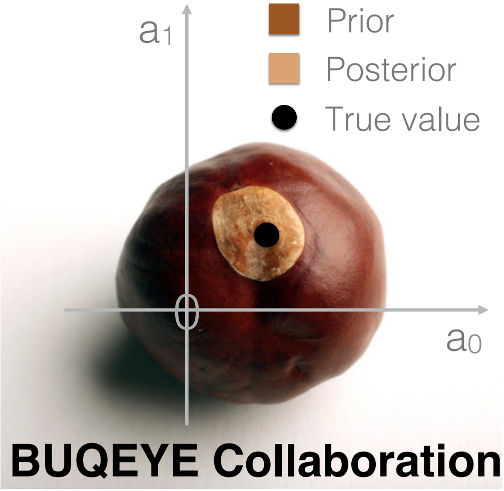
Bayesian analysis of EFTs with Jupyter notebooks

Dick Furnstahl
Virtual DNP Meeting, October 2020

The Ohio State University



Special thanks to my BUQEYE colleagues!

https://buqeye.github.io

This talk: [pptx][pdf]

NSF
U.S. DEPARTMENT OF ENERGY
NUCLEI
Nuclear Computational Low-Energy Initiative

What is a Jupyter notebook? (cf. Mathematica notebook)

- Executes Python (Anaconda recommended; all free!) but also other languages
- Displays in your browser (can run in the cloud through Binder! Example below)
- Tutorials available from datacamp, dataquest, YouTube, …

Sampling of 1d pdfs in Python

Here we show how histogrammed samples become closer to the continuous pdf as the sample size increases.

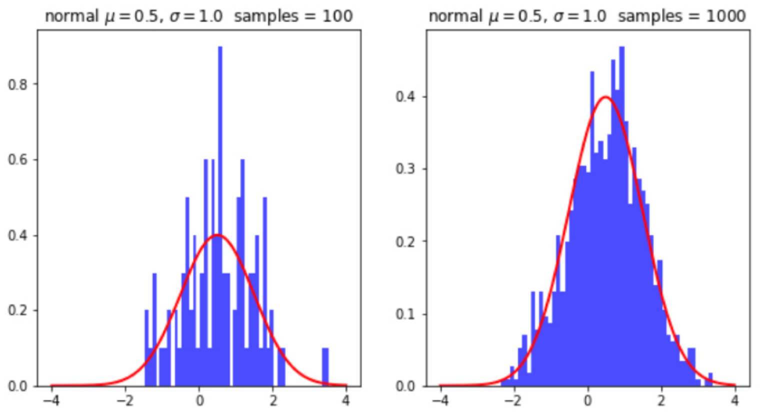
We use a 1d Gaussian distribution:

$$\mathrm{pr}(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

In [1]:
```python
import scipy.stats as stats      # We'll use stats as our source of pdfs
import numpy as np               # numpy for arrays
import matplotlib.pyplot as plt  # matplotlib for plotting
```

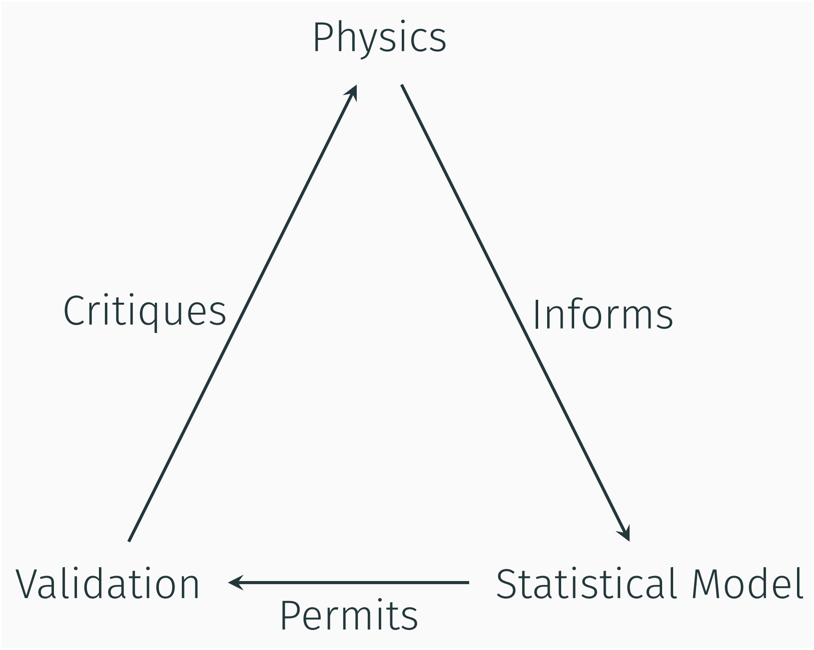
In [2]:
```python
def plot_hist(ax, name, x_dist, dist, num_samples, num_bins):
    """Plot a pdf and a histogram of samples"""
    samples = dist.rvs(size=num_samples)  # draw random samples from the pdf
    # Make a histogram of the random samples
    count, bins, ignored = ax.hist(samples, num_bins, density=True,
                                   color='blue', alpha=0.7)
    ax.plot(x_dist, dist.pdf(x_dist), linewidth=2, color='r') # true pdf
    title_string = name + f'  samples = {num_samples:d}'
    ax.set_title(title_string)


mu, sigma = 0.5, 1 # mean and standard deviation
x_dist = np.linspace(-4, 4, 500) # range of x points
name = rf'normal $\mu=${mu:1.1f}, $\sigma=${sigma:1.1f}' # title for plots
num_bins = 50  # histogram bins
```

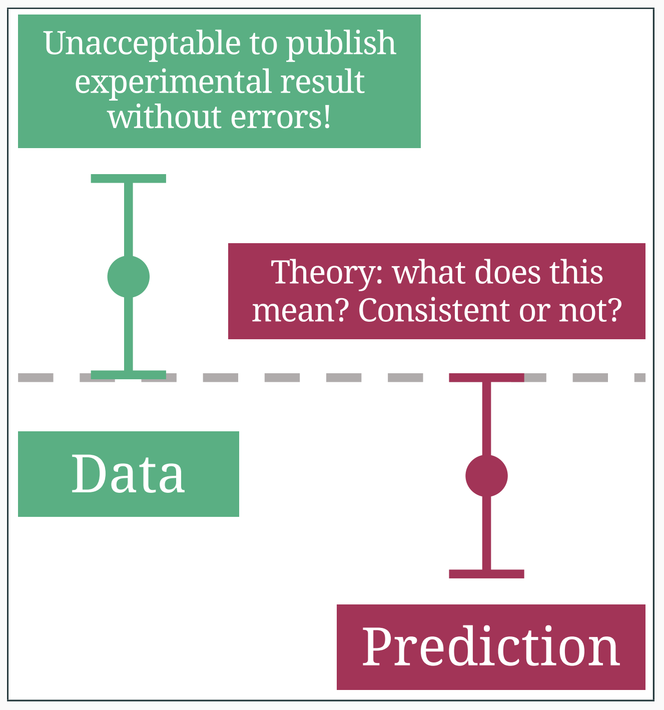
In [3]:
```python
fig = plt.figure(figsize=(15,5))
num_samples = 100
norm_dist = stats.norm(mu, sigma)
ax_1 = fig.add_subplot(1, 3, 1)
plot_hist(ax_1, name, x_dist, norm_dist, num_samples, num_bins)

num_samples = 1000
norm_dist = stats.norm(mu, sigma)
ax_2 = fig.add_subplot(1, 3, 2)
plot_hist(ax_2, name, x_dist, norm_dist, num_samples, num_bins)

```



Overview of Bayesian methods

- Bayesian statistics is a powerful framework for (chiral) EFT uncertainty quantification (UQ). *Everything is a pdf.*





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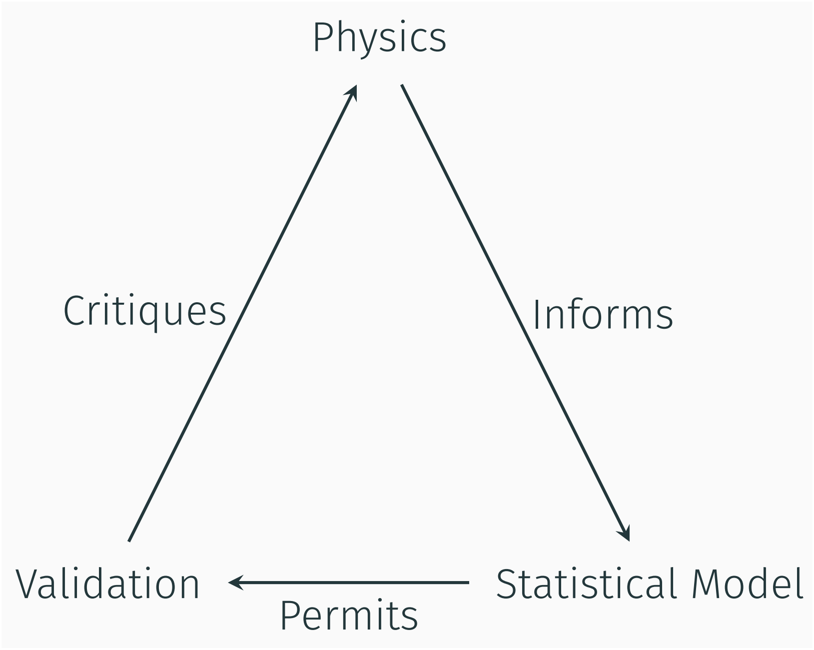

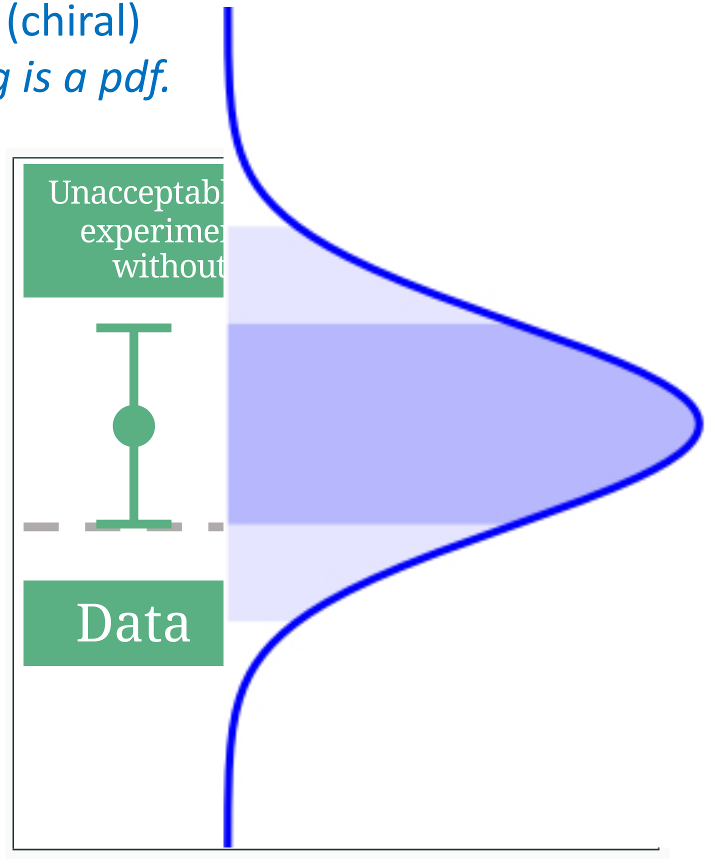

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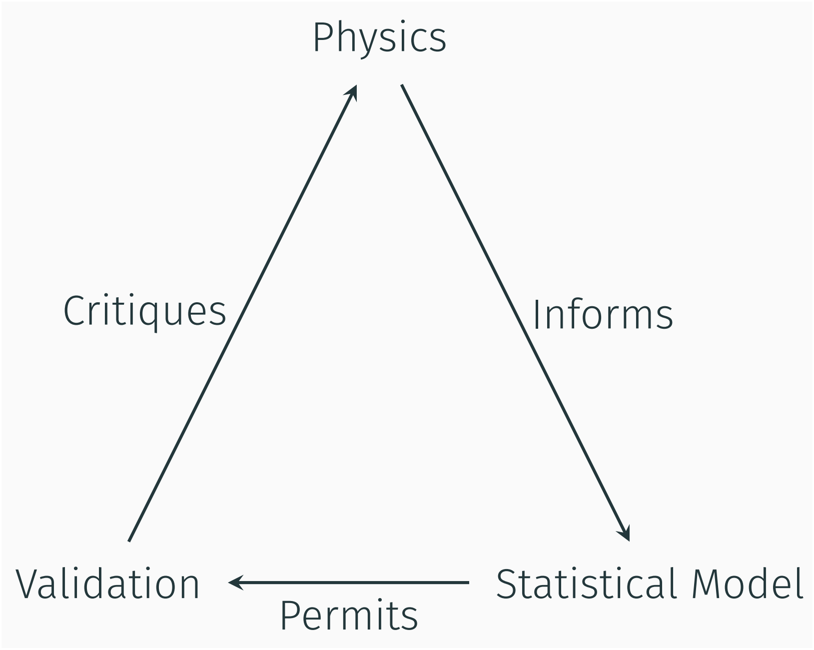

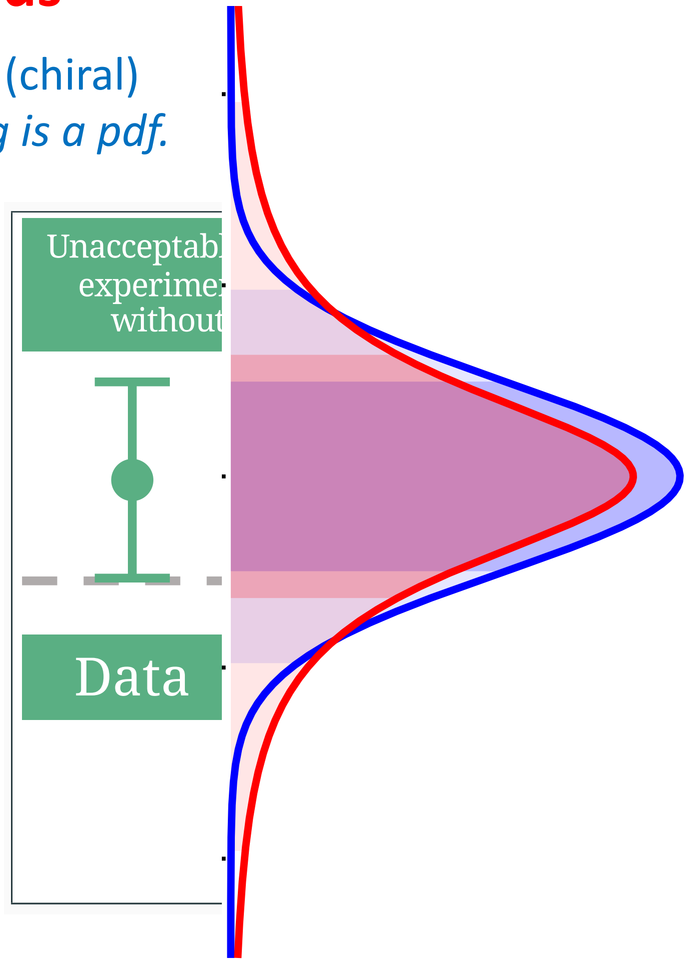

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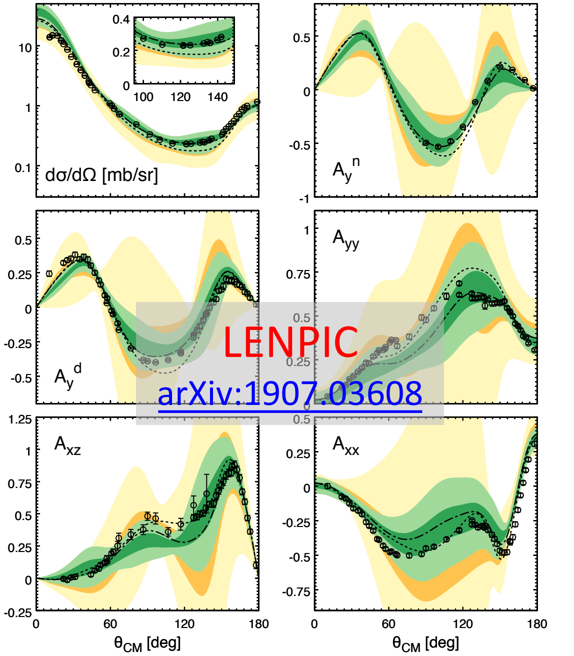

$\mathrm{pr}(\delta \mathbf{y}_{th} \mid \mathbf{y}_{th}, I) \Rightarrow$ pdf of *theory error* $\delta \mathbf{y}_{th}$ given theory calculations $\mathbf{y}_{th}$

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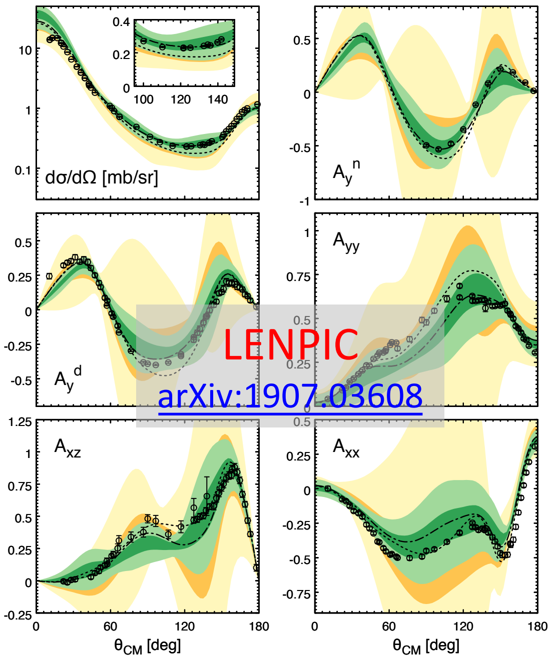

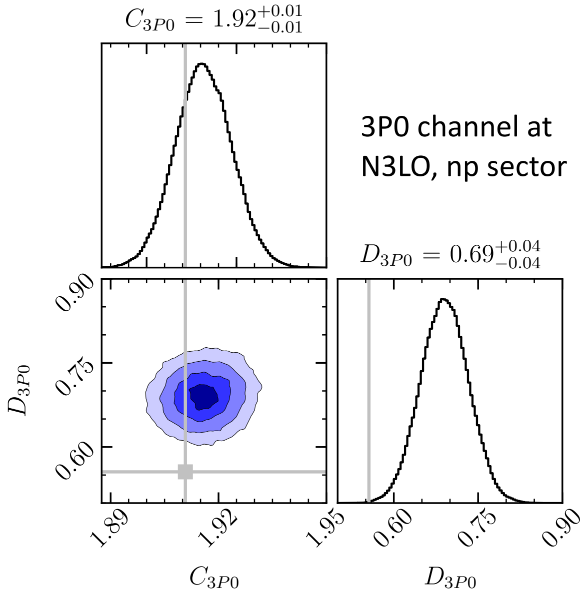

3P0 channel at N3LO, np sector

pr(δ$\mathbf{y}_{th}$ | $\mathbf{y}_{th}$, I) ⇒ pdf of *theory error* δ$\mathbf{y}_{th}$ given theory calculations $\mathbf{y}_{th}$

pr(**θ** | $\mathbf{y}_{exp}$, Σ_{exp} , Σ_{th} , I) ⇒ pdf of model parameters **θ** given data $\mathbf{y}_{exp}$ and experiment/theory errors Σ

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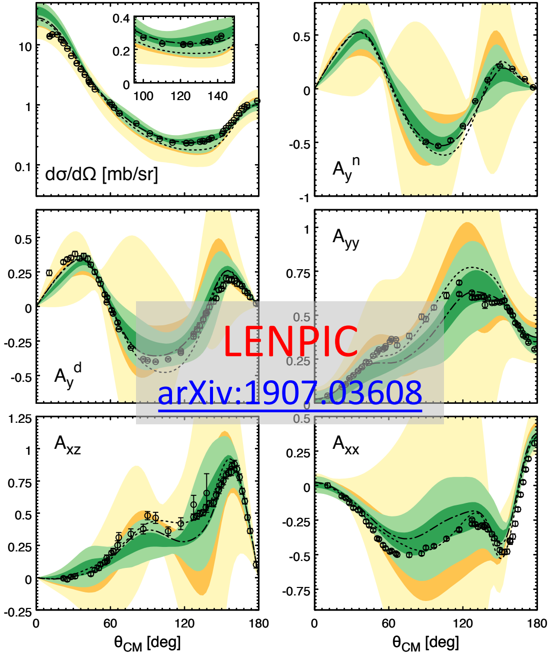

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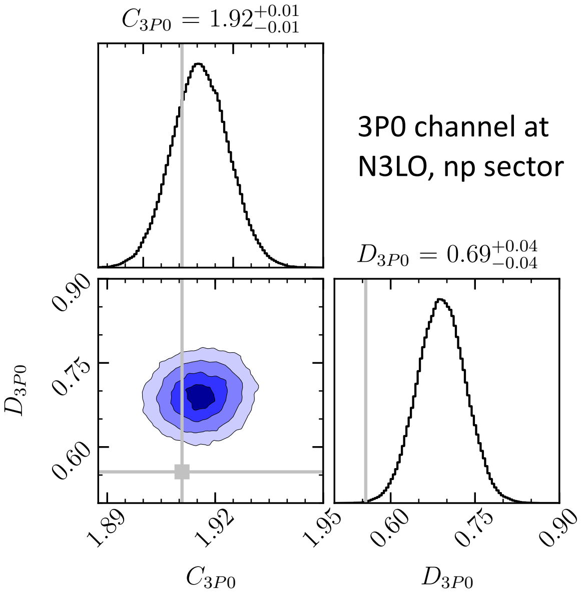

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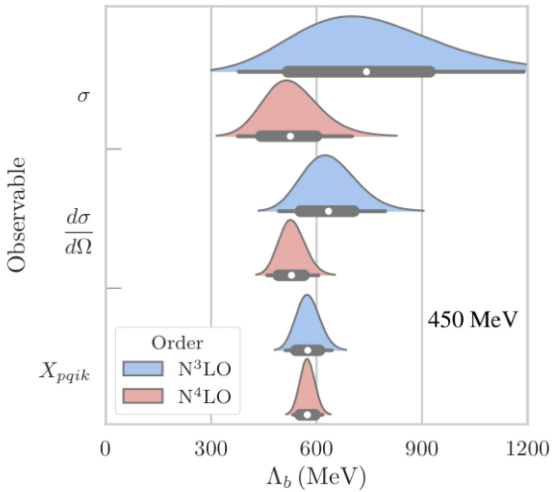
$\text{pr}(\boldsymbol{\theta} \,|\, \mathbf{y}_{exp}, \Sigma_{exp}, \Sigma_{th}, I) \Rightarrow$ pdf of model parameters $\boldsymbol{\theta}$ given data $\mathbf{y}_{exp}$ and experiment/theory errors Σ



$\text{pr}(\Lambda_b \,|\, \mathbf{y}_{th}, I) \Rightarrow$ pdf of breakdown scale of EFT expansion

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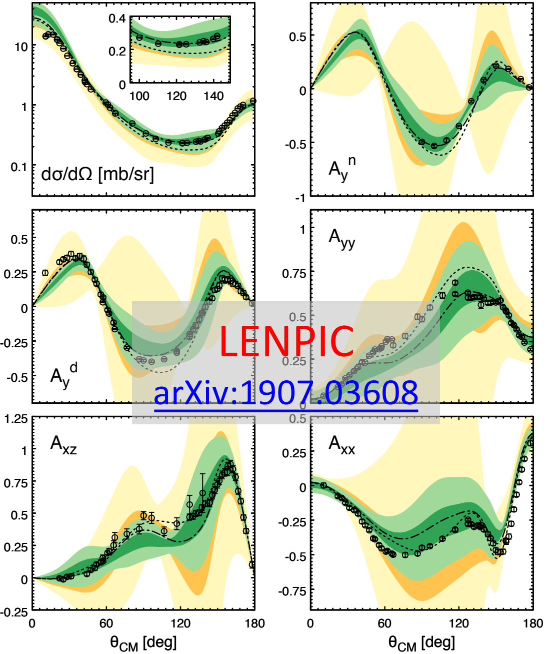

LENPIC
arXiv:1907.03608

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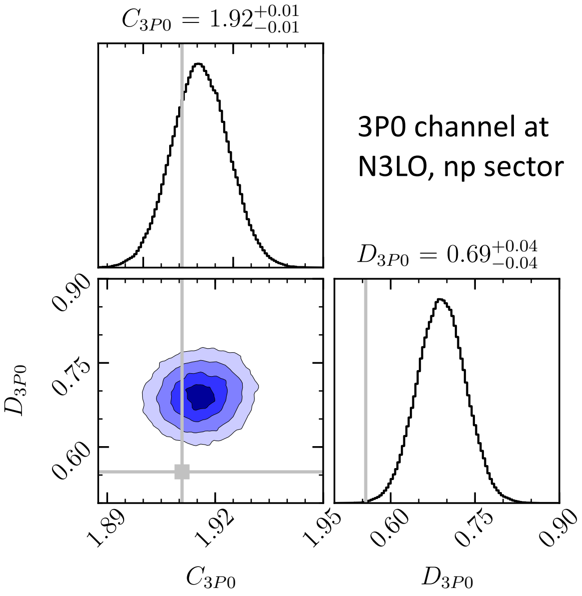

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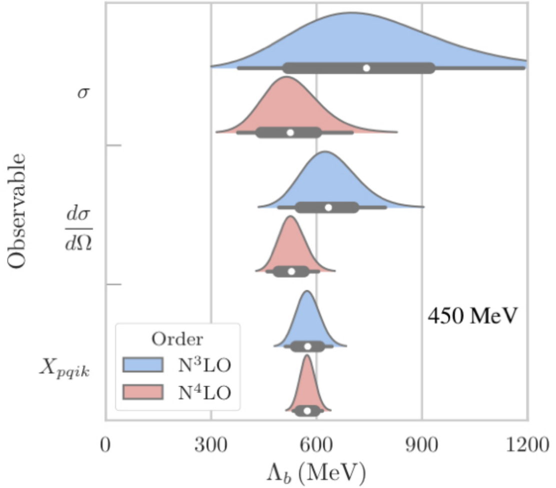

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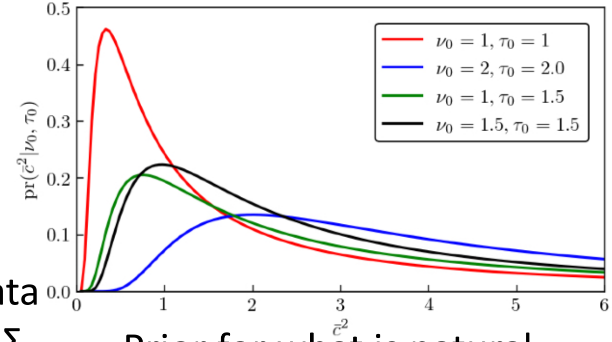

Prior for what is natural

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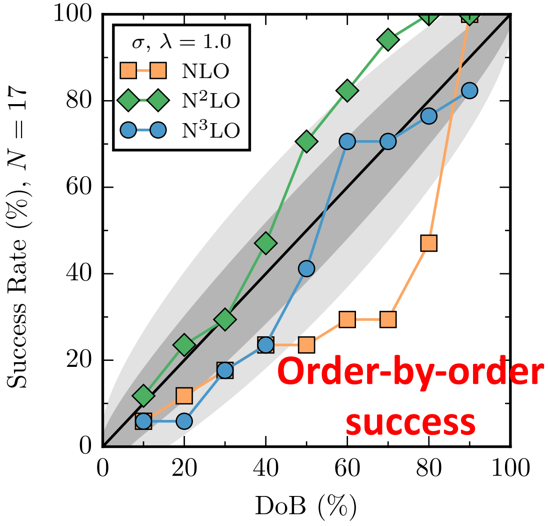

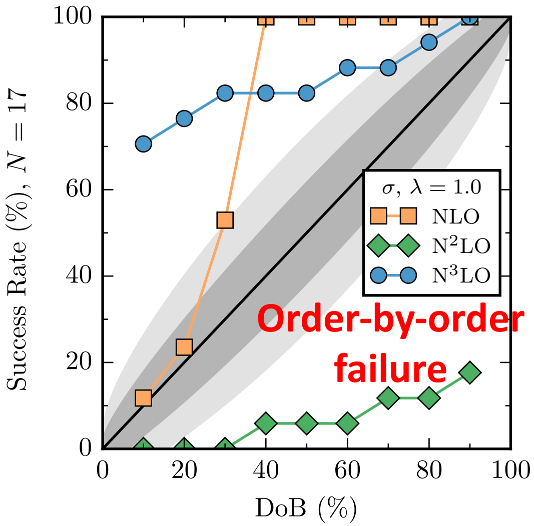

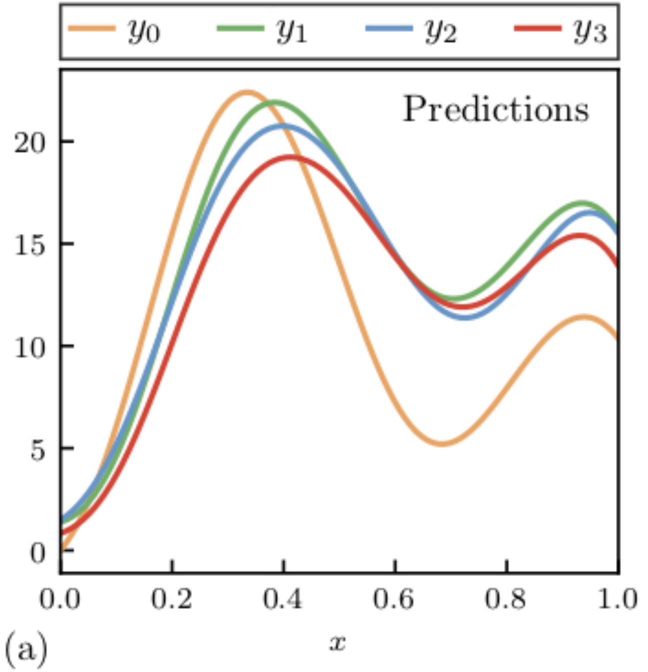

Toy model for an observable *y(x);* e.g., cross section vs. energy, order-by-order in EFT.

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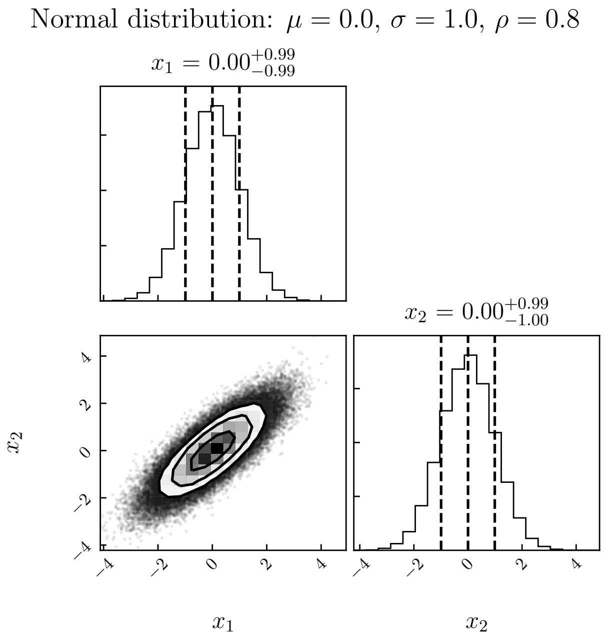

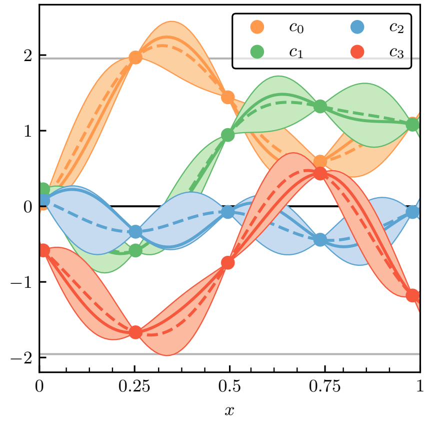

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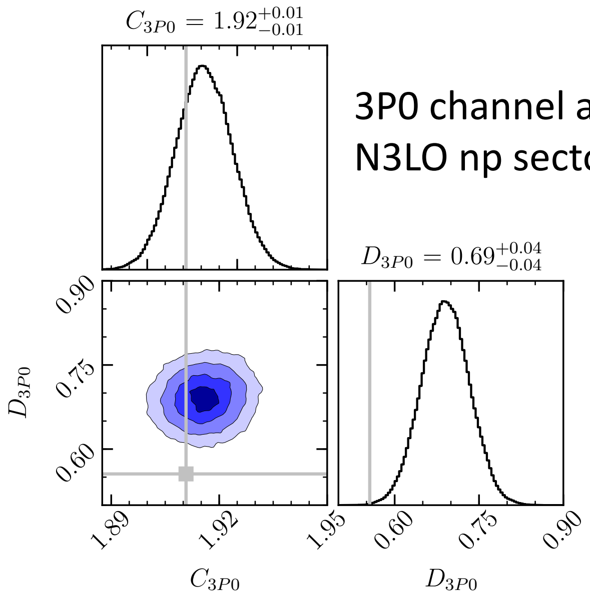

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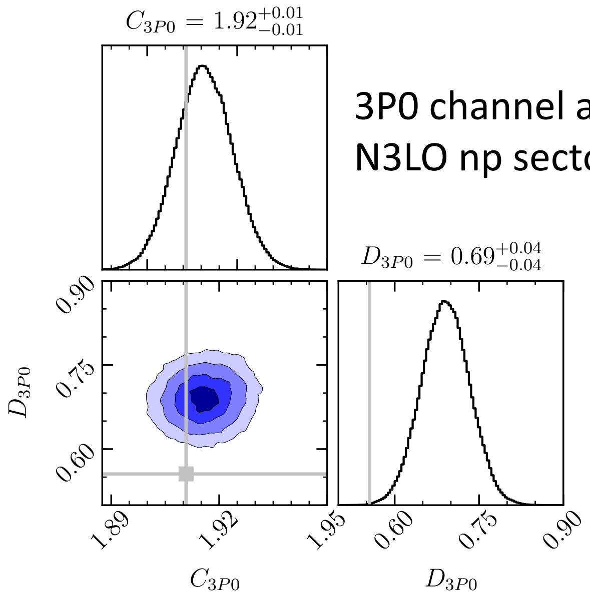

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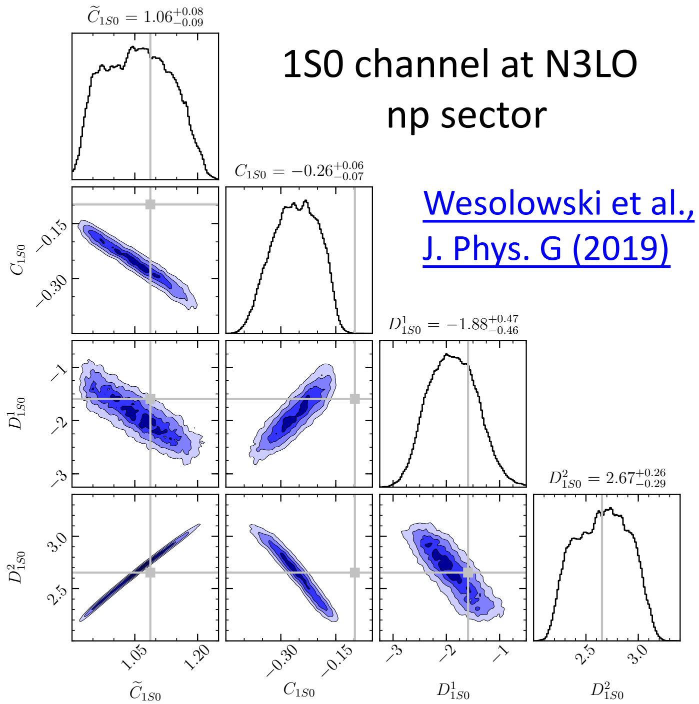
1S0 channel at N3LO
np sector



[Wesolowski et al., J. Phys. G (2019)]

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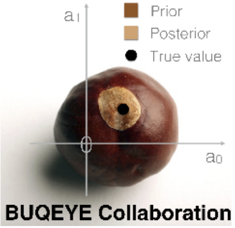
BUQEYE Collaboration ("Bayesian Uncertainty Quantification: Errors for Your EFT")

The buckeye is the state tree of Ohio!



https://buqeye.github.io

Papers and software (including Jupyter notebooks for figures)

BUQEYE philosophy for Bayesian analysis via notebooks:

- All assumptions explicit, with model checking and able to be checked externally
- Jupyter notebook(s) that reproduce all figures in BUQEYE papers (data provided)
- Open source, available on Github (or equivalent). Forks are encouraged!

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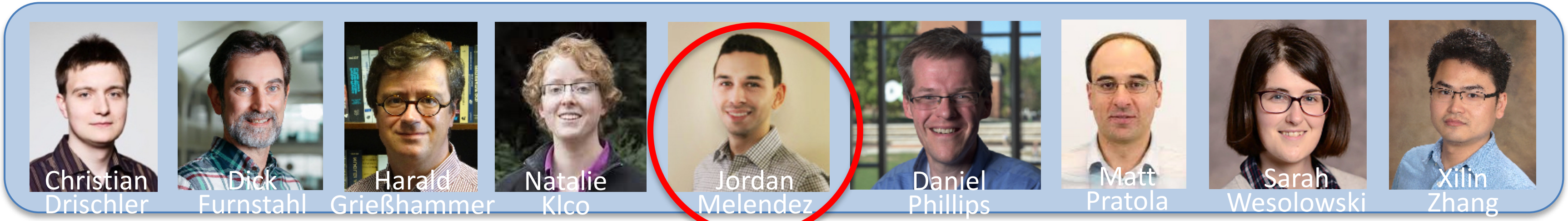

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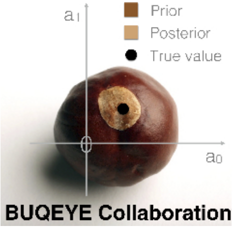

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Recent highlight: "Effective Field Theory Truncation Errors and Why They Matter,"
Jordan Melendez PhD thesis 2021 Dissertation Award in Nuclear Physics (SA.00003 11:42am)

The BUQEYE Cheatsheet for Pointwise Truncation Errors (arXiv:1904.10581)

From observable y, extract coefficients

$$\begin{aligned} \vec{y}_k &\equiv \{y_0, y_1, \cdots, y_k\} \\ \Rightarrow \vec{c}_k &\equiv \{c_0, c_1, \cdots, c_k\} \end{aligned} \tag{A1}$$

Choose ν_0 and τ_0. Update hyperparameters

$$\nu = \nu_0 + n_c \tag{A7}$$

$$\nu\tau^2 = \nu_0\tau_0^2 + \vec{c}_k^{\,2} \tag{A8}$$

Compute posterior

$$\mathrm{pr}(y \mid \vec{y}_k, Q) \sim t_\nu\left[y_k, y_{\mathrm{ref}}^2 \frac{Q^{2(k+1)}}{1-Q^2}\tau^2\right] \tag{A13}$$

```python
import numpy as np
y_ref = 20.0; Q = 0.3; k = 3
y_k = [21.7, 27.3, 25.4, 26.2]
c_k = np.array([y_k[0] / y_ref] + [
  (y_k[n] - y_k[n-1]) / (y_ref * Q**n)
  for n in range(1, k+1)])

nu_0 = 1; tau_0 = 1 # ~Uninformative
nu = nu_0 + len(c_k)
tau_sq = \
  (nu_0 * tau_0**2 + c_k @ c_k) / nu

from scipy.stats import t
scale = y_ref * Q**(k+1) * \
  ( tau_sq / (1 - Q**2) )**0.5
y = t(nu, y_k[-1], scale)
dob = y.interval(0.95) # (25.7, 26.7)
```

Note: If $n_c \gg 1$, the posterior for y becomes a normal distribution.

From https://buqeye.github.io/

The BUQEYE (...)twise Truncation Errors (arXiv:1904.10581)

Reference scale, expansion parameter, order of calculation

From observable y, extract coefficients

$$\vec{y}_k \equiv \{y_0, y_1, \cdots, y_k\} \\ \Rightarrow \vec{c}_k \equiv \{c_0, c_1, \cdots, c_k\} \qquad \text{(A1)}$$

$$\boldsymbol{y}_k = \boldsymbol{y}_{\mathrm{ref}} \sum_{n=0}^{k} c_n Q^n \rightarrow \delta \boldsymbol{y}_{\mathrm{th}} = \boldsymbol{y}_{\mathrm{ref}} \sum_{n=k+1}^{\infty} c_n Q^n$$

$$\chi\mathrm{EFT} \Rightarrow Q = \frac{\{p, m_\pi\}}{\Lambda_b}, \qquad \Lambda_b \approx 600\,\mathrm{MeV}$$

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Order-by-order calculations

Extract coefficients

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Order-by-order calculations

Extract coefficients

Update hyperparameters

Compute posterior and error bands

Note: If $n_c \gg 1$, the posterior for y becomes a normal distribution.

From https://buqeye.github.io/

Recent BUQEYE notebooks for EFT UQ papers

- **Quantifying correlated truncation errors in effective field theory**, J. Melendez, rjf, D. Phillips, M. Pratola, and S. Wesolowski, Phys. Rev. C 100, 044001 (2019) [notebooks]

- **How well do we know the neutron-matter equation of state at the densities inside neutron stars? A Bayesian approach with correlated uncertainties**, C. Drischler, rjf, J. Melendez, and D. Phillips, Phys. Rev. Lett. (in press). [notebooks]

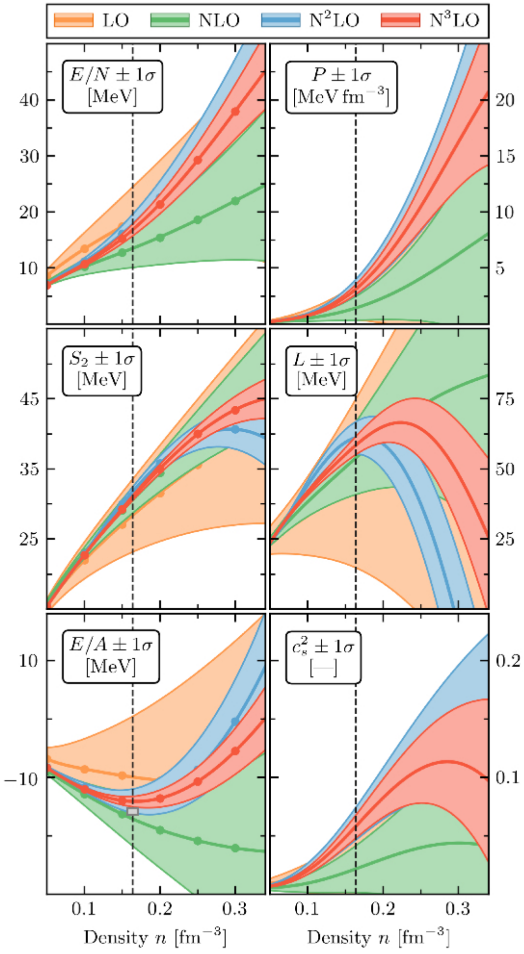
- **Quantifying uncertainties and correlations in the nuclear-matter equation of state**, C. Drischler, J. Melendez, rjf, and D Phillips, Phys. Rev. C (in press). [notebooks]

- **Efficient emulators for scattering using eigenvector continuation**, rjf, A. Garcia, P. Millican, and X. Zhang, Phys. Lett. B 809, 135719 (2020). [notebooks]

- **Designing Optimal Experiments: An Application to Proton Compton Scattering**, J. Melendez, rjf, H. Grießhammer, J. McGovern, D. Phillips, and M.T. Pratola, arXiv:2004.11307. [notebooks]

See Harold Grießhammer talk following this one.

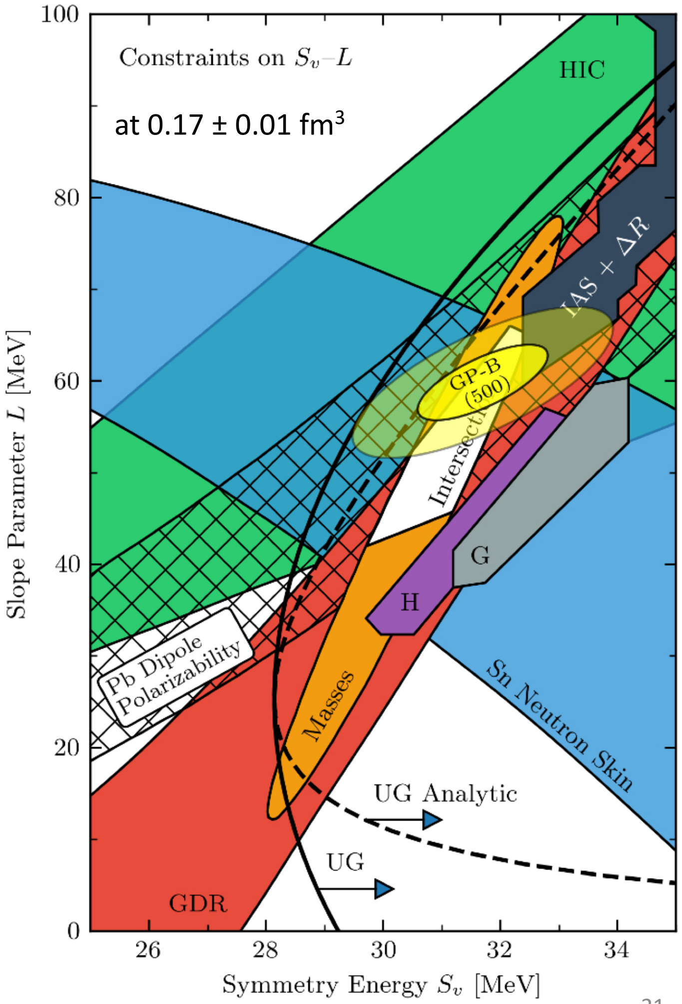
Correlated theory errors for EOS properties



C. Drischler et al.
(arXiv:2004.07232
PRL, in press)
(SD.00006 11:30am)

Correlated GP treatment gives better estimates for truncation errors and clean propagation of uncertainties to derived quantities.

See also comparisons to GW and NICER posteriors!



Summary points and more information

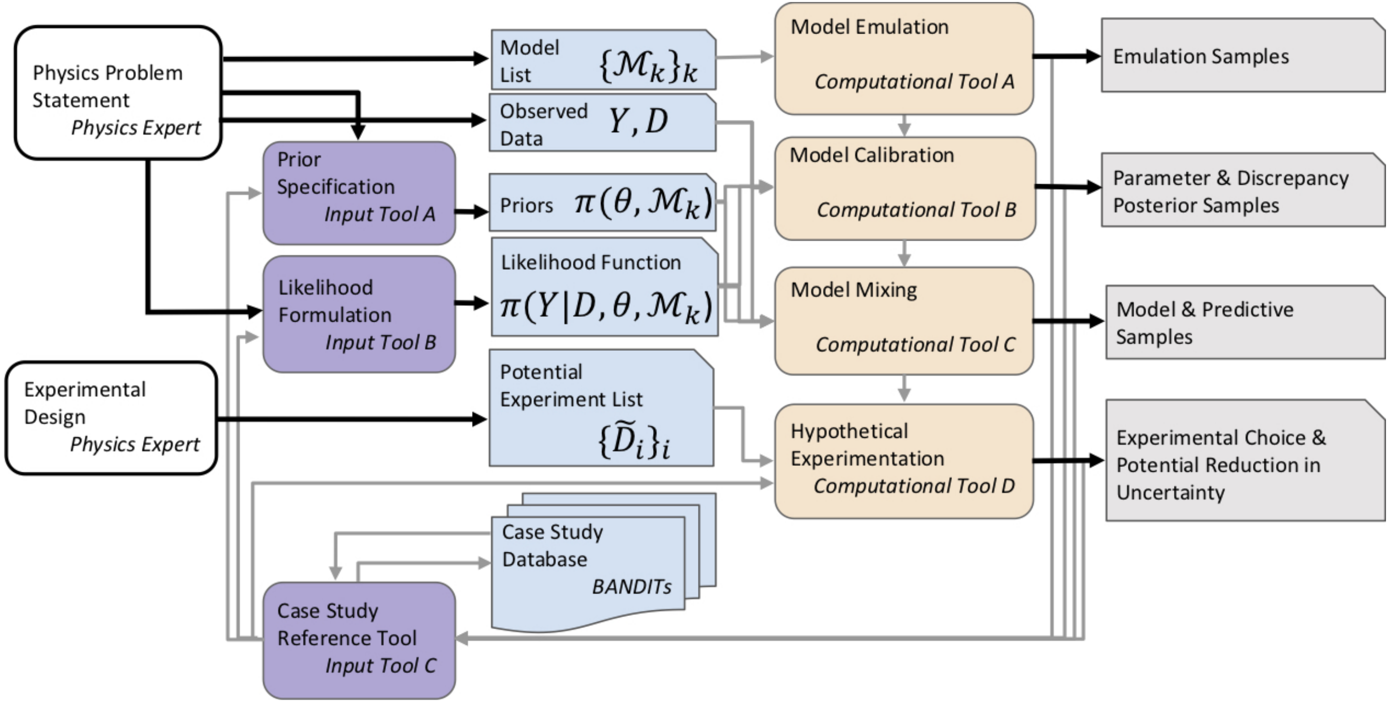
- Jupiter notebooks and Python are great tools for nuclear physics UQ
- Bayesian methods for EFT and other theory errors (combined with experiment)
    - Many examples from the BUQEYE collaboration
- We strongly advocate that *every* paper have a notebook for reproducing figures

- Github repositories with notebooks for learning Bayesian statistics for physics
    - BAYES 2019 (TALENT course): https://nucleartalent.github.io/Bayes2019/
    - Furnstahl course at Ohio State: https://furnstahl.github.io/Physics-8805/

BAND (Bayesian Analysis of Nuclear Dynamics)

An NSF Cyberinfrastructure for Sustained Scientific Innovation (CSSI) Framework (from 7/2020)

Look to https://bandframework.github.io/ over the next five years!



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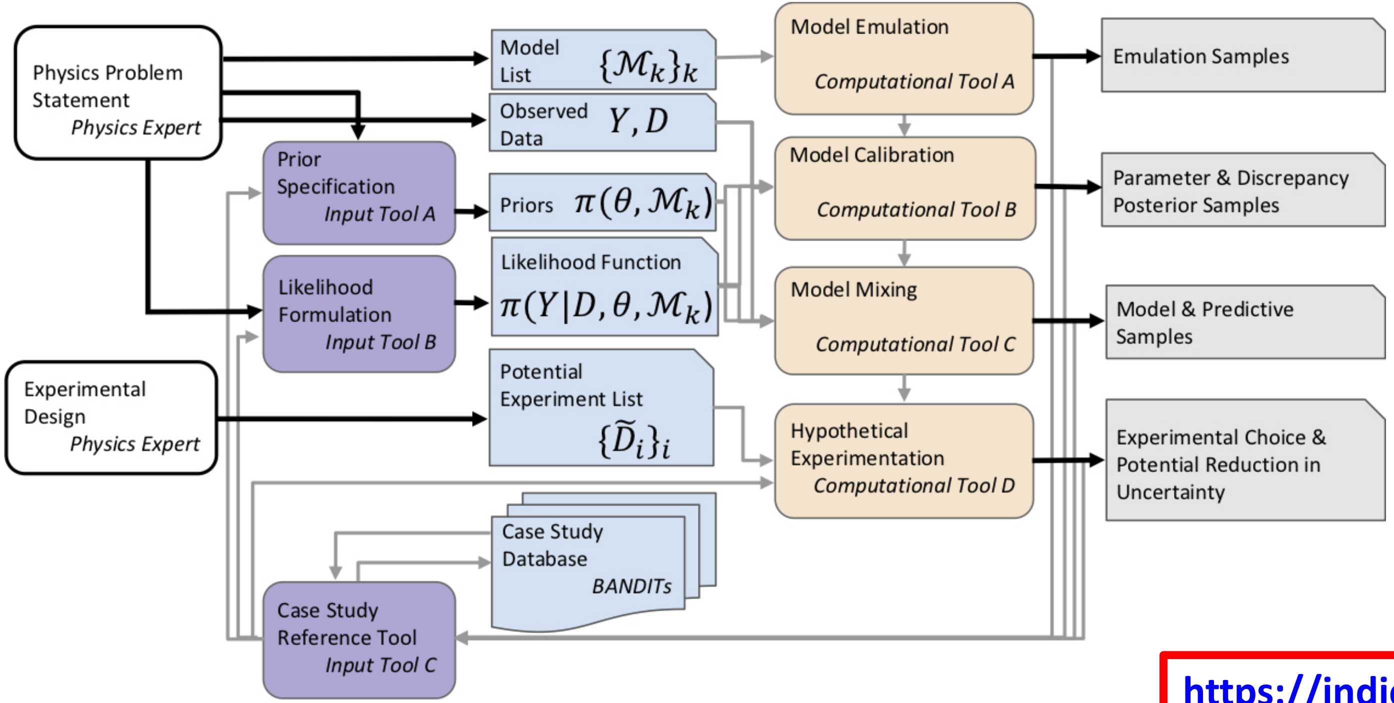

Bayesian Analysis of Nuclear Dynamics

Registration for Virtual ISNET 8 and for the First Annual BAND Camp is open. The website lists confirmed speakers for both events.

https://indico.frib.msu.edu/event/21/

Thank you!