The Bayesian Analysis of Nuclear Dynamics Cyberinfrastructure Framework

Bayesian Analysis of Nuclear Dynamics

https://bandframework.github.io/

Daniel Phillips
Ohio University

Research funded by the NSF's Office of Advanced Cyberinfrastructure

Outline

- Why?
- Who?
- How?
- What?
  - BAND examples
  - BAND tools
- When?

Why? Nuclear Science motivation

Model uncertainty limits our predictions in key problems:

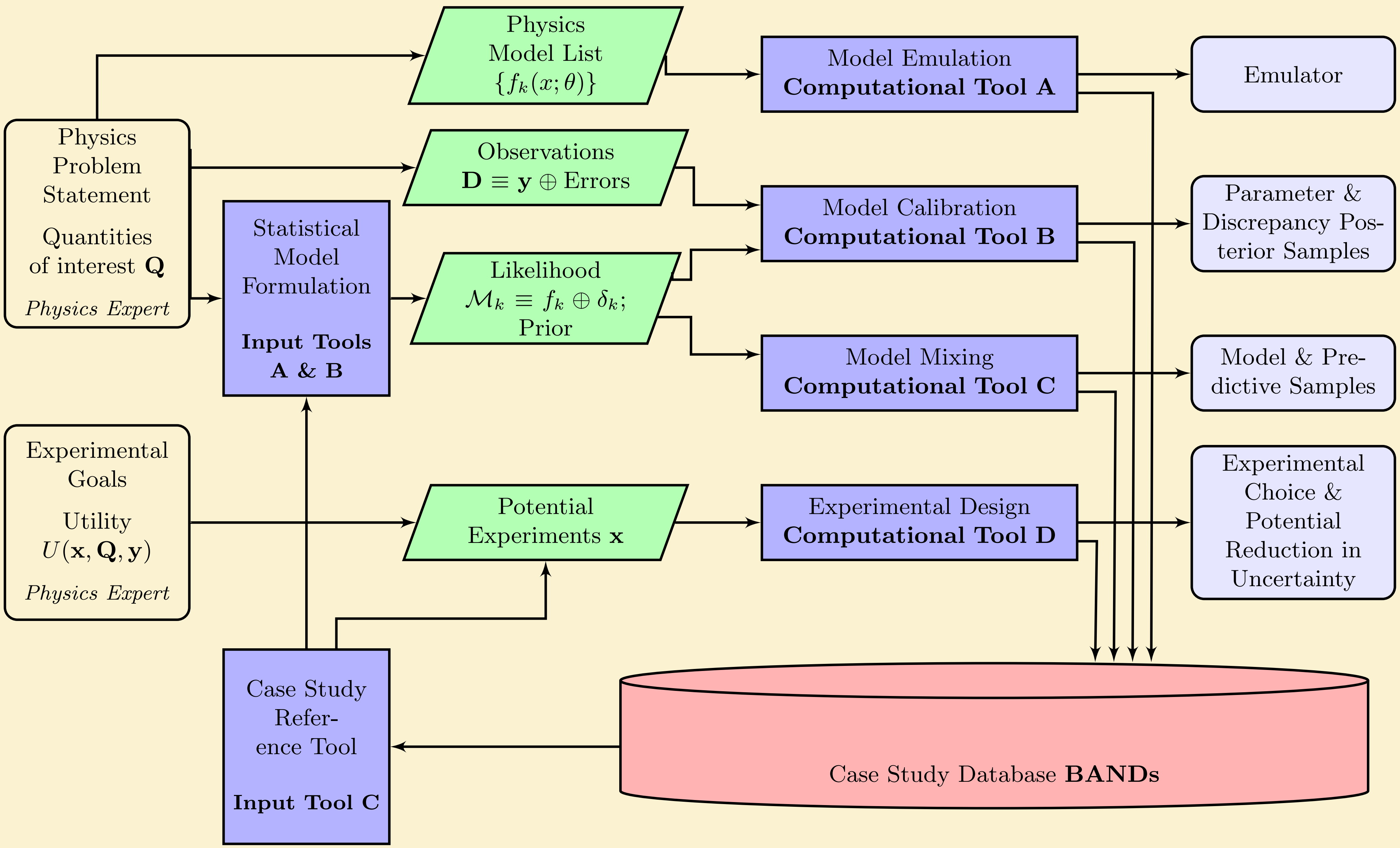
- Neutrinoless double beta decay
- r-process: extrapolation to the dripline and beyond→other nuclear-structure issues
- Heavy-ion Collisions: energy deposition; pre-hydrodynamic stage; conversion of hydrodynamic output to final-state particles
- Different approaches to reaction dynamics→nuclear data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

Researchers and grad students

Moses Chan

Kyle Godbey

Sunil Jaiswal

Jared O'Neal

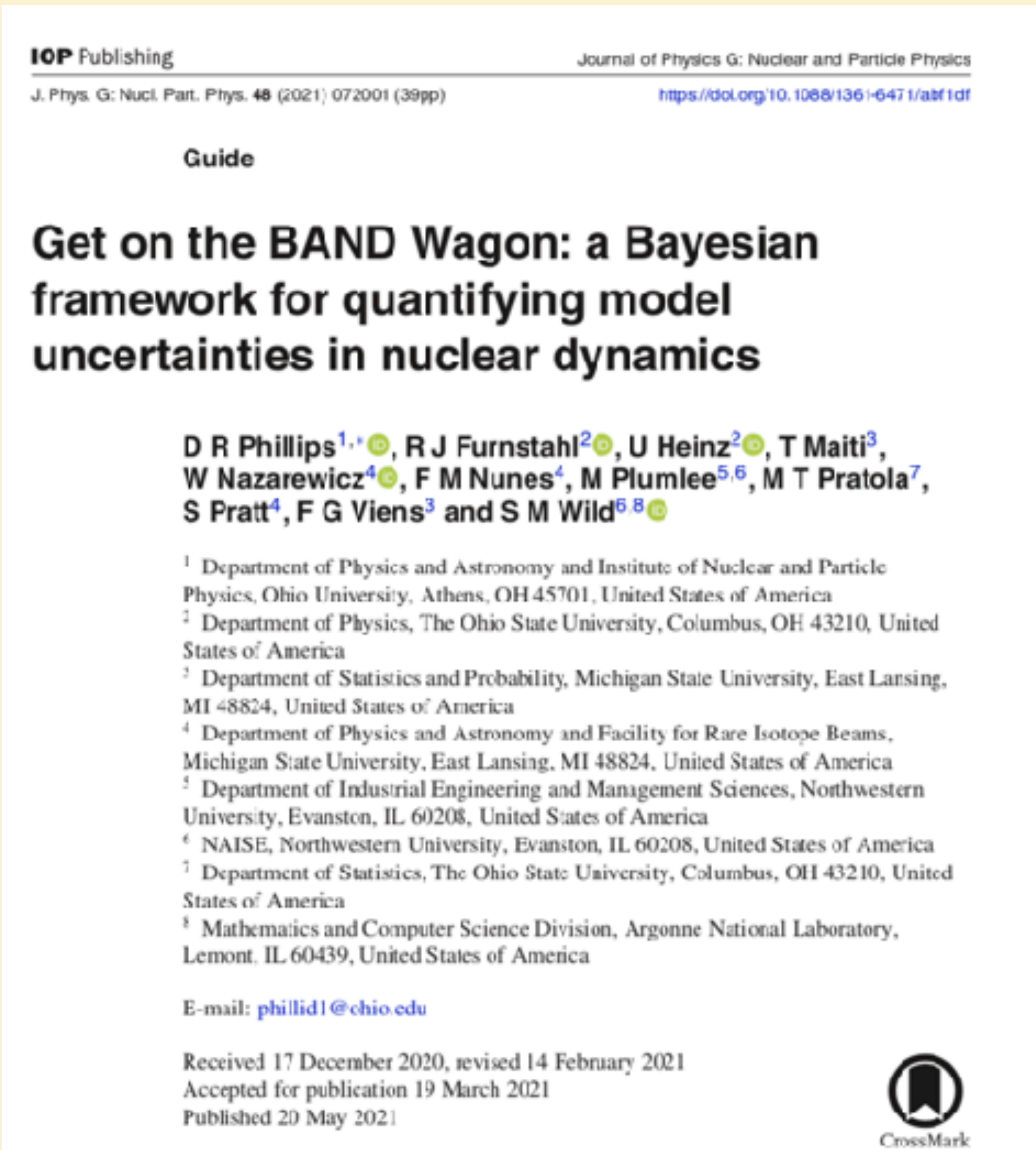
Manuel Catacora-Rios

Alexandra Semposki

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

D R Phillips[1,*], R J Furnstahl[2], U Heinz[2], T Maiti[3], W Nazarewicz[4], F M Nunes[4], M Plumlee[5,6], M T Pratola[7], S Pratt[4], F G Viens[3] and S M Wild[6,8]

[1] Department of Physics and Astronomy and Institute of Nuclear and Particle Physics, Ohio University, Athens, OH 45701, United States of America

[2] Department of Physics, The Ohio State University, Columbus, OH 43210, United States of America

[3] Department of Statistics and Probability, Michigan State University, East Lansing, MI 48824, United States of America

[4] Department of Physics and Astronomy and Facility for Rare Isotope Beams, Michigan State University, East Lansing, MI 48824, United States of America

[5] Department of Industrial Engineering and Management Sciences, Northwestern University, Evanston, IL 60208, United States of America

[6] NAISE, Northwestern University, Evanston, IL 60208, United States of America

[7] Department of Statistics, The Ohio State University, Columbus, OH 43210, United States of America

[8] Mathematics and Computer Science Division, Argonne National Laboratory, Lemont, IL 60439, United States of America

E-mail: phillid1@ohio.edu

Received 17 December 2020, revised 14 February 2021

Accepted for publication 19 March 2021

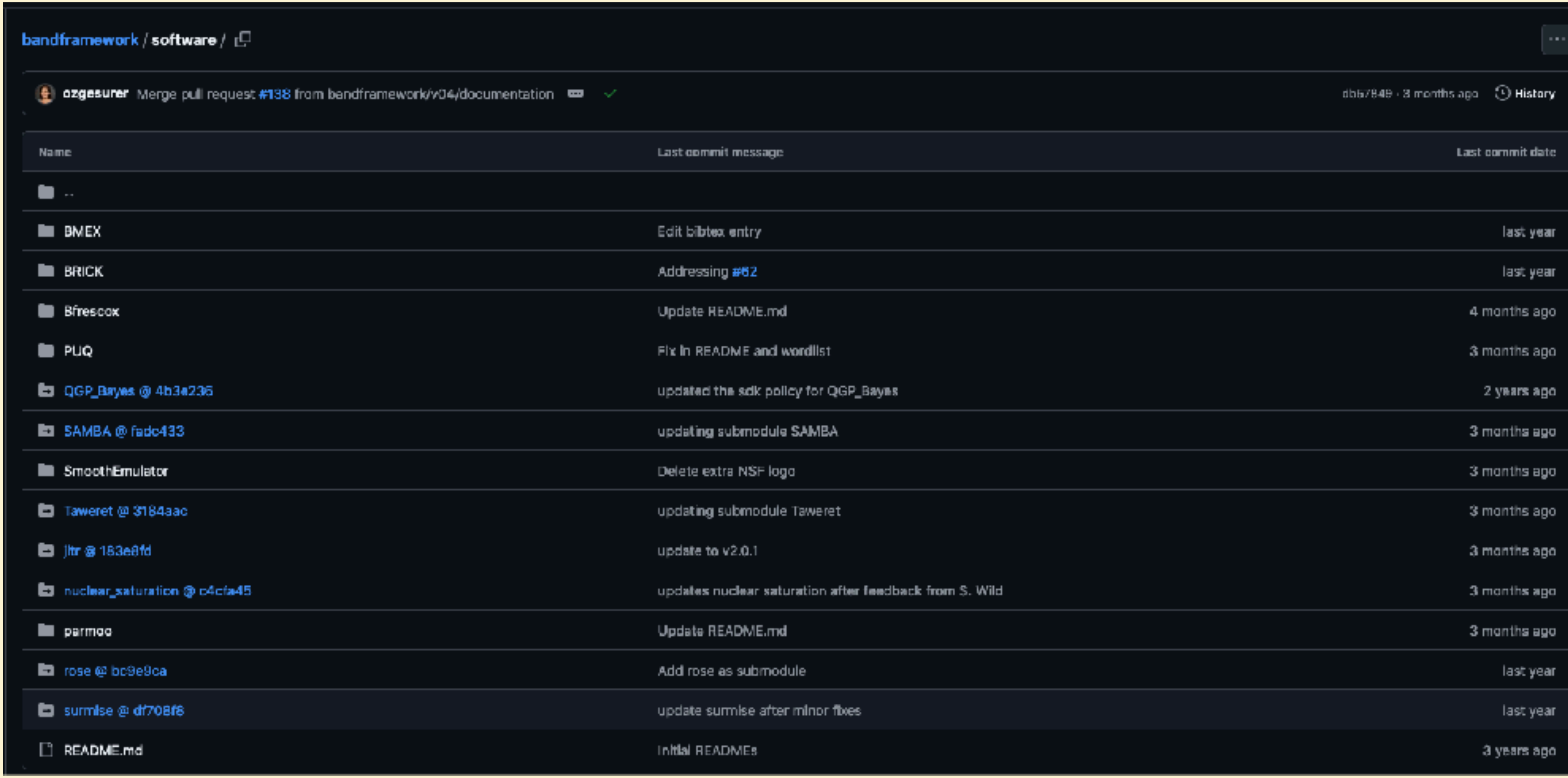
Published 20 May 2021

CrossMark

Full publication list:

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

GitHub repo



bandframework / software /

ozgesurer Merge pull request #138 from bandframework/v04/documentation — db67848 · 3 months ago — History

Name	Last commit message	Last commit date
..		
BMEX	Edit bibtex entry	last year
BRICK	Addressing #62	last year
Bfrescox	Update README.md	4 months ago
PUQ	Fix in README and wordlist	3 months ago
QGP_Bayes @ 4b3a236	updated the sdk policy for QGP_Bayes	2 years ago
SAMBA @ fadc433	updating submodule SAMBA	3 months ago
SmoothEmulator	Delete extra NSF logo	3 months ago
Taweret @ 3184aac	updating submodule Taweret	3 months ago
jitr @ 183e8fd	update to v2.0.1	3 months ago
nuclear_saturation @ c4cfa45	updates nuclear saturation after feedback from S. Wild	3 months ago
parmoo	Update README.md	3 months ago
rose @ bc9e9ca	Add rose as submodule	last year
surmise @ df708f6	update surmise after minor fixes	last year
README.md	Initial READMEs	3 years ago

Presently: v0.4

https://github.com/bandframework/bandframework

BAND Framework v0.4

Now available at https://github.com/bandframework/bandframework

Tools:

- surmise: for model emulation via Gaussian Processes and calibration
- SmoothEmulator: a simplex sampler, emulator trainer, and MCMC explorer
- * rose: A reduced-order scattering emulator
- parMOO: A Python library for multiobjective simulation optimization
- * Taweret: A Python package containing multiple BMM methods
- * PUQ: A Python package for generating experimental design tailored to UQ

Examples:

- * BRICK: Bayesian R-matrix Inference Code Kit
- * BMEX: Bayesian Mass Explorer
- BFRESCOX: Emulation and Bayesian model calibration of coupled-channels treatment of nuclear reactions
- jitr: Lagrange mesh R-matrix solver for reaction-model calibration
- nsat: Bayesian mixture model approach to calibrating saturation

BMEX

Buskirk, Godbey, Nazarewicz, Sajtula, Phys. Rev. C (2023).

- Updates popular "Mass Explorer"
- Masses from EDFs augmented with discrepancy function from a GP

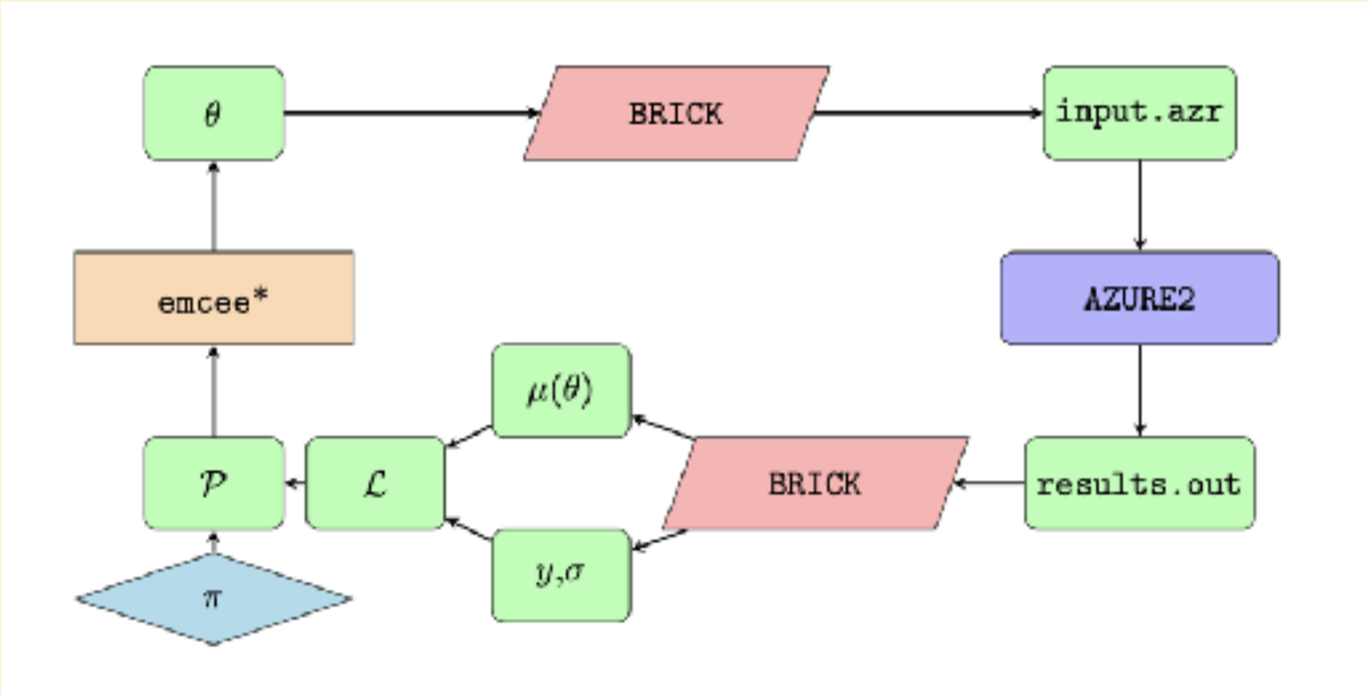
$$M(N,Z) = M_{\mathrm{EDF}\ j} + \delta(N,Z;\ell,\sigma^2)$$

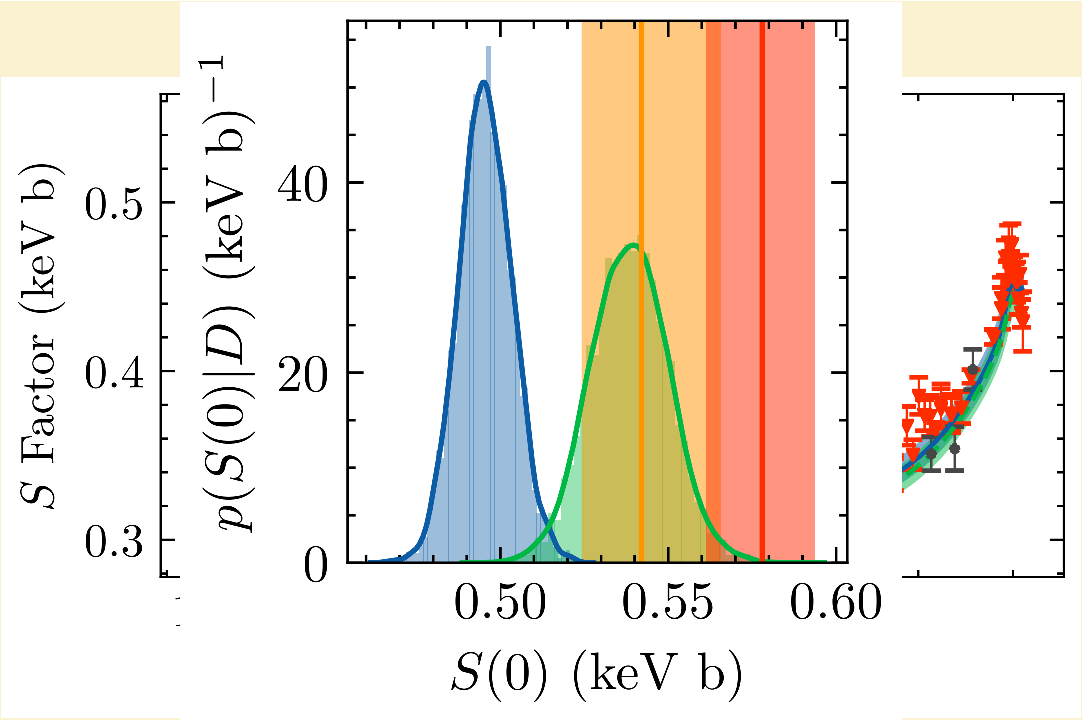
- GP then calibrated to mass data
- https://bmex.dev
- See talk of Kyle Godbey
- Ultimately want to mix different EDFs to get unified prediction
- Model orthogonalization soon

Tin isotopes

BRICK

- 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
- See talk of James de Boer this afternoon

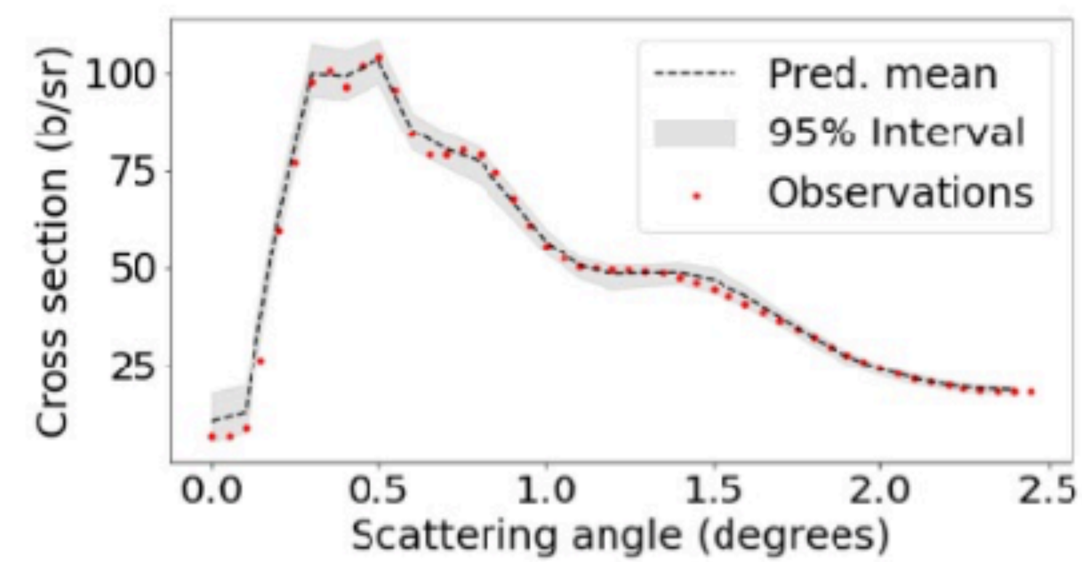




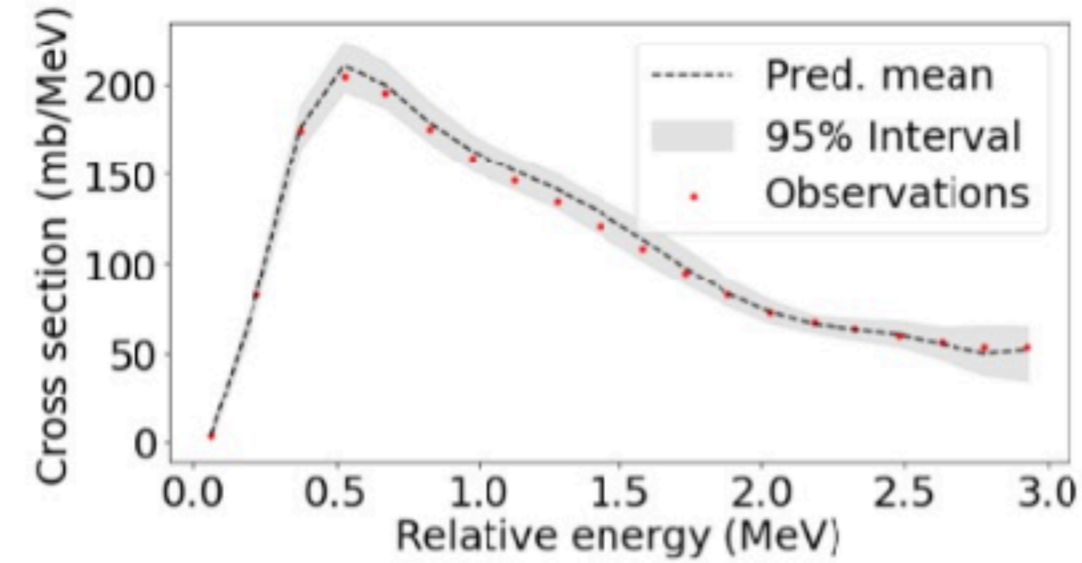
Odell, deBoer, Paneru, Brune, Phillips, Frontiers in Physics (2022)

BFRESCOX

- Measurements of breakup of ^{8}B in collisions with a ^{208}Pb target: important for solar neutrinos
- Computed using CDCC code (in approximation $^{8}B \approx {}^{7}Be + p$): three-body problem
- Emulate CDCC results as a function of ^{7}Be-p optical potential parameters using a Gaussian Process
- Infer parameters of ^{7}Be-p potential, and hence ANC, from data



(a) Angular distribution.



(b) Energy distribution.

Surer, Nunes, Plumlee, Wild Physical Review C (2022)

The Framework

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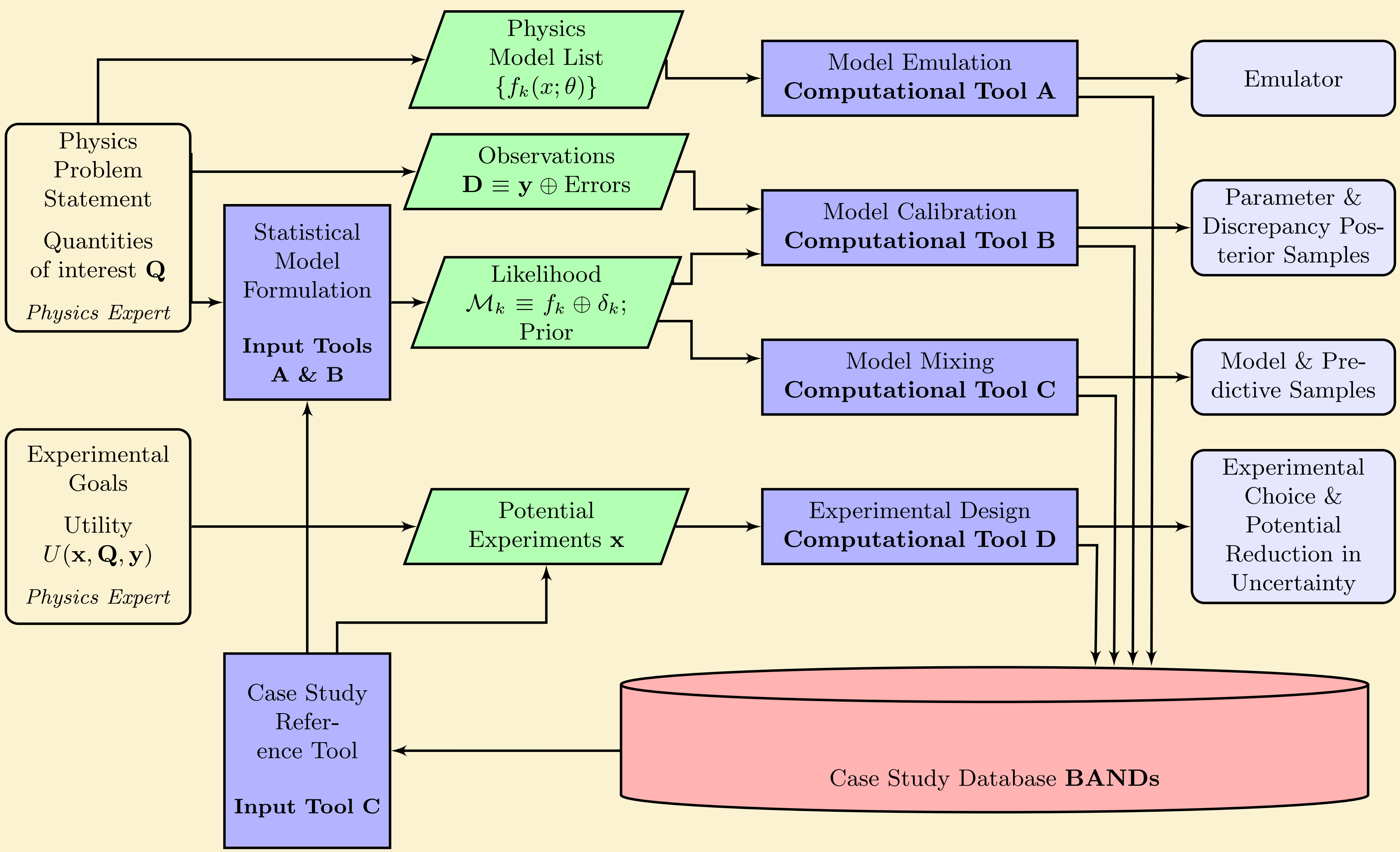


surmise

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". See Kyle Beyer's talk on ROSE for an example of an "intrusive" emulator
- 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
- See talk of Matt Pratola this afternoon

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**.

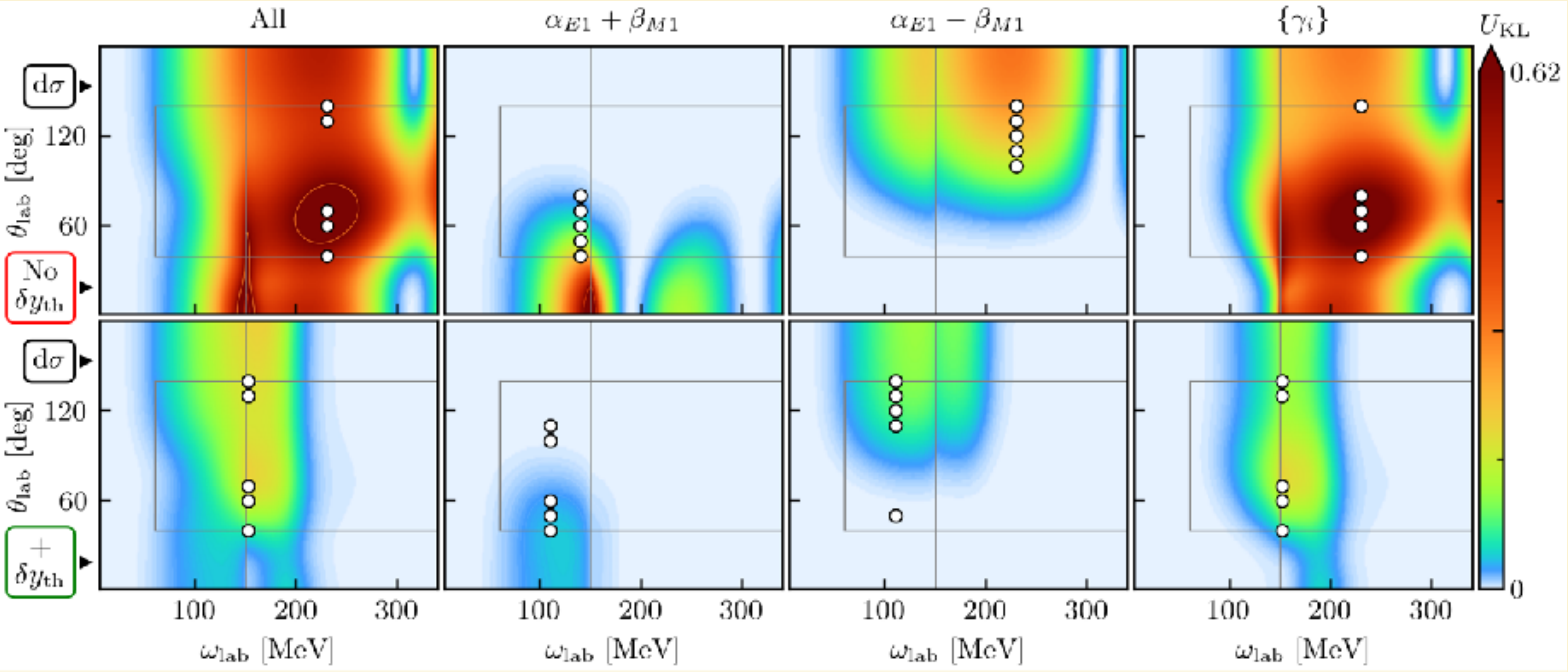
- Seek **x*** that maximizes U(**x**) across space of feasible experimental designs **x**.

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's talk

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
- 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
- Summer 2025: Release of v1.0: full functionality