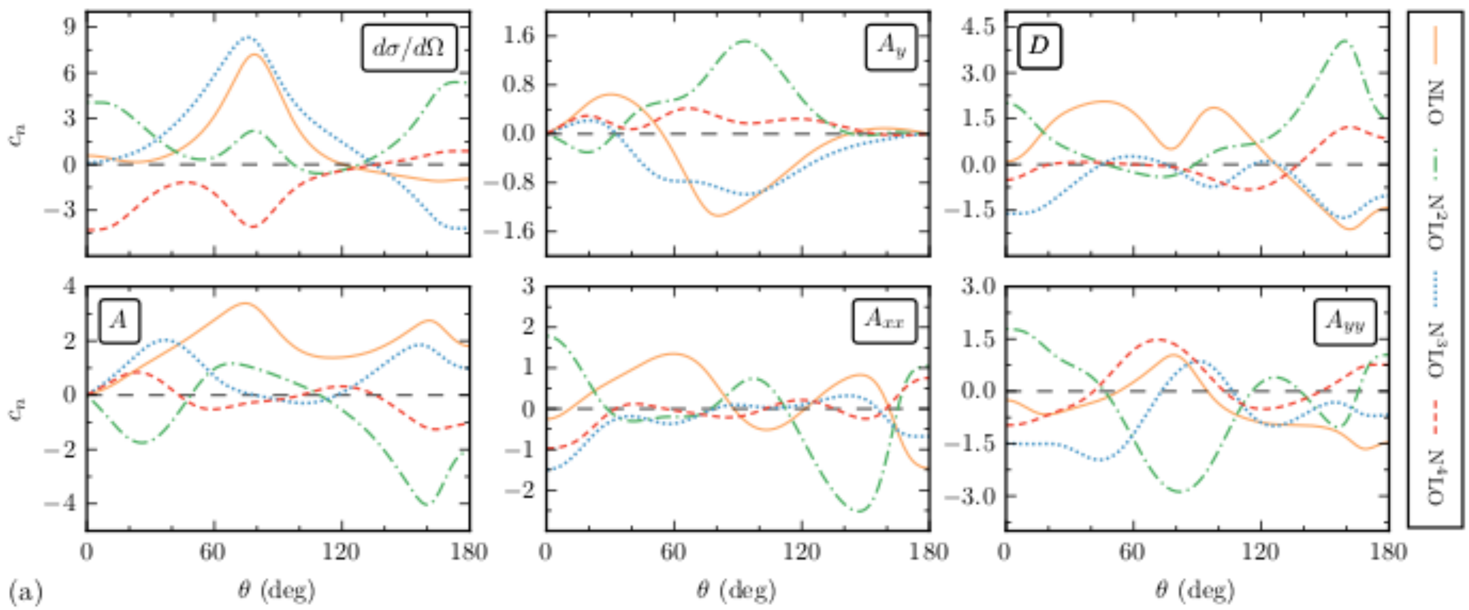
$$y(x) = y_{\rm ref}(x)\sum_{n=0}^{k} c_n(x)Q(x)^n + y_{\rm ref}(x)\sum_{n=k+1}^{\infty} c(x)_n Q(x)^n$$

Still using lower-order convergence to inform missing corrections

E.g., truncation error at $E_{\rm lab} = 50\,\mathrm{MeV}$ won't be too different from $51\,\mathrm{MeV}$

# Status report 2: Truncation error and GPs

Good evidence in NN sector that truncation errors are well-modeled by GPs




Differential cross-section of np scattering, $E_{\text{lab}} = 150\,\text{MeV}$

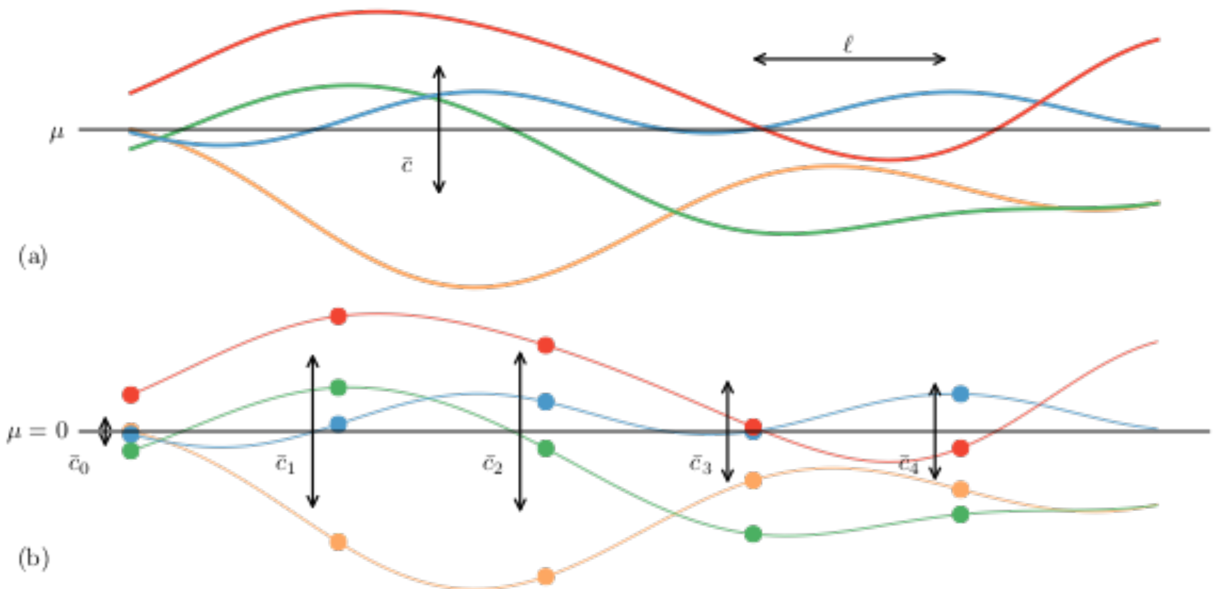
From order-by-order predictions from LO to N$^4$LO (5 orders)

GPs are random curves with some mean function and covariance kernel

J. Melendez, SW, et al. PRC 96 024003 (2017)

# Status report 2: Truncation error and GPs

A correlated vs. pointwise truncation error model
J. Melendez, SW, et al. PRC 100 044001 (2019)

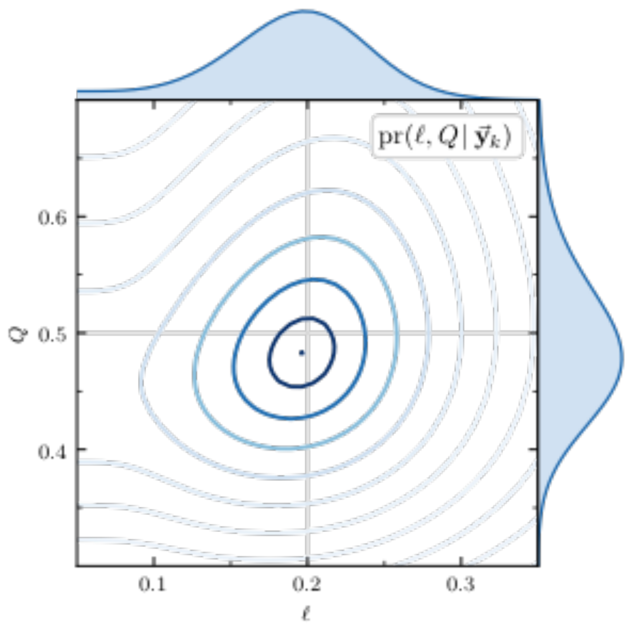



Major feature: can use statistical validation tools to gain physics insight!

# Status report 2: Truncation error and GPs

In preparation: Melendez, SW, et al. (2020)

Use GP model with modern NN potentials to diagnose convergence




This figure: toy problem

Estimate correlation length
and EFT breakdown scale!

Currently applying diagnostics to
modern NN potentials

Package `gsum` freely available to use: buqeye.github.io/software

# More ongoing BUQEYE projects

- Convergence analysis of infinite matter calculations
  Drischler, Melendez, Furnstahl, Phillips
- Bayesian experimental design for proton Compton scattering experiments
  Melendez, Furnstahl, Griesshammer, McGovern, Phillips
- Ongoing questions about Bayesian model selection in EFTs

## See everything at buqeye.github.io

# Summary and status

- Bayesian statistics is the ideal tool for effective field theories
- Build and include physics assumptions explicitly through Bayesian priors
- A data-driven study of theory expectations

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## Gain physics insight from statistical tools

- Continuing need for expertise in statistics and machine learning
- Model selection for EFTs? Power-counting comparison and diagnosis?
  - major bottleneck is observable computation
- Fully quantify uncertainties on EFT predictions
  - understand full correlation/interplay of all errors
  - easily usable approaches for nuclear structure practitioners