

BAND Science Highlight Fast & Accurate Two-Body Scattering Emulator



Problem: Bayesian analysis for experimental design often requires very many calculations with different parameters → too expensive!

Plan: Make computer *models* of calculations → add *emulators* to BAND Framework.

Method: Eigenvector continuation (EC) uses a small set of wave functions in variational calculations → fast & accurate emulators for bound-state matrix elements.

Advance: Here EC has been extended to calculate two-body *scattering observables* directly (i.e., without needing wave functions).

Results: Tests verify the new method is fast, accurate, and versatile. The figure shows an emulation of a cross section depending on 26 parameters. The errors are negligible with a 300-times reduction in CPU time!

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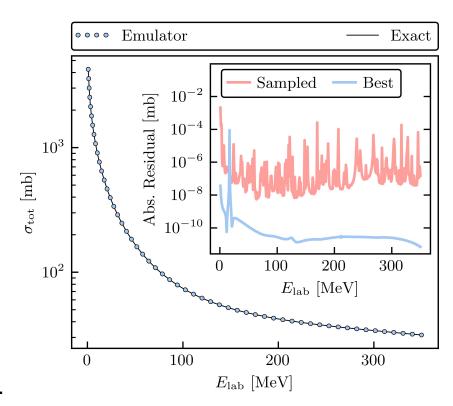


Figure: The total cross section for neutron-proton scattering as a function of energy for a modern chiral NN interaction. The emulator results (circles) are indistinguishable from the exact curve. **Inset:** the mean absolute error for 500 sampled points (red) and the absolute residual for the best-fit parameters (blue).