Eigenvector Continuation Emulators for NN Scattering

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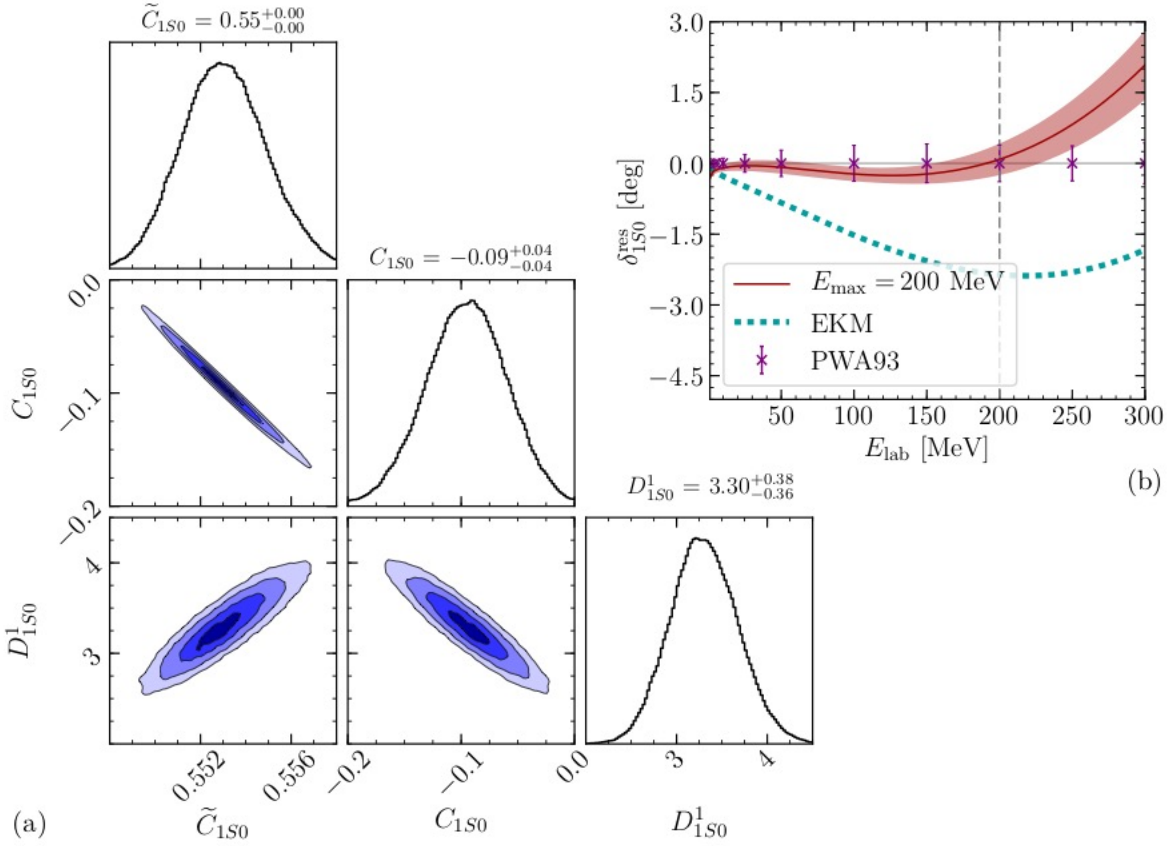
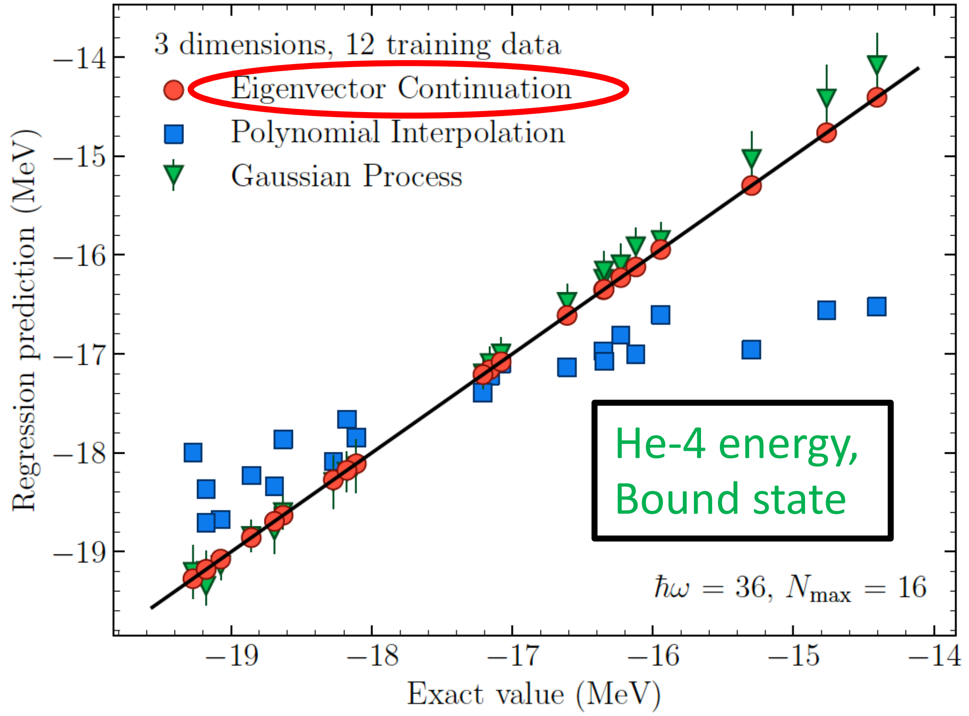
Phase shifts for NN scattering with UQ

- Full sampling for Bayesian UQ can be expensive using direct calculations
- Alternative: sample from a previously trained computer model
- Linear parameter dependence in χEFT allows for fast calculations



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



König et al, *Phys. Lett. B 810, 135814 (2020)*

Chiral EFT potentials for NN scattering

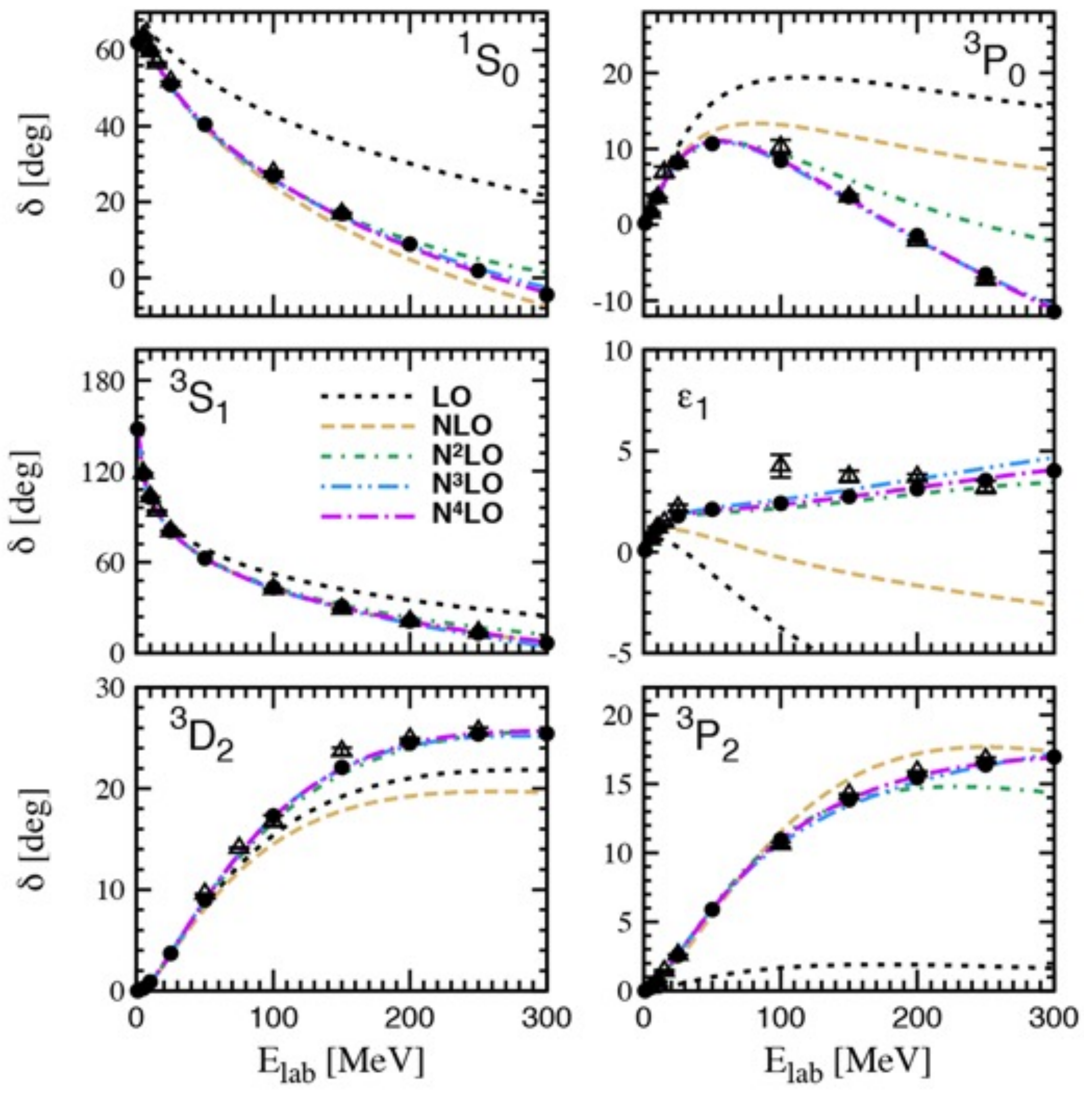
P. Reinert et al., Eur. Phys. J B 54, 86 (2018)

- Here: RKE semi-local momentum-space regularized potential
- Candidate for full Bayesian UQ using eigenvector continuation (EC)
- Can take advantage of linearity between matrix elements and LECs:

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

→ only calculate matrix elements once!

- Test EC neutron-proton *scattering* for the $^1S_0$ channel at cutoff $\Lambda = 450\,MeV$



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Eigenvector continuation (EC) for scattering

Hamiltonian:

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

$\longrightarrow$

Sets of parameters:

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

$\longrightarrow$

K-matrix formulation:

$$\mathcal{K}_\ell(E) = \tan\delta_\ell(E)$$

Kohn variational principle (KVP):

S-wave: $\ell = 0$

$p \equiv \sqrt{2\mu E}$

$$|\psi_{trial}\rangle \underset{r\to\infty}{\longrightarrow} \frac{1}{p}\sin(pr) + \frac{[\mathcal{K}_0(E)]_{trial}}{p}\cos(pr)$$

$$\delta\beta\big[|\psi_{trial}\rangle\big] = \delta\left[\frac{[\mathcal{K}_0(E)]_{trial}}{p} - \frac{2\mu}{\hbar^2}\langle\psi_{trial}|\hat{H}(\boldsymbol{\theta}) - E|\psi_{trial}\rangle\right] = 0 \longrightarrow \beta\big[|\psi_{exact}\rangle\big] = \frac{[\mathcal{K}_0(E)]_{exact}}{p}$$

EC implementation:

$$|\psi_{trial}\rangle = \sum_{i=1}^{N_b} c_i|\psi_E(\boldsymbol{\theta}_i)\rangle \longrightarrow \sum_j \left(\Delta U^T + \Delta U\right)_{ij} c_j = \sum_j \Delta\tilde{U}_{ij}c_j = \frac{\mathcal{K}_0^{(i)}(E)}{p} - \lambda$$

$$\Delta\tilde{U}_{ij} = \frac{2\mu}{\hbar^2}\langle\psi_E(\boldsymbol{\theta}_i)|2\hat{V}(\boldsymbol{\theta}) - \hat{V}(\boldsymbol{\theta}_i) - \hat{V}(\boldsymbol{\theta}_j)|\psi_E(\boldsymbol{\theta}_j)\rangle$$

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

- Simple matrix inversion + cancellation of Coulomb force!
- Stationary approximation to K-matrix (not an upper/lower bound)

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Momentum space implementation

- EC matrix can be calculated using momentum space wave function

$$\Delta \tilde{U}_{ij} = \frac{2\mu}{\hbar^2} \langle \psi_E(\boldsymbol{\theta}_i) | 2\hat{V}(\boldsymbol{\theta}) - \hat{V}(\boldsymbol{\theta}_i) - \hat{V}(\boldsymbol{\theta}_j) | \psi_E(\boldsymbol{\theta}_j) \rangle$$

$$\psi_E(k;\theta) = \frac{1}{k^2}\delta(k - k_0) - \frac{2}{\pi}\mathbb{P}\frac{R(k,k_0;\theta)}{k^2 - k_0^2}$$

- Matrix elements are now calculated using

$$\Delta U_{ij} \equiv \frac{2\mu}{\hbar^2} \iint dk\, dp\, \psi_E(p;\theta_i)\left[V(k,p;\theta) - V_j(k,p)\right]\psi_E(k;\theta_j)$$

- The principal value integrals are evaluated with the same numerical method as conventionally used for the Lippmann-Schwinger equation

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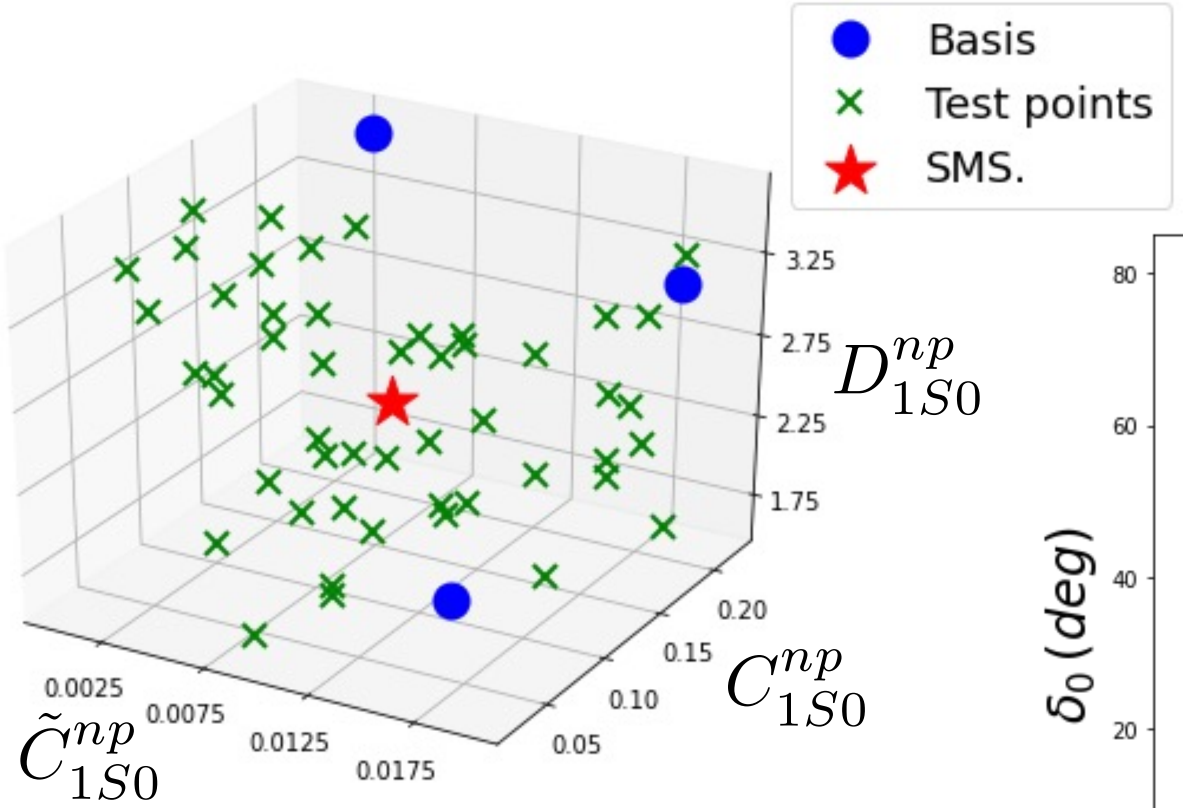
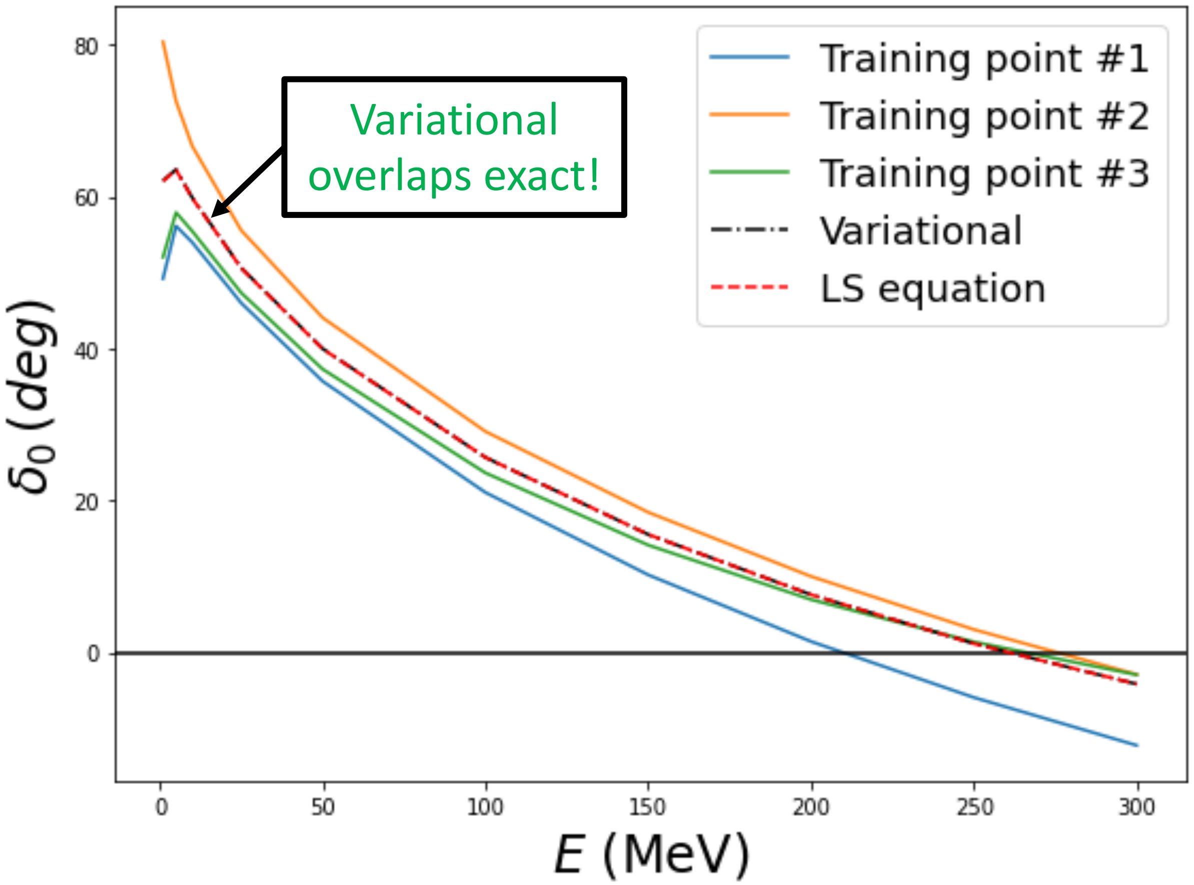
SMS Chiral potential results



$\bigstar = (0.010, 0.121, 2.579)$



- Sampled points in coupling constant space for the 1S0 channel
- 50 test points with best parameters set as a star (Reinert, et al.)

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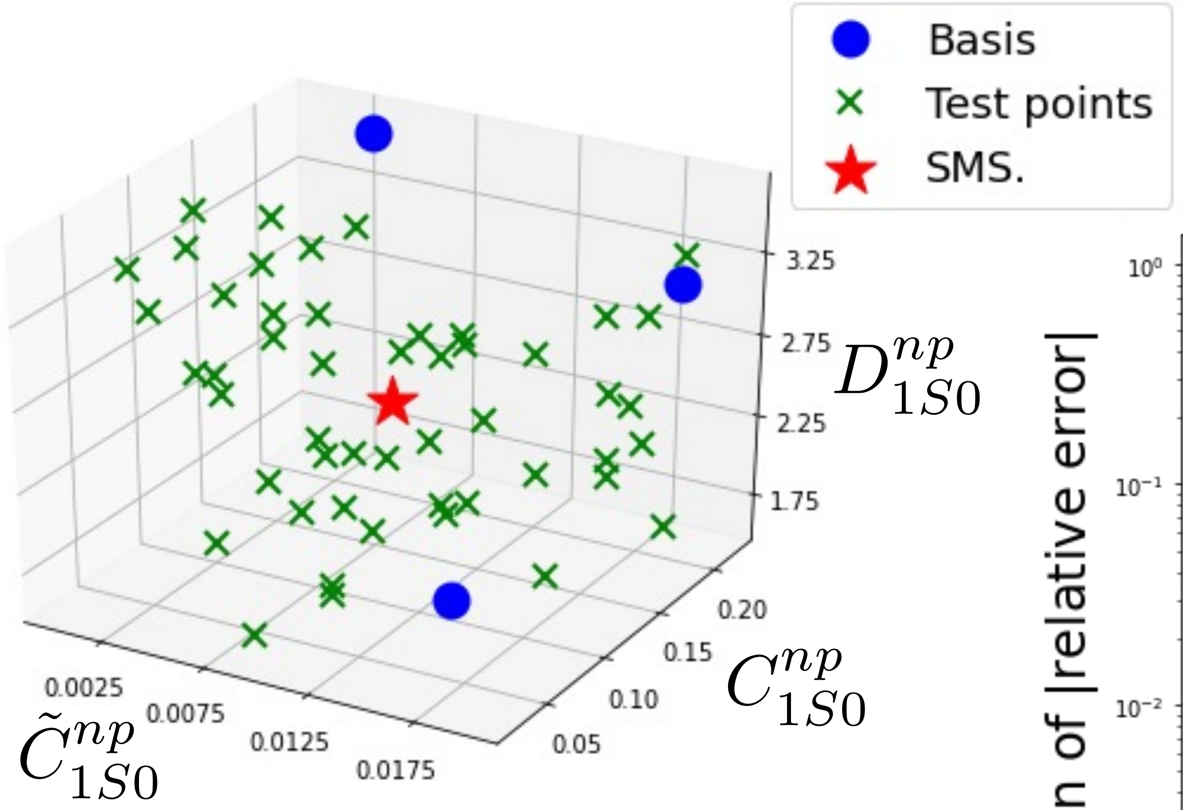
SMS Chiral potential results



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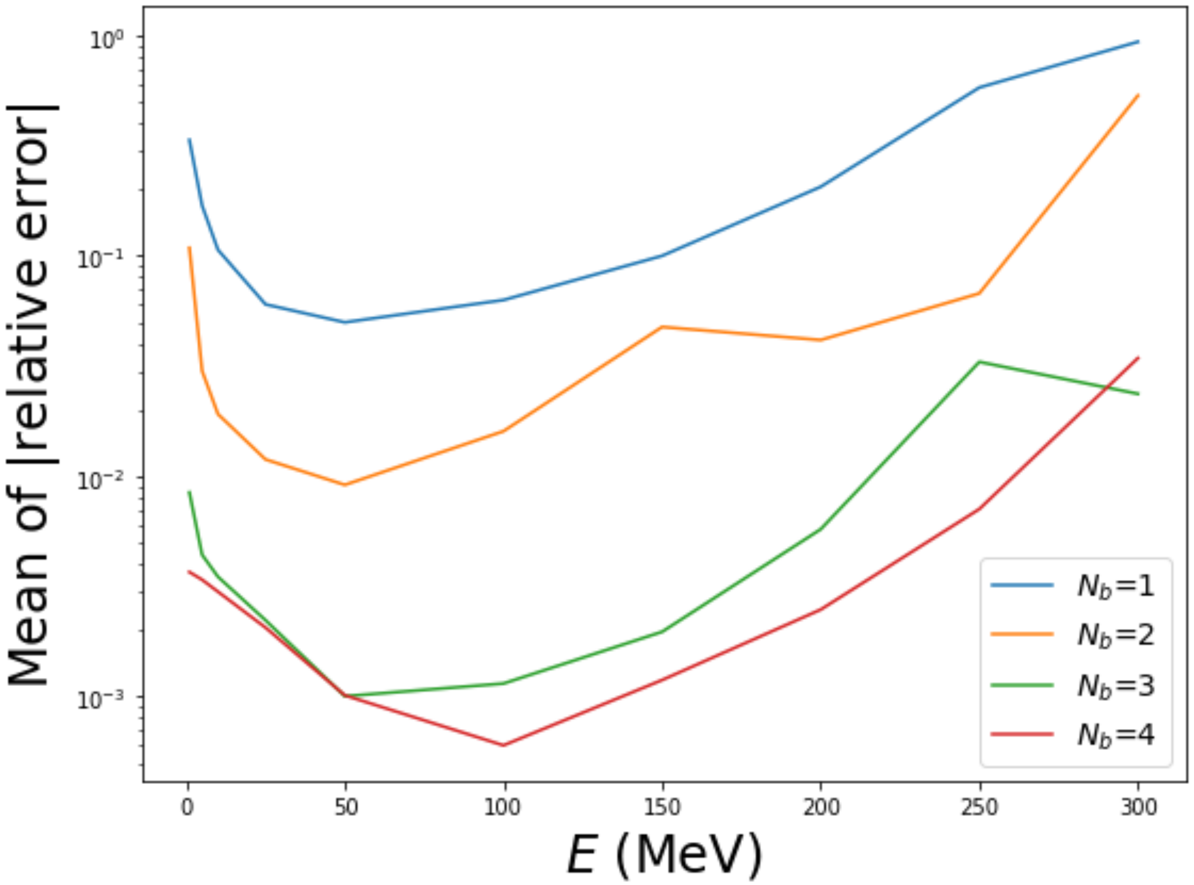

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Numerics currently being studied

- The basis gets close to being linearly dependent with increased size causing the condition number to grow
- Leads to the matrix becoming ill-conditioned
  - Use Moore-Penrose pseudo-inverse with appropriate cutoff
  - Regularize using a “nugget”
- Accuracy currently limited
  - Should get better based on other calculations
- EC calculation for each additional parameter set is 1000x times faster than calculating directly
  - Need to pre-calculate necessary information needed for EC such as wave functions and potentials

Summary

- EC works for momentum space applications (S13.00004: P.J. Millican)
- EC emulators can be used for sampling LECs

Ongoing work

- Understand numerical issues and sensitivity of LECs
- Techniques for a more efficient EC calculation
- Full calculation for all partial waves
- Calculate all observables
- Test EC for different potentials in coordinate and momentum space
- EC applications to three-body scattering (KP01.00027: Xilin Zhang)

Thank you!