Reduced Order Scattering Emulator

Kyle A Beyer

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U.S. DEPARTMENT OF ENERGY | Office of Science

BAND Bayesian Analysis of Nuclear Dynamics

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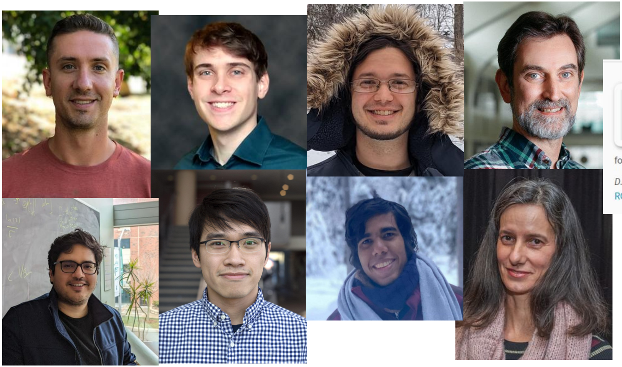
Few Body Reactions Group

ROSE team



ROSE: A reduced-order scattering emulator for optical models

D. Odell,[1,*] P. Giuliani,[2,3,†] K. Beyer,[4,‡] M. Catacora-Rios,[2,5] M. Y.-H. Chan,[6,§] E. Bonilla,[7,¶] R. J. Furnstahl,[8,**] K. Godbey,[2,††] and F. M. Nunes[2,5,‡‡]

Phys. Rev. C **109**, 044612 – **(2024)**

ROSE

The Reduced Order Scattering Emulator (ROSE) is a Python package for building emulators using reduced basis methods for calculating nuclear scattering observables for user-defined interactions, including optical potentials.

D. Odell, P. Giuliani, K. Godbey, K. Beyer, M. Y.-H. Chan

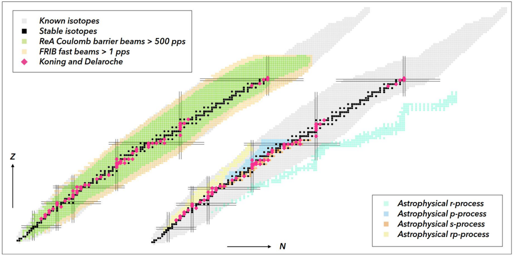
ROSE Github

https://github.com/bandframework/rose

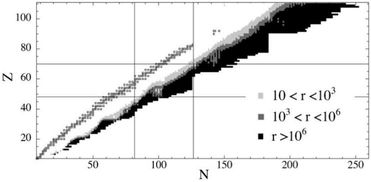
https://pypi.org/project/nuclear-rose/

Outline

We need uncertainty quantified reaction models away from β-stability

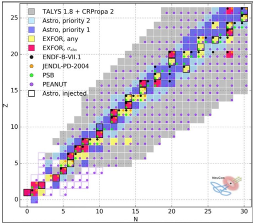


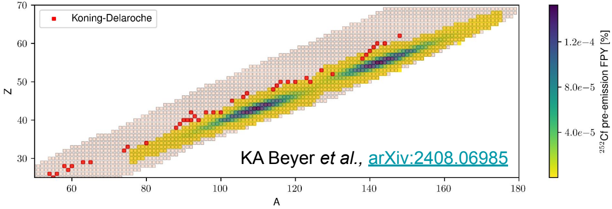
C Hebborn *et al., J. Phys. G: Nucl. Part. Phys.* **50** 060501 (2023)



Goriely & Delaroche, *PLB* 653 178–183 (2007)

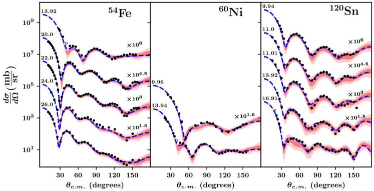
D Boncioli *et al., Sci. Rep.* 7, 4882 (2017)



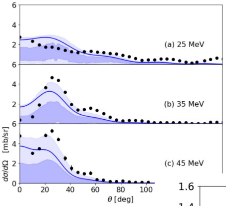


KA Beyer *et al.*, arXiv:2408.06985

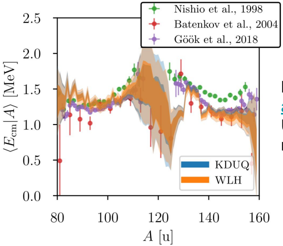
Uncertainty quantification of reaction models



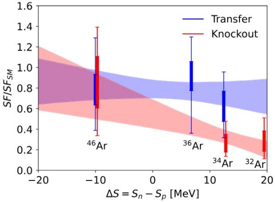
CD Pruitt et al., PRC 107, 014602 (2023)
UQ'ed global optical potential



AJ Smith et al.,
[arXiv:2403.18629](https://arxiv.org/abs/2403.18629)
UQ'ed quasielastic (p,n) cross sections



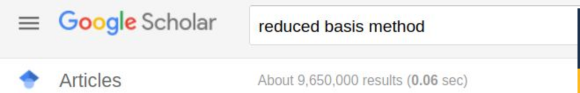
KA Beyer et al.,
[arXiv:2408.06985](https://arxiv.org/abs/2408.06985)
UQ'ed prompt fission neutron spectra

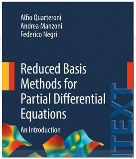


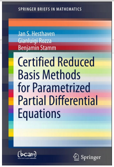
C. Hebborn et al., PRL 131, 212503 (2023)
UQ'ed spectroscopic factors

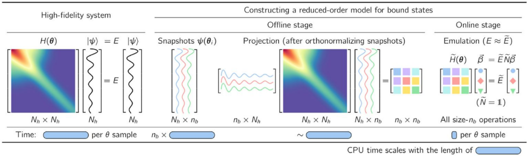
This becomes computationally expensive!

The reduced basis method





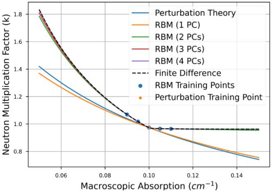




BUQEYE guide to projection-based emulators in nuclear physics

C. Drischler[1,2]*, J. A. Melendez[3], R. J. Furnstahl[3], A. J. Garcia[3] and Xilin Zhang[2]

https://dr.ascsn.net/landing.html



Fast Emulation of the Neutron Diffusion Equation using the Reduced Basis Method

Patrick A. Myers, Connor C. Craig, Kyle Beyer, and Brian C. Kiedrowski

The reduced basis method for reactions

Problem:

- We would like to find a reduced order model for the dimensionless ($s = kr$), parametric system

$$F_{\alpha}[u(s)] = \left(-\frac{d^2}{ds^2} + \frac{l(l+1)}{s^2} + \frac{2\eta}{s} + U(s;\boldsymbol{\alpha}) - 1\right)u(s;\boldsymbol{\alpha}) = 0,$$

with

$$U(s;\boldsymbol{\alpha}) = V(s/k;\boldsymbol{\alpha})2\mu/\hbar^2 k^2,$$

and

$$u(s;\boldsymbol{\alpha}) \rightarrow \frac{i}{2}\left[H_l^-(s,\eta) - S_{\alpha}\, H_l^+(s,\eta)\right]$$

- parameters of interest include

$$\boldsymbol{\alpha} = \{E, V_v, W_v, R_v, a_v, \ldots\}$$

The reduced basis method for reactions

Offline stage:

1. **train**: generate N high-fidelity solutions $\{u_i(s,\alpha_i)\}$ at a training set of parameters $\{\alpha_i\}_{i=0}^{N}$
2. **compress** training snapshots using principal component analysis (PCA)

$$\{u_k\}_{k=1}^{n_u} = \text{PCA}\left[\{u(s,\alpha_m) - u_0(s)\}_{m=1}^{N}\right].$$

3. **project** F_α onto the principal components

$$\langle\psi_j|F_\alpha[\hat{u}]\rangle = \langle\psi_j|F_\alpha|u_0\rangle + \sum_{k=1}^{n_u} a_k\langle\psi_j|F_\alpha|u_k\rangle = 0 \tag{1}$$

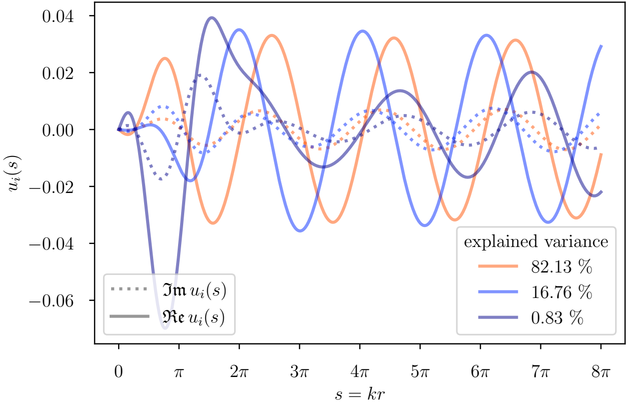
Online stage:

1. **solve** $n_u \times n_u$ reduced system

$$\mathbf{M}(\alpha)\mathbf{a} = \mathbf{c}(\alpha)$$

$$M_{jk} = \langle\psi_j|F_\alpha|u_k\rangle = \int \psi_j^\dagger(s)F_\alpha u_k(s)ds,$$

$$c_j = -\langle\psi_j|F_\alpha|u_0\rangle = -\int \psi_j^\dagger(s)F_\alpha u_0(s)ds.$$



Reduced basis for the S-wave scattering of ^{27}Al(p, p) at 28 MeV. Training space constructed by sampling within $\pm 50\%$ around default Koning-Delaroche parameters

The empirical interpolation method

- we have to be able to pre-compute $\left\langle \psi_j^\dagger \,\middle|\, F_{\boldsymbol{\alpha}} \,\middle|\, u_k(s;\boldsymbol{\alpha}) \right\rangle$
- this is not possible unless F is *affine* in $\boldsymbol{\alpha}$, which is not the case for R_i, a_i in the Woods-Saxon form factor
- so, we make an approximate affine decomposition:

$$U(s,\boldsymbol{\alpha}) \approx \widehat{U}(s,\boldsymbol{\alpha}) = \sum_{i=1}^{n_{EIM}} b_i(\boldsymbol{\alpha}) U_i(s).$$

- we again construct a training space offline and reduce with PCA:

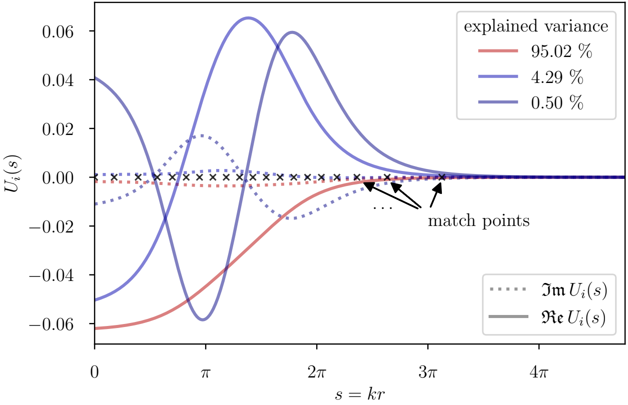
$$\{U_i(s)\}_{i=1}^{n_{EIM}} = \mathrm{PCA}\left[\{U(s,\boldsymbol{\alpha}_m)\}_{m=1}^{N}\right].$$

- we enforce the condition that this decomposition interpolates $U(s,\boldsymbol{\alpha})$, where we choose s_j using a greedy algorithm

$$U(s_j,\boldsymbol{\alpha}) - \sum_{i=1}^{n_{EIM}} b_i(\boldsymbol{\alpha}) U_i(s_j) = 0, \quad \text{for } j \in [1, n_{EIM}].$$

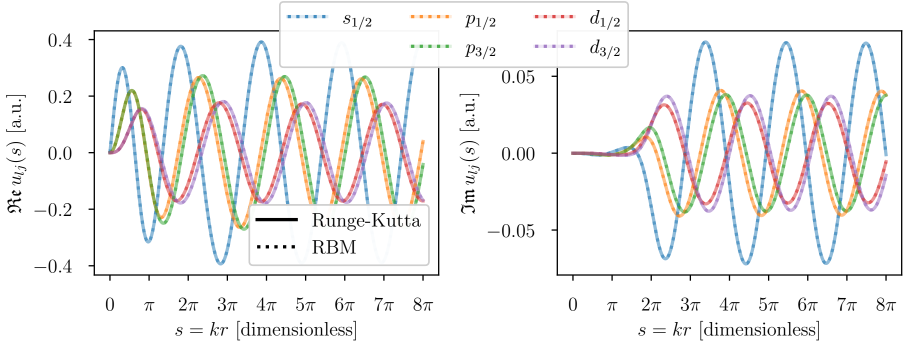
- online, we find the $\mathbf{b}$ by an $n_{EIM} \times n_{EIM}$ matrix multiplication

$$F_{\boldsymbol{\alpha}} \approx \widehat{F}_{\boldsymbol{\alpha}} = F^{(0)} + \sum_{i=1}^{n_{EIM}} b_i(\boldsymbol{\alpha}) F^{(i)},$$



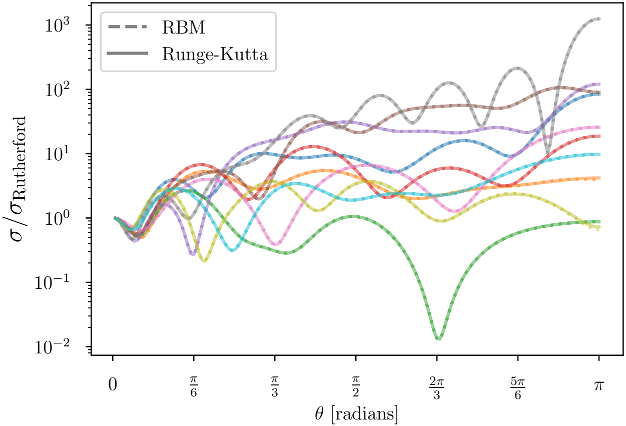
EIM affine decomposition terms for the S-wave scattering of ^{27}Al(p, p) at 28 MeV

RBM results for a local potential



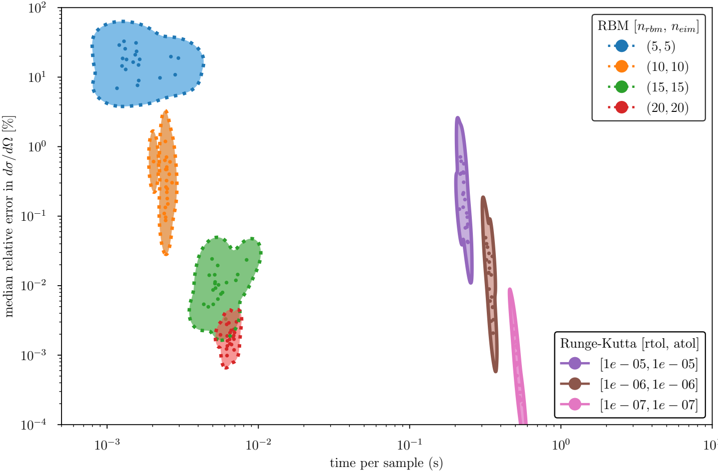
^{27}Al(p,p) at 28 MeV

RBM results for a local potential



^{27}Al(p, p) at 28 MeV

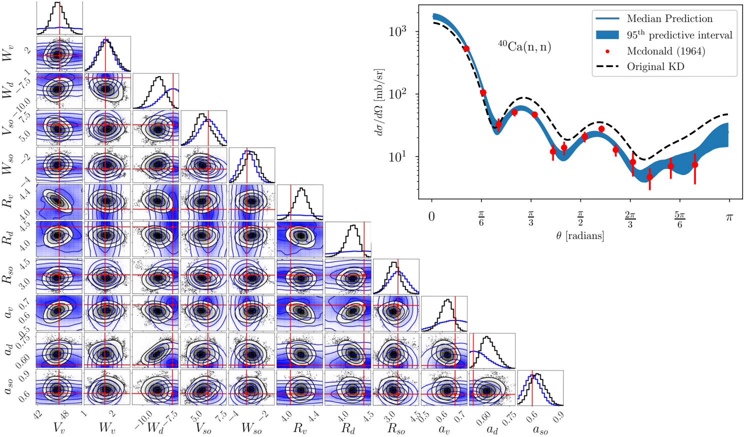
Computational accuracy vs. time



$^{40}\text{Ca}(n, n)$ at 14.1 MeV

Now we can do Bayesian UQ for local optical potentials fast!

800,000 samples in $\sim$ 1 hour



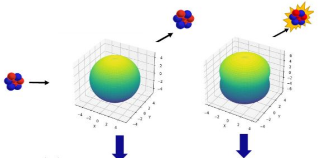
The ROSE software package

All these figures are adapted from the tutorials included in the package!

Features:

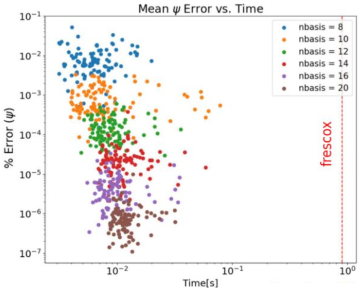
- object oriented Python library
- accepts arbitrary parametric interaction (KDUQ and WLH built in)
- easy convergence and diagnostic of emulator (CAT analysis)
- tutorial demonstrating coupling to Surmise for Bayesian calibration
- testing and continuous integration with `pytest` and github actions
- `https://reduced-order-scattering-emulator.readthedocs.io`
- `pip install nuclear-rose`

Extending ROSE to coupled-channels



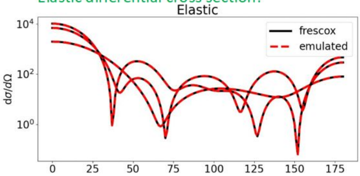
$$\Psi^{\text{tot}} = a_1\phi_1(\xi)\psi_1(R) + a_2\phi_2(\xi)\psi_2(R)$$

*Elastic channel *Inelastic channel

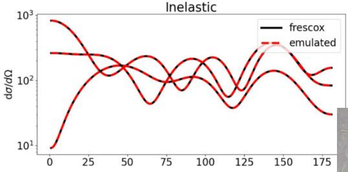


15 RBM basis ^{12}C(n,n') ^{12}C (2^+)@ 10 MeV

Elastic differential cross section:



Inelastic differential cross section:



Developing parametric software

Software paradigms for scientific UQ

	monolithic	modular
plug right into UQ framework	✗	✓
compute only what you need	✗	✓
swap out components for 3^{rd} party libs	✗	✓
fast	✓	up to you

We have the technology. We have the capability to make a modular production-ready library for reaction model UQ. Better... stronger... faster.

Introducing the just-in-time R-Matrix (`jitR`)

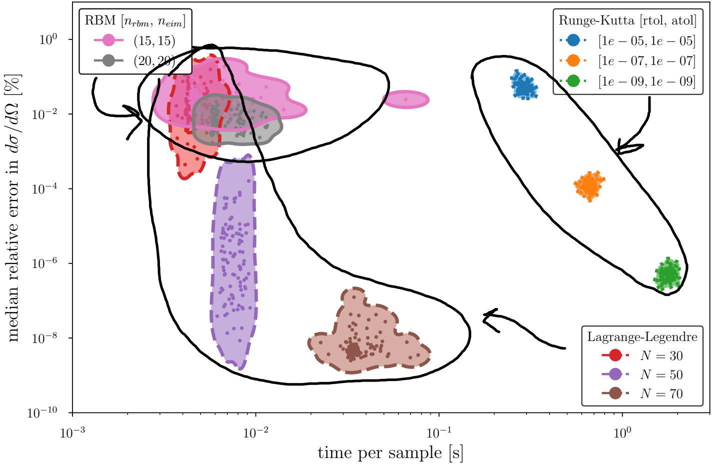
`github.com/beykyle/jitr`

- Lagrange mesh method [Baye, 2015]
- coupled channels
- non-local potentials
- reaction observables with calculable R-Matrix [Descouvemont, 2016]

Why is it so cool?

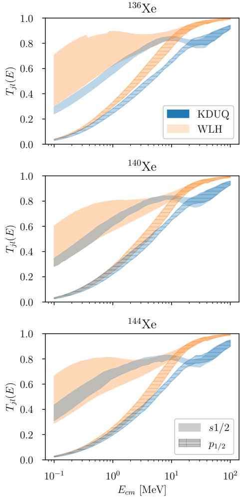
- highly modular - options to precompute most things
- functionality for computing observables
- seamless interoperability with Python stats libraries
- unit testing and continuous integration
- `numba` just-in-time compilation
- heavy use of `numpy`, `scipy`
- core solver functionality only $\sim$750 LOC

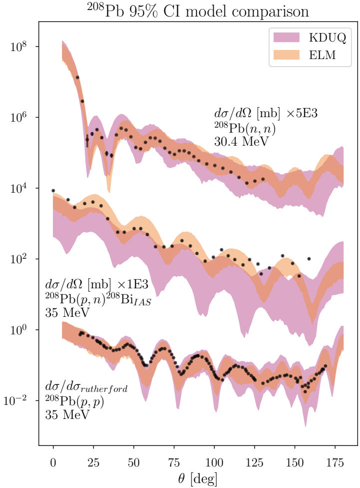
jitR is as fast as an emulator!



Some applications of `jitR`

UQ of transmission coefficients for *n*-evaporation from fission fragments





Global optical potential using quasielastic (p, n)

Summary and path forward

Summary

- RBM-based emulators make UQ of reaction observables more tractable
- ROSE is easy to install and use
- Many advantages to building software from the beginning with UQ in mind

Future work

- pull coupled channels RBM into ROSE
- more Bayesian optical potentials
- apply RBM to continuum-discretized coupled channels for breakup

Thank you for your time!

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References I

Baye, D. (2015).
The lagrange-mesh method.
Physics reports, 565:1–107.

Constantine, P. G., Dow, E., and Wang, Q. (2014).
Active subspace methods in theory and practice: applications to kriging surfaces.
SIAM Journal on Scientific Computing, 36(4):A1500–A1524.

Descouvemont, P. (2016).
An r-matrix package for coupled-channel problems in nuclear physics.
Computer physics communications, 200:199–219.

Pruitt, C., Escher, J., and Rahman, R. (2023).
Uncertainty-quantified phenomenological optical potentials for single-nucleon scattering.
Physical Review C, 107(1):014602.

Sowiński, T. and Garcia-March, M. A. (2022).
Fundamental limitations of the eigenvalue continuation approach.
Physical Review C, 106(2):024002.

Acronyms I

DOM	dispersive optical model
OMP	optical model potential
DSE	dispersive self-energy
RBM	reduced basis method
EIM	empirical interpolation method
PC	principal component
POD	proper orthogonal decomposition
MCMC	Markov-chain Monte Carlo
`ROSE`	Reduced Order Scattering Emulator
`jitR`	just-in-time R-Matrix

What can we precompute and reuse between parametric solves?

- free matrix
- ℓ-independent parts of interaction matrix
- basis functions evaluated at channel radius
- Coulomb functions evaluated at channel radius
- kinematic variables
- compare to: TOMFOOL [Pruitt et al., 2023]

Extending to global optical potentials

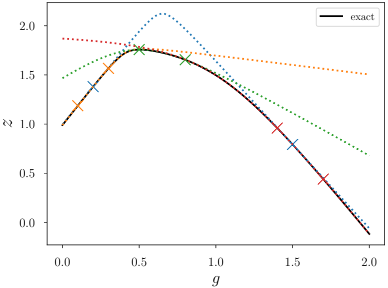
- global potentials we have ($\sim$ 40) sub-parameters $\boldsymbol{\omega}$

$$\boldsymbol{\alpha} = f(A, Z, E, \boldsymbol{\omega}).$$

- the RBM makes a locally-linear tangent space in $\boldsymbol{\alpha}$-space
- when the full manifold is nonlinear, nearby tangent patches may have non-negligible orthogonal components
- toy example adapted rom [Sowiński and Garcia-March, 2022]

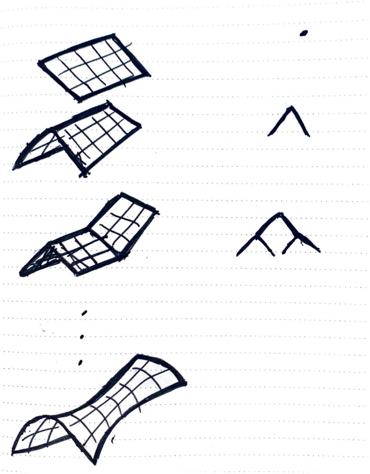
$$(H - z) = 0$$

$$H = \begin{bmatrix} 1.0 & 0.1 & 0.0 \\ 0.1 & 2.0 & 0.5 \\ 0.0 & 0.5 & 4.0 \end{bmatrix} + g \begin{bmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$



Making a quilt: a meshless local reduced basis method

- sample subset of training space to be tangent points
- store in KD-tree
- construct local RBM from neighborhood around each tangent point
- learns the *local* dimensions describing the manifold in each tangent patch, stitches them together into a full "quilt"



The active subspace quilting (ASQ) method I

- **Problem:** there is no guarantee that nearby points in α-space have similar solutions
- **Solution:** define a new metric for distance, that in the *Active Subspace* [Constantine et al., 2014]

- define functional $\mathcal{F}$:

$$\mathcal{F}_{\boldsymbol{\alpha}}\left[u(s;\boldsymbol{\alpha})\right] \equiv \langle \psi_j | F_{\boldsymbol{\alpha}}[u(s;\boldsymbol{\alpha})] \rangle \,.$$

- functional derivative of $\mathcal{F}$ in $\boldsymbol{\alpha}$-space:

$$\left(\nabla_{\boldsymbol{\alpha}} \cdot \hat{\boldsymbol{\alpha}}\right) \mathcal{F}_{\boldsymbol{\alpha}}\left[u(s,\boldsymbol{\alpha})\right] = \lim_{\delta \to 0} \frac{\mathcal{F}_{\boldsymbol{\alpha}}\left[u(s,\boldsymbol{\alpha}+\delta\hat{\boldsymbol{\alpha}})\right] - \mathcal{F}_{\boldsymbol{\alpha}}\left[u(s,\boldsymbol{\alpha})\right]}{\delta}$$

- numerator reduces to matrix element of difference between potentials

$$\begin{aligned}\mathcal{F}_{\boldsymbol{\alpha}}\left[u(s;\boldsymbol{\alpha}')\right] &= \left\langle u^{\dagger}(s;\boldsymbol{\alpha}') \,\middle|\, \left(-\frac{d^2}{ds^2} + \frac{l(l+1)}{s^2} + \frac{2\eta}{s} + U(s;\boldsymbol{\alpha}) - 1\right) \,\middle|\, u(s;\boldsymbol{\alpha}')\right\rangle \\ &= \left\langle u^{\dagger}(s;\boldsymbol{\alpha}') \,\middle|\, U(s;\boldsymbol{\alpha}) - U(s;\boldsymbol{\alpha}') \,\middle|\, u(s;\boldsymbol{\alpha}')\right\rangle\end{aligned}$$

The active subspace quilting (ASQ) method II

- singular value decomposition of samples of $(\nabla_{\boldsymbol{\alpha}} \cdot \hat{\boldsymbol{\alpha}})\, \mathcal{F}_{\boldsymbol{\alpha}}\left[u(s,\boldsymbol{\alpha})\right]$:

$$\mathbf{U} \begin{bmatrix} \ddots & & \\ & s_i & \\ & & \ddots \end{bmatrix} \mathbf{V}^T = \begin{bmatrix} \cdots & \begin{array}{c} | \\ (\nabla_{\boldsymbol{\alpha}} \mathcal{F})_i \\ | \end{array} & \cdots \end{bmatrix}$$

  where s_i are the singular values.

- define the $m \times m$ transformation matrix:

$$\tilde{\ } \equiv \mathbf{U} \begin{bmatrix} \ddots & & \\ & s_i & \\ & & \ddots \end{bmatrix}.$$

- this defines a new metric for distance in $\boldsymbol{\alpha}$-space

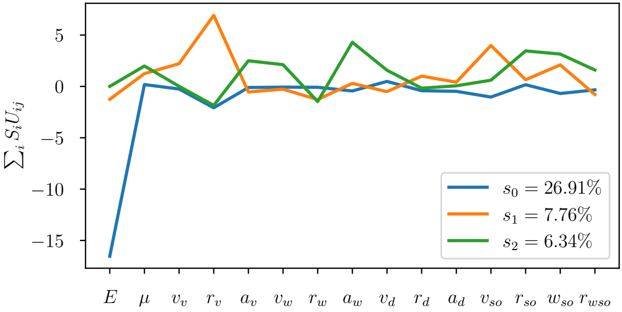
$$|\boldsymbol{\alpha}_i - \boldsymbol{\alpha}_j|^2_{AS} \equiv (\boldsymbol{\alpha}_i - \boldsymbol{\alpha}_j)^T \tilde{\ }^T \tilde{\ } (\boldsymbol{\alpha}_i - \boldsymbol{\alpha}_j).$$

- this metric can easily be implemented for a KD-tree, resulting in nearby points having similar matrix elements $\mathcal{F}$

Preliminary results for the active subspace quilting

Test problem:

- train on 46 isotopes in fission fragments region
- $E \in [0.1, 10]$ MeV
- 1000 training points, 200 tangent points



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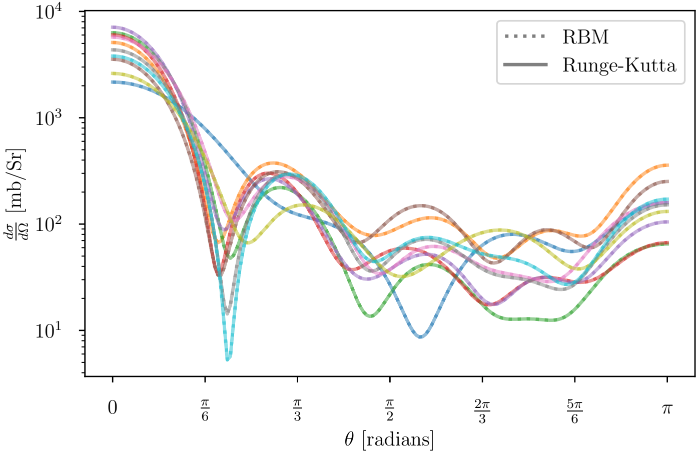

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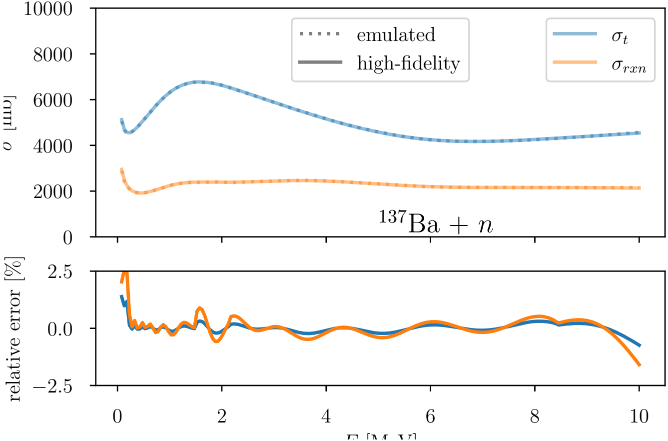

Future work extending the reduced basis method (RBM) to global potentials

problems:

- sensitivity to location of tangent points
- too many tangent points defeats the purpose

applications:

- choose tangent points using greedy algorithm
- Monte Carlo Hauser-Feshbach in `CGMF` with UQ
- put trained online emulator on the internet: BREX?