Active Learning Emulators for Nuclear Two-Body Scattering in Momentum Space

Abhinav Giri
Ohio University, Department of Physics and Astronomy

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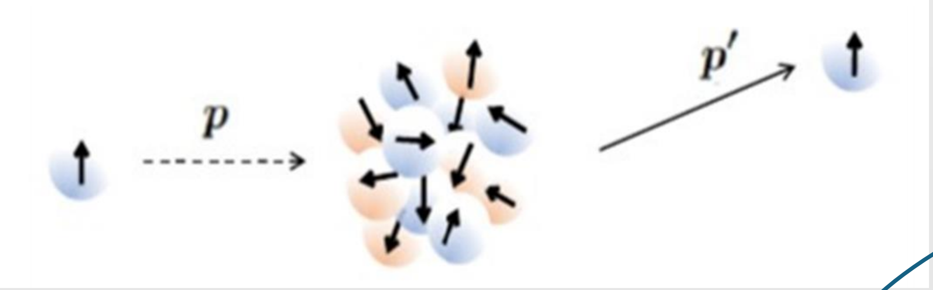
Two-body Nuclear Scattering

OHIO UNIVERSITY

The central computational task: solve the **Lippmann–Schwinger equation** for the t-matrix, from which all scattering observables follow.



Credit: Robert Baker

$$T_{\ell\ell'}(k,k';E_{k_0}) = V_{\ell\ell'}(k,k') + \sum_{\ell''} \lim_{\epsilon\to 0^+} \int_0^\infty dk''\, k''^2 \frac{V_{\ell\ell''}(k,k'')\, T_{\ell''\ell'}(k'',k';E_{k_0})}{E_{k_0} - E'' + i\epsilon}$$

$$A(\boldsymbol{\theta})\,\mathbf{t}(\boldsymbol{\theta}) = \mathbf{V}(\boldsymbol{\theta})$$

Why it stings

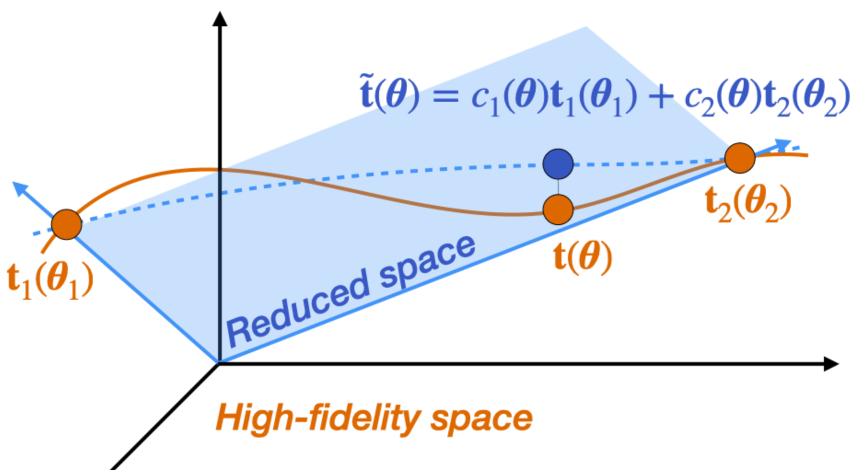
- $(N+1)\times(N+1)$ solve per partial wave
- Coupled channels: $4(N+1)$ x $4(N+1)$ matrix
- Repeat for every energy & every $\boldsymbol{\theta}$

$$V_{\ell,\ell'}(k,k';\theta) = \sum_{a=0}^{n_\theta} h_a^{(\ell,\ell')}(\theta)\, V_a^{(\ell,\ell')}(k,k')$$

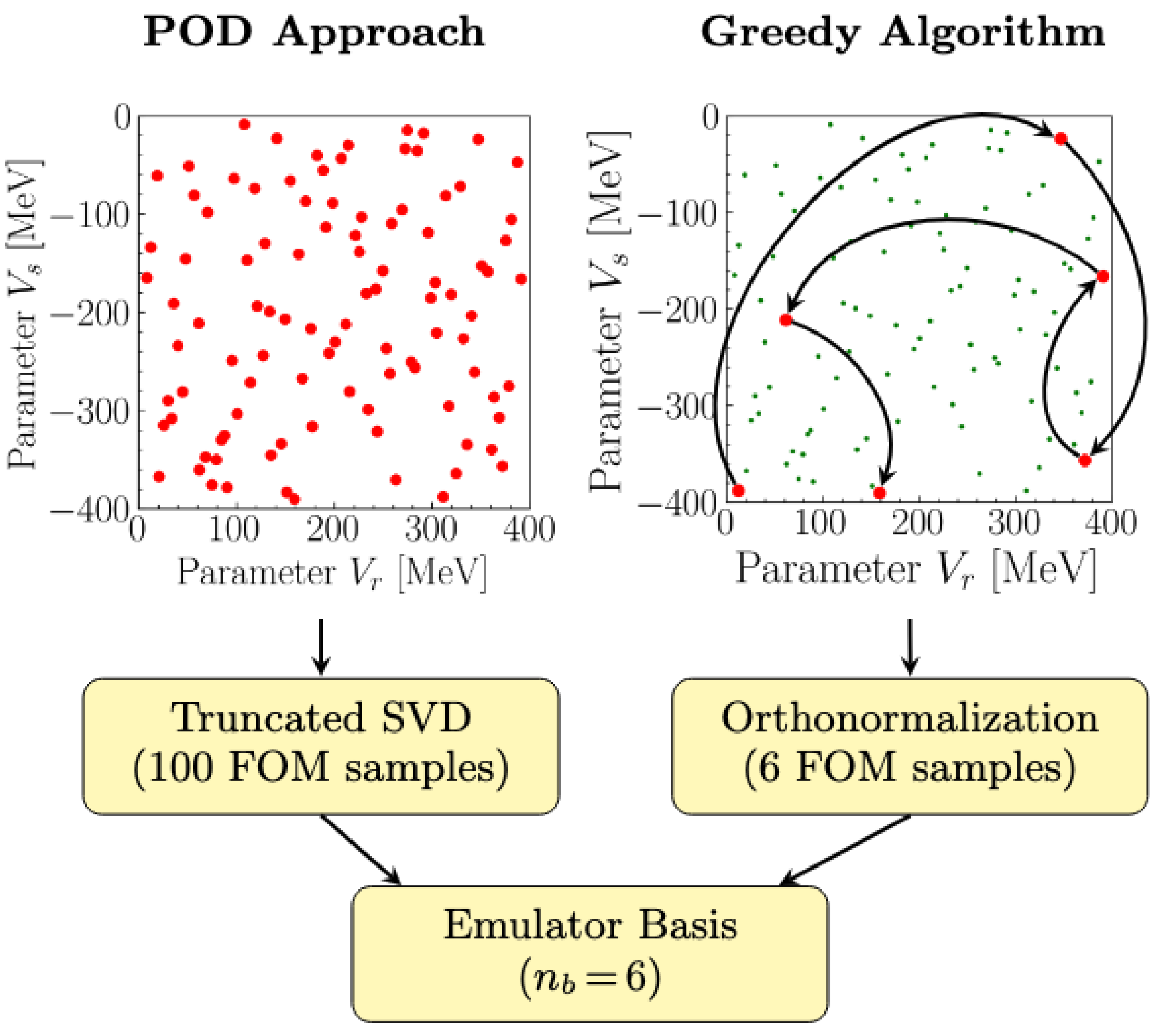
For chiral interactions, the LECs enter *linearly*: $h_a(\boldsymbol{\theta}) = \theta_a$. The index a=0 absorbs all parameter-independent (e.g., pion-exchange) terms.

Solved channel by channel: $^1S_0$, $^3S_1$–$^3D_1$, higher ℓ — phase shifts δ_ℓ compared to data; all observables follow from T.

Reduced Order Models



C. Drischler et al., Front. Phys. **10**, 1365 (2022)



Reduced Basis Methods construct a low-dimensional subspace from high-fidelity solutions called **snapshots**.

Greedy Algorithm aims to **give high accuracy with fewer samples** compared to POD along **with error estimator**

- Offline: expensive basis construction
- Online: fast evaluations for new parameters.

Maldonado et al., PRC **112**, 024002 (2025)

LHC : Latin Hyper Cube **POD : Proper Orthogonal Decomposition** **SVD : Singular Value Decomposition**

Greedy Algorithm in Action (2d Parameter Space)

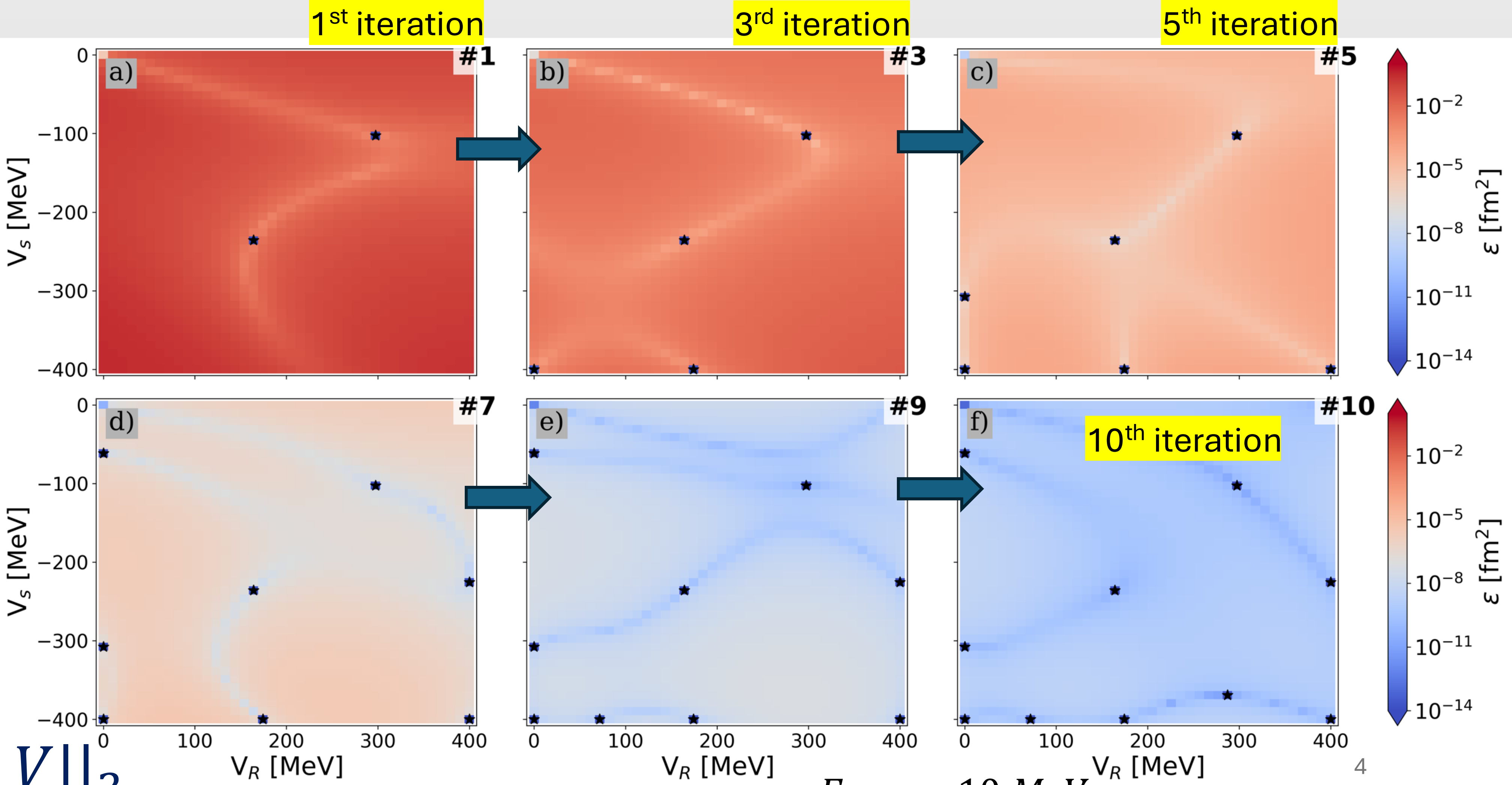
$$V(r;\boldsymbol{\theta}) = \theta_1\, e^{-\kappa_R r^2} + \theta_2\, e^{-\kappa_s r^2}, \qquad \text{where } \boldsymbol{\theta} = (\theta_1, \theta_2) = (V_R, V_s)$$

For demonstration, the Minnesota potential in momentum space is used.

Greedy algorithm chooses **new points where estimated emulator error is largest.**

Stops when **all errors below tolerance.**

$$\varepsilon = ||At_{emu} - V||_2$$



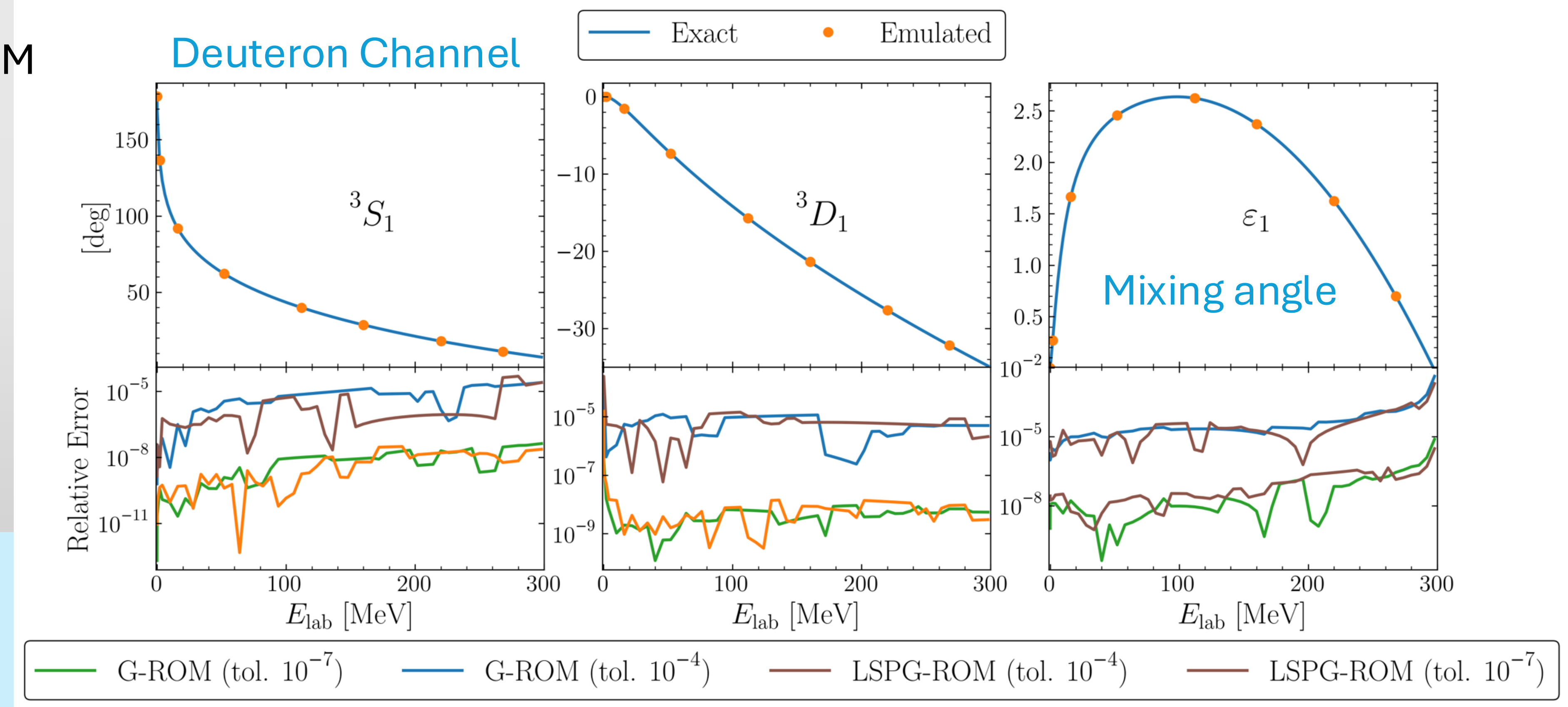
$E_{c.m.} = 10\ MeV$

Phase Shifts

- Obtained from the emulated on-shell t-matrix and compared with exact calculations from the chiral potential at the best-fit LECs

Gezerlis et al., Phys. Rev. C **90**, 054323 (2014)

- The G-ROM and LSPG-ROM were tested at two tolerance levels:
  - $\eta = 10^{-4}$ → relative error mostly below 10^{-5}
  - $\eta = 10^{-7}$ → relative error mostly below 10^{-8}



500 training points per energy

- Both the phase shifts and mixing angle from the emulator **show excellent agreement with the exact *t*-matrix** results

Bayesian Calibration to Total Cross Sections

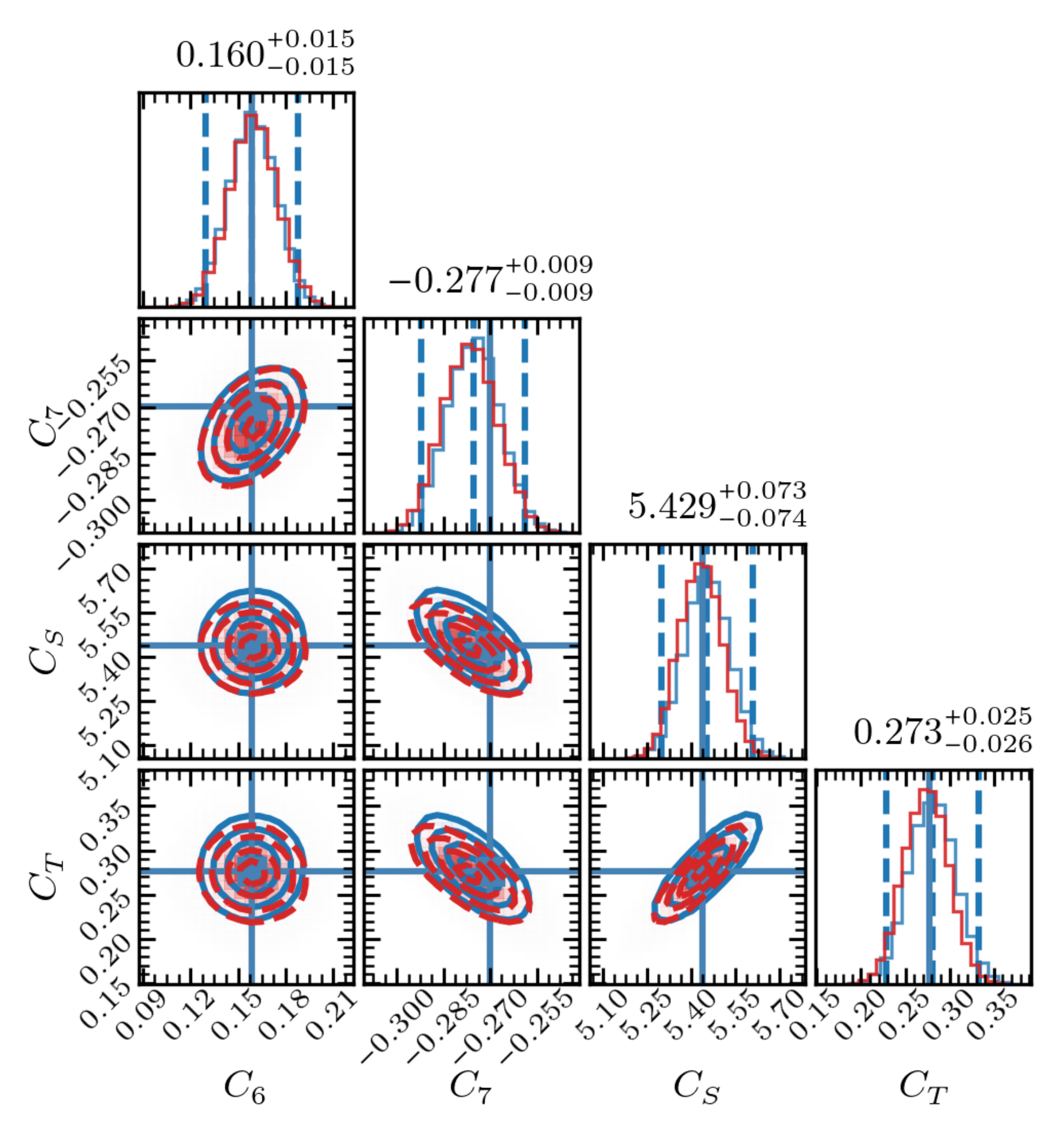
DATA

- PWA93 total *np* cross sections
- 12 energies: 0.1–25.1 MeV + 60 MeV
- Prior: $N(\boldsymbol{\theta}^*, (\kappa\boldsymbol{\theta}^*)^2)$, κ=0.1

SAMPLER

- emcee — 32 walkers
- 5k warm-up + 20k production, thin×15
- MAP-init: basin-hopping + L-BFGS-B

*Even at deliberately loose $\alpha = 10^{-2}$— much looser than the EFT truncation error — the LEC inference is **not distorted**.*



Summary and Outlook

Developed active learning emulators for two-body scattering in momentum space, based on the **Lippmann–Schwinger equation**.

→ **gives access to wide range of chiral NN interactions**

The models reproduce phase shifts and cross sections with errors below 10^{-5} (and 10^{-8}), while conserving unitarity.

Applied Bayesian calibration of chiral NN potential with quantified emulator errors and achieved **26–92× speedup** over the full-order model

Software based on Google JAX made publicly available, setting the stage for calibrating chiral and optical models to scattering experiments

A. Giri et al., Phys. Rev. C **113**, 044001 (2026)

FUTURE WORK:

Extend emulator to all spin-dependent scattering observables + GP truncation error model (SMS only)

Full **Bayesian calibration with SMS** (Δ-less), order-by-order LO→N^4LO^+

Extend to WUSTL for **Δ-full vs Δ-less comparison**