Snapshot-based Emulators for Chiral EFT Observables

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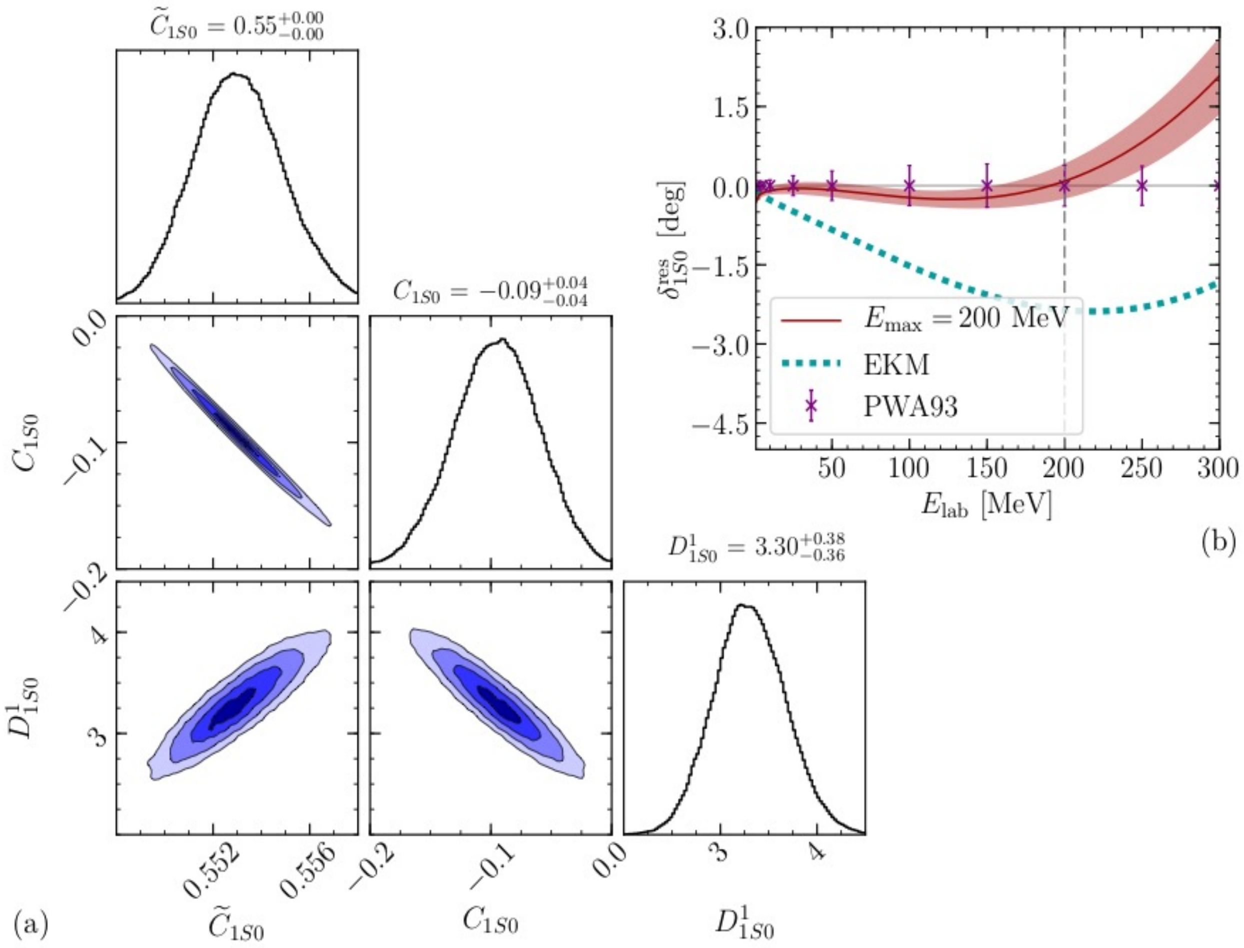
Based on forthcoming pre-print:
Wavefunction-based emulation for nucleon-nucleon scattering in momentum space

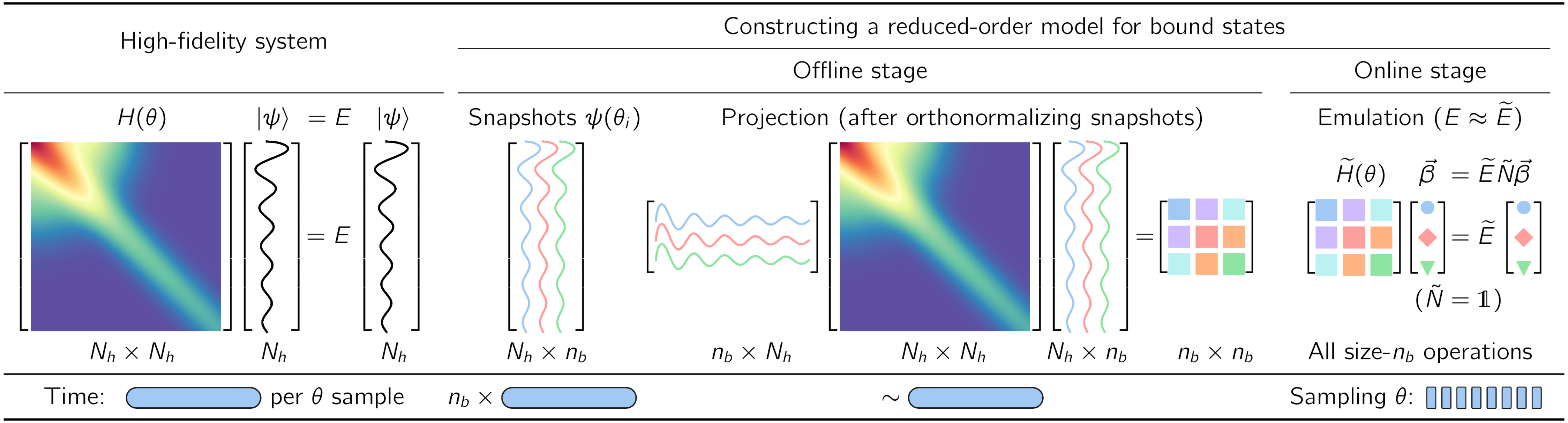
Nucleon-Nucleon (NN) scattering with UQ

- Full sampling for Bayesian UQ can be expensive using direct calculations (high-fidelity system/simulator)
- Must solve high-fidelity system for many sets of parameters
- Alternative: sample from a previously trained surrogate model (emulator)



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

Constructing a reduced-order model (ROM)



High-fidelity system

Constructing a reduced-order model for bound states

Offline stage

Online stage

$H(\theta)$ $|\psi\rangle$ $= E$ $|\psi\rangle$

Snapshots $\psi(\theta_i)$

Projection (after orthonormalizing snapshots)

Emulation ($E \approx \widetilde{E}$)

$\widetilde{H}(\theta)$ $\vec{\beta}$ $= \widetilde{E}\tilde{N}\vec{\beta}$

$= E$

$=$

$= \widetilde{E}$

$(\tilde{N} = \mathbb{1})$

$N_h \times N_h$ N_h N_h $N_h \times n_b$ $n_b \times N_h$ $N_h \times N_h$ $N_h \times n_b$ $n_b \times n_b$

All size-n_b operations

Time: per θ sample $n_b \times$ $\sim$ Sampling θ:

- Offline stage (pre-calculate):
  - Parameter set is chosen (using a greedy algorithm, Latin-hypercube sampling, etc.)
  - Construct basis using snapshots from high-fidelity system (simulator)
  - Project high-fidelity system to small-space using snapshots
- Online stage:
  - Make many predictions fast & accurately (e.g., Bayesian analysis)

Reduced order models:
J. A. Melendez et al., J. Phys. G 49, 102001 (2022)

Reduced basis method:
E. Bonilla, P. Giuliani et al., arXiv:220305284

Chiral EFT potentials for NN scattering

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

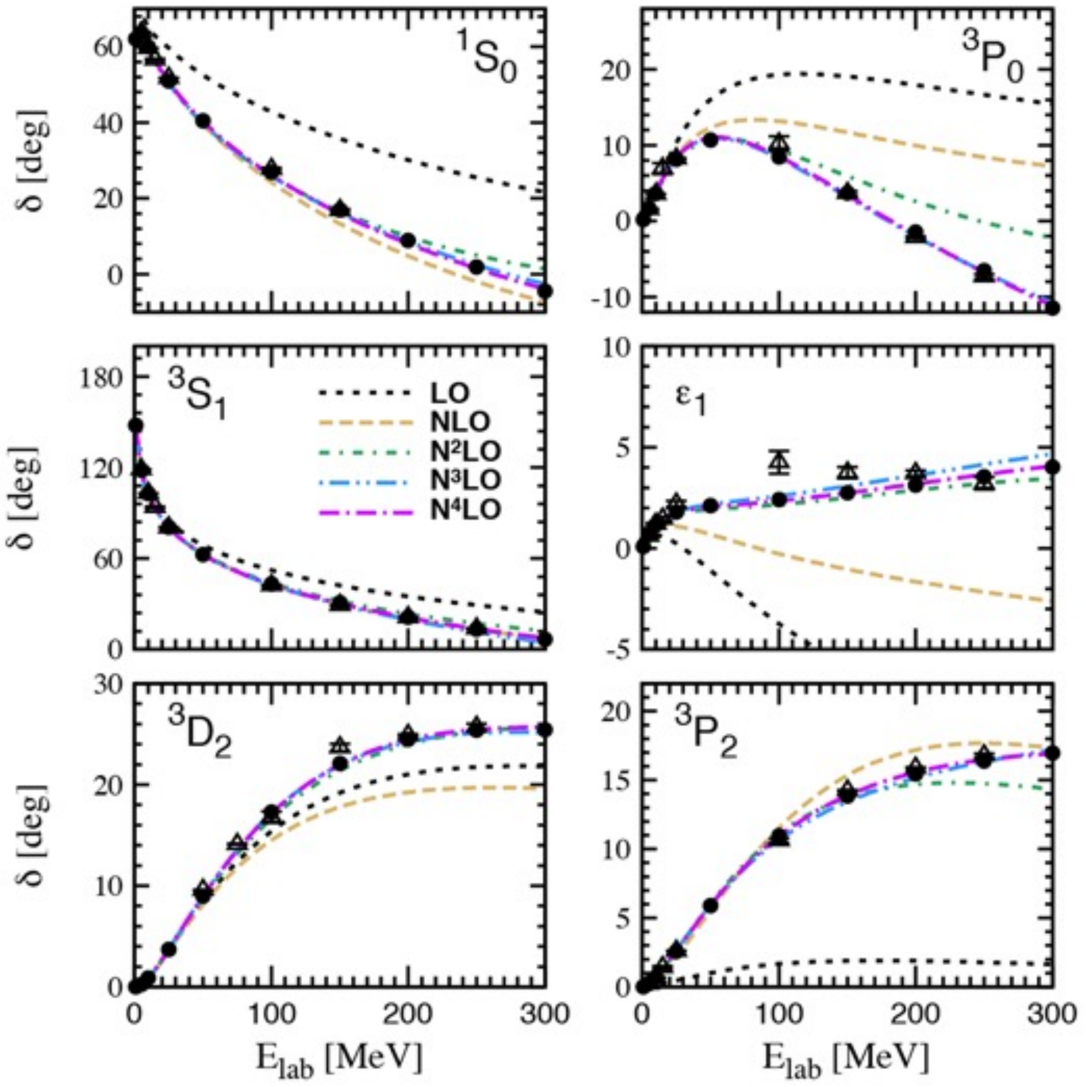
- Here: semi-local momentum-space regularized potential

- Affine dependence on the low-energy couplings (LECs):

$$V(\boldsymbol{\theta}) = V^0 + \boxed{\boldsymbol{\theta}} \cdot \boldsymbol{V}^1$$

→ only calculate matrix elements once!

- Emulate neutron-proton (np) observables at multiple cutoffs



Reduced-order model (ROM) for scattering w/ NVP

LS equation:

Training set:

K-matrix formulation:

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

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

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

Newton variational principle (NVP):

$$\mathcal{K}[\tilde{K}] = V + VG_0\tilde{K} + \tilde{K}G_0V - \tilde{K}G_0\tilde{K} + \tilde{K}G_0VG_0\tilde{K}$$

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

Implementation:

Snapshots

$$\tilde{K}(\vec{\beta}) = \sum_{i=1}^{n_t} \beta_i K_i$$

Basis weights

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

→ Linear algebra in small-space!

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

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Reduced-order model (ROM) for scattering w/ KVP

Hamiltonian:

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

Training set:

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

K-matrix formulation:

$$K_s(E) = \tan \delta_s(E)$$

$$E = k_0^2/2\mu$$

Generalized Kohn variational principle (KVP):

$$\mathcal{L}[\widetilde{\psi}] = L^{ss'}(E) - \frac{2\mu}{\det \boldsymbol{u}} \langle \widetilde{\psi}^{st} | [\widehat{H}(\boldsymbol{\theta}) - E]^{tt'} | \widetilde{\psi}^{t's'} \rangle$$

$$\mathcal{L}[\psi_{\text{exact}}] = L_{\text{exact}} + \mathcal{O}(\delta L^2)$$

Here momentum space implementation.

For coordinate space implementation:

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

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

Implementation:

Snapshots

$$|\widetilde{\psi}^{tt'}\rangle \equiv \sum_{i=1}^{N_b} \beta_i |(\psi_i)^{tt'}\rangle$$

Basis weights

$$\Delta \tilde{U}_{ij}(\boldsymbol{\theta}) = \frac{2\mu}{\det \boldsymbol{u}} [\langle (\psi_i)^{st} | [V(\boldsymbol{\theta}) - V_j]^{tt'} | (\psi_j)^{t's'} \rangle + (i \leftrightarrow j)]$$

$$\mathcal{L}[\vec{\beta}] = \beta_i L_i^{ss'} - \frac{k_0}{2} \beta_i \Delta \tilde{U}_{ij} \beta_j$$

→ Linear algebra in small-space!

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Emulating multiple boundary conditions w/ KVP

- Examples of **u** matrices

$$\boldsymbol{u}_K = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; \boldsymbol{u}_{K^{-1}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; \boldsymbol{u}_T = \begin{pmatrix} 1 & 0 \\ i & 1 \end{pmatrix}$$

1. Rescale functional quantities

$$\Delta\tilde{U}^{(\boldsymbol{u}')} = C'^{-1}(L_i)C'^{-1}(L_j)\frac{\det \boldsymbol{u}}{\det \boldsymbol{u}'}\Delta\tilde{U}^{(\boldsymbol{u})} \qquad C'(L) = \frac{\det \boldsymbol{u}}{\det \boldsymbol{u}'}\frac{u'_{11} - u'_{10}K(L)}{u_{11} - u_{10}K(L)}$$

$$L'(L) = \frac{-u'_{01} + u'_{00}K(L)}{u'_{11} - u'_{10}K(L)}$$

2. Convert back into K-matrix form

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

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Mitigating Kohn anomalies w/ KVP

1. Relative residuals between the emulator predictions of all the KVPs

$$\gamma_{\rm rel}(L_1, L_2) = \max\left\{\left|\frac{S(L_1)}{S(L_2)} - 1\right|, \left|\frac{S(L_2)}{S(L_1)} - 1\right|\right\}$$

2. Apply relative consistency check

$$\gamma_{\rm rel} < \epsilon_{\rm rel} = 10^{-1}$$

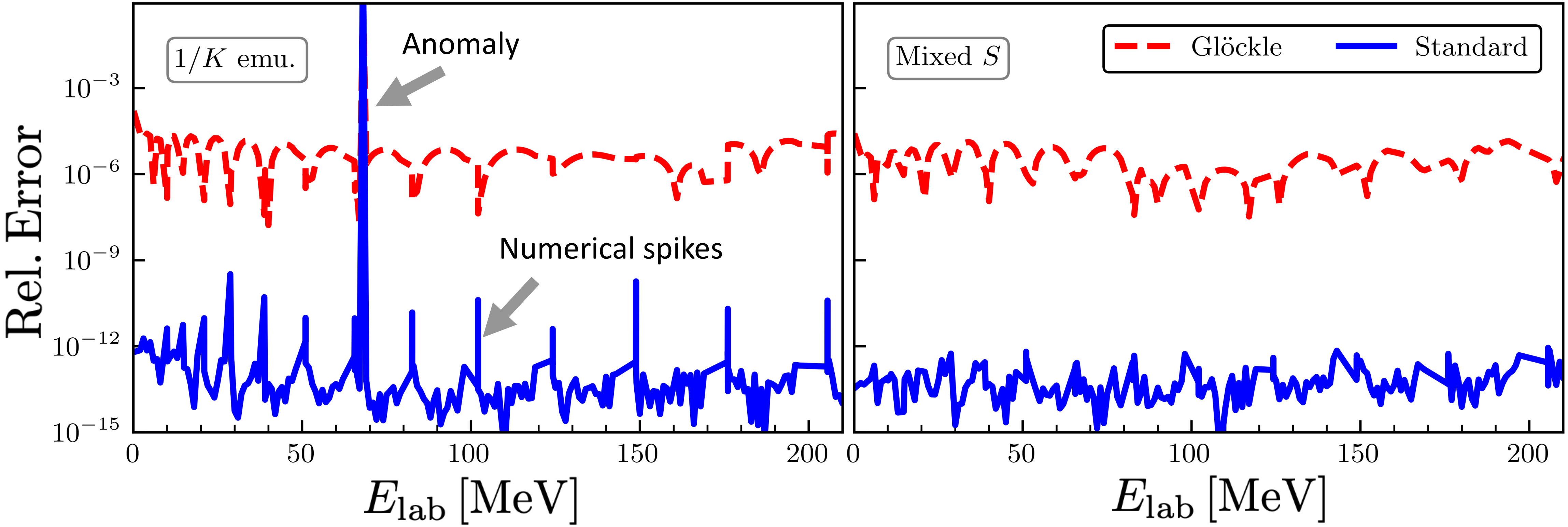
3. Estimate S-matrix

$$[S]^{(\rm mixed)}_{\rm KVP} = \sum_{(\rm L_1, L_2) \in \mathcal{P}} \omega(L_1, L_2) \frac{S(L_1) + S(L_2)}{2}, \quad \omega(L_1, L_2) = \frac{\gamma_{\rm rel}(L_1, L_2)^{-1}}{\sum_{(\rm L_1', L_2') \in \mathcal{P}} \gamma_{\rm rel}(L_1', L_2')^{-1}}$$

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

Anomalies example

- Kohn anomalies mitigated!
- Mesh-induced spikes in high-fidelity LS equation detected and removed



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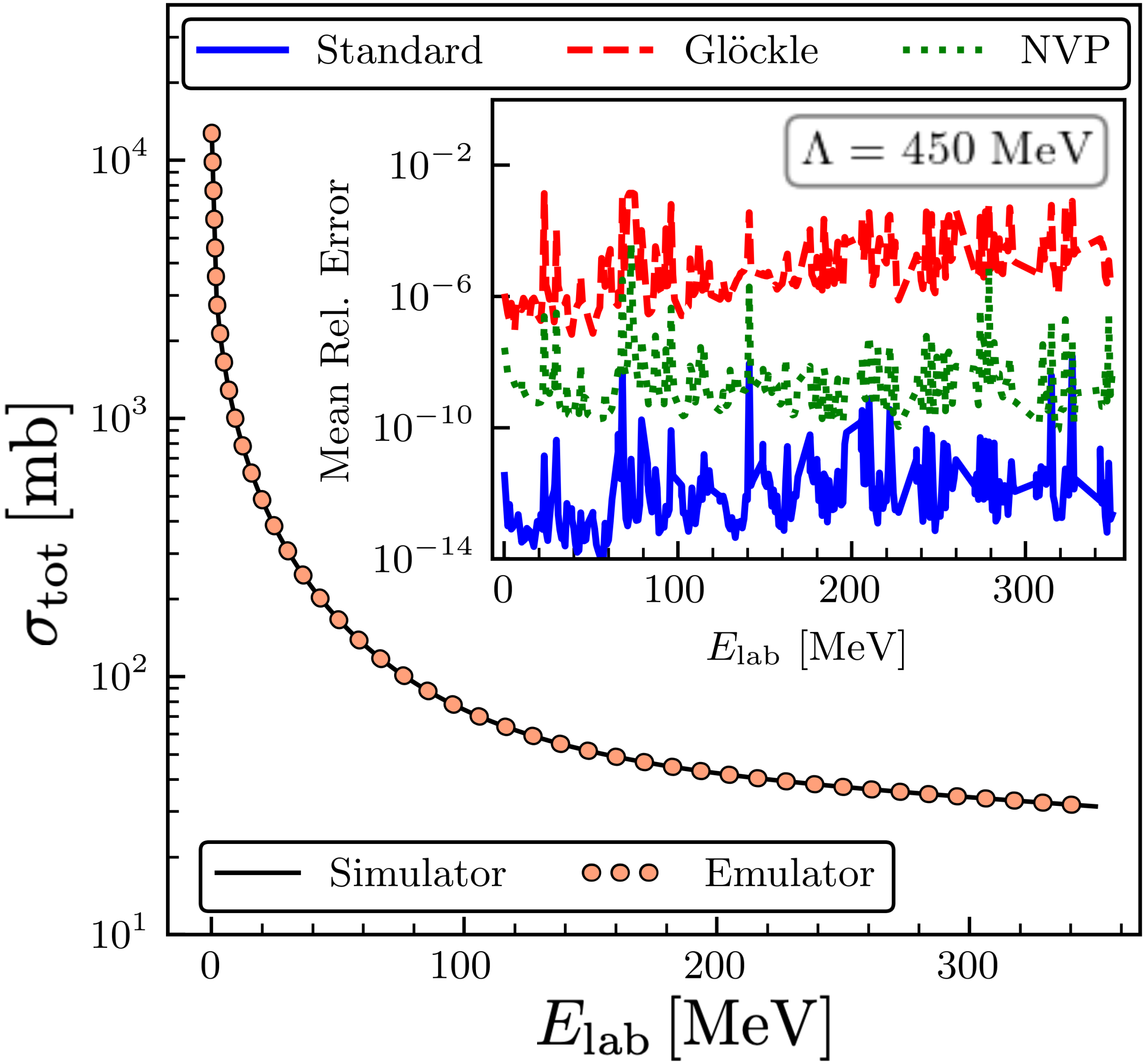
Total cross section emulation

- Partial waves up to $j = 20$
- Used LHS to sample 500 parameter sets in an interval of [-5, 5]
- Glöckle spline interpolation:
  $$\sum_k f(k)S_k(k_0) \rightarrow f(k_0)$$
- Errors negligible compared to other uncertainties
- Speed is highly implementation-dependent!
- Consistent for $\Lambda = 400 - 550\,\mathrm{MeV}$
- Kohn anomalies mitigated!



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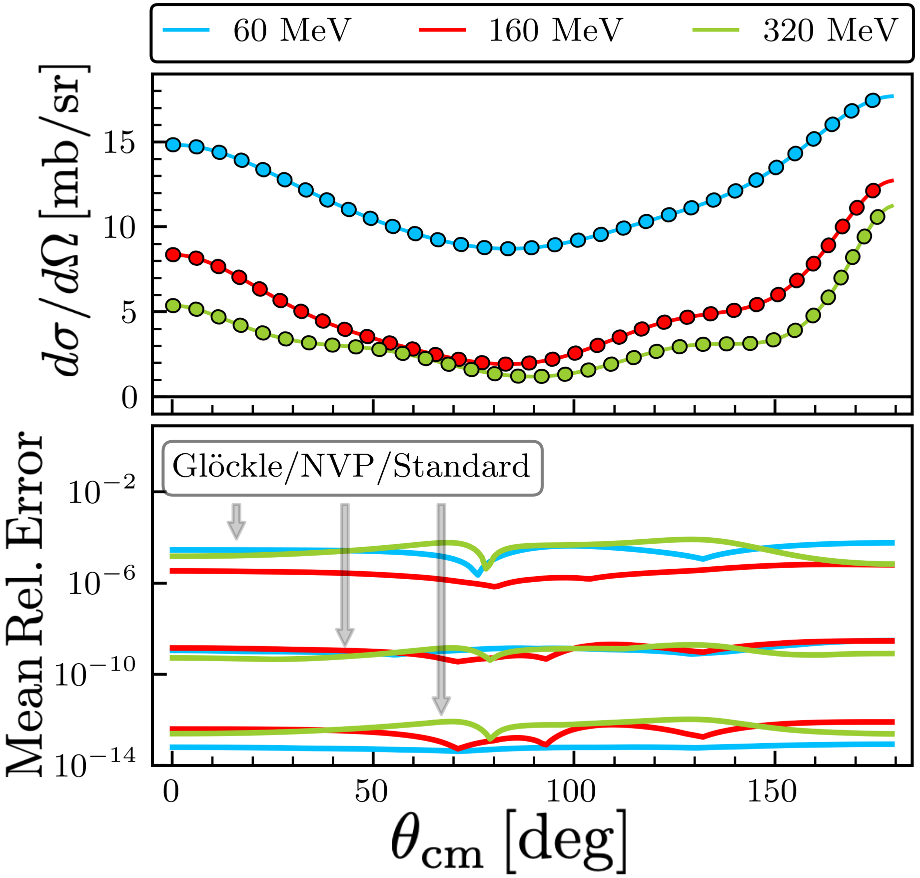
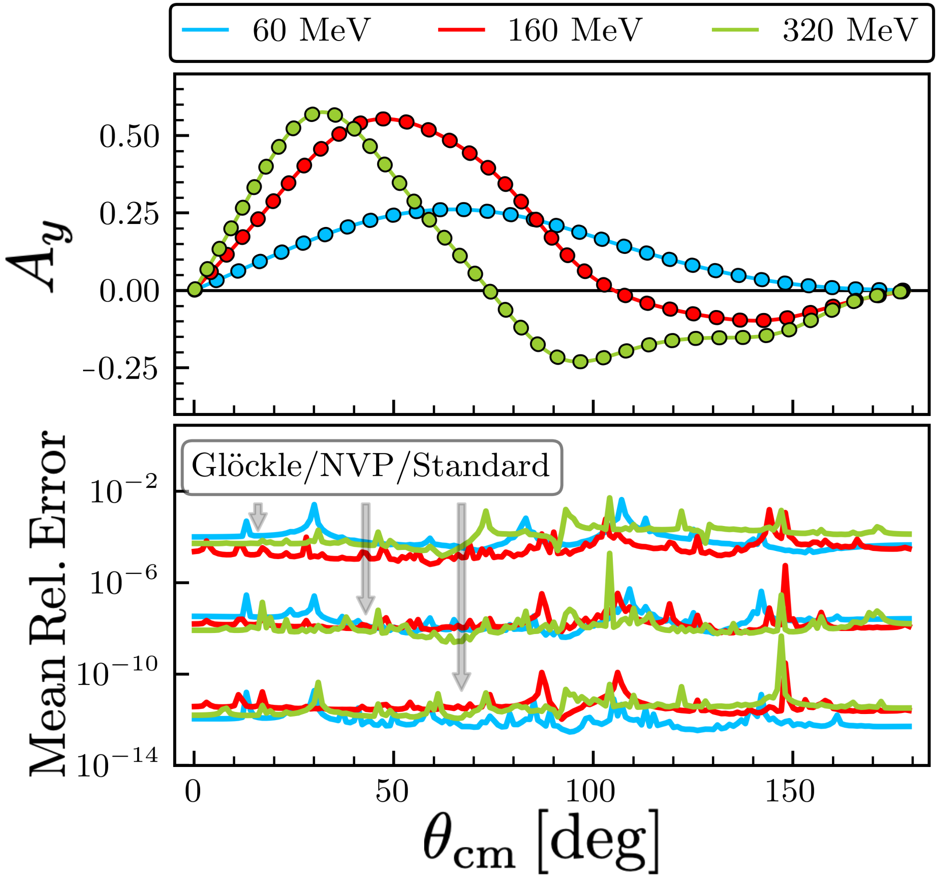
Emulation of other observables





- Partial waves up to $j = 20$
- Used LHS to sample 500 parameter sets in an interval of [-5, 5]

- Errors negligible compared to other uncertainties
- Consistent for all energies and cutoffs

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Summary

- NVP/KVP provides a general method of creating emulators for predicting observables
- Successfully mitigated Kohn anomalies in the observables for the KVP
- KVP and NVP emulators errors are negligible compared to other uncertainties
- Emulators are faster than the simulator, but how much is implementation-dependent
- Efficient Bayesian parameter estimation is now feasible

Ongoing work

- Pre-print and codes on the way!
- Full Bayesian parameter estimation for chiral NN potential
- Emulator applications to three-body scattering

Thank you!

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$$\sum_k f(k) S_k(k_0) \to f(k_0)$$

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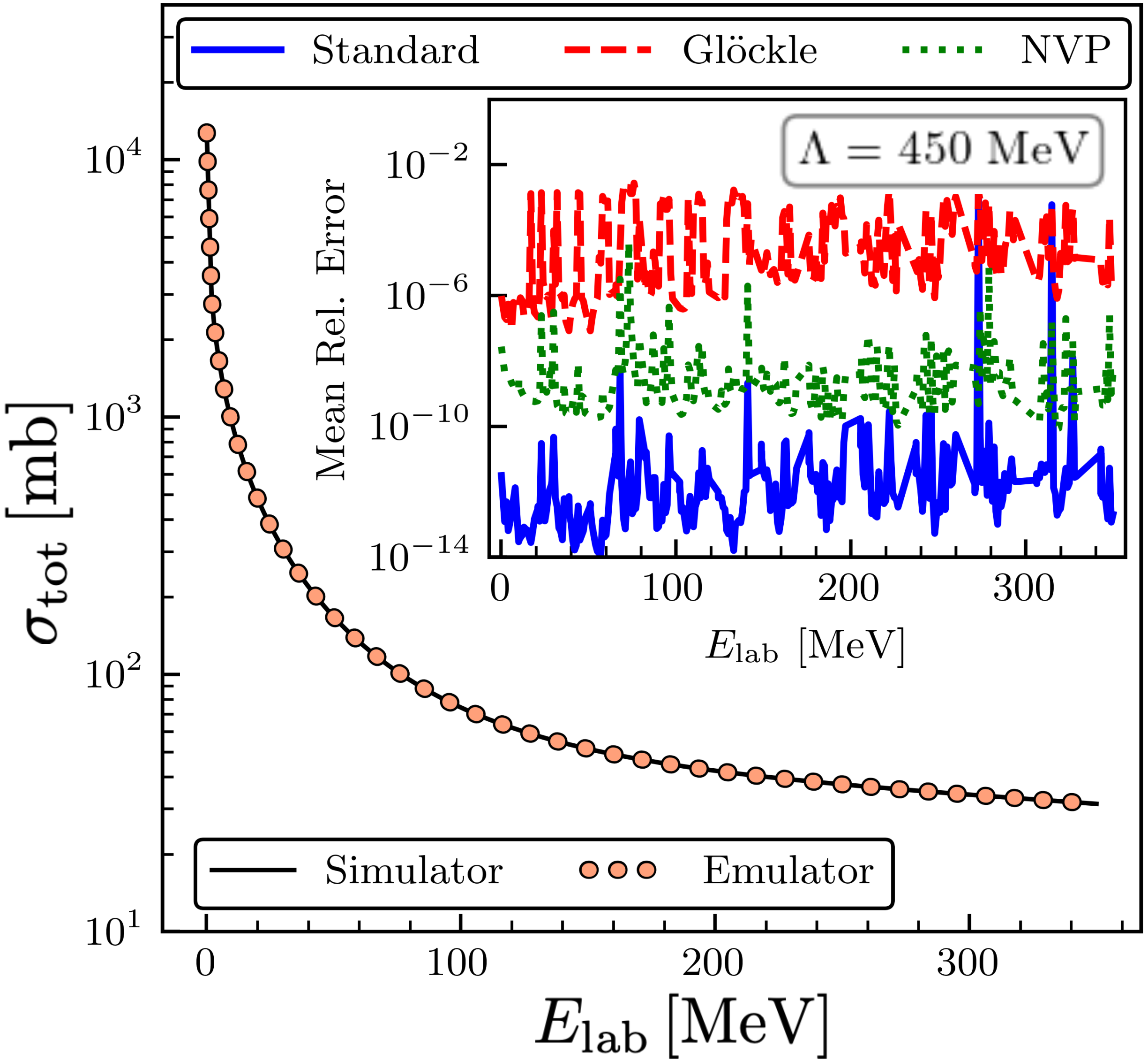

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Total cross section emulation

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- Consistent for $\Lambda = 400 - 550\,\mathrm{MeV}$

- Different cutoff!

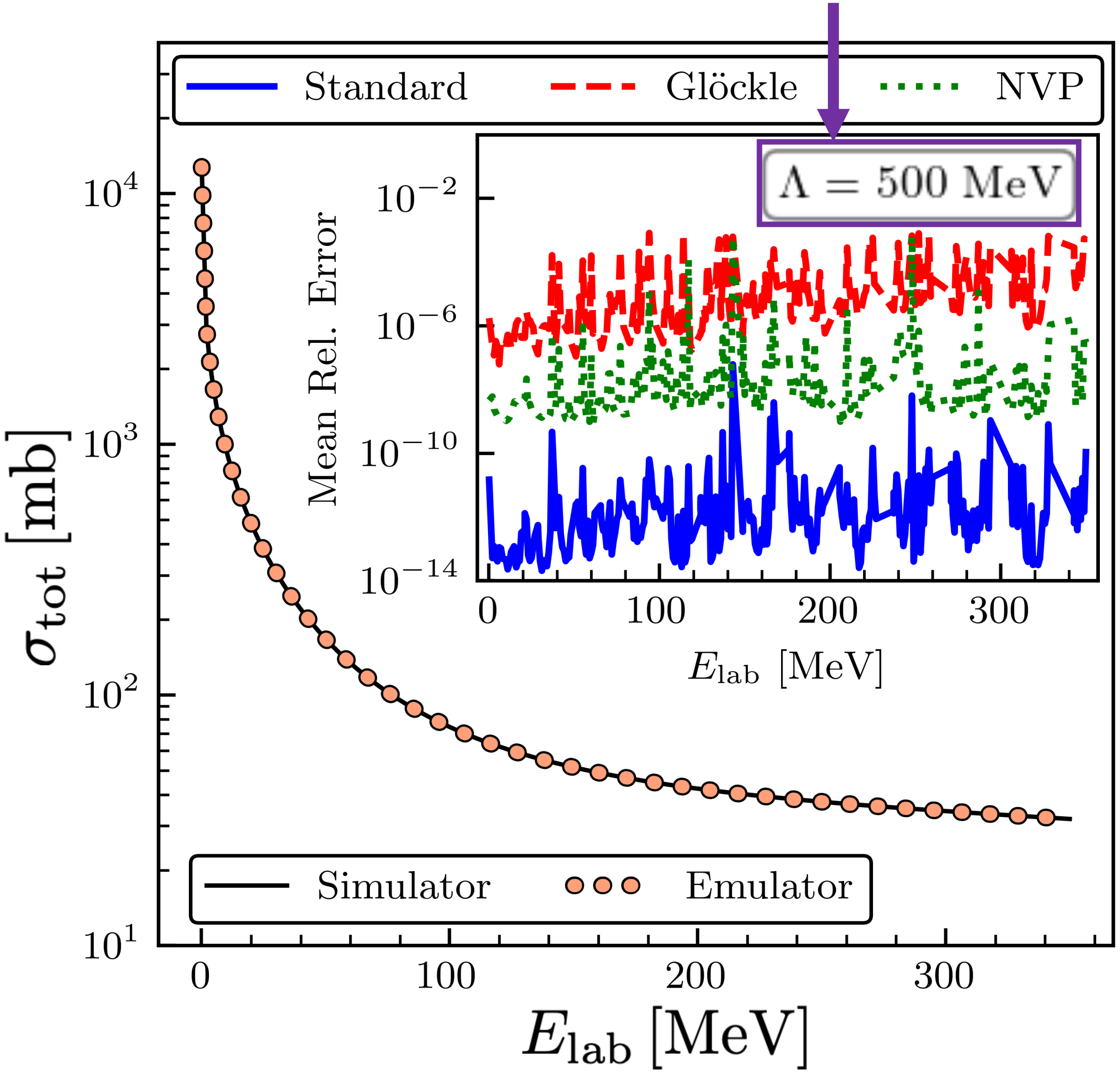

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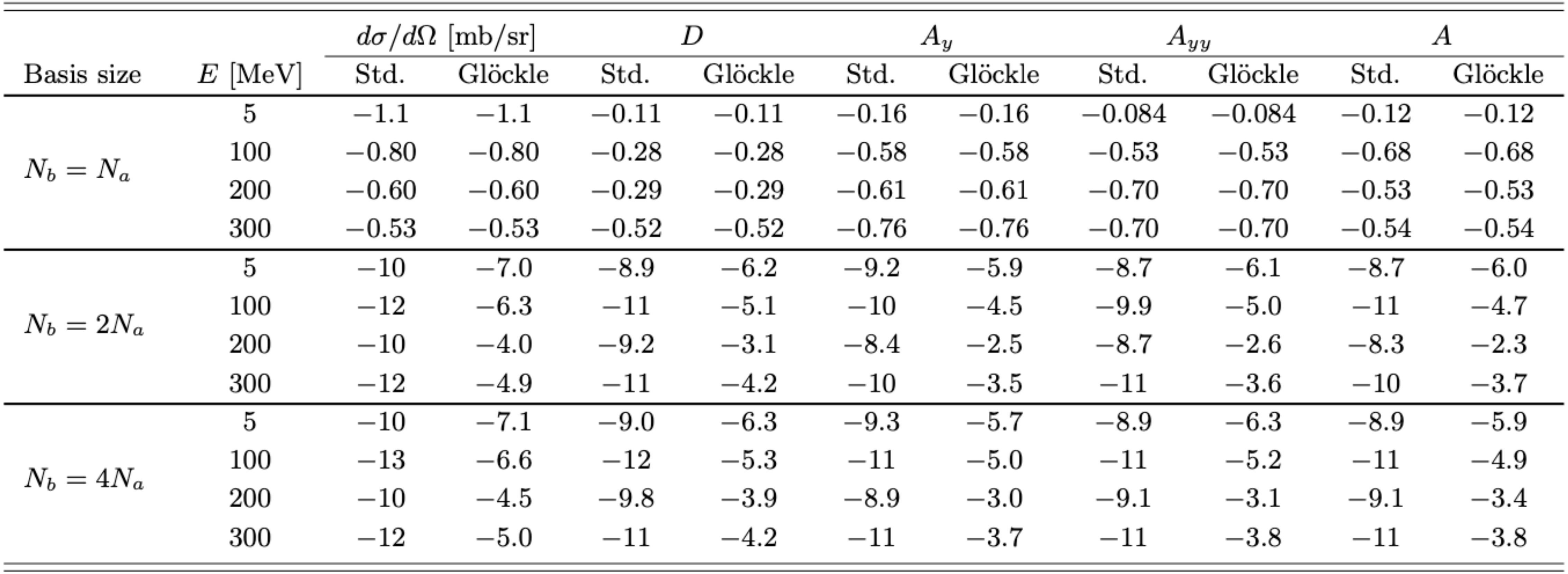
Table of spin observables emulation



		$d\sigma/d\Omega$ [mb/sr]		D		A_y		A_{yy}		A	
Basis size	E [MeV]	Std.	Glöckle	Std.	Glöckle	Std.	Glöckle	Std.	Glöckle	Std.	Glöckle
$N_b = N_a$	5	-1.1	-1.1	-0.11	-0.11	-0.16	-0.16	-0.084	-0.084	-0.12	-0.12
	100	-0.80	-0.80	-0.28	-0.28	-0.58	-0.58	-0.53	-0.53	-0.68	-0.68
	200	-0.60	-0.60	-0.29	-0.29	-0.61	-0.61	-0.70	-0.70	-0.53	-0.53
	300	-0.53	-0.53	-0.52	-0.52	-0.76	-0.76	-0.70	-0.70	-0.54	-0.54
$N_b = 2N_a$	5	-10	-7.0	-8.9	-6.2	-9.2	-5.9	-8.7	-6.1	-8.7	-6.0
	100	-12	-6.3	-11	-5.1	-10	-4.5	-9.9	-5.0	-11	-4.7
	200	-10	-4.0	-9.2	-3.1	-8.4	-2.5	-8.7	-2.6	-8.3	-2.3
	300	-12	-4.9	-11	-4.2	-10	-3.5	-11	-3.6	-10	-3.7
$N_b = 4N_a$	5	-10	-7.1	-9.0	-6.3	-9.3	-5.7	-8.9	-6.3	-8.9	-5.9
	100	-13	-6.6	-12	-5.3	-11	-5.0	-11	-5.2	-11	-4.9
	200	-10	-4.5	-9.8	-3.9	-8.9	-3.0	-9.1	-3.1	-9.1	-3.4
	300	-12	-5.0	-11	-4.2	-11	-3.7	-11	-3.8	-11	-3.8

$\Lambda = 450\ \mathrm{MeV}$

- Angle-averaged relative errors (base-10 logarithm)
- Different basis size
- Consistent for $\Lambda = 400 - 550\,\mathrm{MeV}$