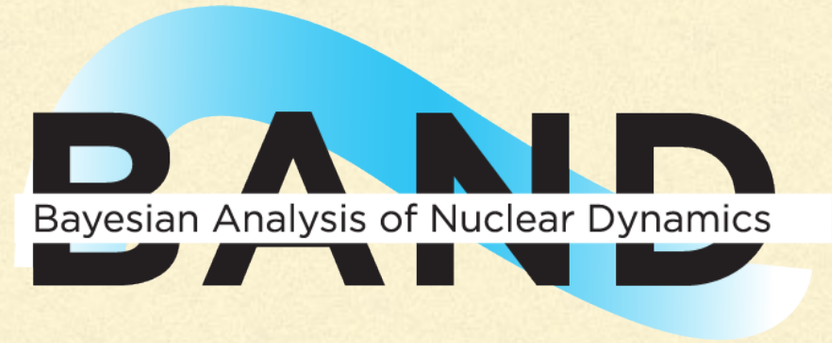
The Bayesian Analysis of Nuclear Dynamics CI Framework

https://bandframework.github.io/



Daniel Phillips, Ohio University

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Outline

- Why?
- Who?
- How?
- What?
- When?

Why? Nuclear Science motivation

Model uncertainty limits our predictions in key problems:

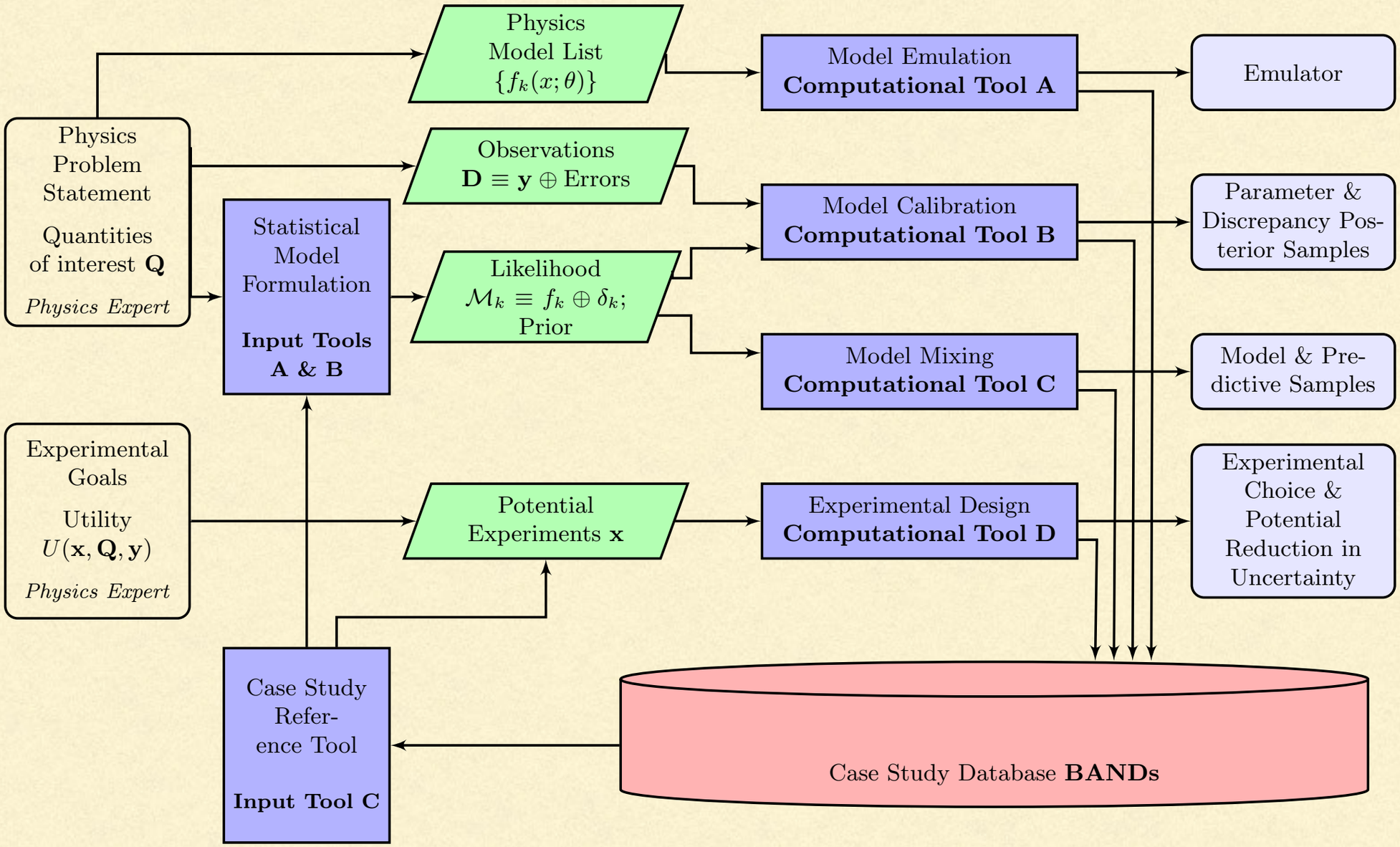
- Neutrinoless double beta decay
- r-process: extrapolation to the dripline and beyond → other nuclear-structure issues
- Heavy-ion Collisions: energy deposition; pre-hydrodynamic stage; conversion of hydrodynamic output to final-state particles
- Different approaches to reaction dynamics → nuclear data
- Experimental planning

Goal is to build framework that is *generally useful* for full (including model) UQ in nuclear physics and provide examples of its use

The Framework

https://bandframework.github.io/

Goal: *Facilitate principled Uncertainty Quantification in Nuclear Physics*



Who: Senior Investigators

- Indiana University: Matt Pratola, statistics
- Miami University: Özge Sürer, statistics
- Michigan State University: Filomena Nunes (co-PI), Witek Nazarewicz, Scott Pratt, nuclear theory
- Northwestern University: Stefan Wild (co-PI), computational science & applied mathematics
- Ohio State University: Dick Furnstahl (co-PI), Uli Heinz, nuclear theory
- Ohio University: Daniel Phillips (PI), nuclear theory
- Rice University: Frederi Viens (co-PI), statistics

Researchers and graduate students

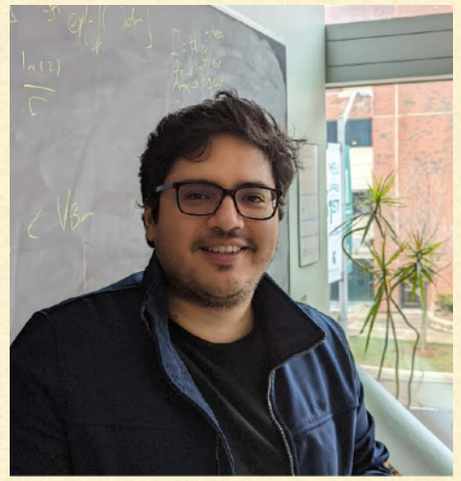
Kyle Beyer

Moses Chan

Kyle Godbey

Sunil Jaiswal

Jared O'Neal



Manuel Catacora Rios

plus five other graduate students who did Ph.D. projects with BAND and have now graduated

How?

BAND Manifesto: J. Phys. G **48**, 072001 (2021)

https://iopscience.iop.org/article/10.1088/1361-6471/abf1df

IOP Publishing Journal of Physics G: Nuclear and Particle Physics

J. Phys. G: Nucl. Part. Phys. **48** (2021) 072001 (39pp) https://doi.org/10.1088/1361-6471/abf1df

Guide

Get on the BAND Wagon: a Bayesian framework for quantifying model uncertainties in nuclear dynamics

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CrossMark

Full publication list:

https://bandframework.github.io/publications/

GitHub repo

GitHub repo

bandframework / **bandframework** Public

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Code | Issues 6 | Pull requests 1 | Actions | Security | Insights

main | 9 Branches | 4 Tags | Go to file | Code

wildsm Merge pull request #188 from bandframework/v05release — ac0cb02 · 2 weeks ago — 924 Commits

.github	Update URL checker blacklist in CI workflow	2 weeks ago
BANDsoftware_uses	Modernize Bfrescox tutorial notes for release	2 weeks ago
examples	Minor update to examples/README.md	2 weeks ago
resources	Linking to rose bandsdk	2 weeks ago
software	Update README.md	2 weeks ago
.gitmodules	Added rose via submodule. v1.1.7 already reviewed, see #167	3 weeks ago
AUTHORS	Update AUTHORS	3 weeks ago
CHANGELOG.rst	Link points to release branch instead of develop	2 weeks ago
CODE_OF_CONDUCT.md	Update CODE_OF_CONDUCT.md	3 years ago
CONTRIBUTING.rst	Update CONTRIBUTING.rst	2 years ago
LICENSE	Initial commit	5 years ago
README.md	Update README.md	2 weeks ago

About

This contains the public repository for the BAND framework project.

Readme
BSD-2-Clause license
Code of conduct
Contributing
Activity
Custom properties
29 stars
2 watching
9 forks
Report repository

Releases 4

Release 0.5.0 Latest
2 weeks ago

+ 3 releases

Packages

Presently: v0.5

https://github.com/bandframework/bandframework

BAND Framework v0.5

Bayesian Analysis of Nuclear Dynamics

Software tools:

- † Bfrescox: A Python wrapper for the Frescox reaction code.
- † jitr: A Python package containing a Lagrange mesh R-matrix solver for parametric reaction model calibration.
- LCGP: Gaussian process surrogate model for emulating stochastic outputs.
- parMOO: A Python library for multiobjective simulation optimization
- * PUQ: A Python package for generating for generating experimental designs tailored for UQ
- pybmc: A Python package for performing Bayesian model combination on various predictive models.
- † rose: A reduced-order scattering emulator.
- SmoothEmulator: a simplex sampler, emulator trainer, and MCMC explorer
- * surmise: for model emulation via Gaussian Processes and calibration
- * Taweret: A Python package containing multiple BMM methods

Plus 7 examples of principled Bayesian UQ for nuclear physics problems. E.g.:

- * BRICK: Bayesian R-matrix Inference Code Kit
- BMEX: Bayesian Mass Explorer

surmise

Chan, Sürer, Plumlee, Wild

- surmise provides a surrogate model interface for emulation, calibration, and sensitivity analysis
- Your calibration never has to interact directly with "simulation code"
- Instead you provide training data at a set of input values $\{x_i\}$, and parameter vectors $\{\boldsymbol{\theta}_\alpha\}$ and surmise will construct an emulator
- (Which you should then check against testing data, closure tests, etc.)
- Various emulation capabilities are built into surmise (e.g. PCGP, but also PCGP "with missingness"). You can fork the repo and add your own.
- So far these are "black-box emulators".
- Basic calibration capabilities are also built in
- Tutorial available on Google Colab

Taweret

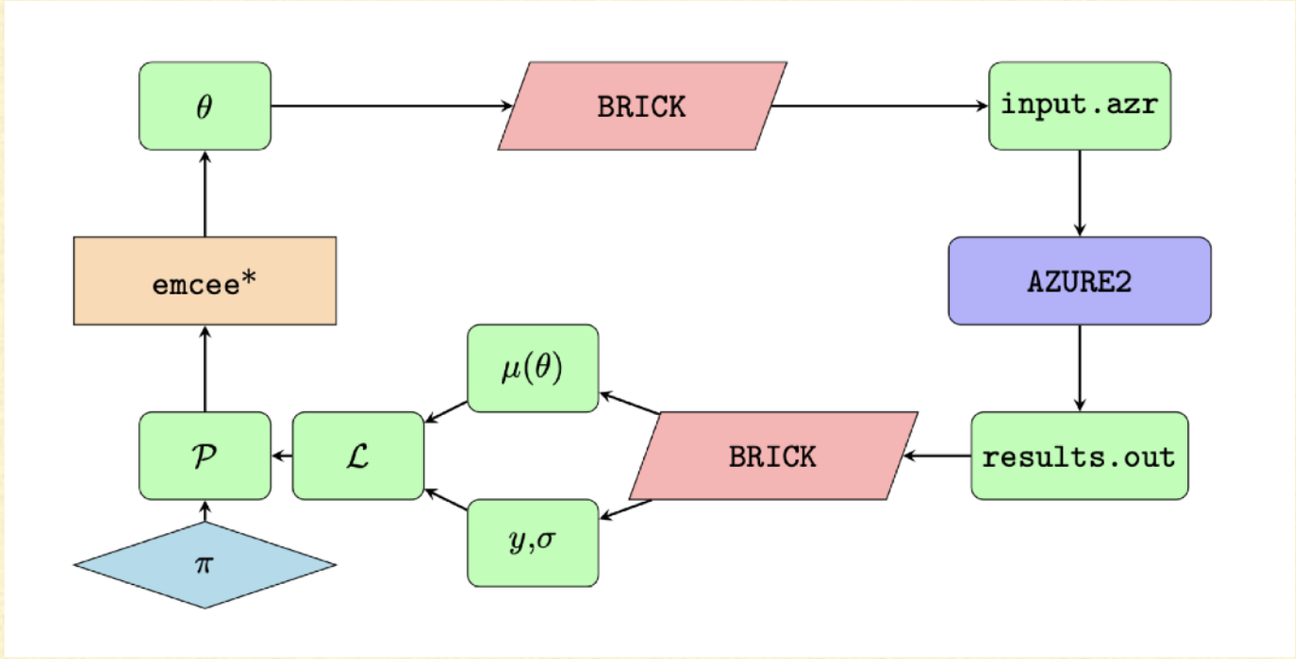
K. Ingles, D. Liyanage, A. Semposki, J. Yannotty,
https://joss.theoj.org/papers/10.21105/joss.06175

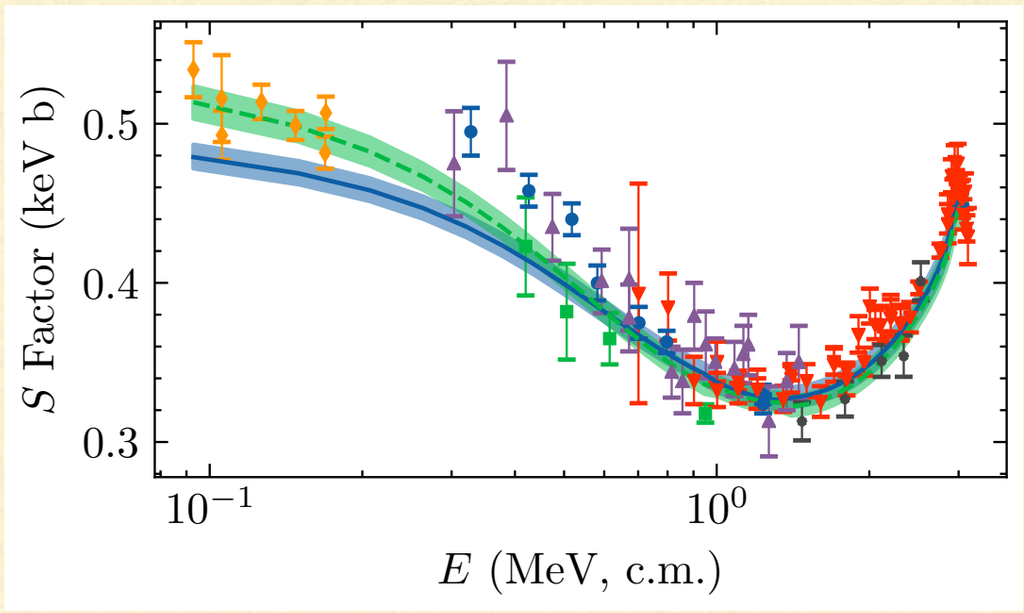
- Generalized Bayesian Model Mixing package
- At present the package implements the following methods:
  - Linear mixing of pdfs of different models
  - Multivariate BMM
  - Bayesian trees
- Designed to be able to mix a variety of models
- Also designed to be extensible to other mixing methods

BRICK

Odell, deBoer, Paneru, Brune, Phillips, Frontiers in Physics (2022)

- Bayesian R-matrix Inference Code Kit
- Main piece is a mediator between AZURE2 and a sampler (emcee originally)
- https://github.com/odell/brick
- Constrain R-matrix parameters from data using emcee, then propagate samples to extrapolate





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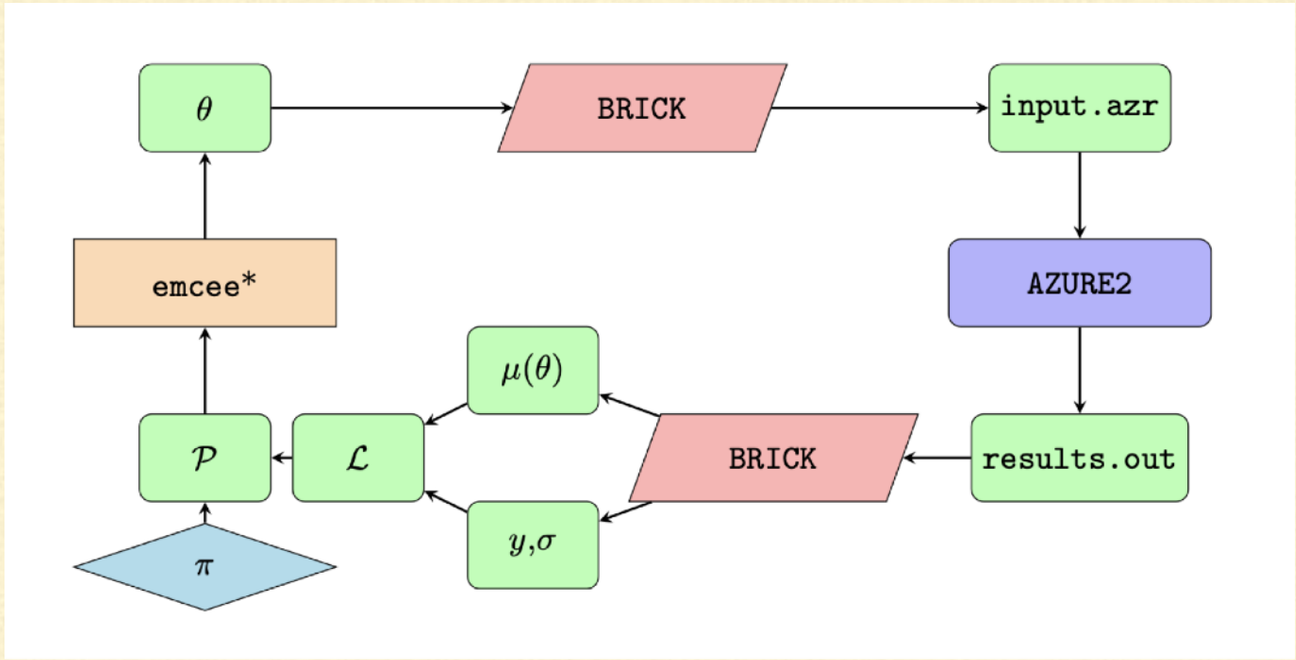
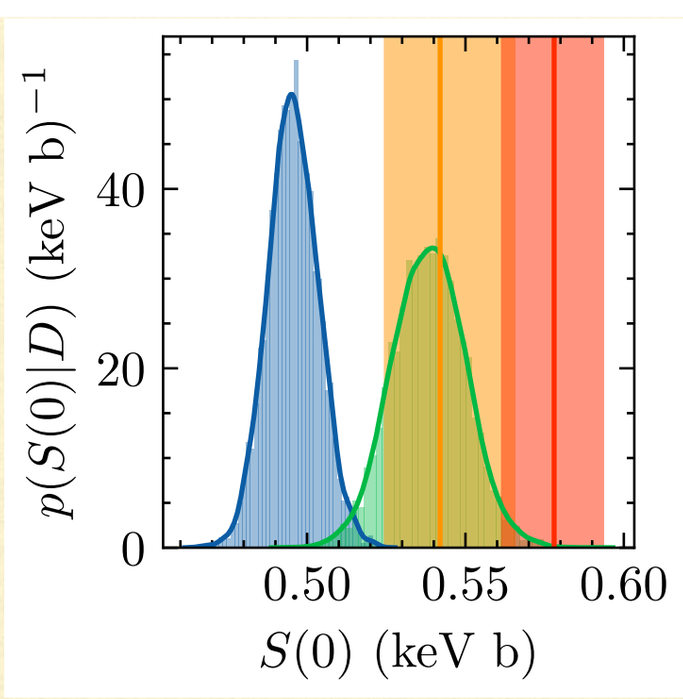




Experimental Design

An example Melendez, Furnstahl, Griesshammer, McGovern, DP, Pratola, Eur. Phys, J. A 57, 81 (2021)

- Encode experimental goal as utility function (design criterion): U(**x**), that is function of "design points" (observables, experimental conditions) **x**.

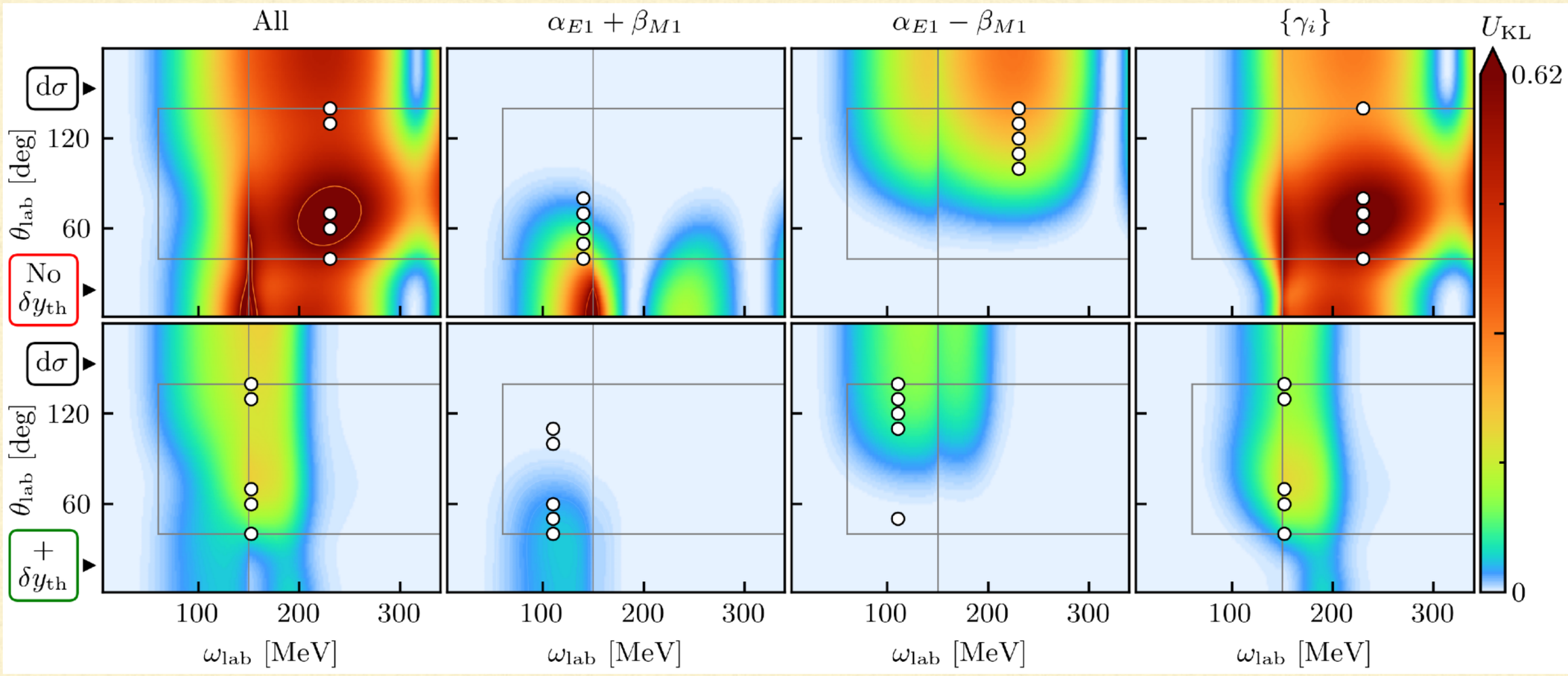
- Seek $\mathbf{x}^*$ that maximizes U(**x**) across space of feasible experimental designs **x**.

  If we choose to assess using gain in Shannon information cf. prior (=KL divergence between prior and posterior for θ) then we have:

$$U_{KL}(\mathbf{x}) = \int \left\{ \ln \left[\frac{\mathrm{pr}(\theta \,|\, \mathbf{y}, \mathbf{x})}{\mathrm{pr}(\theta)} \right] \mathrm{pr}(\theta \,|\, \mathbf{y}, \mathbf{x}) d\theta \right\} \mathrm{pr}(\mathbf{y} \,|\, \mathbf{x}) d\mathbf{y}$$

- Reduces to log of ratio of prior & posterior volumes of parameter hyperellipsoids ("shrinkage") if model $\mathbf{y}(\mathbf{x}; \theta)$ is linear in θ

Compton Scattering Application



- Determine angles at energies and angles for γp scattering experiment that maximize improvement in knowledge of proton (scalar & spin) electromagnetic polarizabilties, or—if one prefers —any subset thereof

Expensive computer experiments using PUQ (Özge Sürer)

When? BAND timeline

- July 2020: beginning of grant from NSF OAC
- December 2020: virtual BAND camp
- December 2021: hybrid BAND camp
- Summer 2022: Release of v0.2
- May 2023: in-person BAND camp prior to ISNET-9 at WUSTL
- Summer 2023: Release of v0.3, including additional model-mixing methods, emulators (ROSE), and additional physics examples, e.g., BMEX
- Summer 2024: Release of v0.4, including computational experimental-design capability and additional physics examples
- Fall 2025: Release of v0.5: includes versions of all software in framework
- Summer 2026: v1.0 release, final publication
- Fall 2026: BAND camp prior to ISNET-12 at UC Berkeley