BAND
Bayesian Analysis of Nuclear Dynamics

NSF

Reduced Basis Methods & Scattering

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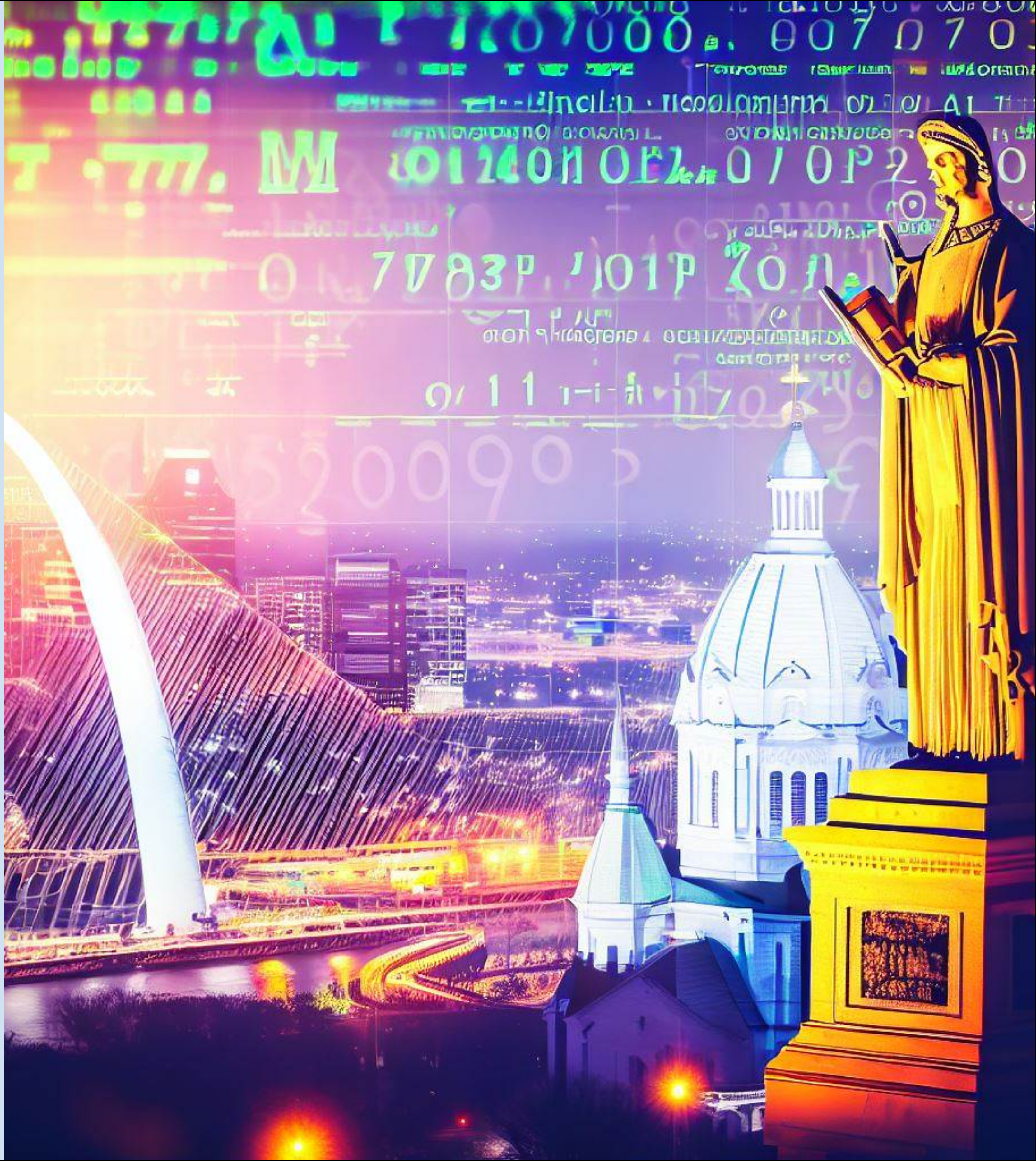
ISNET 2023-05-25

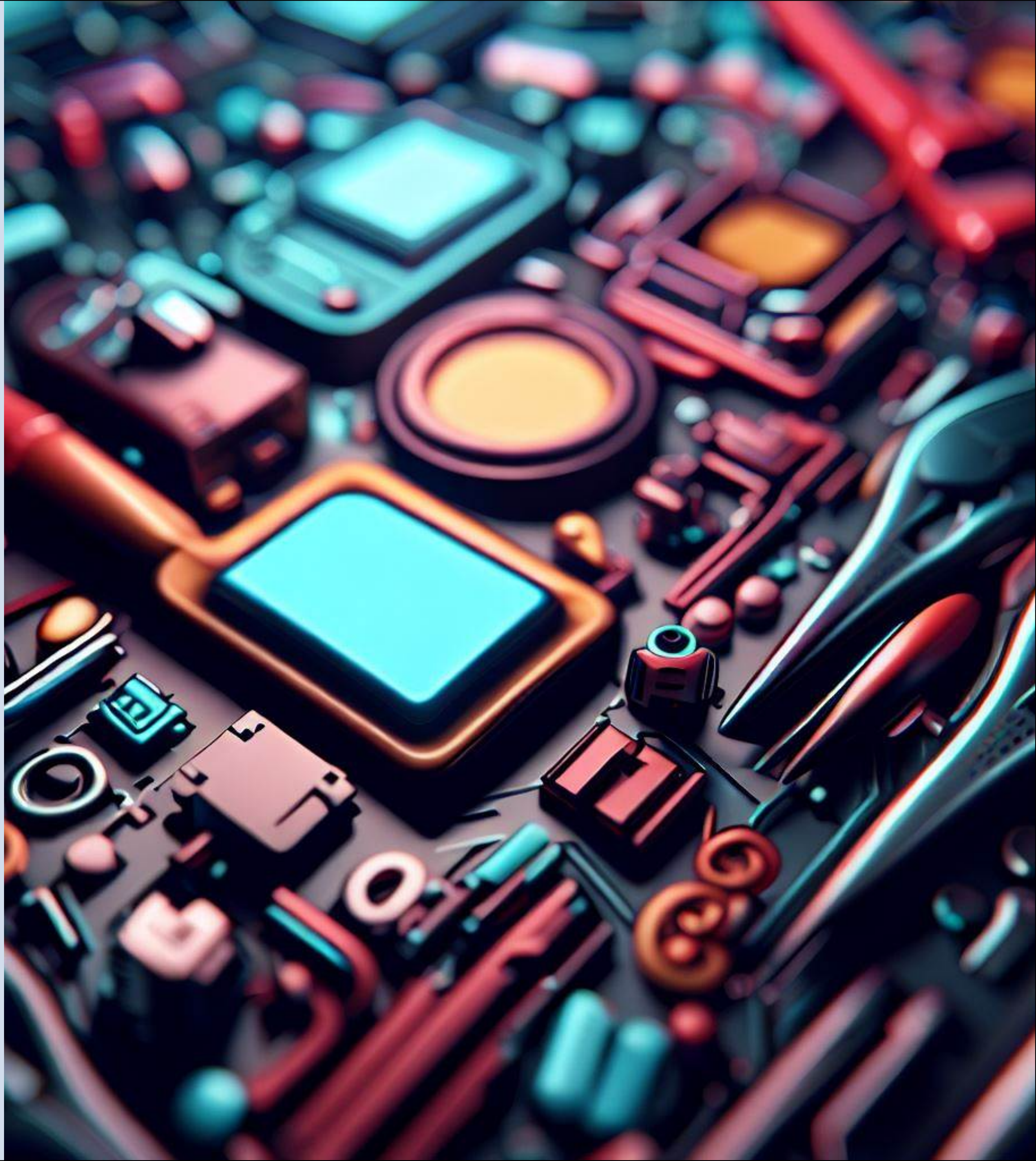
Rigorous UQ is good.

But it can be expensive.



Emulators significantly reduce this cost.

Building them is nontrivial.



BAND 🎸📈🥁📊

Choose a problem:

Optical Potentials

Build a tool:

`rose`

rose

Reduced-Basis Methods

Presenting ROSE, a Reduced Order Scattering Emulator

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2-Body Scattering

We're solving the Schrödinger Equation (SE),

$$F(\phi) = \left[-\frac{d^2}{ds^2} + \frac{\ell(\ell+1)}{s^2} + \frac{2\eta}{s} + U(s, \alpha, k) - 1\right] \phi(s) = 0$$

But we're going to solve it in a clever way – using a "well-informed" basis,

$$\langle \psi | F_\alpha(\hat{\phi}) \rangle = 0$$

where

$$\hat{\phi} = \phi_0 + \sum_{j=0}^{n-1} x_j f_j \approx \phi$$

2-Body Scattering

What are we going to use for the basis states (and judges/weights)?

$$f_j = \mathrm{PC}(\phi_\alpha - \phi_0)$$

The projection is defined as (these are stored in `rose`)

$$\langle \psi_i | F(f_j) \rangle = \int_0^\infty ds\, \psi_i(s)\, F(f_j(s))$$

Finally, we have a straightforward inversion problem,

$$\sum_{j=0}^{n-1} A_{ij} x_j = b_i$$

in n space.

rose

- **R**educed-**O**rder **S**cattering **E**mulator
- Python
- BAND Framework v0.3
- Supports local, complex, non-affine interactions.
- Designed to be user-friendly.
  - See pseudo-code ➡
  - Supports user-supplied solutions

```
import rose

def potential(r, alpha):
    alpha0, alpha1, … = alpha
    return alpha0 *
        woods_saxon(
            r, alpha1, alpha2
        ) + 1j*…

interaction = InteractionEIM(
    potential,
    num_params,
    reduced_mass,
    energy, Z_1, Z_2,
    is_complex=True
)

sae = ScatteringAmplitudeEmulator(
    interaction,
    training_points,
    l_max
)

cross_section = sae.emulate(alpha)
```

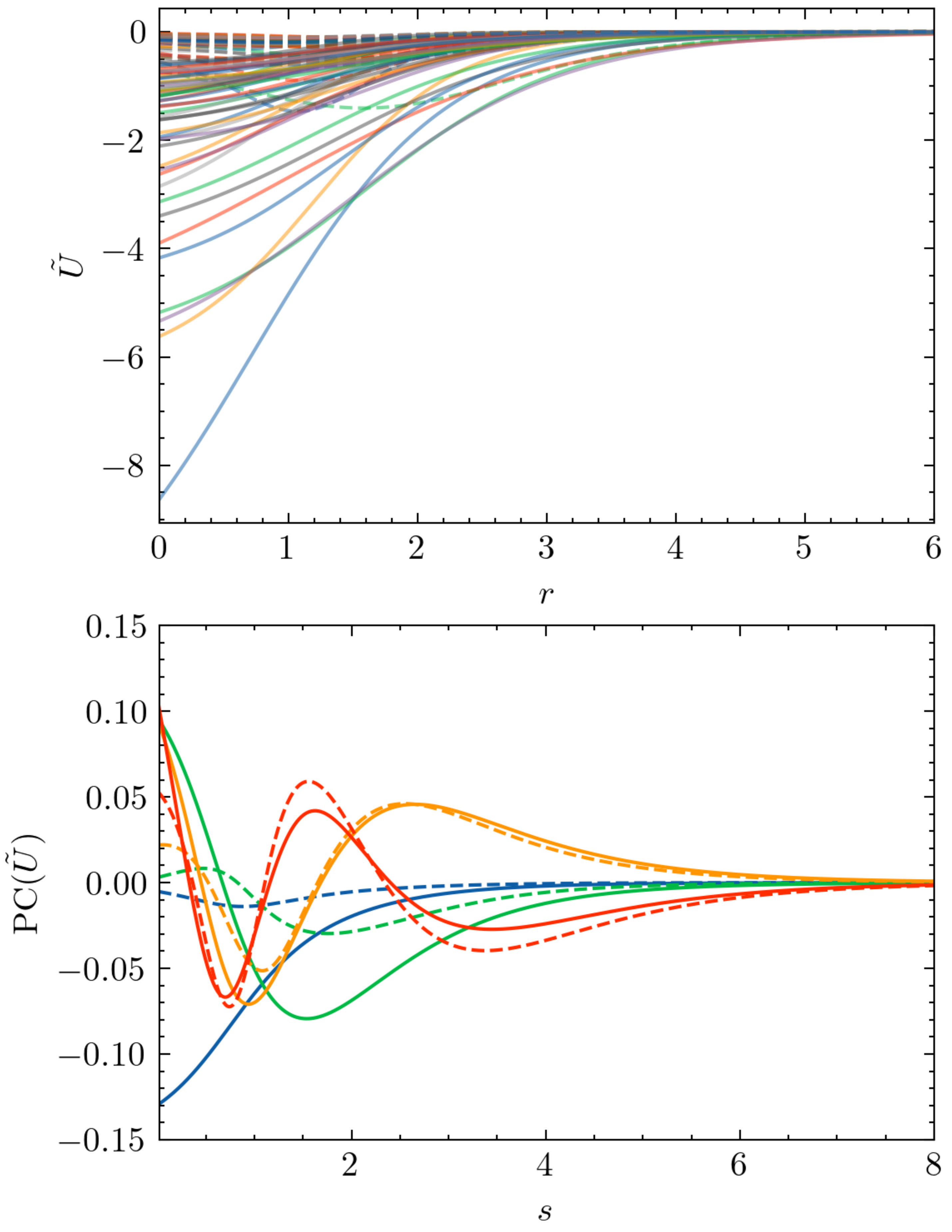
Empirical Interpolation Method

How do we handle non-affine potentials?

$$\tilde{U}(\alpha) \approx \sum_{j=0}^{n-1} \beta_j(\alpha) u_j$$

where

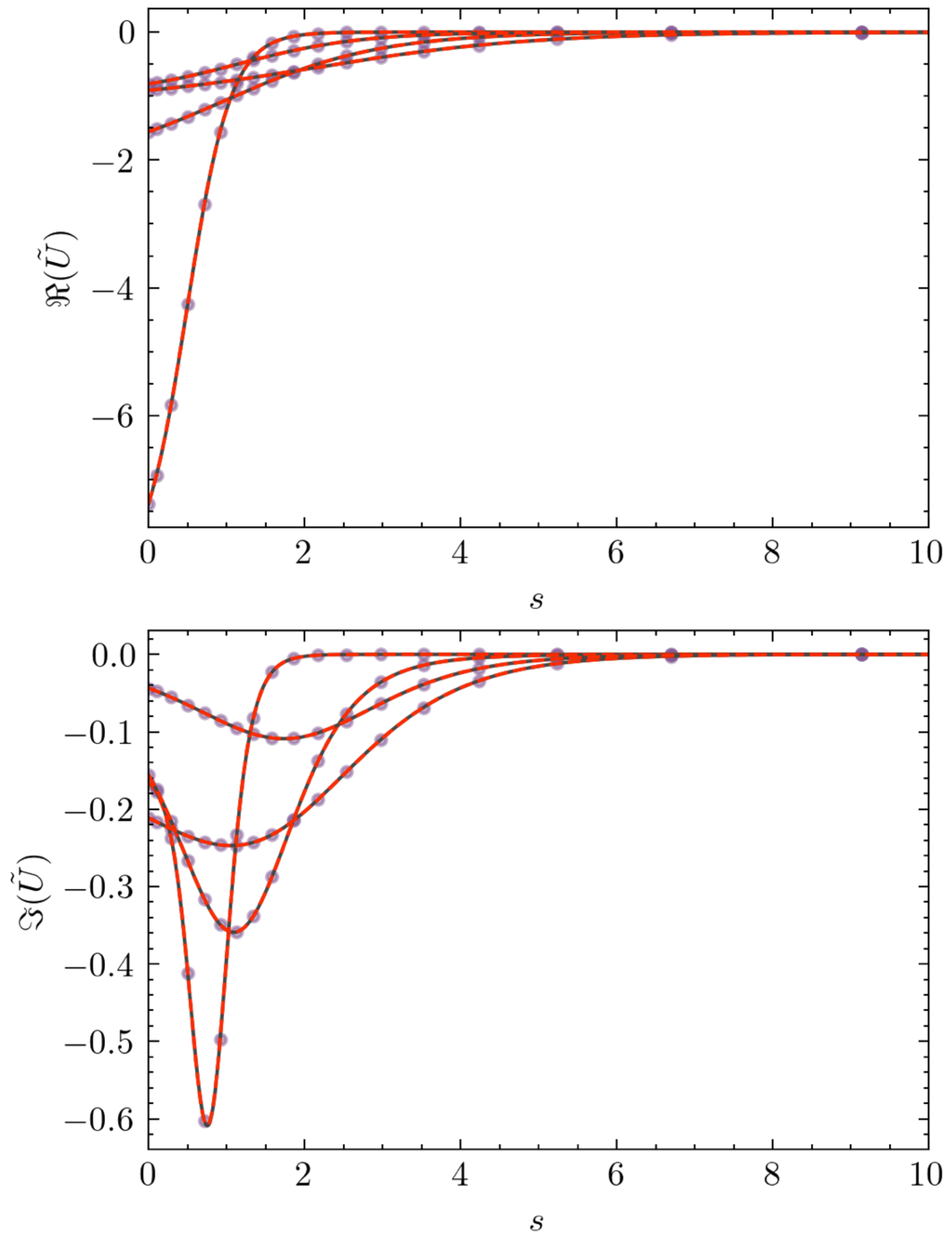
$$u_j = \mathrm{PC}(\tilde{U}_\omega)$$



EIM

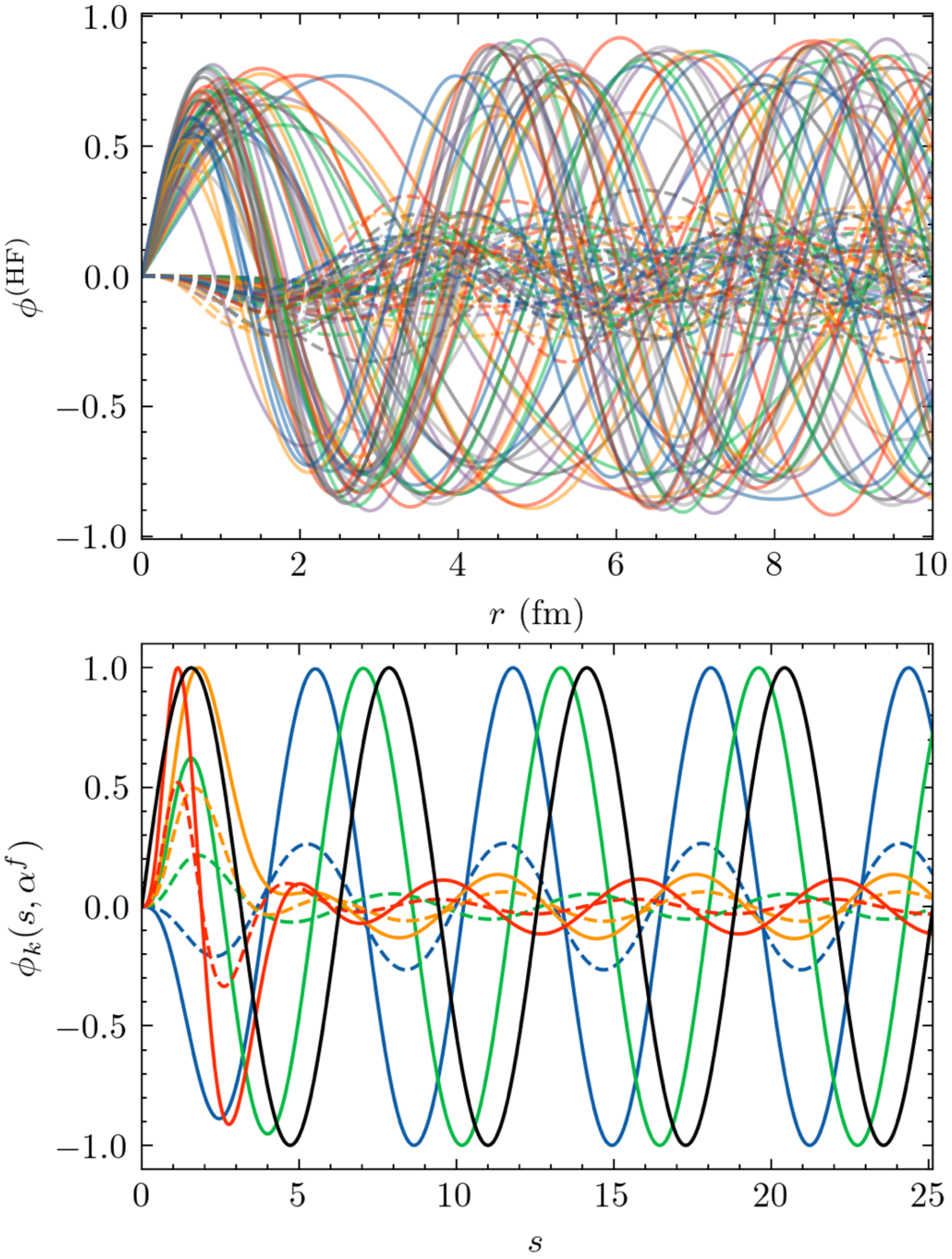
How do we ensure that $\tilde{U}$ is accurately reproduced?

$$\sum_{j=0}^{n-1} \beta_j u_j(r_i) = \tilde{U}(r_i)$$



RBM

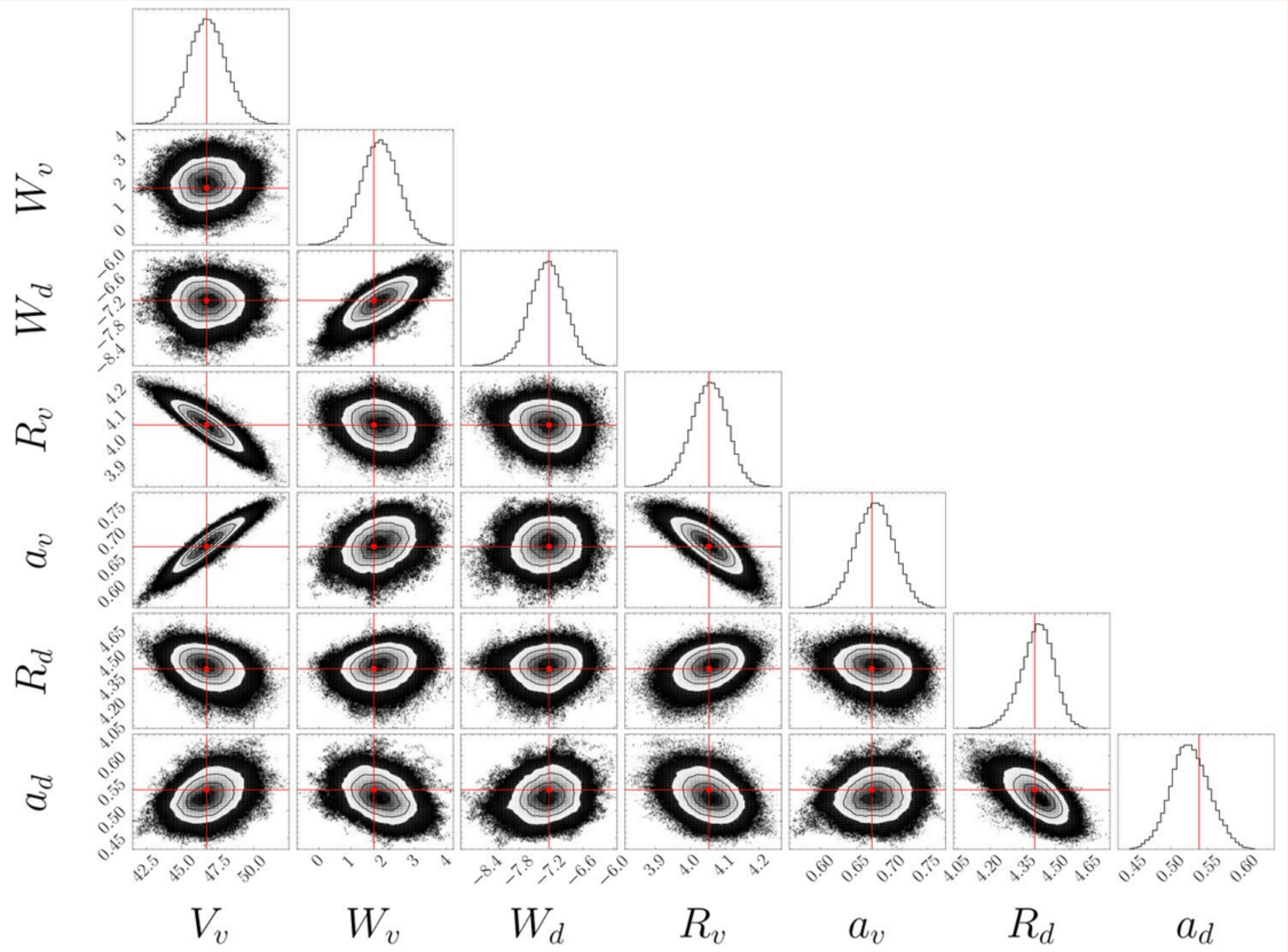
- different frequencies
  - E is just* another parameter
- PCs capture intricate behavior very well

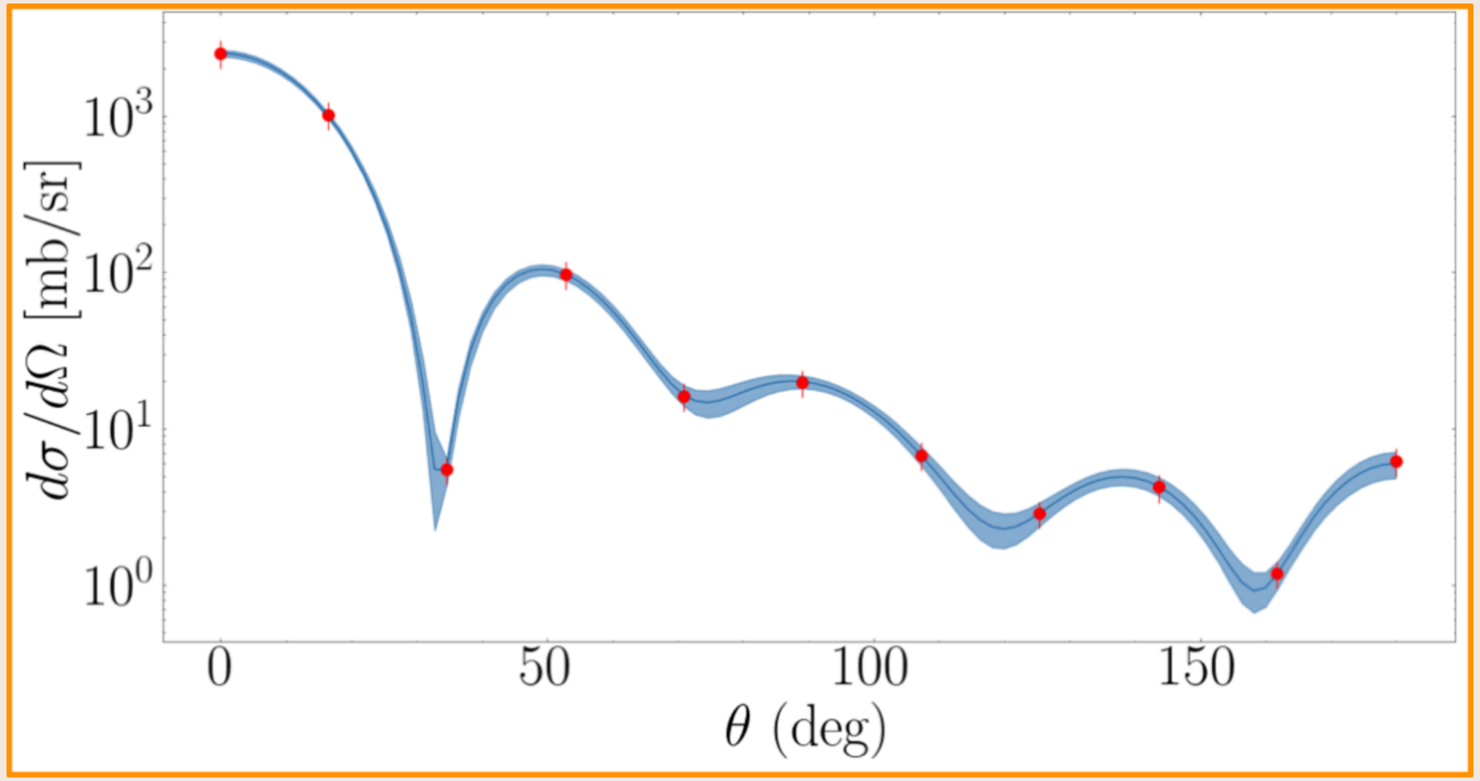


Results

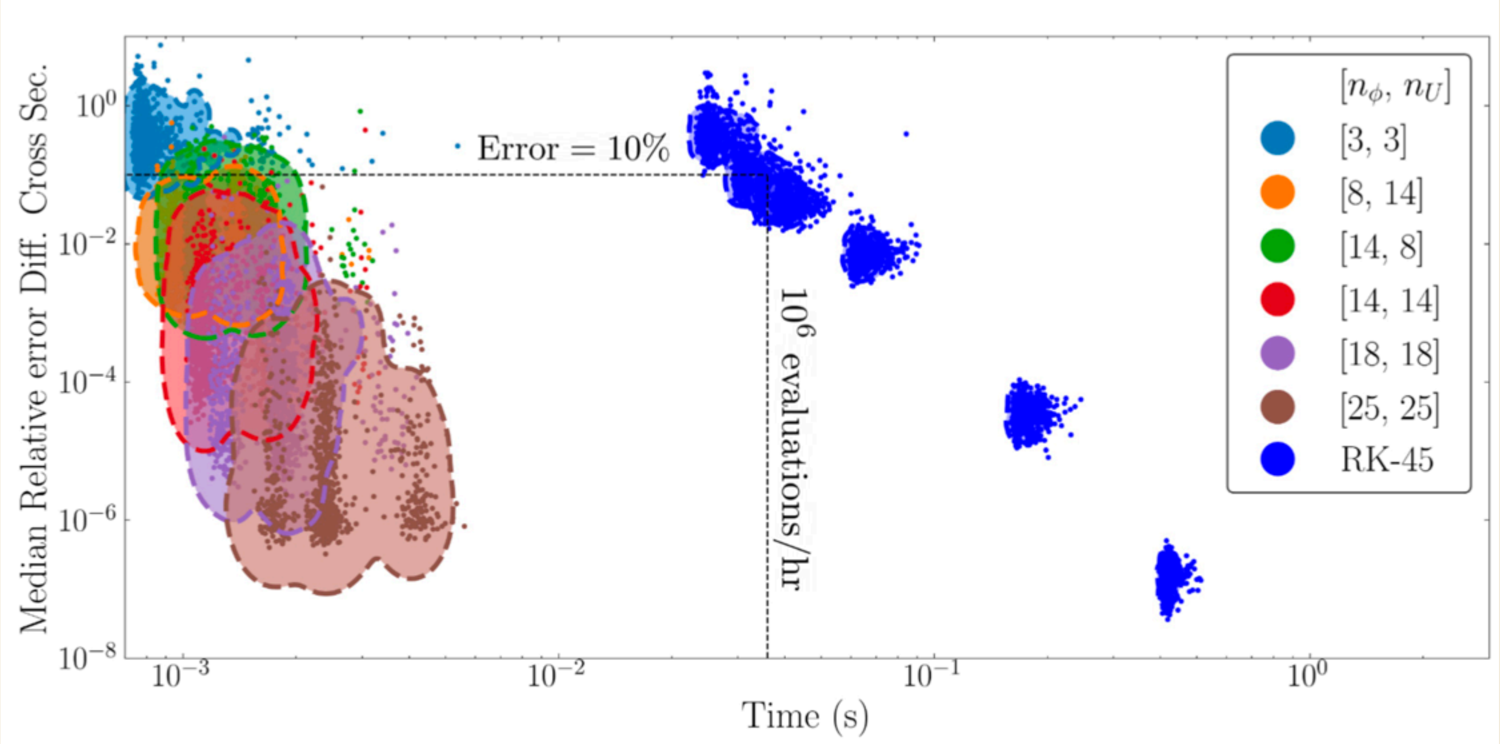
$^{40}\mathrm{Ca}(n,n)$

- 10% error bars
- $V_{\mathrm{KD}}(r)$ is non-affine in R_v, R_d, a_v, and a_d.
- 1.2M samples in $\approx$ 20 min (vs 11 days)





Computational Accuracy vs Time (CAT)

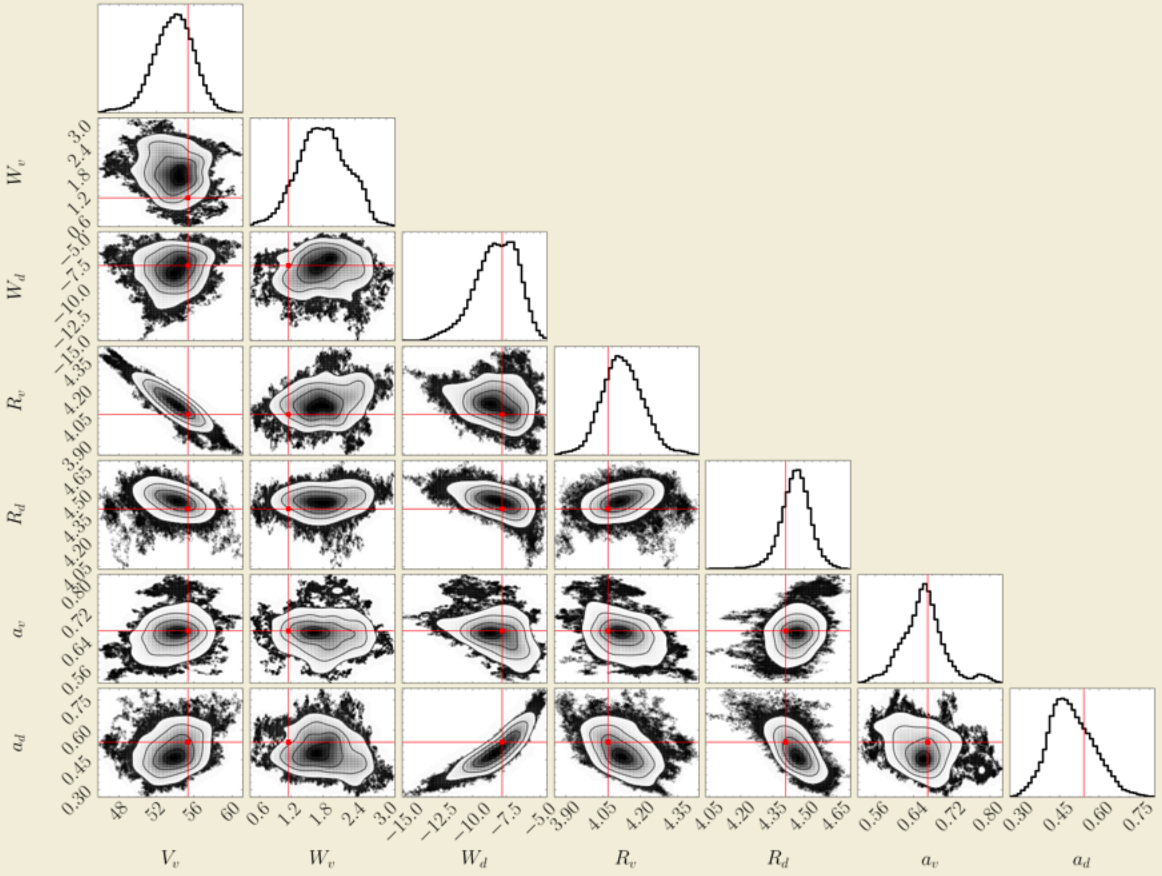


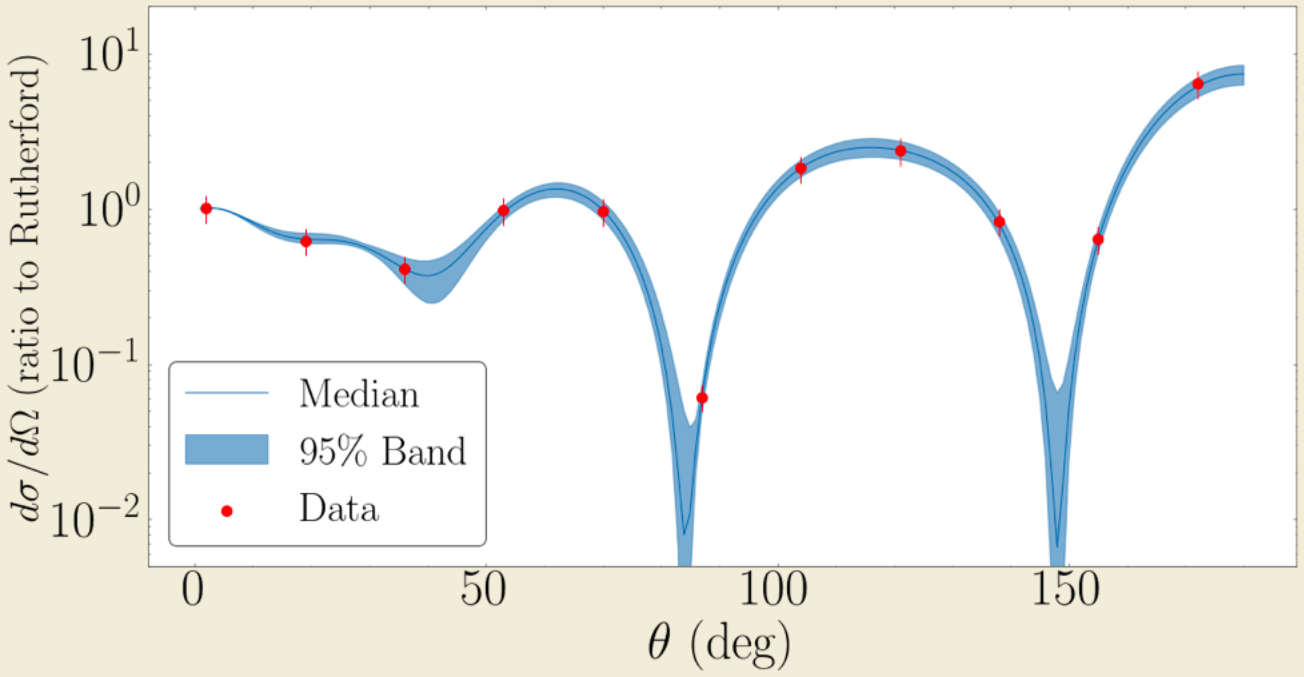
- Speedups are useful, but incomplete.
  - Highly implementation-dependent.
- Sacrificing HF accuracy **will not catch the emulator**.

Results

$^{40}\mathrm{Ca}(p,p)$

- 10% error bars
- Similar agreement with true values
- Similar speedup



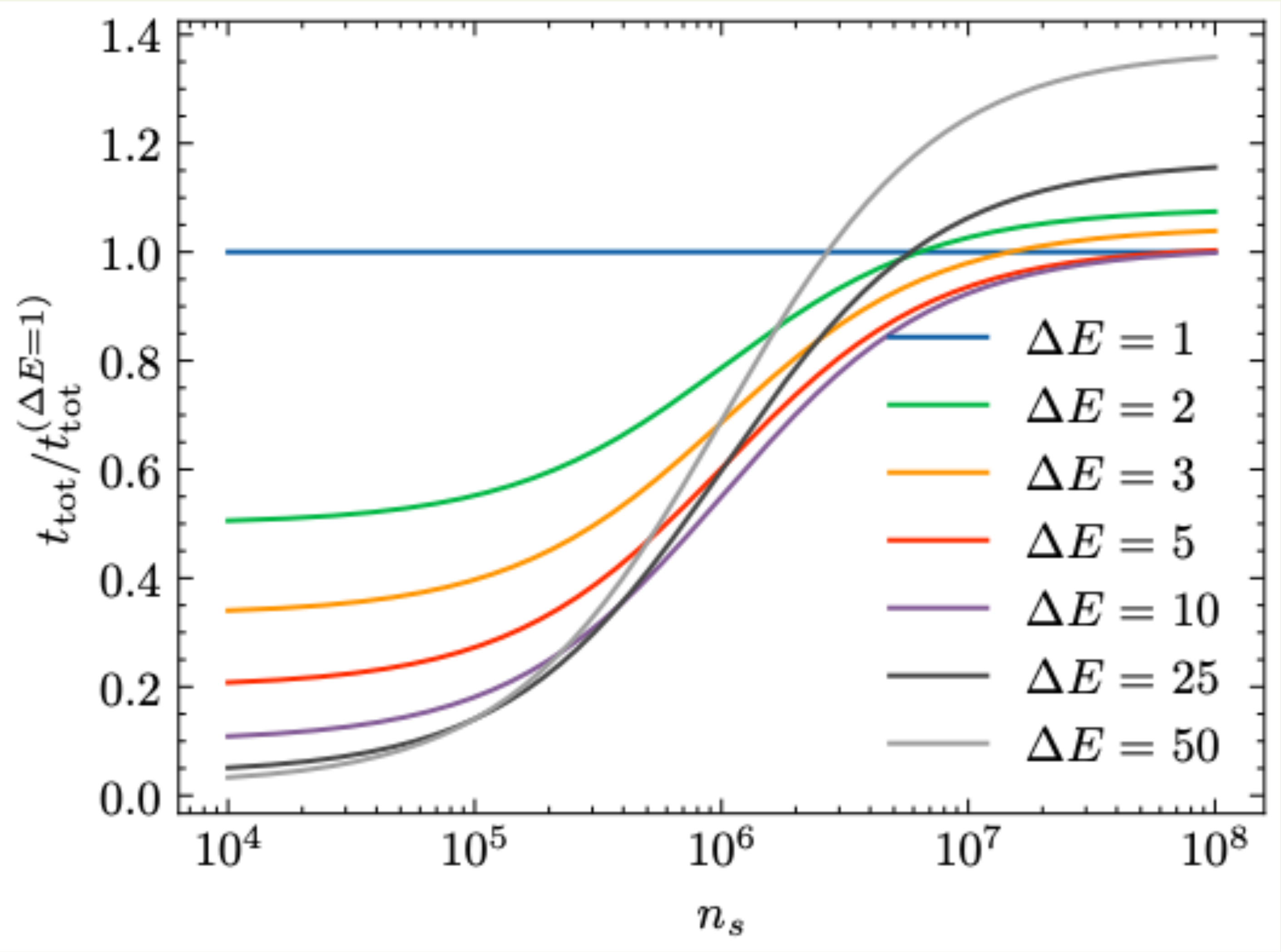


Energy Emulation

Cost

- neutrons-only (for now)
- $E = [5, 55]$ MeV
- Energy emulation *reduces* offline time, *increases* online time.
- Gain depends on n_s. Winner(n_s)
- E emulation allows you to evaluate at different E
  .
- $\Delta E = 50$ is *much* smaller
  - $\mathcal{O}(10^2)$ MB

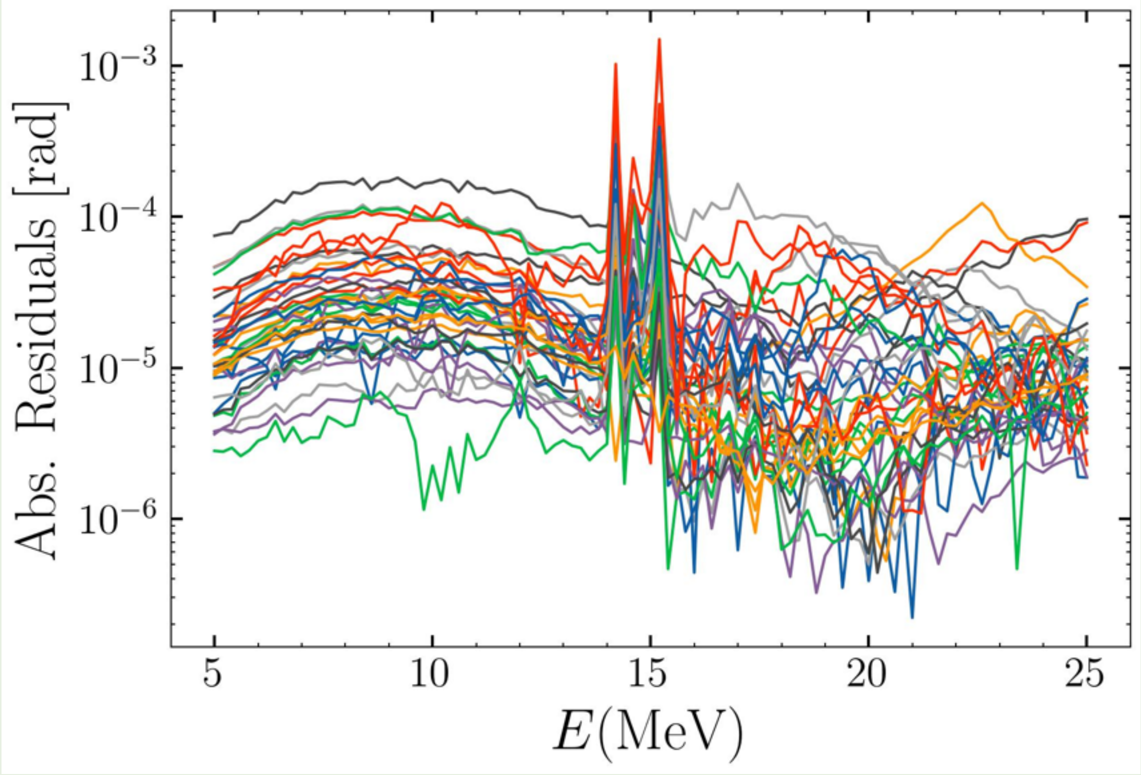
Maximum Energy-Optimized Window (MEOW?) Plot

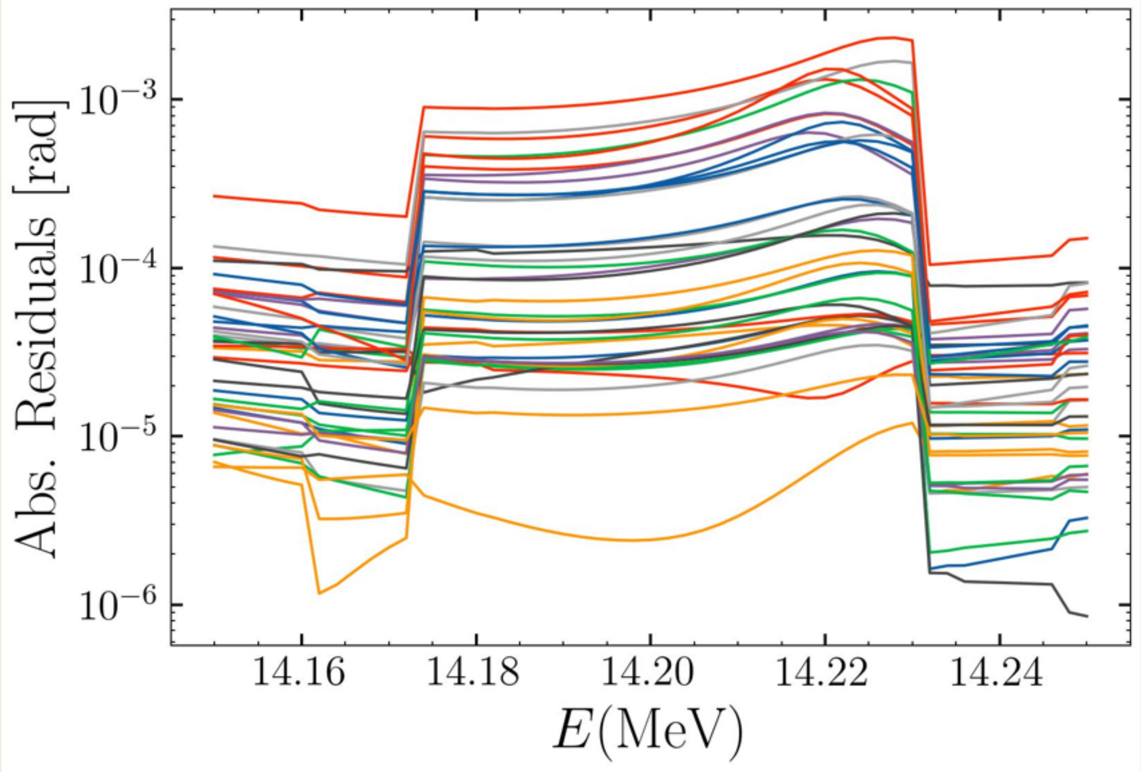


Anomalies

Manuel Catacora-Rios

- See Drischler et al. PLB 823, 136777 (2021).
- Local maxima, not singularities.





Summary

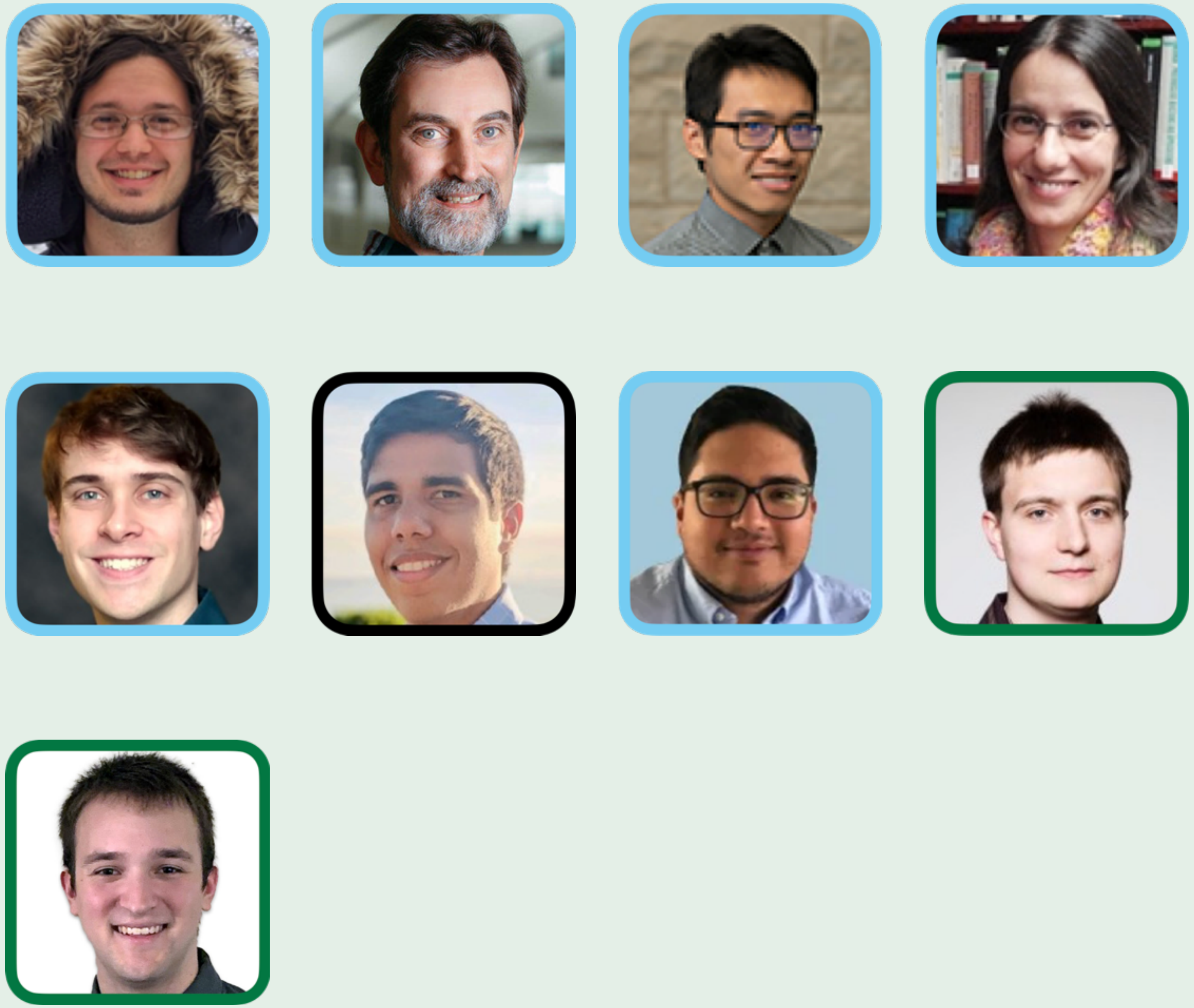
RBM treatment of 2-body scattering produces fast & accurate™, anomaly-free* (MCR) emulators.

github.com/odell/rose

github.com/bandframework/bandframework

Future

- E emulation with Coulomb
  - works below threshold (AB)
- nonlocal potentials
- 3-body scattering (💵): $T = tP + tPG_0T$



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