Emulating Observables from Chiral EFT potentials

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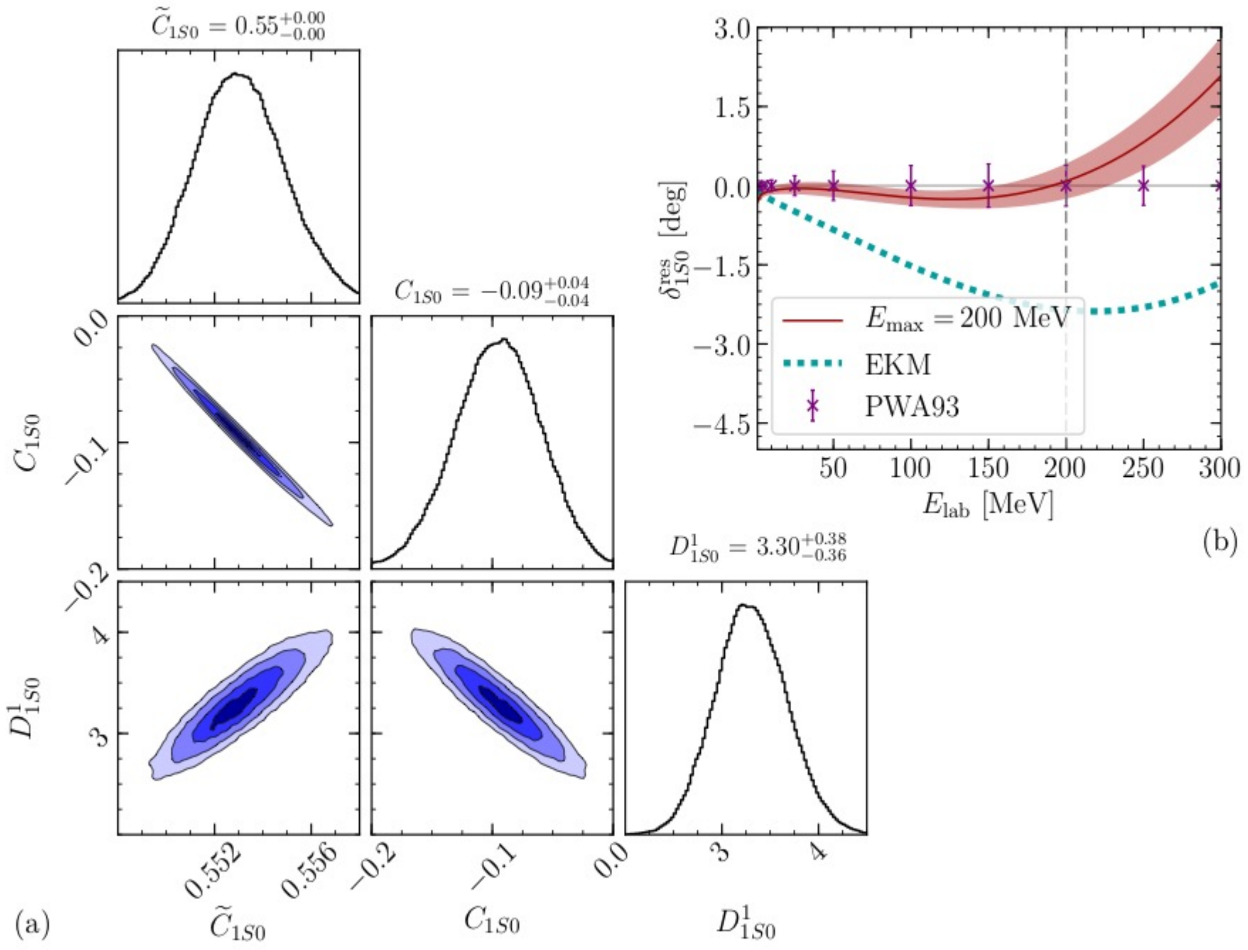
Nucleon-Nucleon (NN) scattering with UQ

- Full sampling for Bayesian UQ can be expensive using direct calculations
- Alternative: sample from a previously trained surrogate model (emulator)



S. Wesolowski et al., J. Phys. G 46, 045102 (2019)

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Model order reduction (MOR)

J. A. Melendez et al., arXiv:2203.05528

- Constructing a reduced-order model (ROM)
- Reduction schemes:
  - Data-driven: interpolate output of high-fidelity model w/o understanding → non-intrusive
  - Examples: Gaussian processes, neural networks

  - Model-driven: derive reduced-order equations from high-fidelity equations → intrusive
  - Is often projection-based (requires writing new code)
  - Examples: physics-based, respects underlying structure
- Reduced Basis (RB) method:
  - Parameter set is often chosen by using a greedy algorithm
  - A basis is constructed out of snapshots and orthonormalized
  - RB model is built from a global basis projection

Chiral EFT potentials for NN scattering

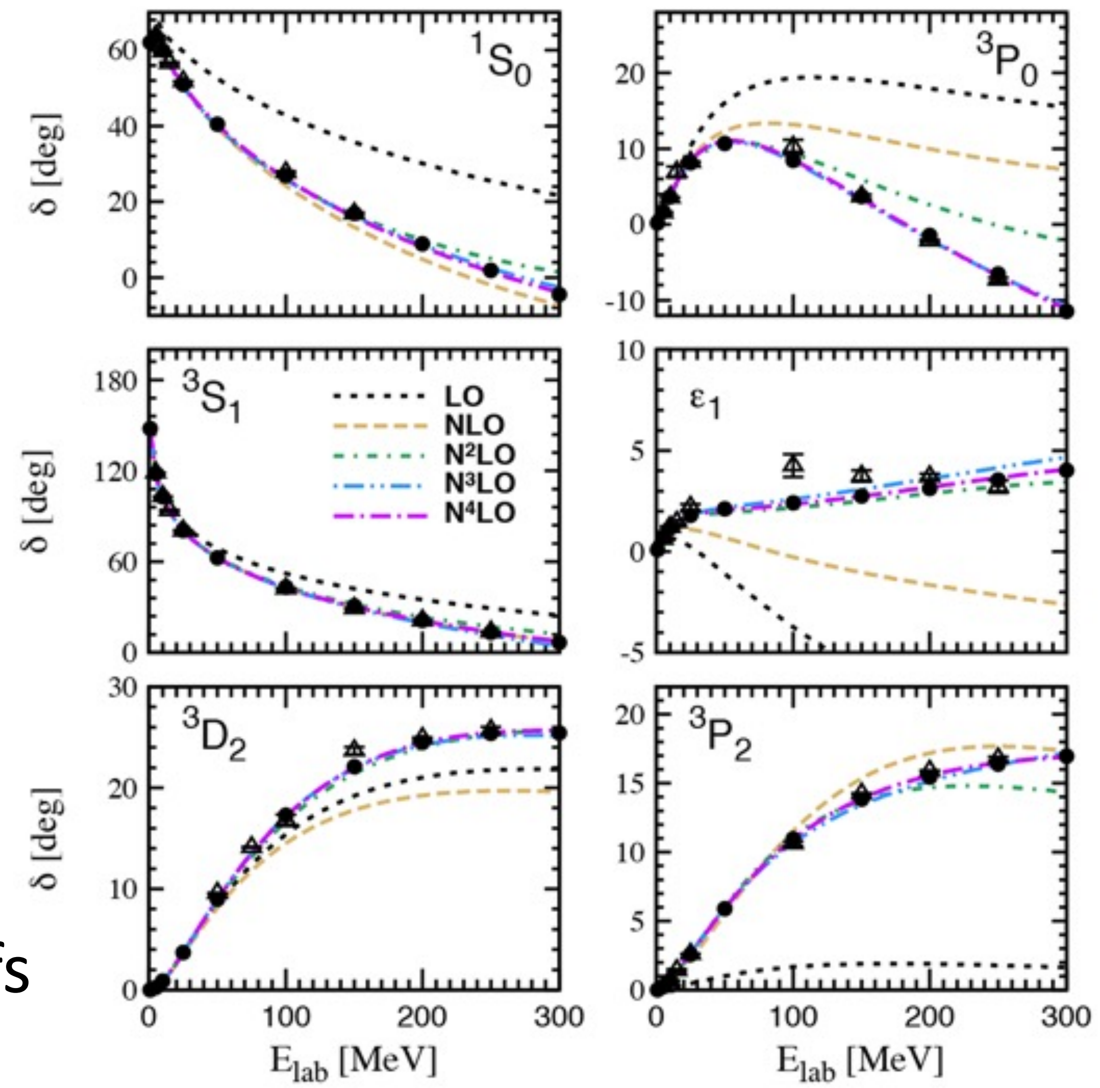
- Here: semi-local momentum-space regularized potential
- Affine dependence on the low-energy couplings (LECs):

$$V = \boxed{C_0} V^{(0)} + \boxed{C_2} V^{(2)} + \boxed{C_4} V^{(4)}$$

→ only calculate matrix elements once!

- Emulate neutron-proton (np) total *scattering* cross section at multiple cutoffs

P. Reinert et al., Eur. Phys. J B 54, 86 (2018)



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Reduced-order model (ROM) for scattering

Hamiltonian:

$$\widehat{H}(\boldsymbol{\theta}) = \widehat{T} + \widehat{V}(\boldsymbol{\theta}) \rightarrow$$

Parameters:

$$\{(\boldsymbol{\theta})_i\} \rightarrow$$

K-matrix formulation:

$$K^{\ell\ell'}(k_0) = -\tan\delta^{\ell\ell'}(k_0)$$

$$k_0 \equiv \sqrt{\frac{2\mu E}{\hbar^2}}$$

Kohn variational principle (KVP):

$$I = \langle \varphi_t^{\ell\ell'} | \widehat{H}(\boldsymbol{\theta}) - E | \varphi_t^{\ell\ell'} \rangle \rightarrow |\varphi_t^{\ell\ell'}\rangle = \frac{1}{k^2}\delta(k-k_0)\delta^{\ell\ell'} - \frac{2}{\pi}\mathbb{P}\frac{K_t^{\ell\ell'}(k,k_0)}{k^2-k_0^2}$$

$$\delta I\left[|\varphi_t^{\ell\ell'}\rangle\right] = \delta\left[\frac{K_t^{\ell\ell'}(k_0)}{k_0} - \frac{2\mu}{\hbar^2}\langle\varphi_t^{\ell\ell'}|\hat{H}(\boldsymbol{\theta}) - E|\varphi_t^{\ell\ell'}\rangle\right] = 0 \rightarrow I\left[|\varphi_{\text{ex}}^{\ell\ell'}\rangle\right] = \frac{K_{\text{ex}}^{\ell\ell'}(k_0)}{k_0}$$

Building the ROM:

$$|\varphi_t^{\ell\ell'}\rangle = \sum_{i=1}^{N_b} c_i |\varphi_E^{\ell\ell'}(\boldsymbol{\theta}_i)\rangle \rightarrow \sum_j \left(\Delta U^T + \Delta U\right)_{ij} c_j = \sum_j \Delta\tilde{U}_{ij} c_j = \frac{K_i^{\ell\ell'}(E)}{p} - \lambda$$

$$\Delta U_{ij} \equiv \frac{2\mu}{\hbar^2}\iint dk dp\, k^2 p^2 \left(\varphi_i^{\ell_0\ell'}(k)\right)^T V_{\boldsymbol{\theta},j}^{\ell'\ell''}\varphi_j^{\ell''\ell}(p) \rightarrow V_{\boldsymbol{\theta},j}^{\ell'\ell''}(k,p) \equiv V^{\ell'\ell''}(k,p;\boldsymbol{\theta}) - V_j^{\ell'\ell''}(k,p)$$

$$V^{\ell'\ell''}(k,p;\boldsymbol{\theta}) = V_0^{\ell'\ell''}(k,p) + \boldsymbol{\theta}\cdot\vec{V}_1^{\ell'\ell''}(k,p) \rightarrow \Delta U_{ij}(\boldsymbol{\theta}) = \Delta U_{ij}^0 + \boldsymbol{\theta}\cdot\Delta\vec{U}_{ij}^1$$

For coordinate space implementation:

Furnstahl et al., Phys. Lett. B 809, 135719 (2020)

Drischler et al., Phys. Lett. B 823, 136777 (2021)

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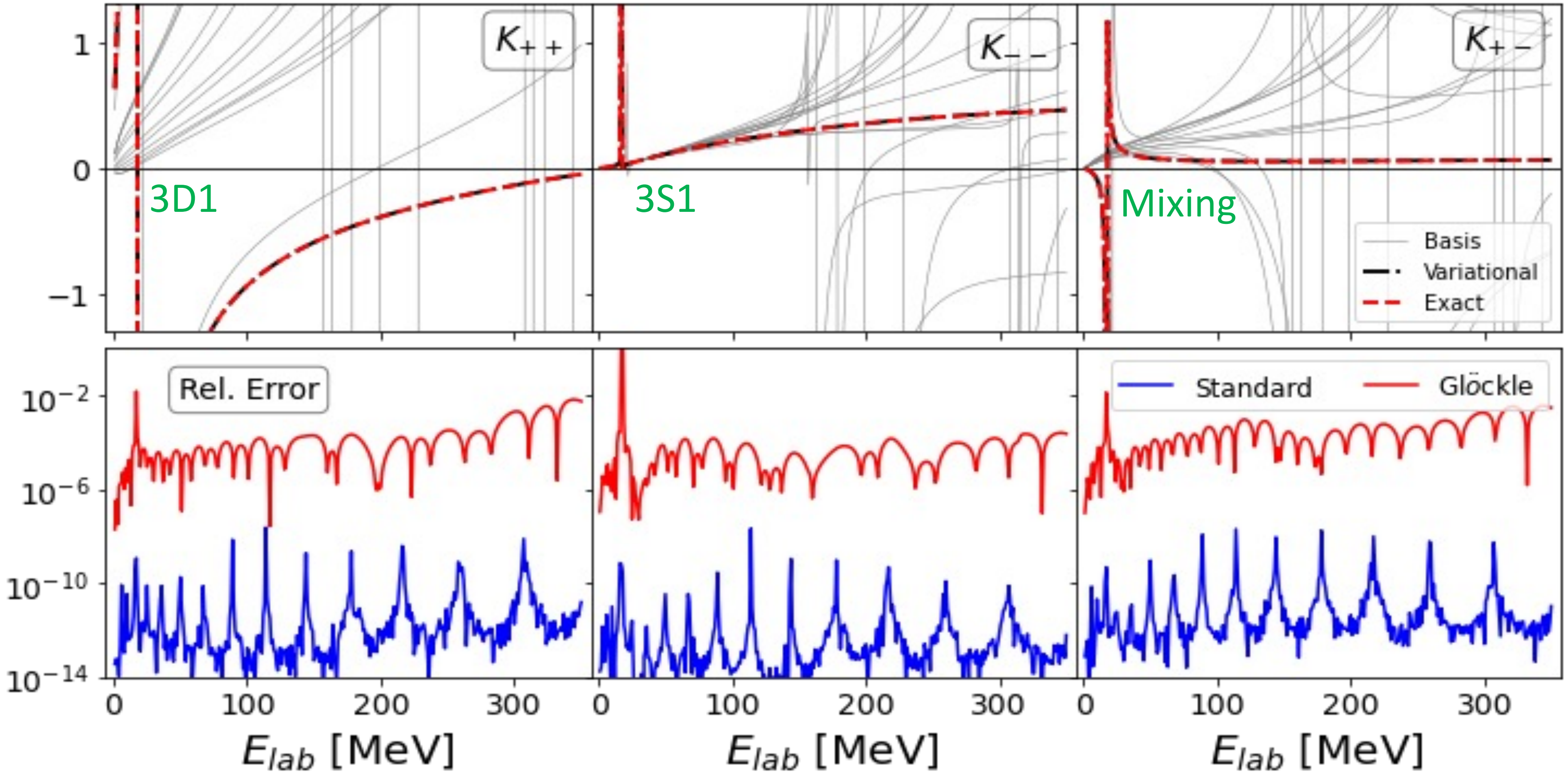
Emulation of the coupled channel

- Basis size of $N_b = 12$ at $\mathrm{N^4LO+}$
- Sampled in a range of [-5, 5] using Latin hypercube sampling (LHS)
- Glöckle interpolation:
  $$\sum_k f(k) S_k(k_0) \rightarrow f(k_0)$$



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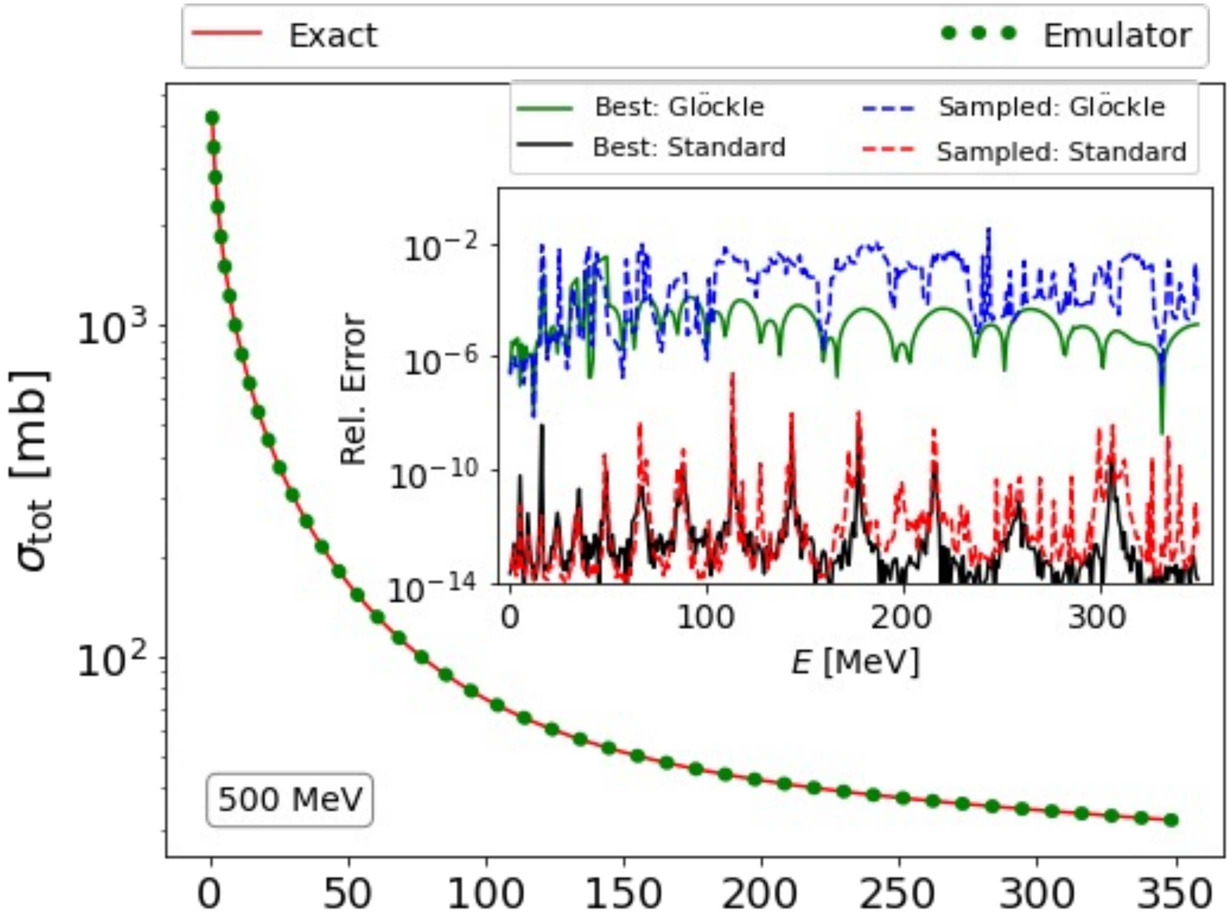
KVP emulation: total cross section

- Partial waves up to $j = 20$
- Used LHS to sample 100 parameter sets in an interval of [-5, 5]

Dealing with anomalies:
Drischler et al., Phys. Lett. B 823, 136777 (2021)

- Errors negligible compared to other uncertainties for standard method
- Glöckle method simulator is 15x faster than standard method
- Speed up of > 86x when comparing emulation to exact calculation for standard method
- >6x when comparing emulation to exact calculation for Glöckle method



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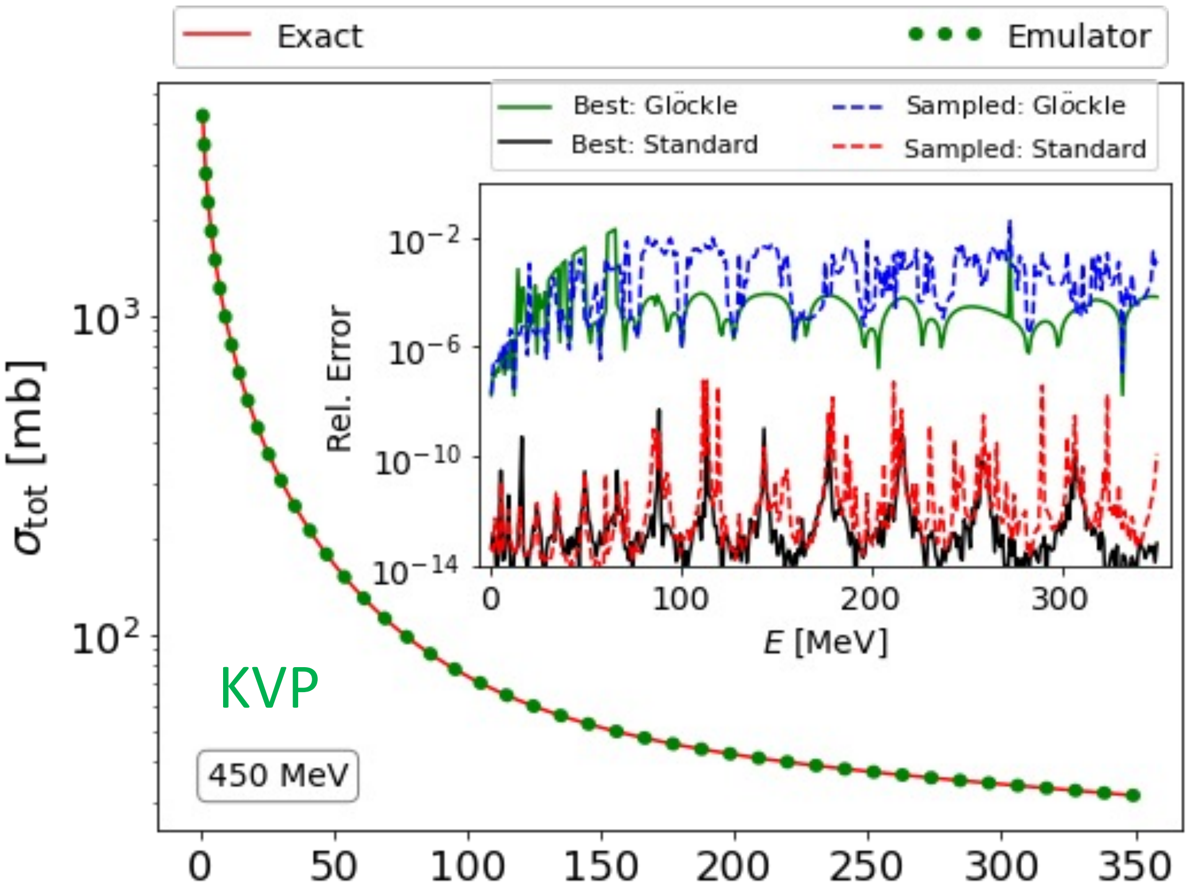
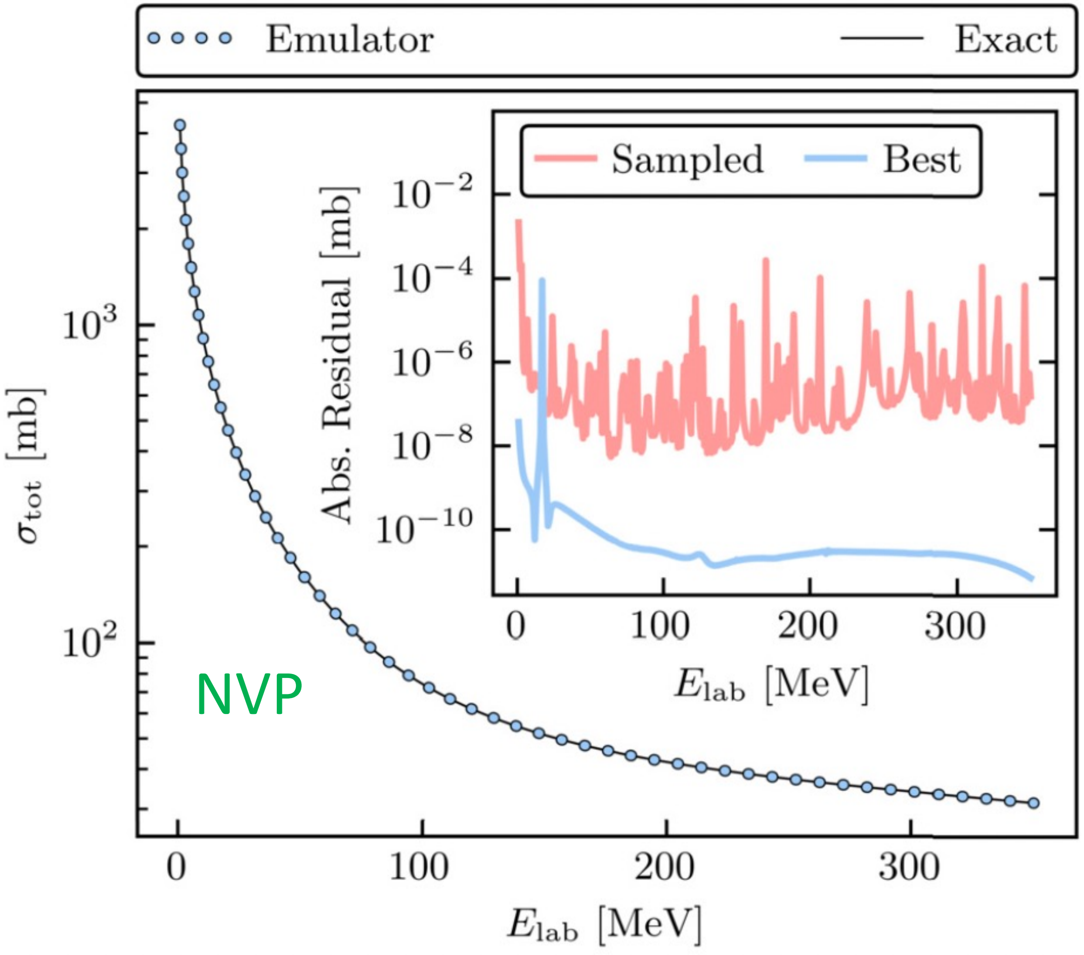
Comparing emulators

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





- Errors: KVP is more accurate when using standard approach
- Timing: NVP emulator is faster by about a factor of 3.

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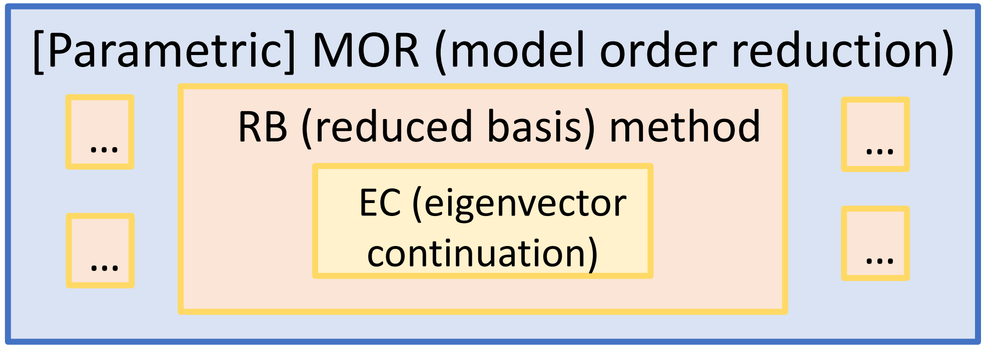
Summary

- Eigenvector continuation is part of a general class of models known as reduced-order models (ROM)
- KVP provides a general method of creating emulators for predicting scattering observables
- KVP and NVP emulators are similar in accuracy for total cross section emulation



Ongoing work

- Emulation of spin-dependent observables
- Better timing comparison between NVP and KVP
- Full Bayesian parameter estimation for chiral NN potential
- Emulator applications to three-body scattering

Thank you!

Scattering: coordinate vs. momentum space

Coordinate space:

W. Kohn, Phys. Rev. 74 (1948)

$$\psi_E^{\ell\ell'}(r) \underset{r\to\infty}{\longrightarrow} \frac{1}{k_0}\sin\left(k_0 r - \frac{\ell\pi}{2}\right)\delta^{\ell\ell'} - K^{\ell\ell'}(k_0)\cos\left(k_0 r - \frac{\ell\pi}{2}\right)$$

- Extends over infinite regions of space, but finite everywhere
- Can get complicated when including correlations between particles

Momentum space:

$$\varphi_E^{\ell\ell'}(k) = \frac{1}{k^2}\delta(k-k_0)\delta^{\ell\ell'} - \frac{2}{\pi}\mathbb{P}\frac{K^{\ell\ell'}(k,k_0)}{k^2-k_0^2}$$

- Vanishes at infinity, but contains multiple singularities

Asymptotic behavior of coordinate space wave function is reflected in the singularities of momentum space wave function!

Emulating the Lippmann-Schwinger (LS) equation

LS equation:

$$K(\vec{a}) = V(\vec{a}) + V(\vec{a})\, G_0(E_q)\, K(\vec{a})$$

→

Sets of parameters:

$$\{\vec{a}_i\}$$

→

K-matrix formulation:

$$K_\ell(E_q) = -\tan\delta_\ell(E_q)$$

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

Newton variational principle (NVP):

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

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

Implementation:

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

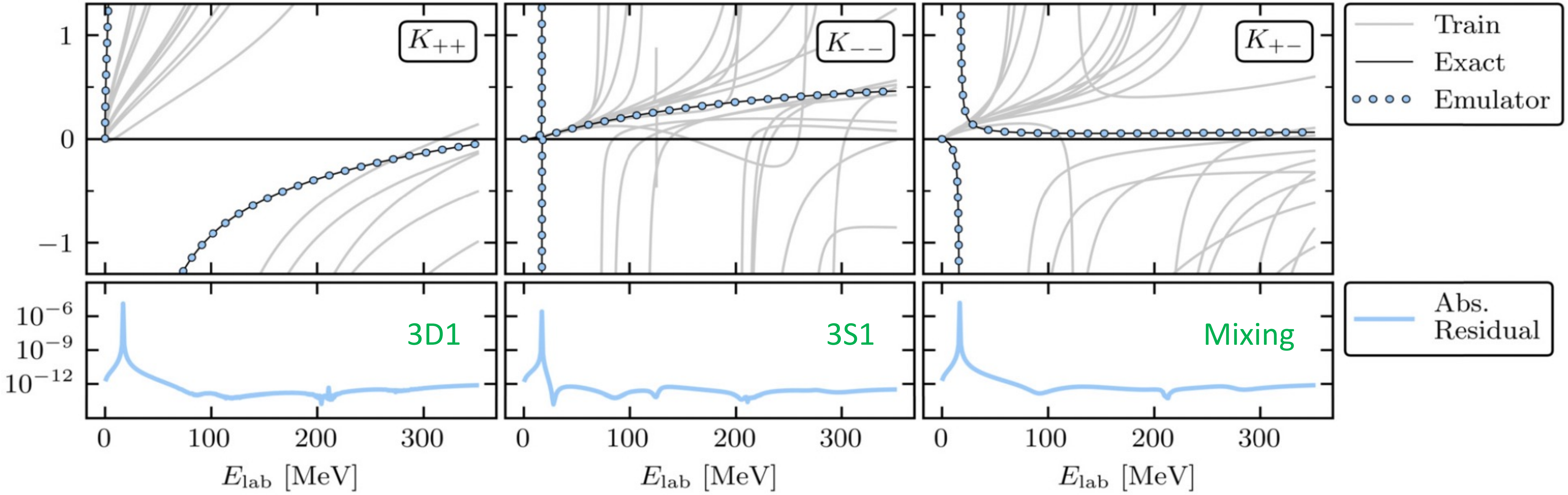
J. A. Melendez et al., Phys. Lett. B 821, 136608 (2021)

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

NVP emulation: SMS chiral potential

- Emulation of 3S1-3D1 coupled channel
- Basis size of 12 $\{\vec{a}_i\}$ at $\mathrm{N^4LO+}$
- Randomly sampled in a range of [-5, 5]

Dealing with anomalies:
C. Drischler et al.,
arXiv: 2108.08269 (2021)
Wednesday: session LM.00006



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