# Emulators for Bayesian Inference in Chiral EFT


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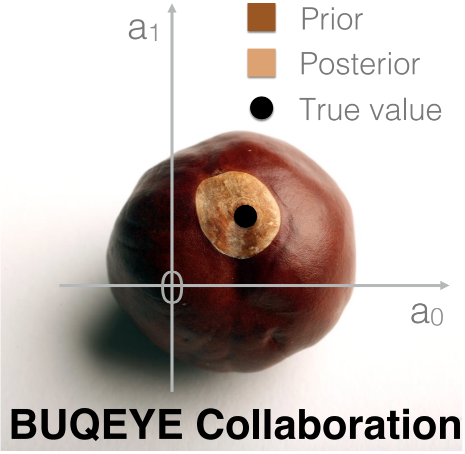
LENPIC Meeting, August 2022

The Ohio State University


References:




https://buqeye.github.io/

Jupyter notebooks here!

LENPIC

https://www.lenpic.org/

NUCLEI
Nuclear Computational Low-Energy Initiative

https://nuclei.mps.ohio-state.edu/

BAND
Bayesian Analysis of Nuclear Dynamics

https://bandframework.github.io/

U.S. DEPARTMENT OF ENERGY

NSF

# What would we like to use Bayesian inference for?

In order of complexity . . .

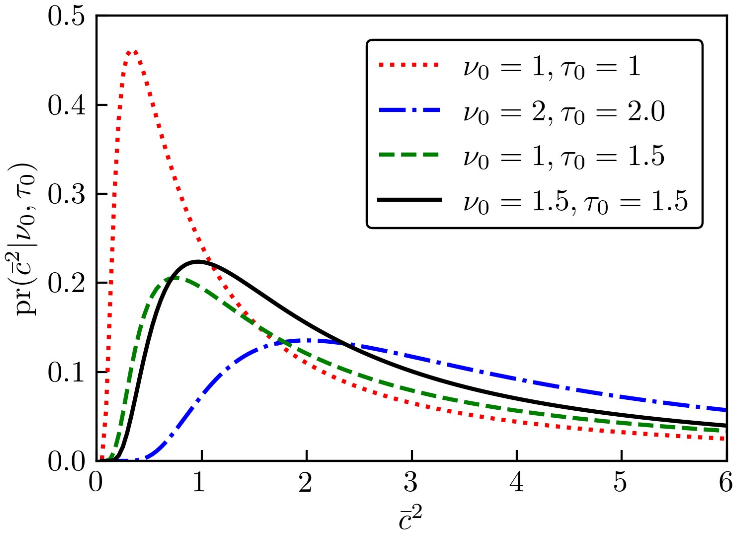
1. Forward UQ (e.g., propagate errors using already-sampled posteriors)

2. Inverse UQ (e.g., parameter estimation including theory errors)

3. Experimental Design (guide to experiment: which data are most likely to provide the largest information gain; both theory uncertainty *and* the expected pattern of experimental errors must be considered)

# Barrier to using Bayesian methods: Computational cost

Calculating Bayesian pdfs and expectation values can be prohibitively costly for expensive likelihood. What can we do to mitigate the cost?




→ 1. **Use conjugate priors:** for some likelihoods, posterior pdf is in same family as prior pdf → analytical updating of posterior. Example: the EFT truncation variance (used in LENPIC papers):

$$\underbrace{\mathrm{pr}(\bar{c}^2|\{c_n\})}_{\sim\chi^{-2}(\nu,\tau^2)} \propto \underbrace{\mathrm{pr}(\{c_n\}|\bar{c}^2)}_{\sim\mathcal{N}(0,\bar{c}^2)}\ \underbrace{\mathrm{pr}(\bar{c}^2)}_{\chi^{-2}(\nu_0,\tau_0^2)} \quad \longleftarrow \quad \nu = \nu_0 + n_c, \quad \nu\tau^2 = \nu_0\tau_0^2 + \sum_n c_n^2$$

2. **Gaussian approximation** (data >> model complexity)

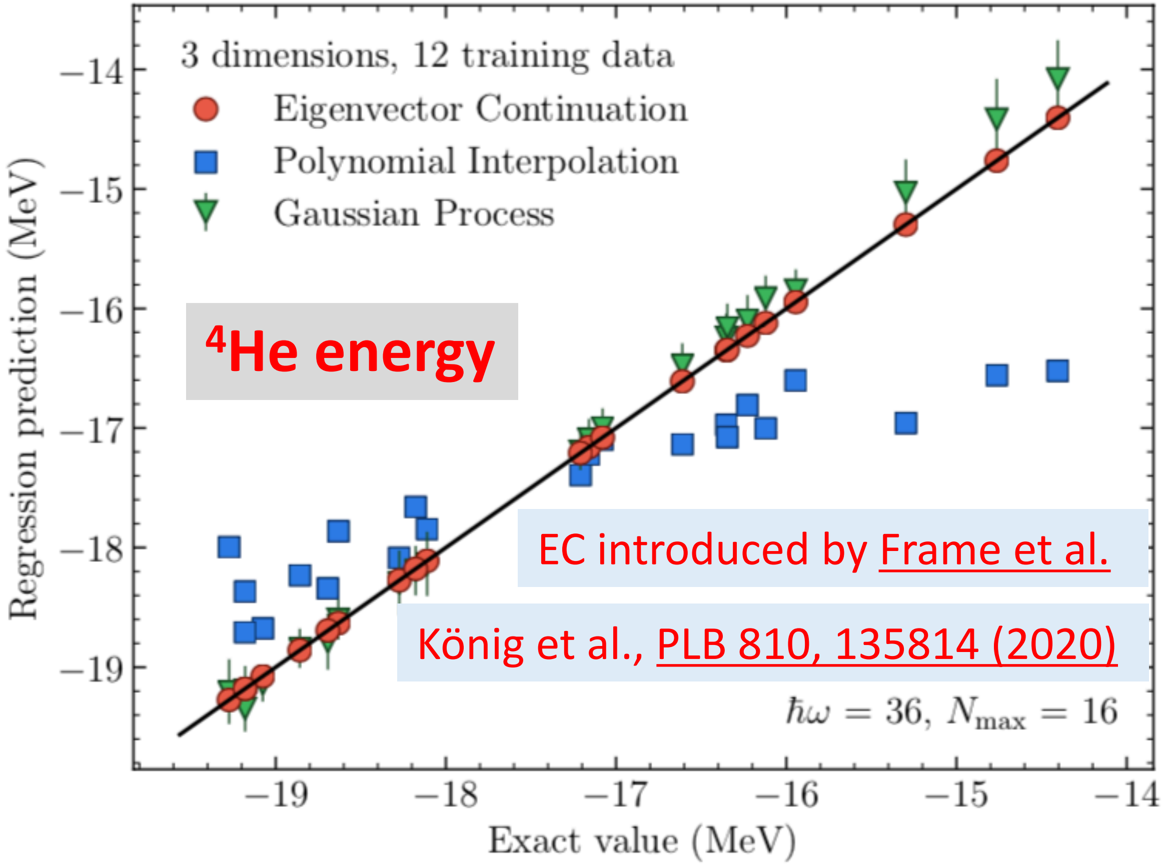
3. **Variational Bayesian Inference or VBI** (approximate the posterior)

→ 4. Sample with Markov chain Monte Carlo (MCMC) using an ***emulator***
   → *Make a computer model of your calculation*
   - Gaussian process model emulators [e.g., learn your residuals]
   - Eigenvector continuation (EC) and extensions [König et al., PLB 810, 135814 (2020)]

See also Witala et al., arXiv:2103.13237

# Eigenvector continuation emulators for few-nucleon observables

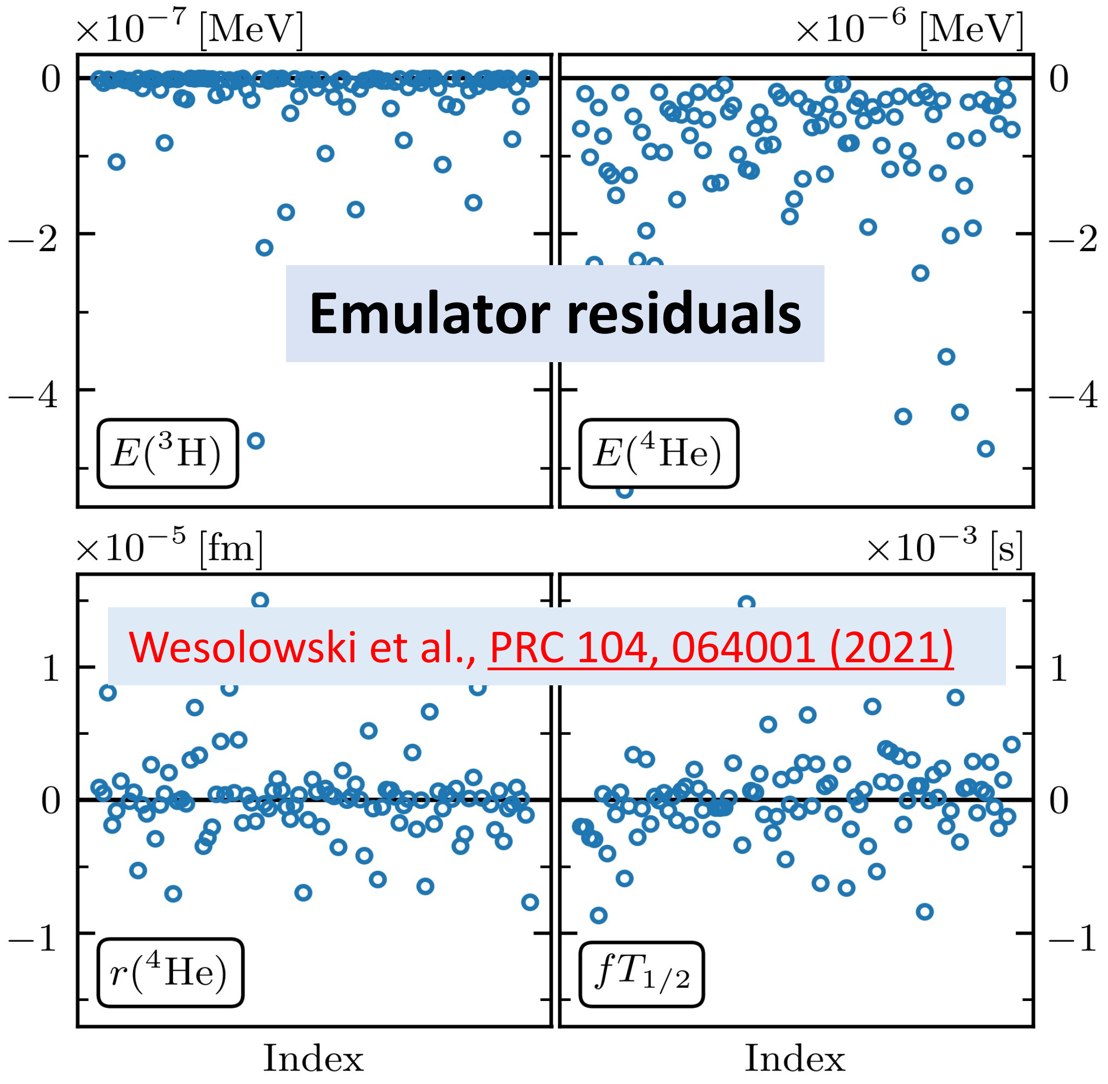
**Basic idea:** a small # of ground-state eigenvectors from a selection of parameter sets is an extremely effective variational basis for other parameter sets.
**Characteristics:** fast and accurate!




$^4$He energy

EC introduced by Frame et al.

König et al., PLB 810, 135814 (2020)



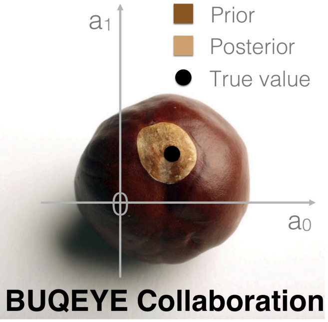

**Emulator residuals**

Wesolowski et al., PRC 104, 064001 (2021)

Works well for transitions, too!

# *Rigorous constraints on three-nucleon forces in chiral effective field theory from fast and accurate calculations of few-body observables*

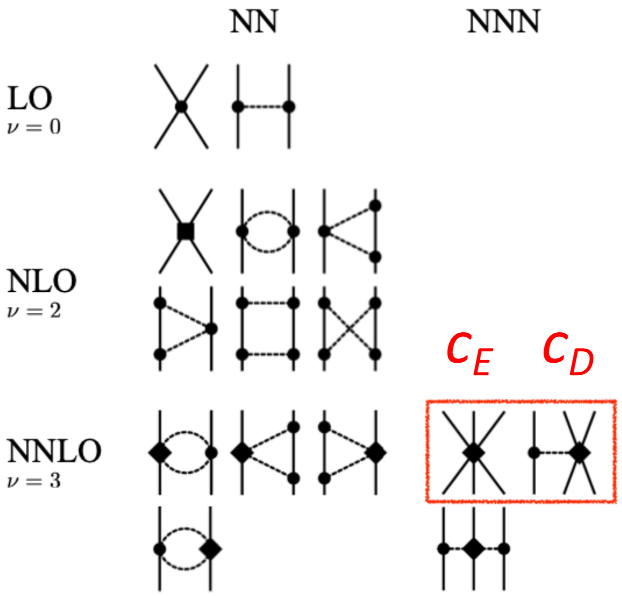
S. Wesolowski, I. Svensson, A. Ekström, C. Forssén, rjf, J. A. Melendez, and D. R. Phillips




**BUQEYE Collaboration**

Notebook with all figures at
[https://buqeye.github.io](https://buqeye.github.io)

**Original title:** *Fast & rigorous constraints on chiral three-nucleon forces from few-body observables*
arXiv:2104.04441 PRC **104**, 064001 (2021)




**Fast:** uses eigenvector continuation emulators for observables

**Rigorous:** statistical best practices for parameter estimation

**Chiral 3N forces:** estimate constraints on $c_D$ and $c_E$

**Few-body observables (cf. other possibilities):**

$^3$H ground-state energy; $^3$H β-decay half-life;
$^4$He ground-state energy; $^4$He charge radius

# (almost) Full Bayesian approach to constraining parameters

Experimental data

Other info (EFT scheme/scale, etc.)

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 \,|\, \mathbf{y}_{\rm exp}, I) \propto \mathrm{pr}(\mathbf{y}_{\rm exp} \,|\, \vec{a}, \Sigma, I)\; \mathrm{pr}(\vec{a}\,|\,I)\;\; \mathrm{pr}(\bar{c}^2\,|\,Q, \vec{a}, I)\;\; \mathrm{pr}(Q\,|\,\vec{a}, I)$$

NN *and* 3N LECs

EFT expansion parameter

Truncation error variance

**Everything has priors!**

All experiment and theory errors

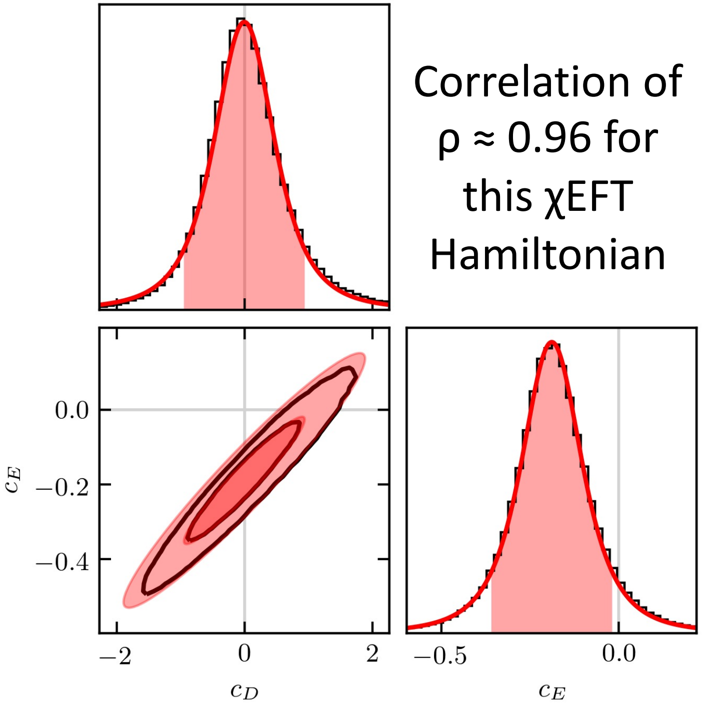
Likelihood: $\mathrm{pr}(\mathbf{y}_{\rm exp} \,|\, \vec{a}, \Sigma, I) \sim \mathcal{N}(\mathbf{y}_{\rm th}(\vec{a}),\; \Sigma_{\rm exp} + \Sigma_{\rm method} + \Sigma_{\rm th})$

Uses NNLO chiral EFT without Δ's based on Carlsson et al. PRX **6**, 011019 (2016), but methods are general (other regulators, Δ's, other observables)

Sample pdf with MCMC over 15 dimensions (11 NN LECs + $c_D$, $c_E$ + $Q$, $\bar{c}^2$)
→ marginalize (integrate out) what you are not considering

# Posteriors from “*Fast & Rigorous*” (arXiv:2104.04441)

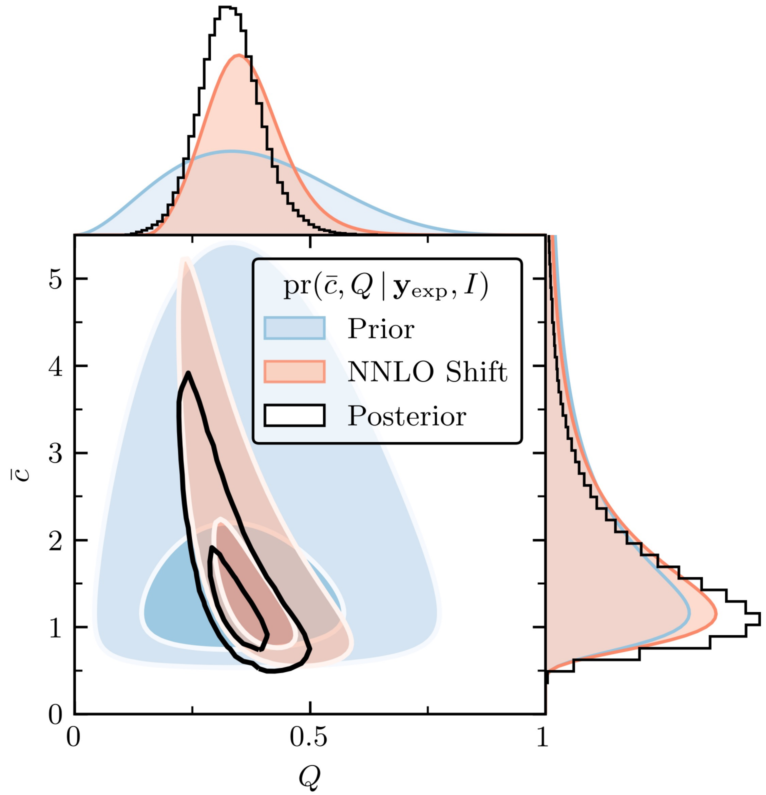
## Posterior for $c_D$ and $c_E$




Correlation of ρ ≈ 0.96 for this χEFT Hamiltonian

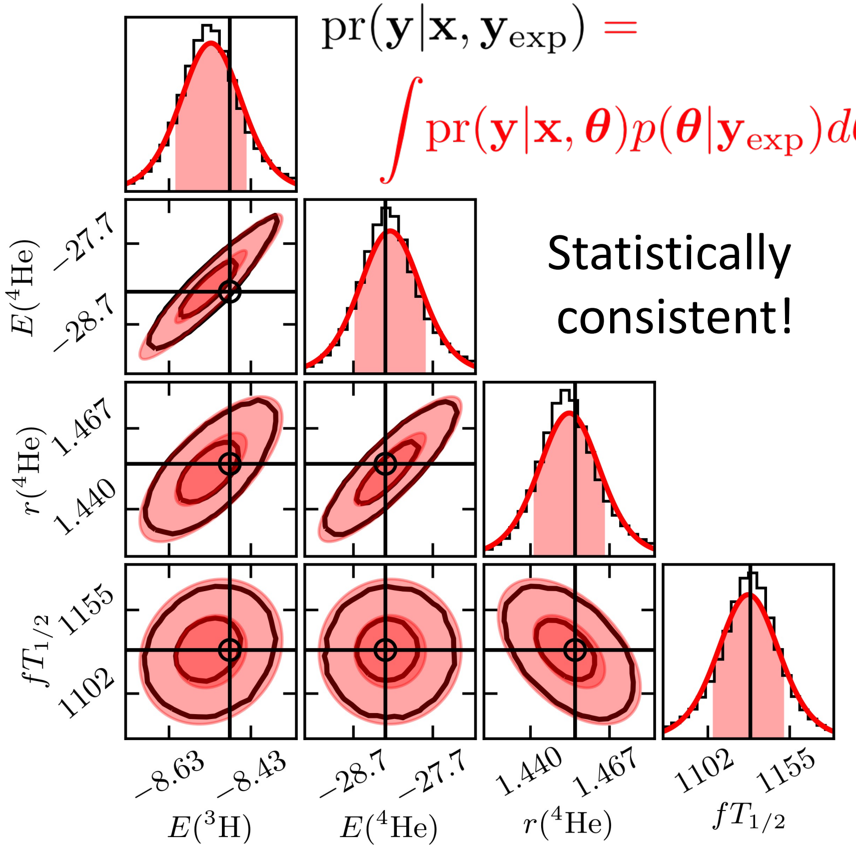
Tails are *not* well approximated by a Gaussian! (But do look like t’s!)

## Posterior for $Q$ and $\bar{c}$




## Posterior predictive distribution

$$\mathrm{pr}(\mathbf{y}|\mathbf{x}, \mathbf{y}_{\mathrm{exp}}) = \int \mathrm{pr}(\mathbf{y}|\mathbf{x}, \boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathbf{y}_{\mathrm{exp}}) d\boldsymbol{\theta}$$




Statistically consistent!

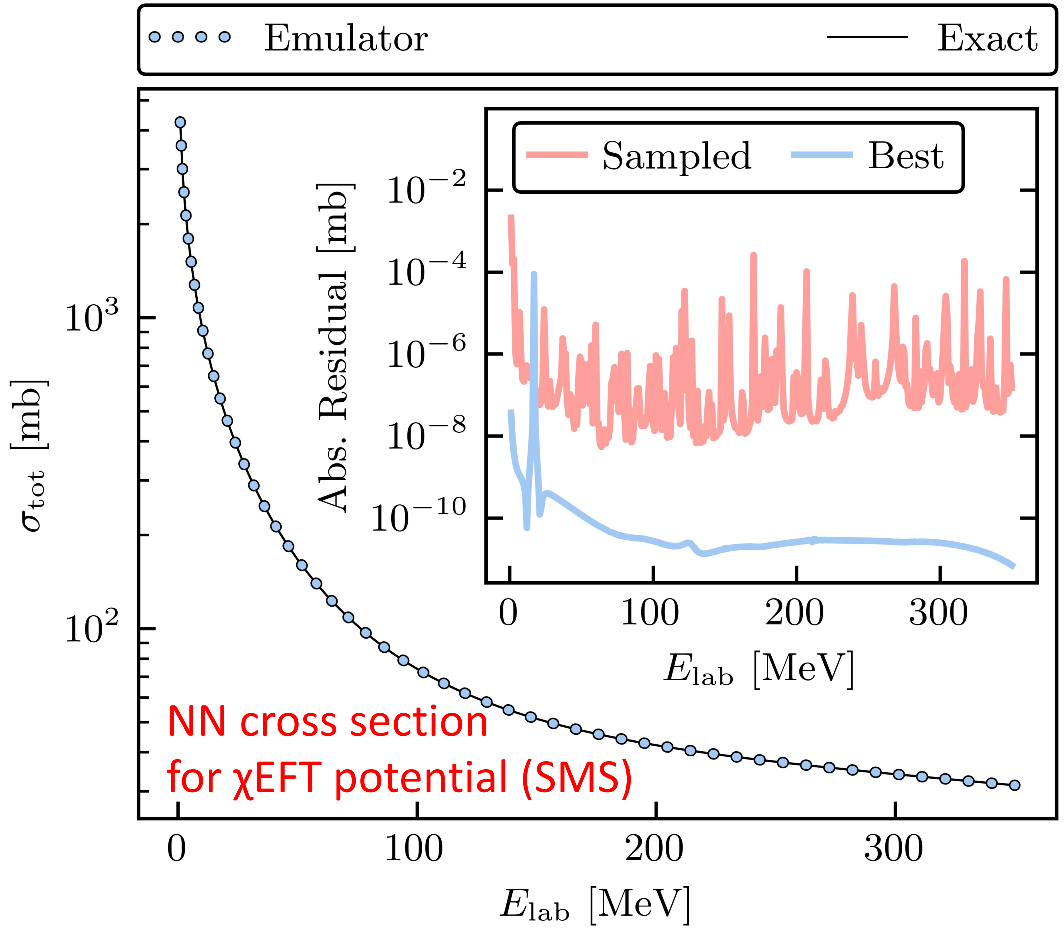
Truncation error for observables:

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 | \mathbf{y}_{\mathrm{exp}}, I) \;, \qquad y_{\mathrm{k}} = y_{\mathrm{ref}} \sum_{n=1}^{k} c_n Q^k \;, \qquad \bar{c}^2 \text{ variance for } c_n\text{'s}$$

Sample pdf with MCMC over 11 NN LECs + $c_D$, $c_E$ + $Q$, $\bar{c}^2$ → marginalize (integrate out) what you are not considering

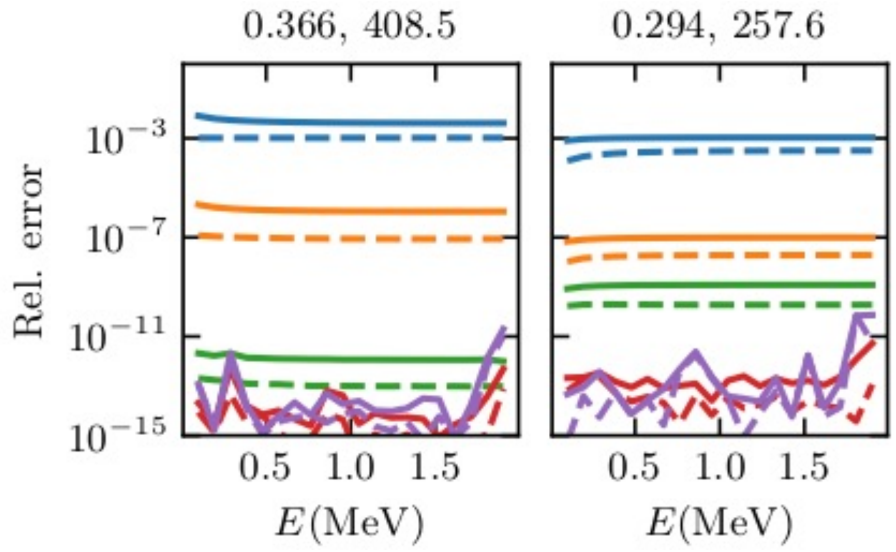
# EC emulators for NN and 3N scattering

- EC extended to 2-body scattering by rjf et al., PLB (2020) using the Kohn variational principle.
- Method improved by Drischler et al., PLB (2021) (e.g., mitigate Kohn anomalies).
- Two-body emulation w/o wfs by Melendez et al., PLB (2021) (Newton variational method).




NN cross section for χEFT potential (SMS)

What about 3-body scattering emulators?
Most useful for Bayesian χEFT LEC estimation.
→ Xilin Zhang proof of principle w/KVP (2022).




3-body S-matrix errors for basis size 3, 6, 9, 12, 14 with schematic potential for two test LEC points.

See also Sarkar and Lee, PRL 126 (2021) and PR Res. 4 (2022) and Krakow group for Faddeev emulator, EPJA 57 (2021).

# Eigenvector continuation (EC) for bound states

$$\widehat{H}(\boldsymbol{\theta}) = \widehat{T} + \widehat{V}(\boldsymbol{\theta}) = \widehat{T} + \sum_a \theta^{(a)} \mathcal{O}^{(a)} \text{ with LECs } \boldsymbol{\theta} = \{\theta^{(a)}\}$$

*Affine* dependence (could be chiral EFT or AV18 or …)

Ground-state variational: $\delta\Big[\langle\psi_{\rm trial}|\widehat{H}(\boldsymbol{\theta})|\psi_{\rm trial}\rangle - \lambda\big(\langle\psi_{\rm trial}|\psi_{\rm trial}\rangle - 1\big)\Big] = 0$

EC: $|\psi_{\rm trial}\rangle = \sum_{i=1}^{N} c_i|\psi_{\rm gs}(\boldsymbol{\theta}_i)\rangle \implies$ gen. eig. problem: $\lambda_{min} \approx E_{\rm gs}, \ \{c_i\} \to |\psi_{\rm gs}(\boldsymbol{\theta})\rangle$

- Use regularization to deal with ill-conditioning of norm matrix
- EC works for local or non-local potentials, r-space or k-space, many body

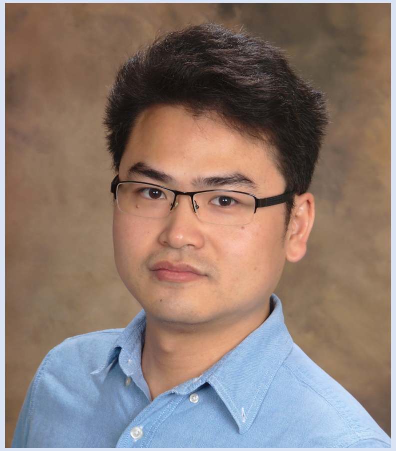
# Eigenvector continuation (EC) for scattering

$$\widehat{H}(\boldsymbol{\theta}) = \widehat{T} + \widehat{V}(\boldsymbol{\theta}) = \widehat{T} + \sum_a \theta^{(a)} \mathcal{O}^{(a)} \text{ with LECs } \boldsymbol{\theta} = \{\theta^{(a)}\}$$

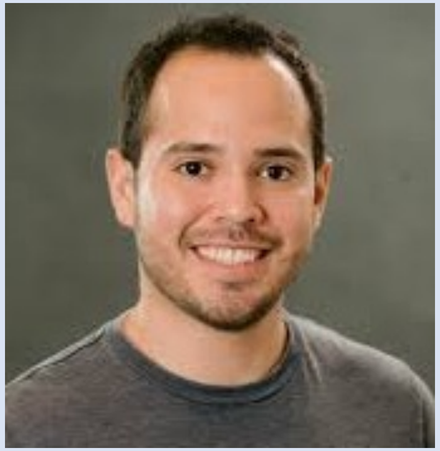
*Affine* dependence (here chiral)

K matrix: $k_\ell(E) = \tan\delta_\ell(E) \quad [\text{cf. } s_\ell(E) = e^{2i\delta_\ell(E)}] \quad \text{Take } \ell = 0 \text{ here, } p \equiv \sqrt{2\mu E}$

Kohn: $\delta\left[\frac{[k_0(E)]_{\text{trial}}}{p} - \frac{2\mu}{\hbar^2}\langle\psi_{\text{trial}}|\widehat{H}(\boldsymbol{\theta}) - E|\psi_{\text{trial}}\rangle\right] = 0 \text{ with } |\psi_{\text{trial}}\rangle \xrightarrow[r\to\infty]{} \frac{1}{p}\sin(pr) + \frac{k_0(E)}{p}\cos(pr)$



Xilin Zhang



Alberto Garcia

Patrick Millican

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Could be chiral EFT or AV18 or …

K matrix: $k_\ell(E) = \tan\delta_\ell(E)$ $\quad$ [cf. $s_\ell(E) = e^{2i\delta_\ell(E)}$] $\quad$ Take $\ell = 0$ here, $p \equiv \sqrt{2\mu E}$

Kohn: $\delta\left[\frac{[k_0(E)]_{\rm trial}}{p} - \frac{2\mu}{\hbar^2}\langle\psi_{\rm trial}|\widehat{H}(\boldsymbol{\theta}) - E|\psi_{\rm trial}\rangle\right] = 0$ with $|\psi_{\rm trial}\rangle \underset{r\to\infty}{\longrightarrow} \frac{1}{p}\sin(pr) + \frac{k_0(E)}{p}\cos(pr)$

EC: $|\psi_{\rm trial}\rangle = \sum_{i=1}^{N} c_i |\psi_E(\boldsymbol{\theta}_i)\rangle \implies c_i = \sum_j (\Delta\widetilde{U})^{-1}_{ij}([k_0/p]_j - \lambda)$ and $\lambda = \frac{\sum_{ij}(\Delta\widetilde{U})^{-1}_{ij}([k_0/p]_j - 1)}{\sum_{ij}(\Delta\widetilde{U})^{-1}_{ij}}$

with $\Delta\widetilde{U}_{ij}(E) \equiv \frac{2\mu}{\hbar^2}\langle\psi_E(\boldsymbol{\theta}_i)|2\widehat{V}(\boldsymbol{\theta}) - \widehat{V}(\boldsymbol{\theta}_i) - \widehat{V}(\boldsymbol{\theta}_j)|\psi_E(\boldsymbol{\theta}_j)\rangle$ ← Coulomb cancels!

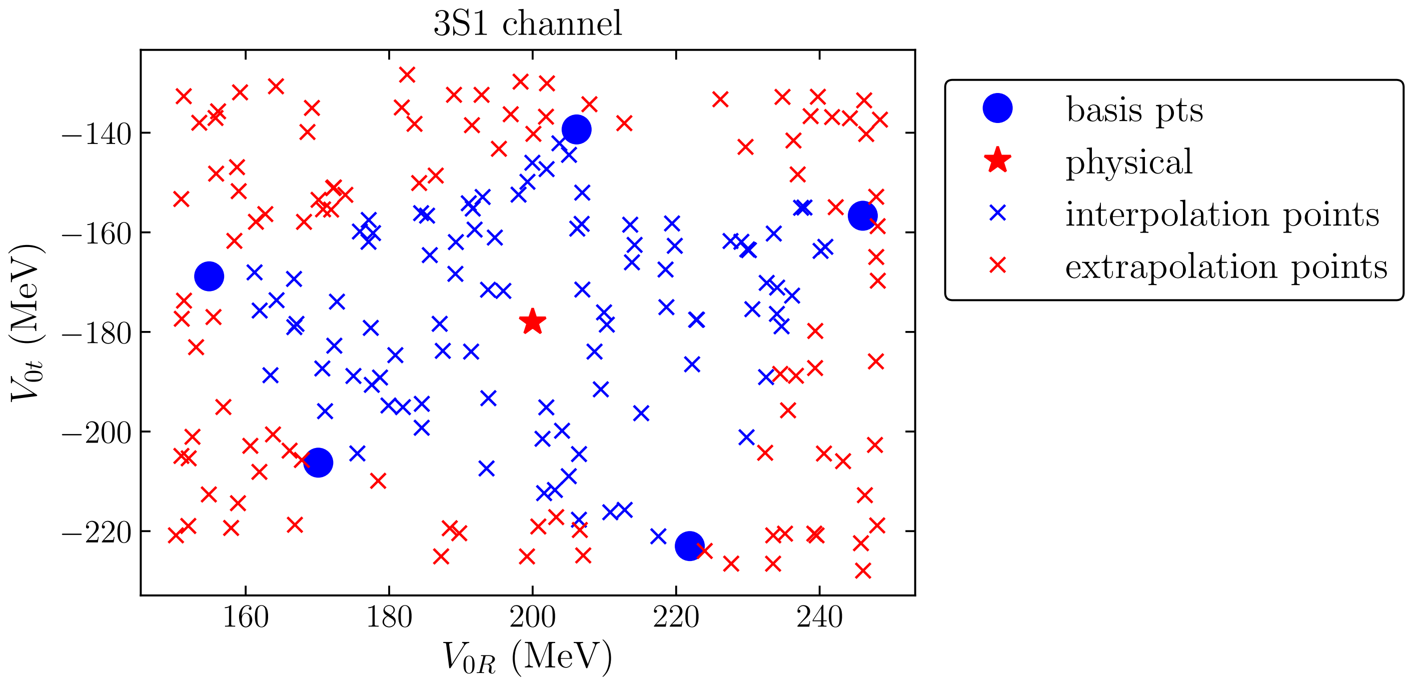
- Stationary functional for $k_l(E)$ but not an upper (or lower bound) → still works!
- Use nugget regularization to deal with ill-conditioning and/or mix boundary conditions
- EC works for local or non-local potentials, r-space or k-space, complex potentials, 3-body
- More recent: also works for complex *E* and extrapolating in *E* *(Xilin Zhang)*

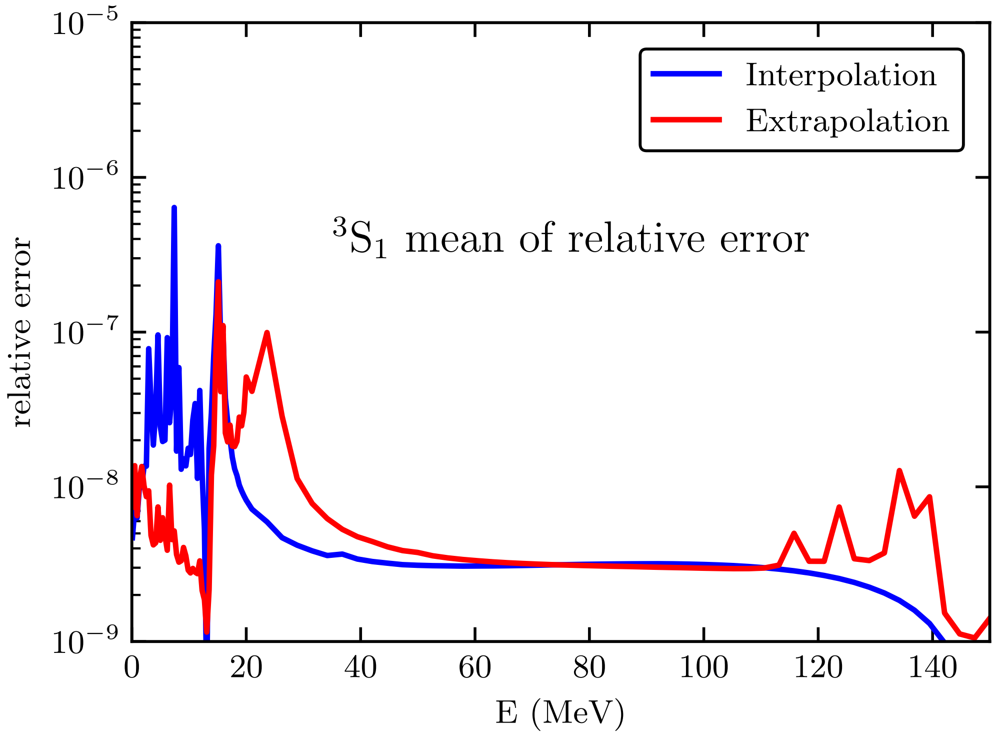
# Testing eigenvector continuation (EC) for scattering

Many different model problems tested: square well, + Coulomb, Yamaguchi potential, …
→ one example: Minnesota potential in $^3S_1$ channel (other plots available with notebooks)

$$V_{^3S_1}(r) = V_{0R}\, e^{-\kappa_R r^2} + V_{0t}\, e^{-\kappa_t r^2} \;\text{ with } \kappa_R = 1.487\,\text{fm}^{-2} \kappa_t = 0.639\,\text{fm}^{-2} \;\text{(fixed)}$$

$$\boldsymbol{\theta} = \{V_{0R}, V_{0t}\} \underset{\text{“physical”}}{\longrightarrow} \{200\,\text{MeV}, -178\,\text{MeV}\}$$




Future: choose basis points by “greedy algorithm”

# Emulating the Lippmann-Schwinger (LS) equation

LS equation: Sets of parameters: K-matrix formulation:

$$K(\vec{a}) = V(\vec{a}) + V(\vec{a})\, G_0(E_q)\, K(\vec{a}) \rightarrow \{\vec{a}_i\} \rightarrow K_\ell(E_q) = -\tan\delta_\ell(E_q)$$

$$E_q = q^2/2\mu$$

Newton variational principle (NVP):

$$\tilde{K}(\vec{\beta}) = \sum_{i=1}^{n_t} \beta_i K_i \longrightarrow \mathcal{K}[\tilde{K}] = V + VG_0\tilde{K} + \tilde{K}G_0V - \tilde{K}G_0\tilde{K} + \tilde{K}G_0VG_0\tilde{K}$$

$$\mathcal{K}[K_{\mathrm{exact}} + \delta K] = K_{\mathrm{exact}} + (\delta K)^2$$

Implementation:

$$\langle\phi'|\mathcal{K}(\vec{a},\vec{\beta})|\phi\rangle = \langle\phi'|V(\vec{a})|\phi\rangle + \vec{\beta}^T\vec{m}(\vec{a}) - \frac{1}{2}\vec{\beta}^T M(\vec{a})\vec{\beta}$$

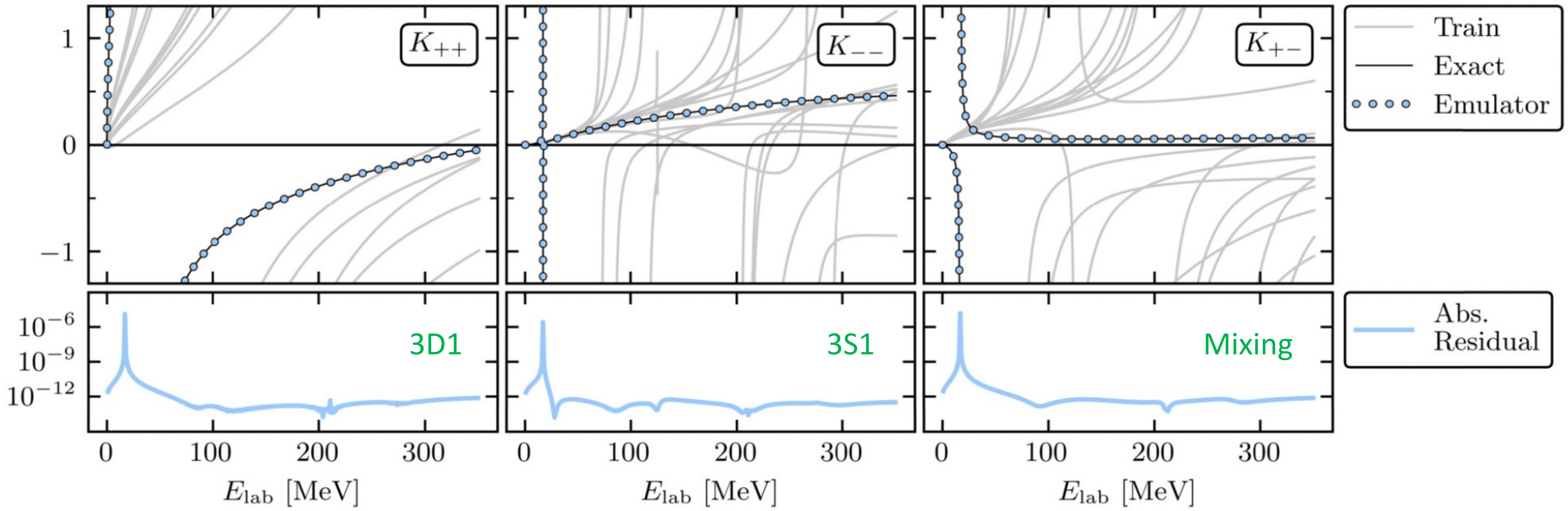
*J. A. Melendez et al., Phys. Lett. B 821, 136608 (2021)*

$$\frac{d\mathcal{K}}{d\vec{\beta}} = 0 \rightarrow \langle\phi'|\mathcal{K}(\vec{a},\vec{\beta})|\phi\rangle \approx \langle\phi'|V(\vec{a})|\phi\rangle + \frac{1}{2}\vec{m}^T M^{-1}(\vec{a})\,\vec{m}$$

# NVP emulation: SMS chiral potential

- Emulation of 3S1-3D1 coupled channel
- Basis size of 12 at $\mathrm{N^4LO+}$

*Dealing with anomalies/singularities: C. Drischler et al., arXiv: 2108.08269 (2021)*



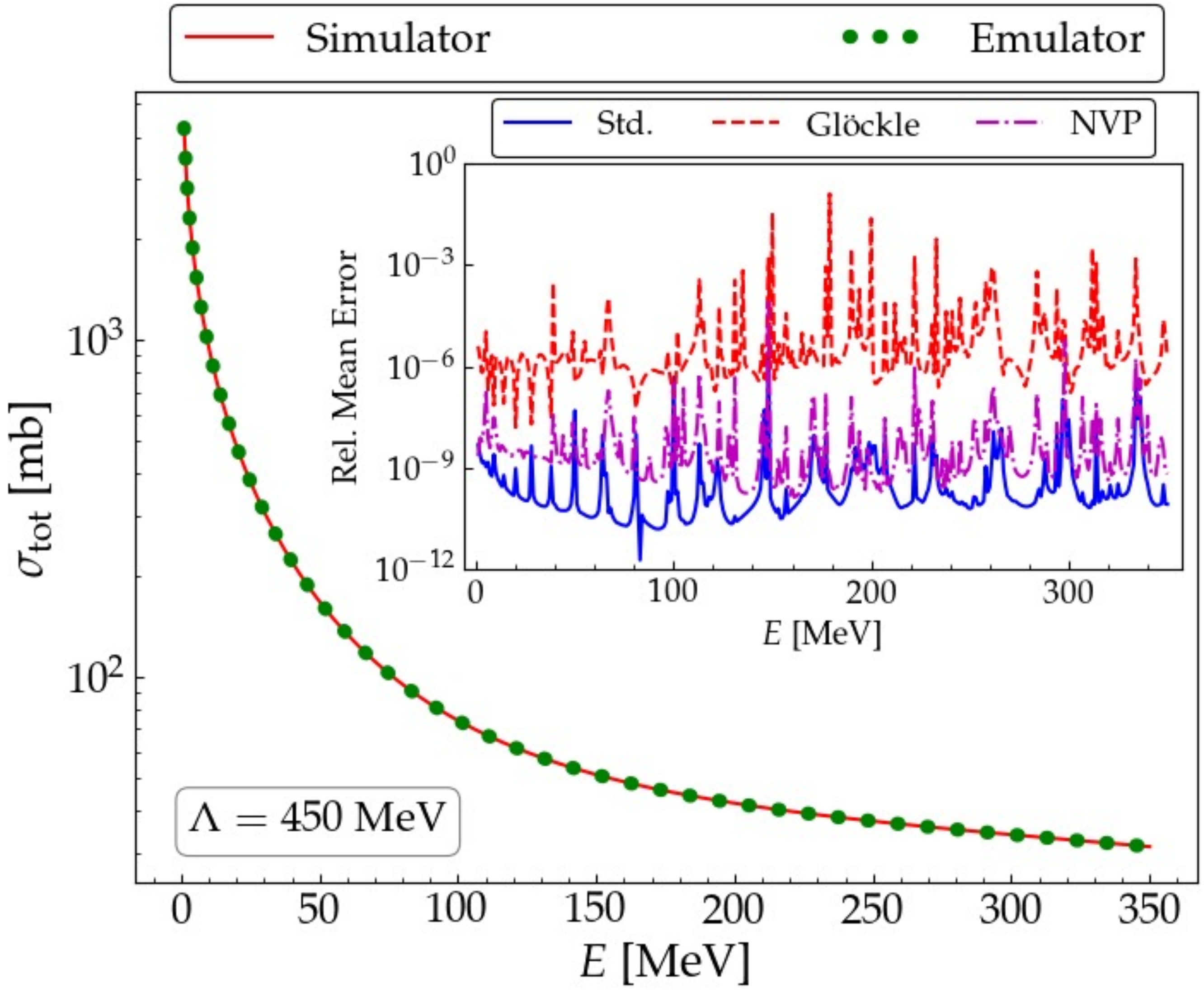

*J. A. Melendez et al., Phys. Lett. B 821, 136608 (2021)*

# In progress: Comparison of emulators for SMS chiral [A. Garcia]

- Observables: Total cross section, differential cross section, $A_y$ for partial waves up to $j = 20$
- Sampling: randomly chose values in an interval of [-10, 10]; 2 x #LECs pts
- Three different methods compared: NVP and two KVP momentum-space

- Errors: consistent for different cutoffs; vary with method but mostly negligible compared to other uncertainties

- Timing: NVP speed up of > 300x compared to "exact" calculation
- >1000x if mesh size is doubled



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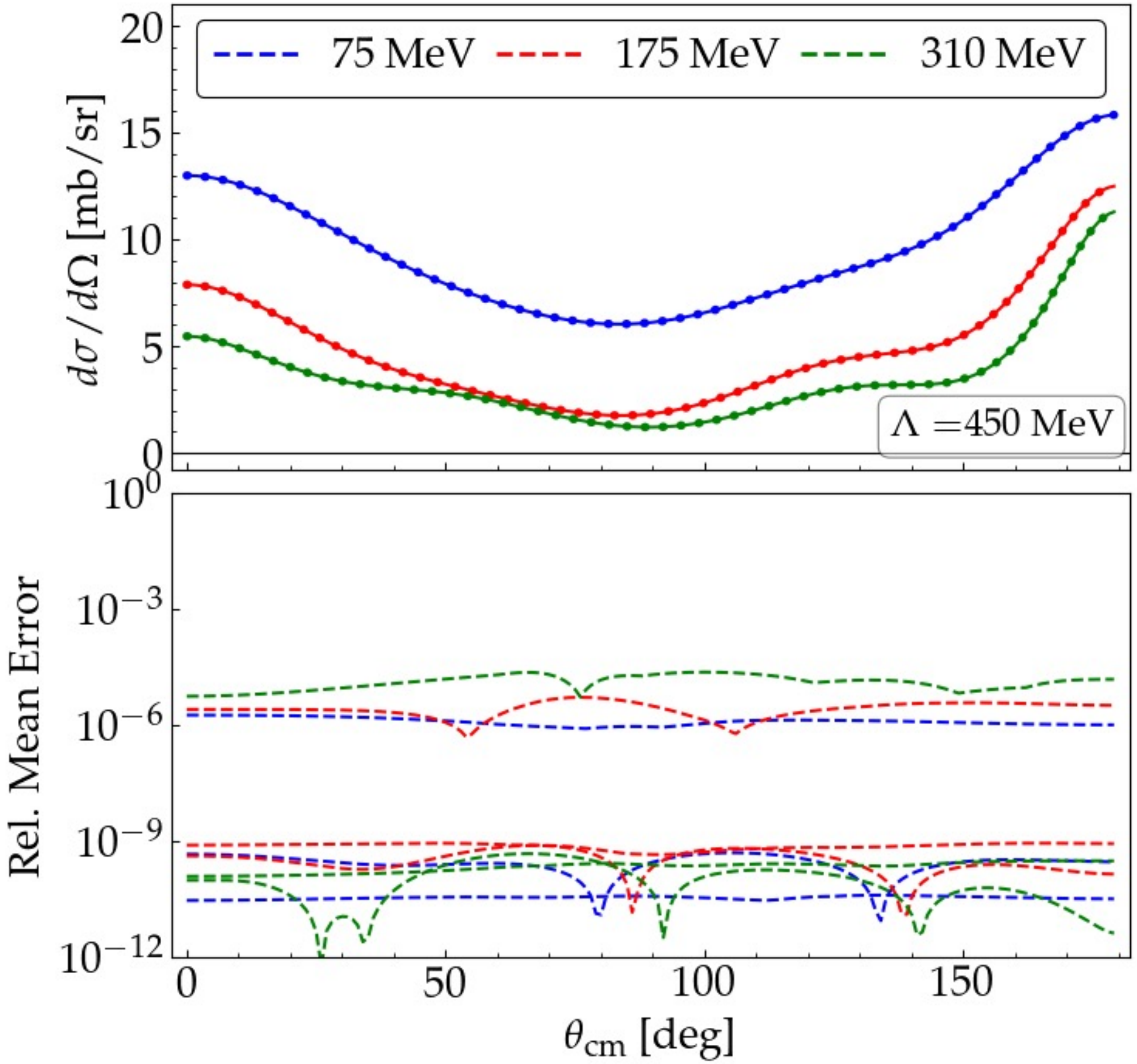

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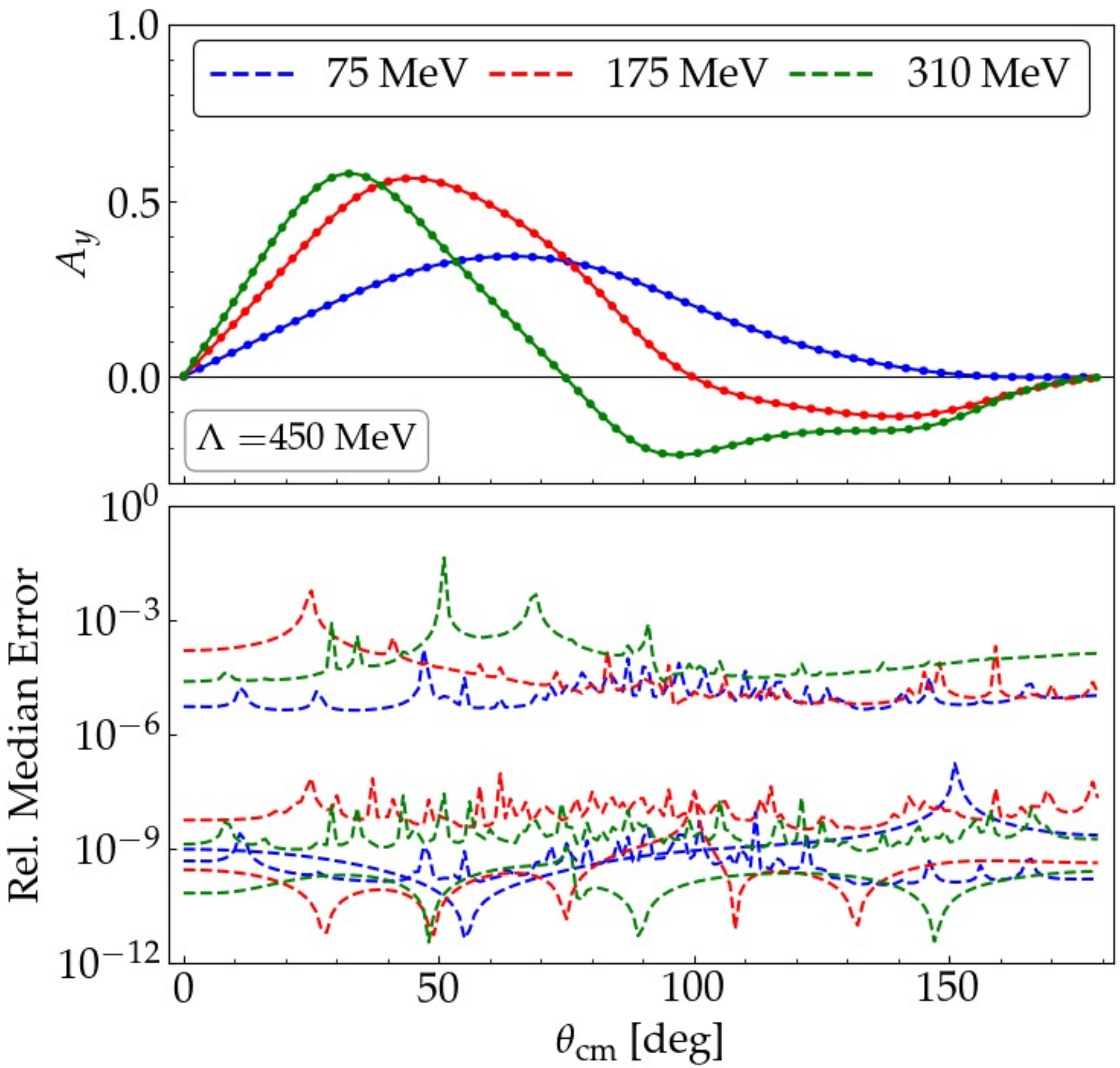


# Summary and outlook for EC-style emulators

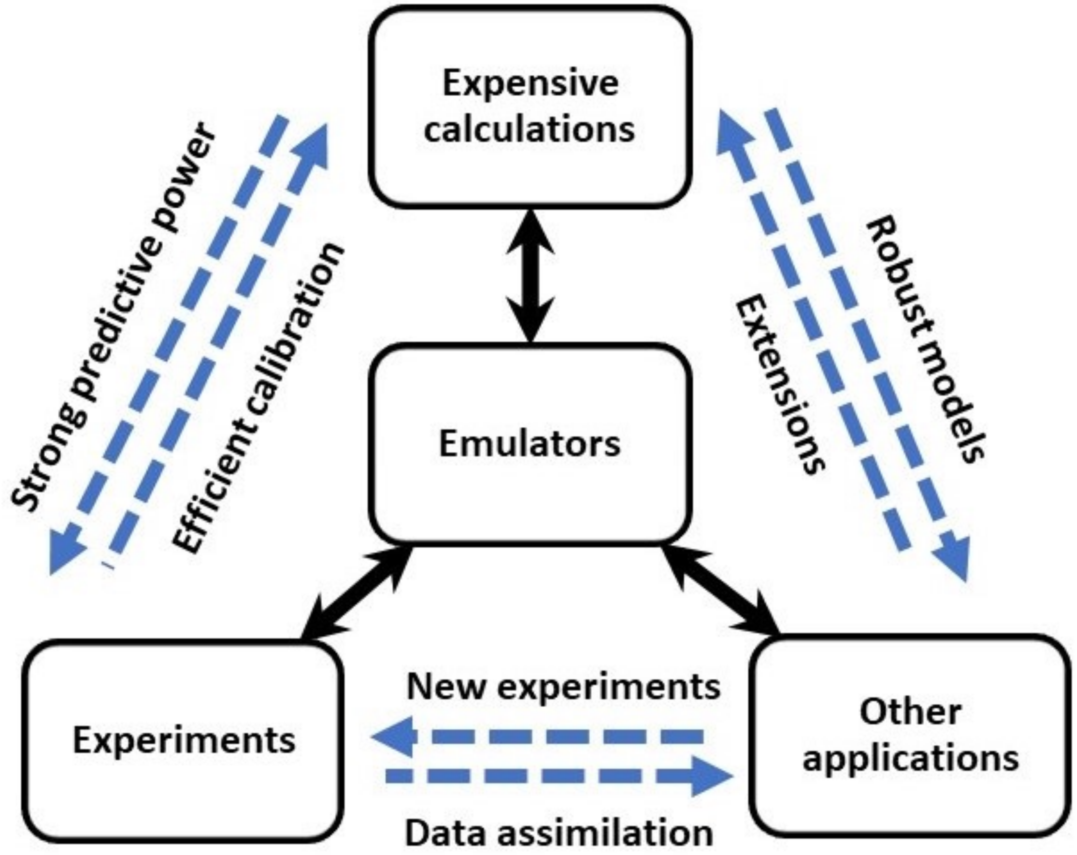
- General traits of emulators for chiral EFT applications:
  - Based on stationary functionals → but do not need to give upper bound
  - Trial functions are “snapshots” → wfs, etc. for a collection of parameter sets
  - Fast, because all the expensive calculations (for training) are done “offline”
  - Accurate for both interpolation and extrapolation
  - Applications (so far) to few-body bound-state energies and radii including 3N, transition matrix elements, NN scattering, many-body up to oxygen, …

- Work in progress for chiral EFT applications:
  - Three-body scattering
  - Active learning of training points
  - Uncertainty quantification
  - Full Bayesian parameter estimation
  - Model mixing of pionless and chiral EFT

# Bonus slides

# Role of emulators: new workflows (cf. Lu Meng's talk)

From Xilin Zhang, rjf, *Fast emulation of quantum three-body scattering*, Phys. Rev. C **105**, 064004 (2022).




If you can create a fast & accurate™ emulator for observables, you can bypass the expert knowledge and expensive resources needed for the calculations!

# Model reduction methods for nuclear emulators

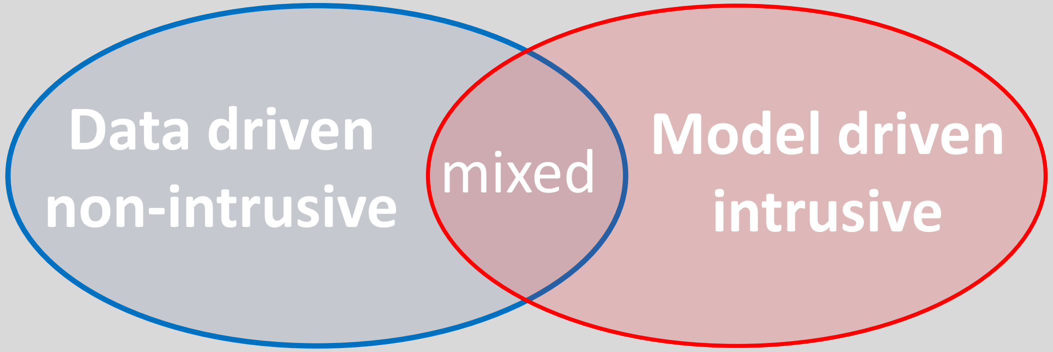
J. Melendez, C. Drischler, rjf, A. Garcia, X. Zhang, **arXiv:2203.05528** → **many great references**

**Need:** to vary parameters for design, control, optimization, UQ.

**Exploit:** much information in high-fidelity models is superfluous.

**Solution:** reduced-order model (ROM) → emulator (fast & accurate™).

General classification of ROMs




**Data driven:** interpolate output of high-fidelity model w/o understanding → *non-intrusive*

Examples: Gaussian processes; artificial neural network; see also hybrid ML approaches

**Model driven:** derive reduced-order equations from high-fidelity equations → *intrusive*

Features: physics-based, respects underlying structure → can extrapolate; often uses projection

# Setting the stage

Vast range of problems have been attacked with MOR in science and engineering, including heat transfer, fluid dynamics, electronic DFT, …→ coupled ode's and pde's (incl. time-dependent and nonlinear); eigenvalue problems; and more!

**There's likely something out there in the MOR literature analogous to what you do!**

Projection-based emulator for solution $\psi$ of $D(\psi;\boldsymbol{\theta}) = 0 \underbrace{\text{in } \Omega}_{\text{domain}};\ B(\psi;\boldsymbol{\theta}) = 0 \underbrace{\text{on } \Lambda}_{\text{boundary}}$

D and B are operators (or $H(\boldsymbol{\theta})|\psi\rangle = E|\psi\rangle$).

Large speed-ups from ***offline-online* paradigm** if heavy compute resources are offline.

→ move size-$\psi$ operations offline so that emulation varying **θ** online is efficient.

Key: exploit *affine* parameter dependence in operators, e.g., $H(\boldsymbol{\theta}) = \sum_n h_n(\boldsymbol{\theta}) H_n$

For non-linear systems and non-affine parameters, use *hyper-reduction* methods.

***Projection-based:*** *(i)* choose *low-dimensional* rep. of $\psi$ and *(ii)* write in integral form.

For *(i)*: $\tilde{\psi}(\boldsymbol{\theta}) \equiv \sum_{i=1}^{N_b} \beta_i \psi_i = X\vec{\beta}, \quad X \equiv [\psi_1\, \psi_2\, \cdots\, \psi_{N_b}]$ with *X* found offline.

***Snapshot* approaches:** construct *X* from high-fidelity solutions $\psi_i = \psi(\boldsymbol{\theta}_i)$ at set $\{\boldsymbol{\theta}_i\}$.

# Variational and Galerkin emulators by concrete example

Emulator → $\psi(\boldsymbol{\theta}) \approx \widetilde{\psi}(\boldsymbol{\theta}) = X\vec{\beta}_*, \quad X \equiv [\psi_1\, \psi_2\, \cdots\, \psi_{N_b}]$ find optimal $\vec{\beta}_*$ cheaply online

E.g., Poisson equation with Neumann BCs → $[-\nabla^2\psi = g(\boldsymbol{\theta})]_\Omega$ with $[\frac{\partial\psi}{\partial n} = f(\boldsymbol{\theta})]_\Gamma$

## Variational (Ritz)

$$S[\psi] = \int_\Omega d\Omega\, (\tfrac{1}{2}\nabla\psi\cdot\nabla\psi - g\psi) - \int_\Gamma d\Gamma\, f\psi$$

$$\Longrightarrow \delta S = \int_\Omega d\Omega\, \delta\psi(-\nabla^2\psi - g) + \int_\Gamma d\Gamma\, \delta\psi\Big(\frac{\partial\psi}{\partial n} - f\Big)$$

So $\delta S = 0$ gives the Poisson eq. and BCs. Emulate $\psi(\boldsymbol{\theta})$:

$S[\widetilde{\psi}] \to \delta S[\widetilde{\psi}] = \sum_{i=1}^{N_b} \frac{\partial S}{\partial \beta_i}\delta\beta_i = 0$ → $N_b$ equations for $\vec{\beta}_*$

If linear (as here) → $\widetilde{A}\vec{\beta}_* = \vec{g} + \vec{f}, \quad \widetilde{A}_{ij} = \int_\Omega \nabla\psi_i\cdot\nabla\psi_j,$
$g_i = \int_\Omega g(\boldsymbol{\theta})\psi_i, \quad f_i = \int_\Gamma f(\boldsymbol{\theta})\psi_i$

If affine g(**θ**), f(**θ**) → calculate high-fidelity offline.
If nonlinear or nonaffine → hyper-reduction, etc.

## Ritz-Galerkin

Weak formulation rather than variational
→ multiply each equation by *test function*

$$\int_\Omega d\Omega\, \phi(-\nabla^2\psi - g) + \int_\Gamma d\Gamma\, \phi\Big(\frac{\partial\psi}{\partial n} - f\Big) = 0$$

$$\Longrightarrow \int_\Omega d\Omega\, (\nabla\phi\cdot\nabla\psi - g\phi) - \int_\Gamma d\Gamma\, f\phi = 0$$

Assert holds for $\psi \to \widetilde{\psi} = X\vec{\beta}$ and $\phi = \sum_{i=1}^{N_b} \delta\beta_i\psi_i$

$$\delta\beta_i\Big[\int_\Omega d\Omega\, (\nabla\psi_i\cdot\nabla\psi_j\beta_j - g\psi_i) - \int_\Gamma d\Gamma\, f\psi_i\Big] = 0$$

Same result as variational here (but Galerkin is more general). If $\varphi_i \neq \psi_i$, then *Petrov-Galerkin*.

# Parametric MOR emulator workflow

Bird's eye view but still for projection-based PMOR only (i.e., not an exhaustive set!)

**(1) Sampling across range of parameters θ for $N_{sample}$ candidate snapshots → $\{\theta_i\}$**

- E.g., space-filling design (like latin hypercube) or center near emulated values.
- Want $N_b \leq N_{sample}$ snapshots; locate wisely based on basis construction method.

**(2) Generating a basis *X* from the snapshots to create.** Multiple options, including:

- *Proper Orthogonal Decomposition* (POD) [cf. PCA] → extract most important basis vectors. Compute all $N_{sample}$ snapshots $\psi(\boldsymbol{\theta}_i)$ but keep $N_b$ based on SVD.
- *Greedy algorithm* is an iterative approach: next location $\boldsymbol{\theta}_i$ from *fast* estimated emulator error at $N_{sample}$ values and choose value with largest expected error.
- For time-dependent case, sample also in time or frequency. Many options here!

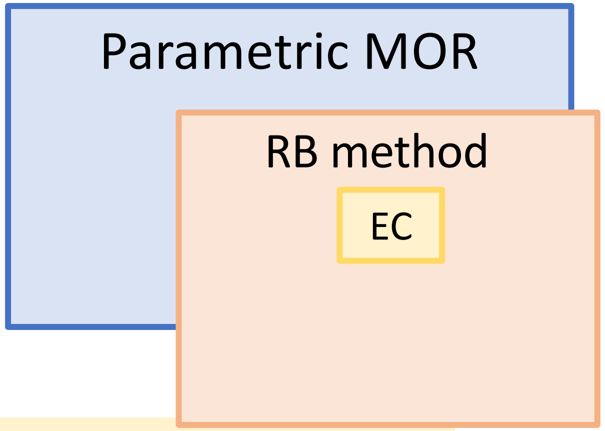
**(3) Construct the reduced system.** Single basis ***X*** or multiple bases across **θ**

- Linear system and affine operators → projecting to single basis works well.
- If non-linear or non-affine → *hyper-reduction* approaches: e.g., empirical interpolation method EIM or DEIM, which finds an affine (separable) expansion.

# Some model reduction methods in context

*Reduced Basis* method (1980) widely used to emulate PDEs in reduced-order approach. Specific choices in MOR framework:

- Parameter set chosen using greedy algorithm (or POD)
- Single basis *X* constructed from snapshots
- RB model built from global basis projection



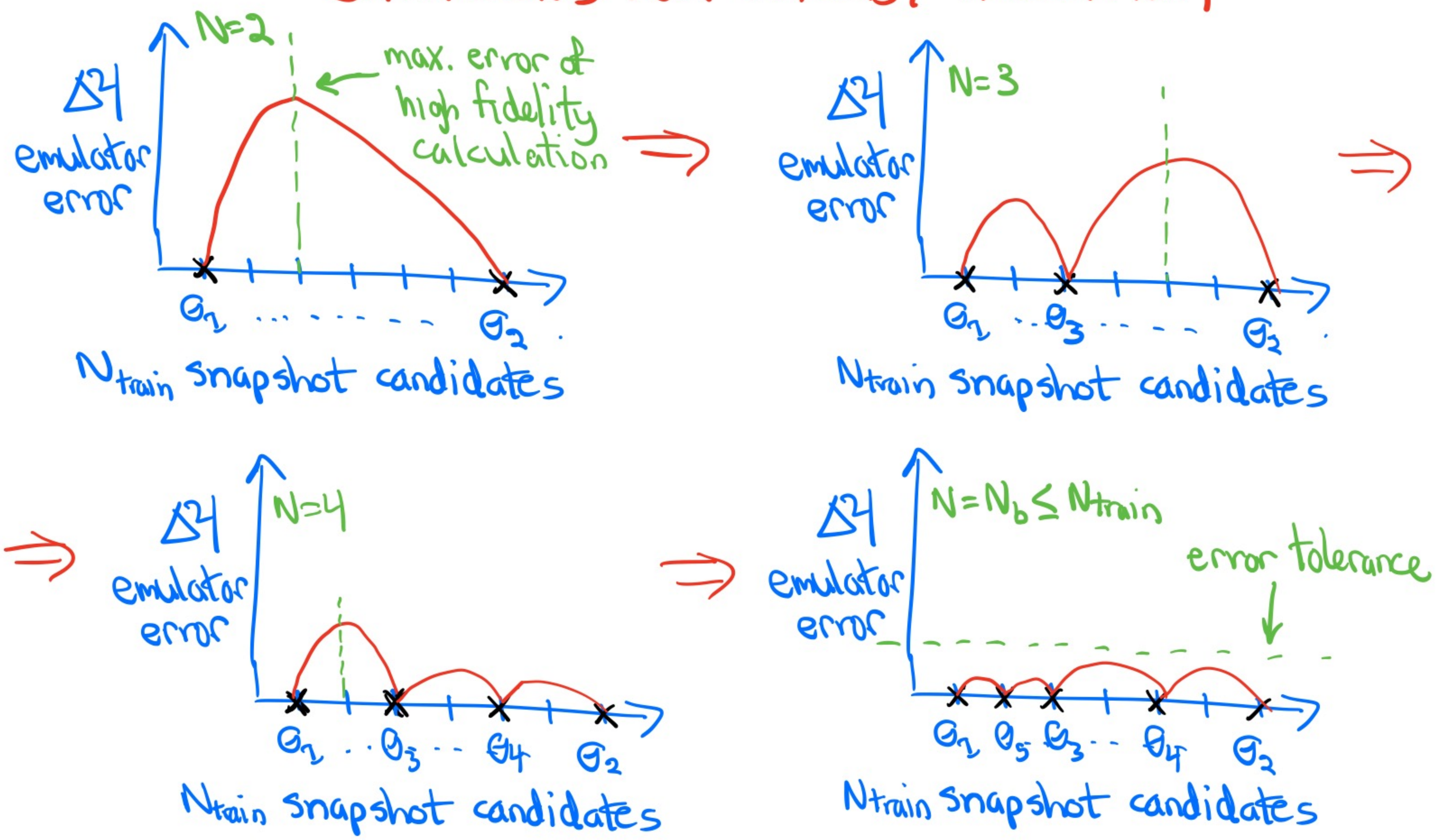

*Eigenvector continuation* (EC) is a particular implementation of the RB method
→ parametric reduced-order model for an eigenvalue problem (lots of prior art)

- Global basis constructed with snapshot-based POD approach
- "Active learning" by Sarkar and Lee adds greedy sampling algorithm for next $\boldsymbol{\theta}_i$

**Summary:** general features of *good* reduced-order emulators

- System dependent → works best when QOI lies in low-D manifold and operations on $\psi$ can be avoided during online phase
- Relative smoothness of parameter dependence
- Affine parameter dependence (or effective hyper-reduction or other approach)

# CARTOONS FOR GREEDY ALGORITHM




Stop once desired error tolerance reached (or given # steps)

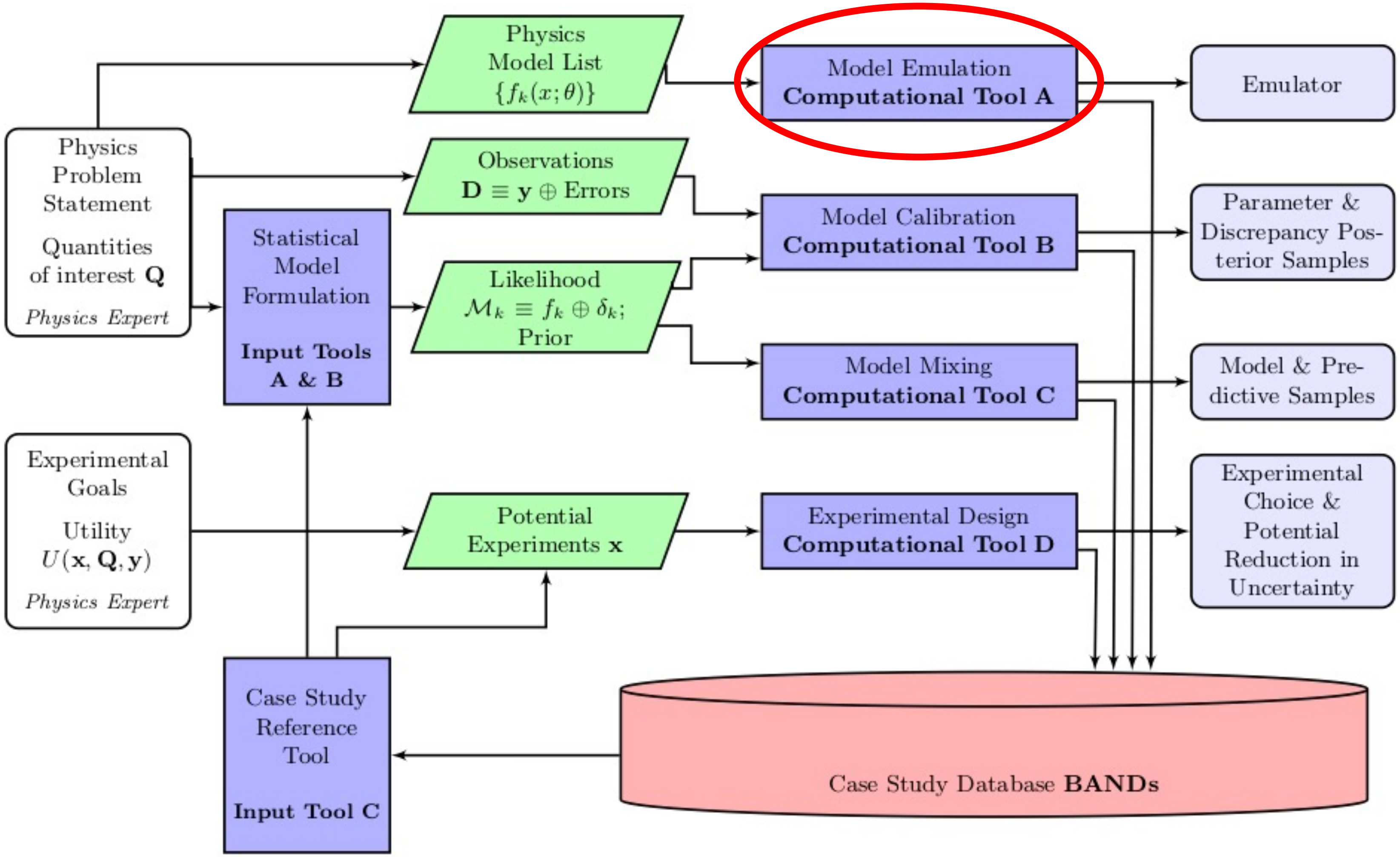
# Thank you!

# Extra slides

# 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 coming years!




Bayesian Analysis of Nuclear Dynamics

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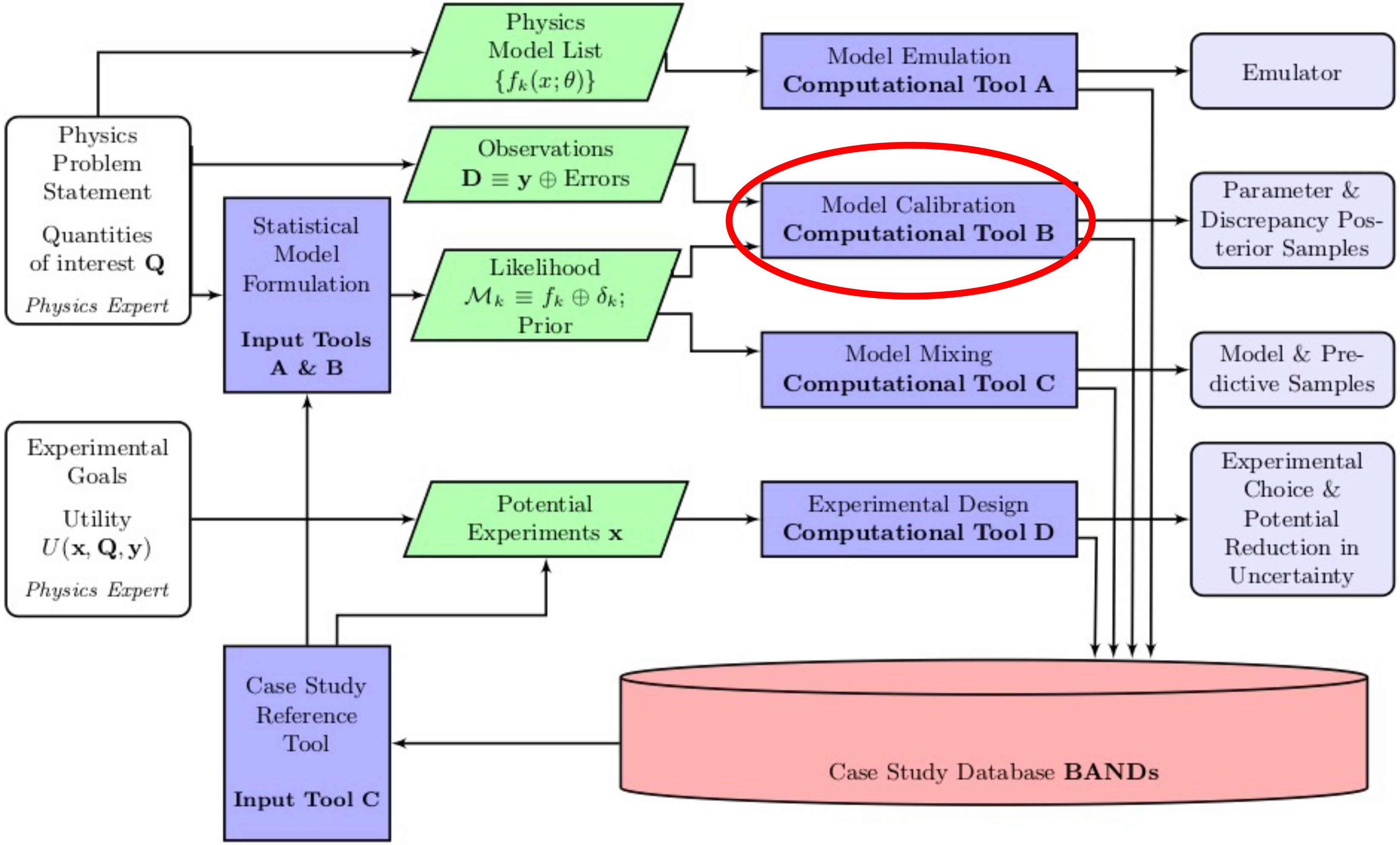

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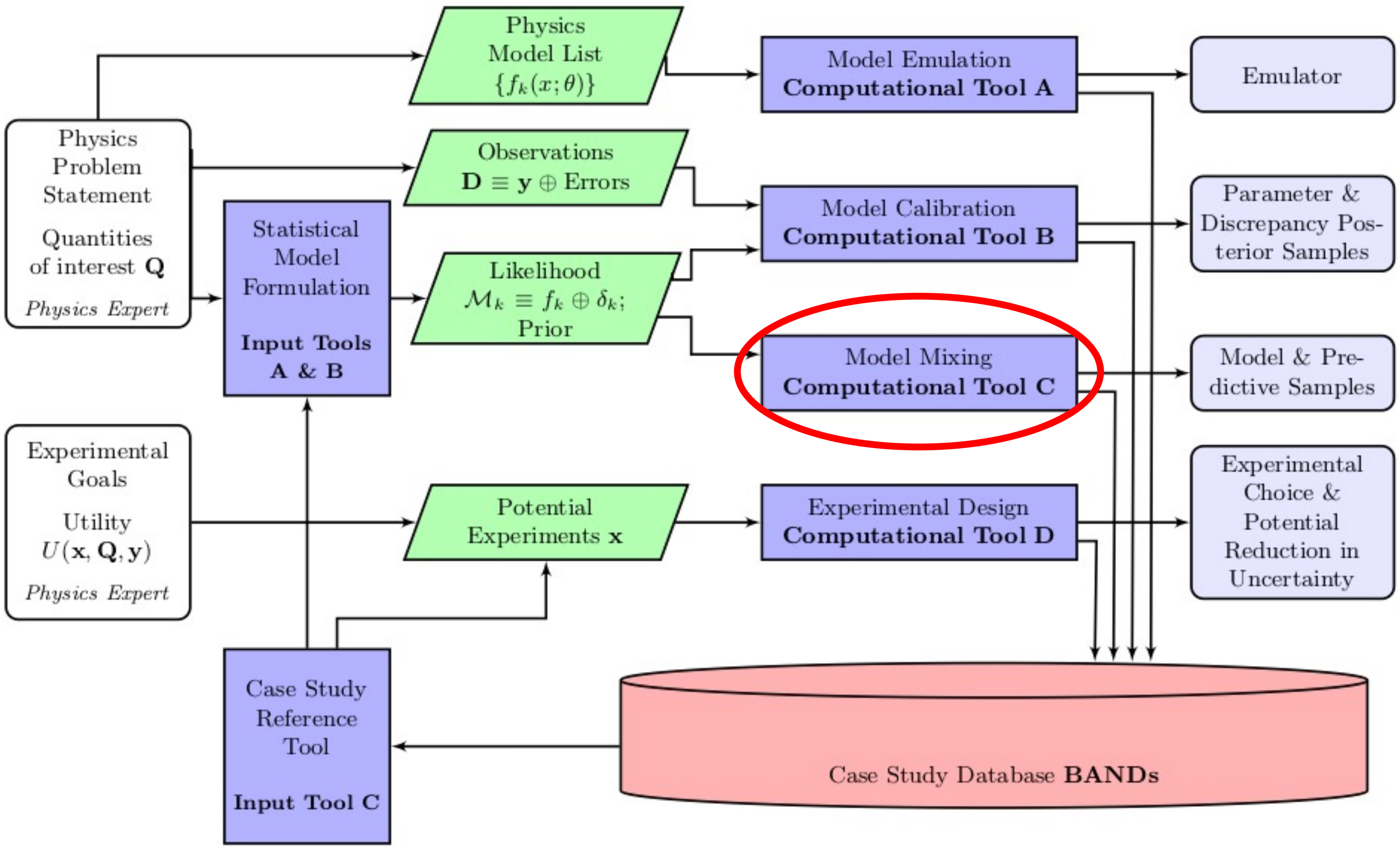


Model-mixing example: A. Semposki et al., arXiv:2206.04116
Matching expansions of a toy model at small and large coupling, with GP filling the gap. Future: mixing pionless+chiral EFT

# Propaganda: Jupyter notebooks for Bayesian UQ

- Jupyter notebooks and Python are great tools for nuclear physics UQ
- E.g., Bayesian methods for EFT and other theory errors (combined with experiment)
    - Many examples from the BUQEYE collaboration [see https://buqeye.github.io/]
- Aspiration: *every* paper should provide a notebook for reproducing figures

- Github repositories with notebooks for learning Bayesian statistics for physics
    - ➢ BAYES 2019 (TALENT course): https://nucleartalent.github.io/Bayes2019/
      [developed by Christian Forssén, rjf, Daniel Phillips]
    - ➢ Christian Forssén's course at Chalmers in Jupyter Book format with notebooks:
      https://physics-chalmers.github.io/tif285/doc/LectureNotes/_build/html/
    - ➢ rjf course at Ohio State with notebooks: https://furnstahl.github.io/Physics-8820/
      [Jupyter Book based on BAYES 2019 and updates by rjf and C. Forssén]

# Lexicon for Model Order Reduction (MOR)

| Term | Definition or usage |
|---|---|
| *High fidelity* | Highly accurate, usually for costly calculation [Full-Order Model (FOM)] |
| *Reduced-order model* | General name for an emulator resulting from applying MOR techniques. |
| *Intrusive* | Non-intrusive treats FOM as black box; intrusive requires coding. |
| *Offline-online paradigm* | Heavy compute done once (offline); cheap to vary parameters (online). |
| *Affine* | Parameter dependence factors from operators, e.g., $H(\boldsymbol{\theta}) = \sum_n h_n(\boldsymbol{\theta}) H_n$ |
| *Snapshots* | High-fidelity calculations at a set of parameters and/or times. |
| *Proper Orthogonal Decomposition* (POD) | Generically the term POD is used for PCA-type reduction via SVD. In snapshot context, PCA is applied to reduce/orthogonalize snapshot basis. |
| *Greedy algorithm* | Serially find snapshot locations $\boldsymbol{\theta}_i$ at largest expected error (fast approx.). |
| *Reduced basis methods* | Or RBMs. Implement snapshot-based projection methods. |
| *Hyper-reduction methods* | Approximations to non-linearity or non-affineness (e.g., EIM). |