BAND: Recap and coming attractions

Dick Furnstahl
BAND Camp at ISNET-9
May 22, 2023

Bayesian Analysis of Nuclear Dynamics

https://bandframework.github.io/

Research funded by the NSF's Office of Advanced Cyberinfrastructure

Michigan State University · Miami University · The Ohio State University · Ohio University · Northwestern University

Why? Nuclear Science motivation

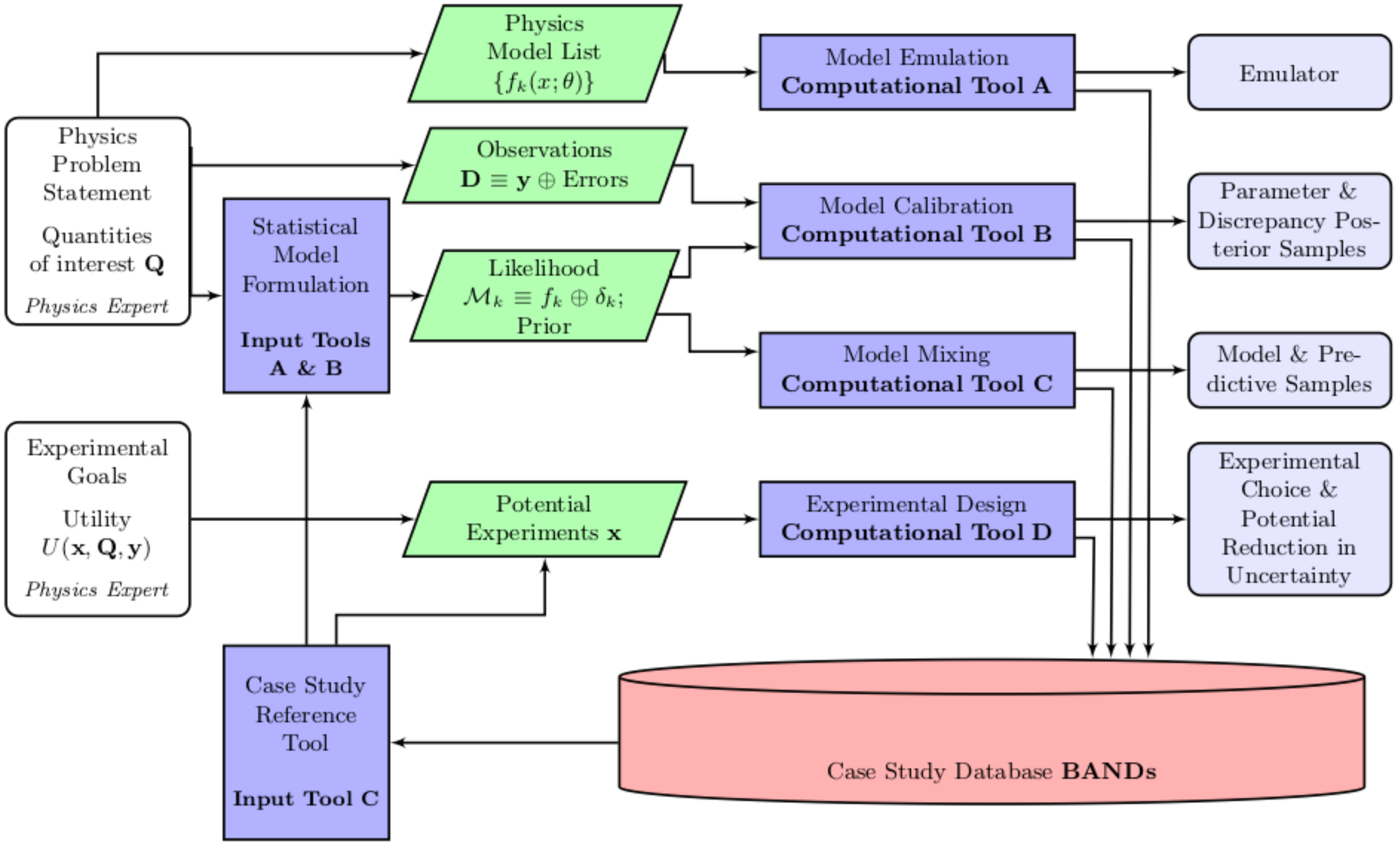
Model uncertainty limits our predictions in key problems:

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

BAND Framework

Goal: *Facilitate principled Uncertainty Quantification in Nuclear Physics*



Bayesian Analysis of Nuclear Dynamics

An NSF CSSI Framework (5 years from 7/2020)

Look to https://bandframework.github.io/ for papers, talks, and software!

v0.3 coming soon!

Guide to the BAND Cyberinfrastructure Framework

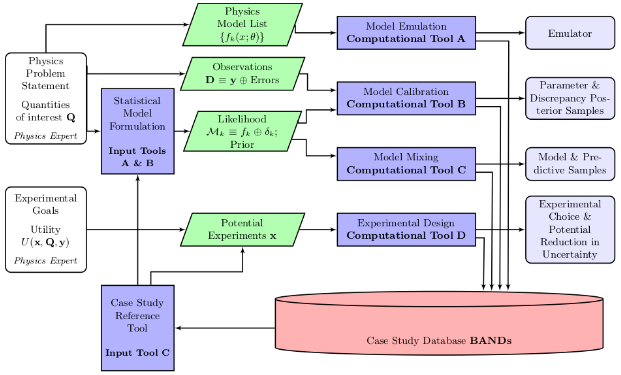
IOP Publishing
Journal of Physics G: Nuclear and Particle Physics
J. Phys. G: Nucl. Part. Phys. **48** (2021) 072001 (39pp)
https://doi.org/10.1088/1361-6471/abf1df

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

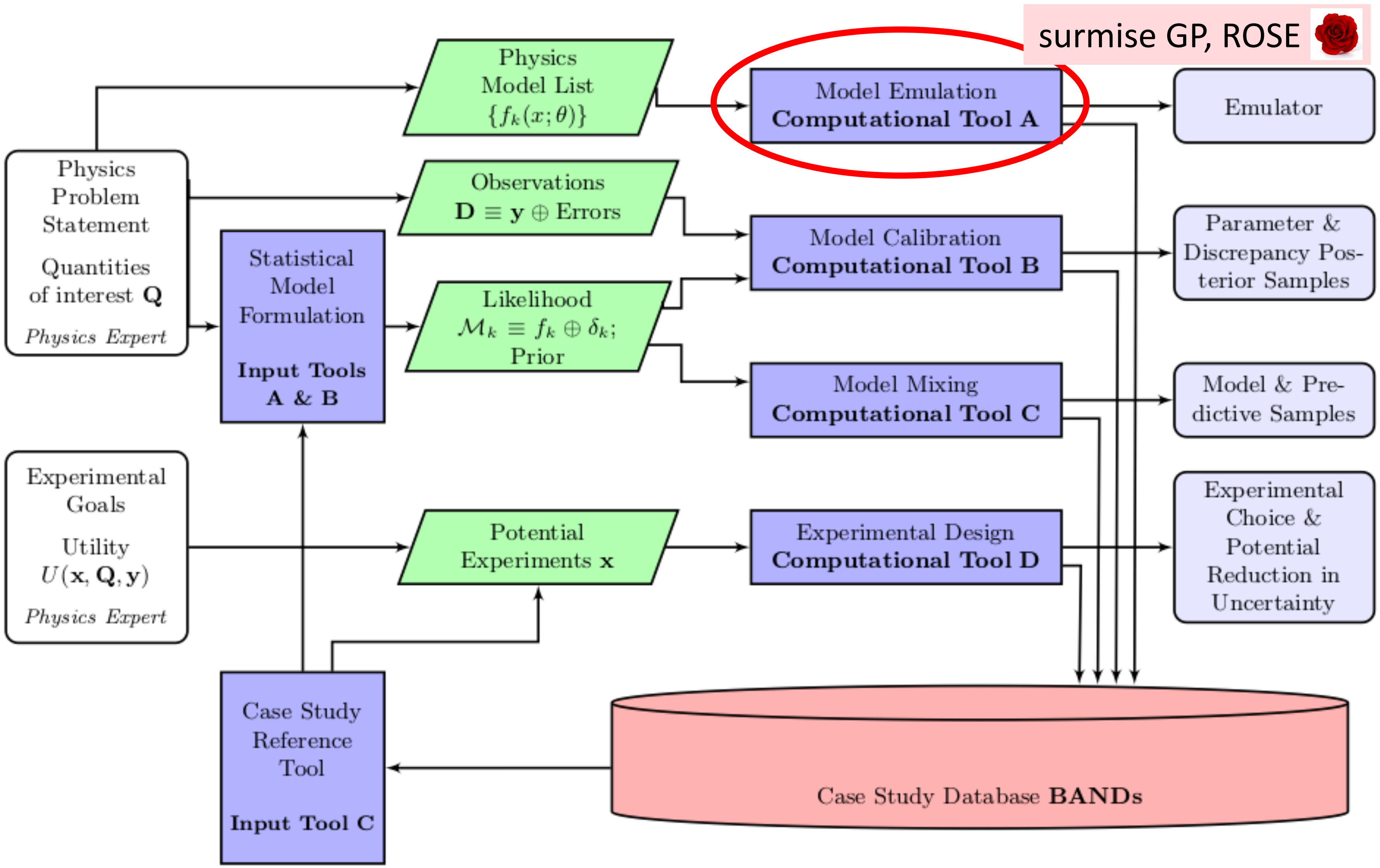


BAND Manifesto:
J. Phys. G 48, 072001 (2021)

Full publication list:
https://bandframework.github.io/publications/

BAND (Bayesian Analysis of Nuclear Dynamics)

High-fidelity models may be too expensive → use an emulator instead!



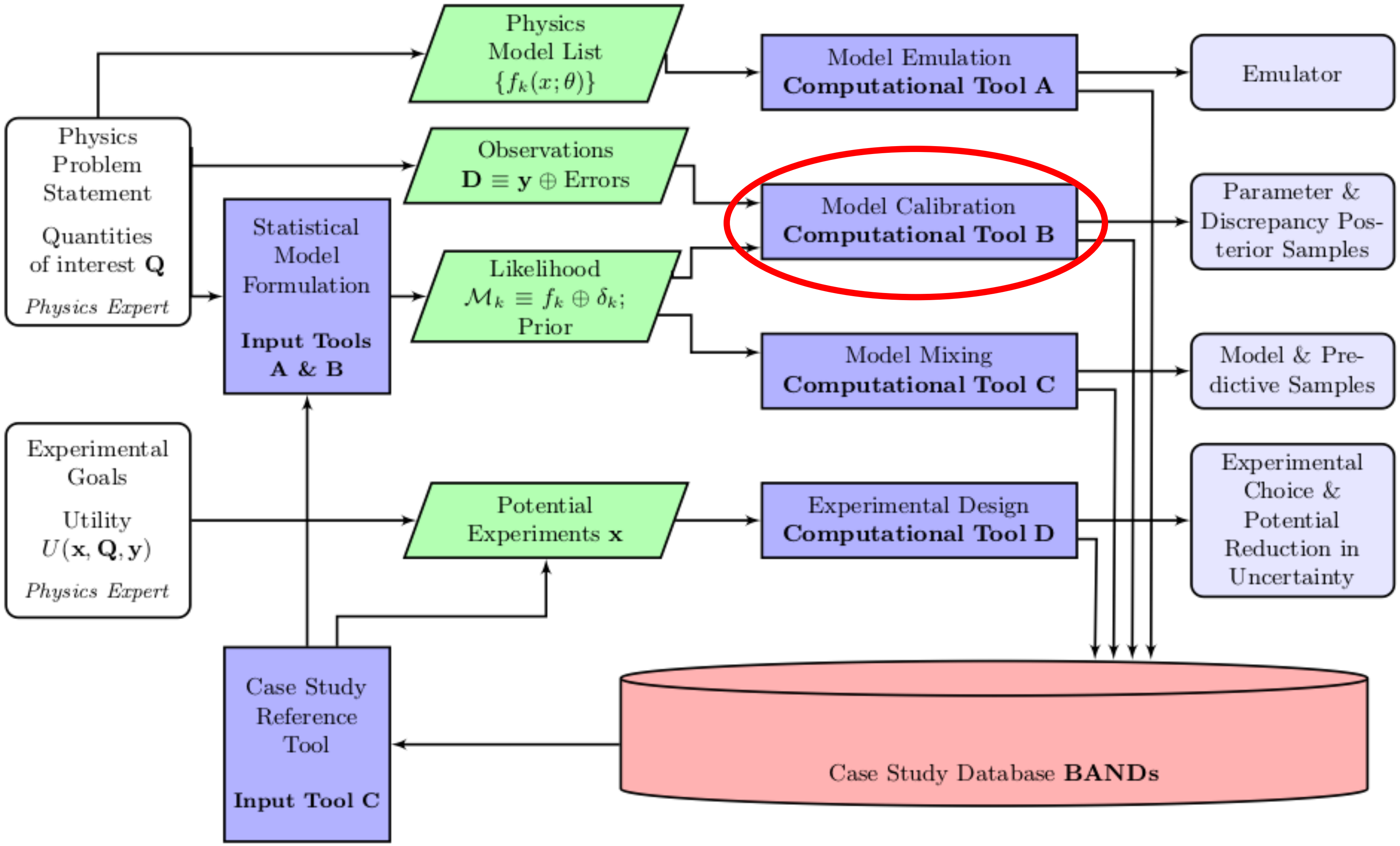
Thursday: Emulators!

Pablo Giuliani, *Quantification for a covariant energy density functional emulated by the reduced basis method*

Daniel Odell, *Reduced basis methods and scattering*

BAND (Bayesian Analysis of Nuclear Dynamics)

Calibrating a model means to update distributions of its parameters based on data.

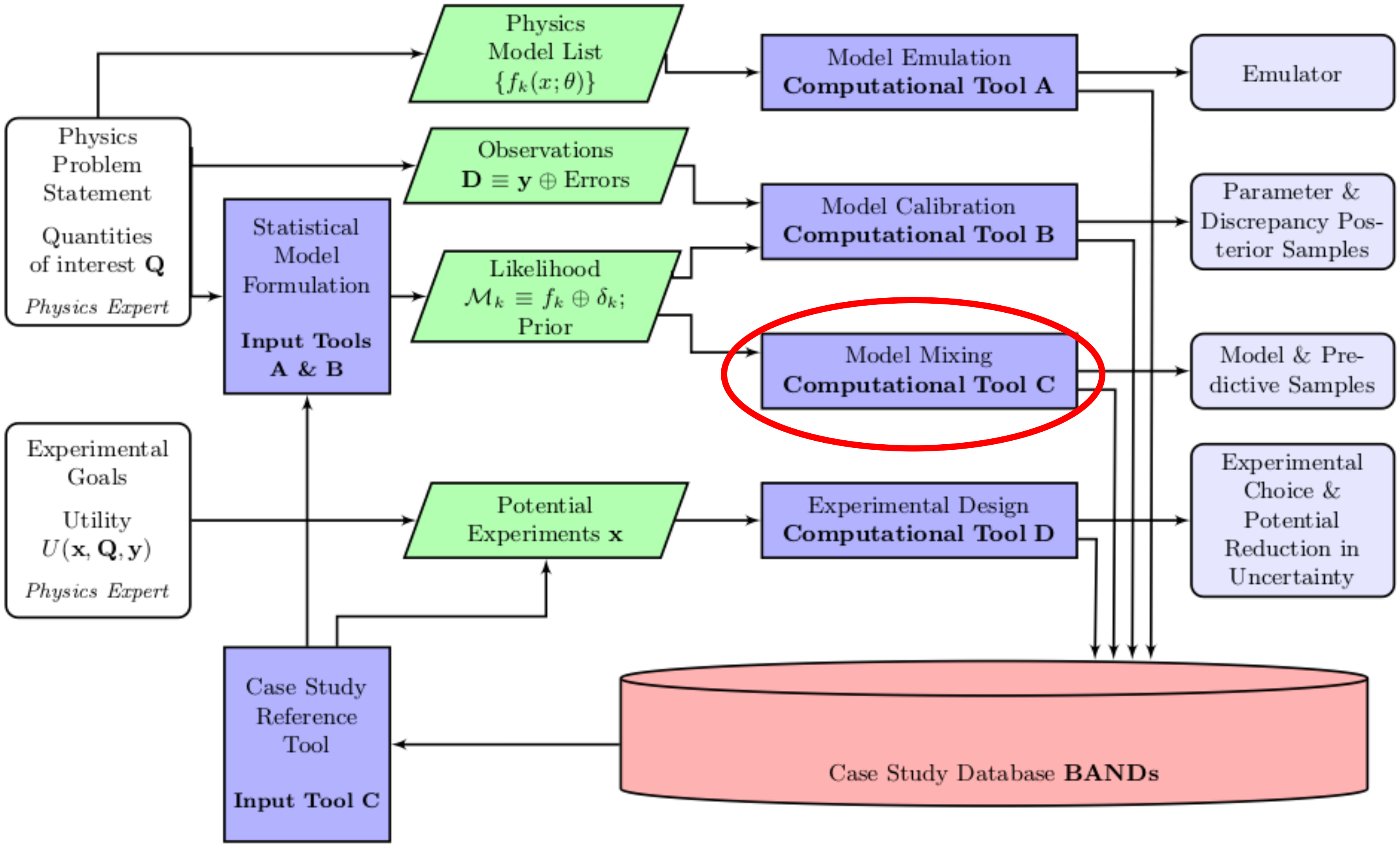


Future: full Bayesian parameter estimation and uncertainty propagation (see ISNET talks)

Tuesday: Dan Liyanage, *Bayesian calibration of viscous anisotropic hydrodynamic simulations of heavy-ion collisions*

BAND (Bayesian Analysis of Nuclear Dynamics)

Multiple models predict an observable: how to combine for the *best* prediction?



Bayesian Analysis of Nuclear Dynamics

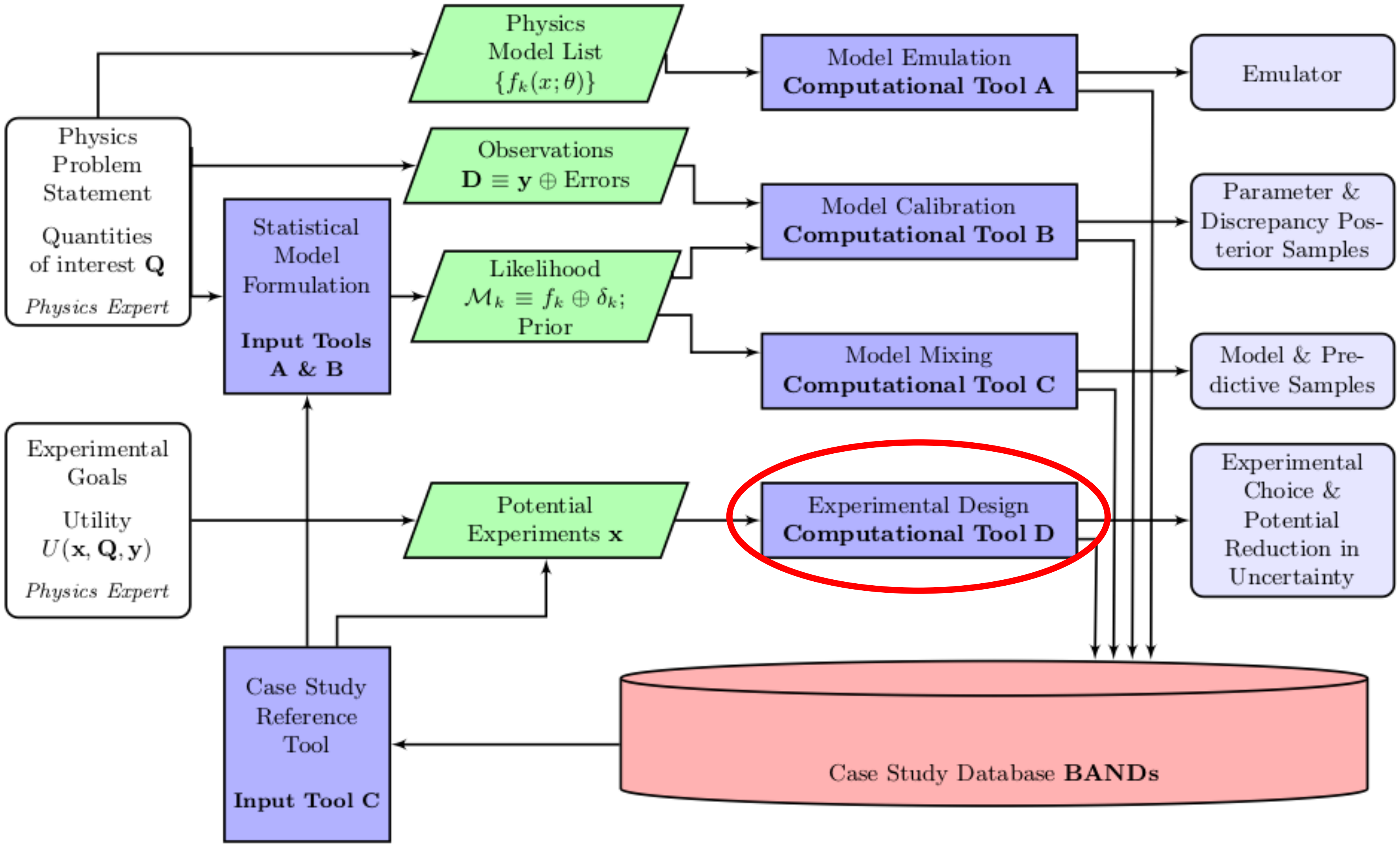
Future: Applications using BAND Taweret software

Example applications:

- Relativistic heavy-ion dynamics;
- Nuclear equation-of-state (EOS): e.g., χEFT and pQCD;
- Effective field theories (EFT): e.g., pionless and chiral EFT, different scales/schemes.

BAND (Bayesian Analysis of Nuclear Dynamics)

Experimental design requires uncertainties from both experiment and models

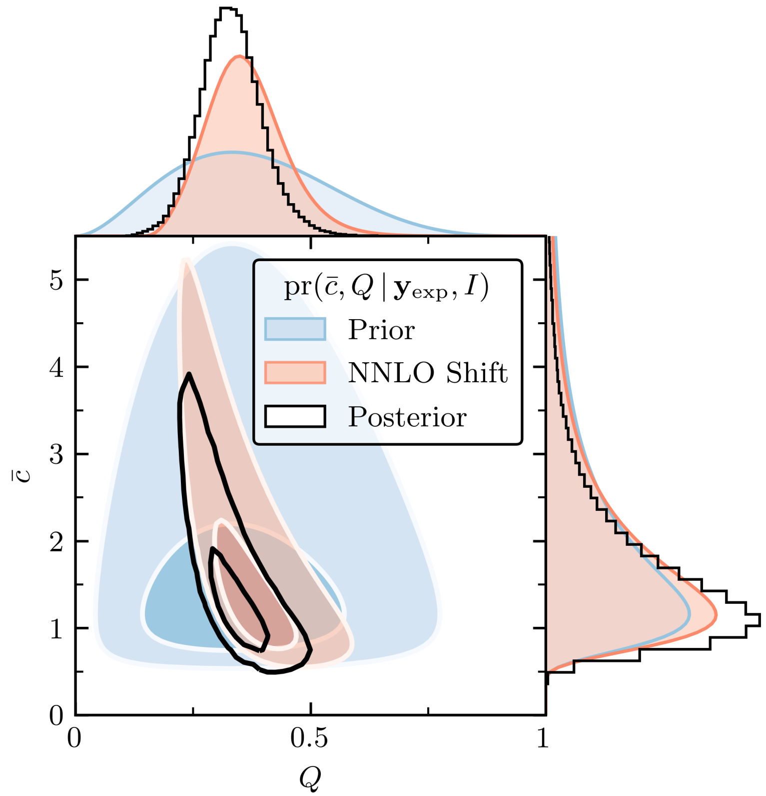


Tuesday: Ozge Sürer, *Sequential Bayesian experimental design for calibration of expensive physics models*

Future: explore alternative approaches; *enabled* by emulators, calibration, model mixing

Basic ideas of experimental design

- Goals of experiment encoded in a *utility* function and averaged over potential experimental results from each particular *design*
  - Design might be beam energies and detector positions
  - Maximize expectation of utility function over designs
- Possible goals:
  - Accurate observation of some quantity
  - Discriminate between competing models
  - Precisely constrain parameters of the theory (here $\vec{a}$)



What designs shrink the prior most?

Utility of **design**: information gain averaged over **parameters** and **measurements**

$$U_{\mathrm{KL}}(\mathbf{d}) = \int \left\{ \ln\left[\frac{\mathrm{pr}(\vec{a}\,|\,\mathbf{y},\mathbf{d})}{\mathrm{pr}(\vec{a})}\right] \mathrm{pr}(\vec{a}\,|\,\mathbf{y},\mathbf{d})\,d\vec{a} \right\} \mathrm{pr}(\mathbf{y}\,|\,\mathbf{d})\,d\mathbf{y} \quad \text{(cf. entropy)}$$

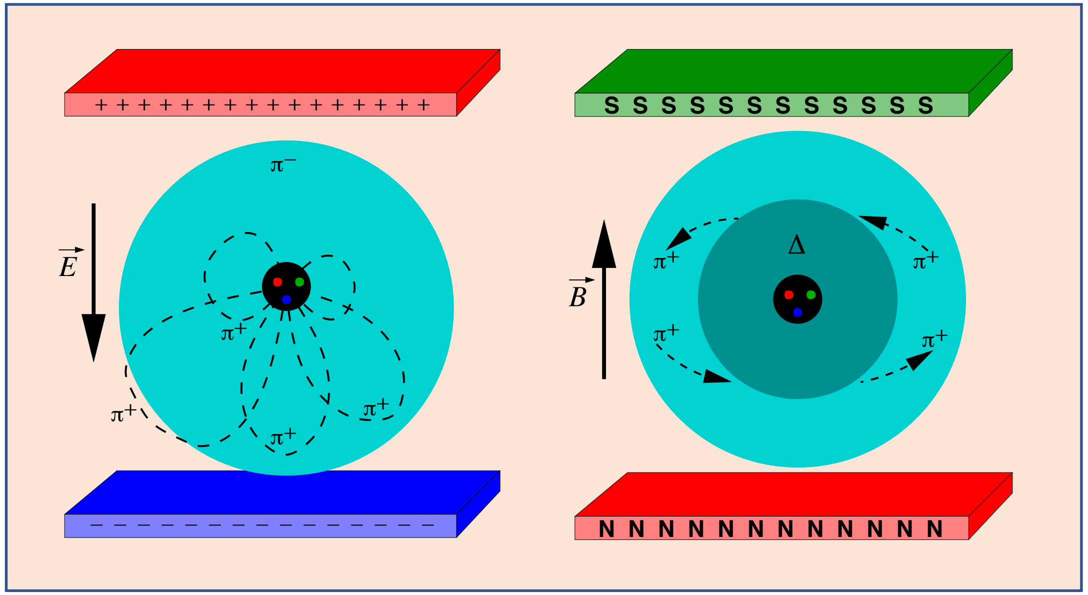
Here: gain in *Shannon information* from prior to posterior

Goal: maximize benefits – minimize cost (time, money, workforce)

Example: Design of future γp Compton scattering experiments

What experimental (ω, θ) are most useful for constraining polarizabilities and testing theory?

Given: (1) Present polarizability error bars; (2) experimental constraints; (3) χEFT accuracy decreases as ω↑.



Nucleon polarizabilities from Compton scattering with χEFT

Griesshammer, McGovern, Phillips, EPJA (2018)

Experiments: HIγS; A2@MAMI
→ tension with χEFT valid range

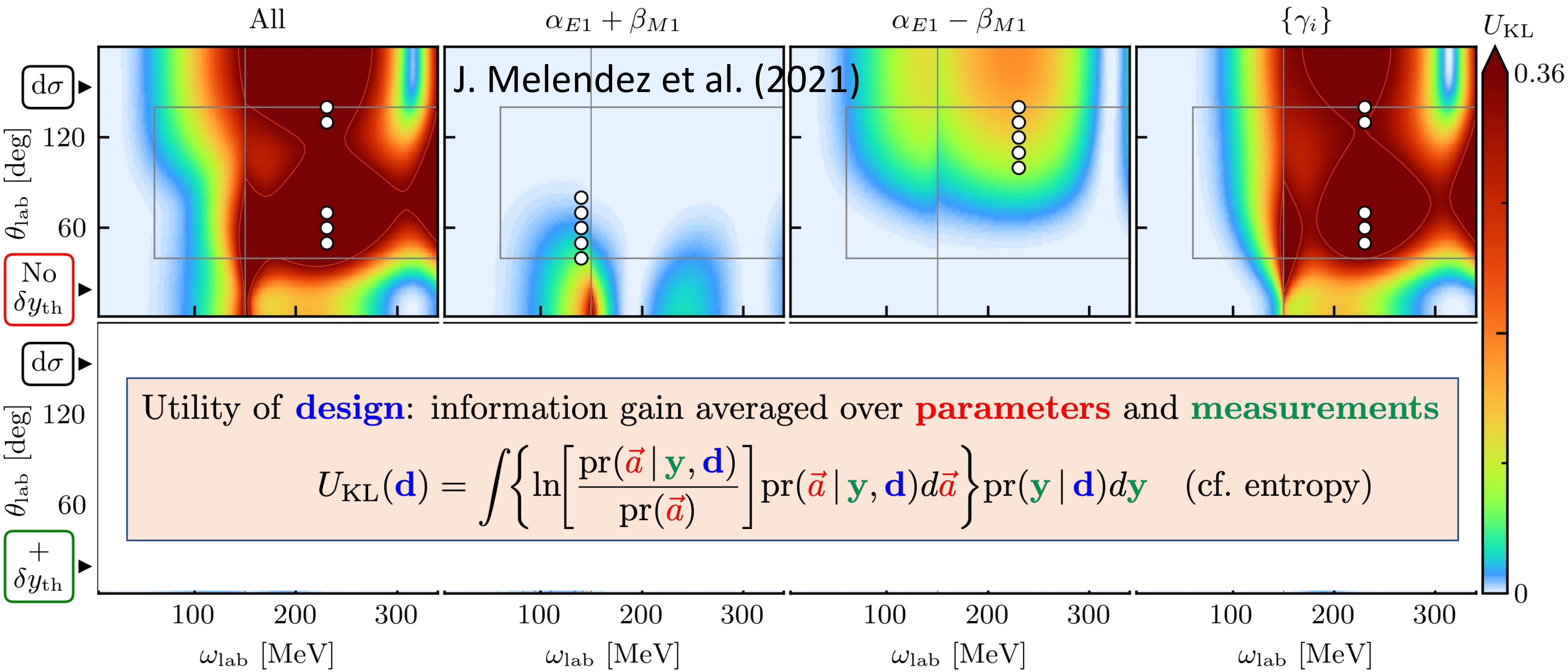
What does a Bayesian analysis of experimental design look like?

[J. Melendez et al, Eur. Phys. J. A **57,** 3 (2021)]

Example: Design of future γp Compton scattering experiments

What experimental (ω, θ) are most useful for constraining polarizabilities and testing theory?

Given: (1) Present polarizability error bars; (2) experimental constraints; (3) χEFT accuracy decreases as ω↑.



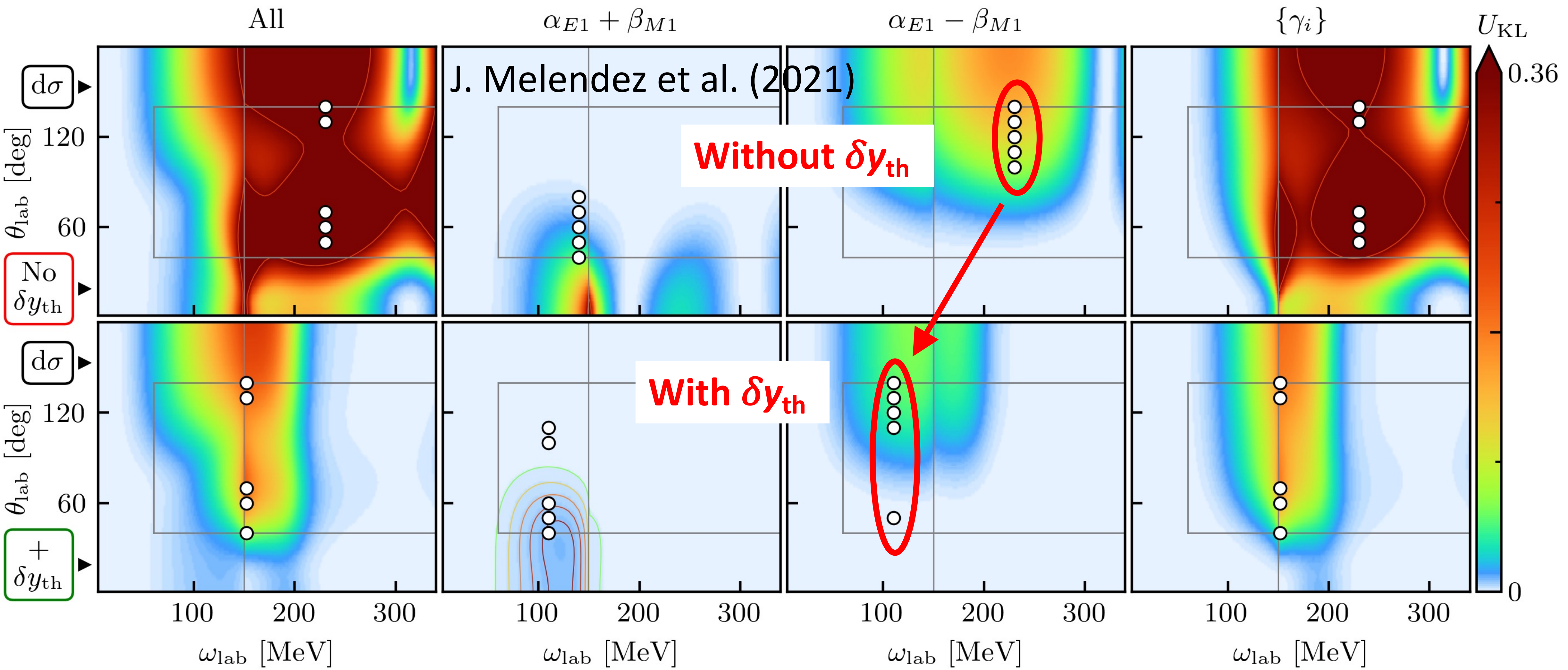
Utility of **design**: information gain averaged over **parameters** and **measurements**

$$U_{\mathrm{KL}}(\mathbf{d}) = \int \left\{ \ln\left[\frac{\mathrm{pr}(\vec{a} \mid \mathbf{y}, \mathbf{d})}{\mathrm{pr}(\vec{a})}\right] \mathrm{pr}(\vec{a} \mid \mathbf{y}, \mathbf{d}) d\vec{a} \right\} \mathrm{pr}(\mathbf{y} \mid \mathbf{d}) d\mathbf{y} \quad \text{(cf. entropy)}$$

Example: Design of future γp Compton scattering experiments

What experimental (ω, θ) are most useful for constraining polarizabilities and testing theory?

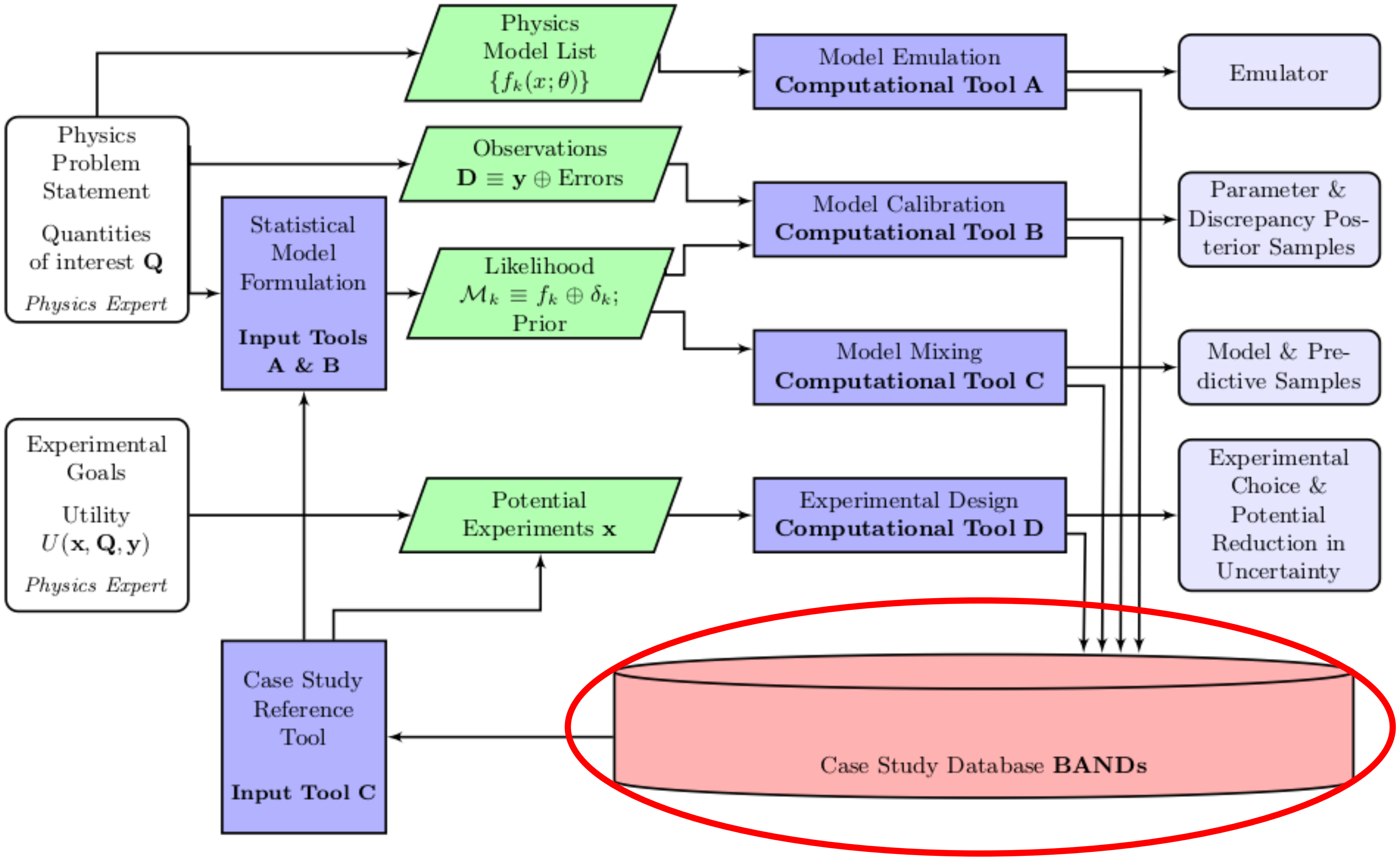
Given: (1) Present polarizability error bars; (2) experimental constraints; (3) χEFT accuracy decreases as ω↑.



Compare utility without-to-with model discrepancy δy_{th} ⇒ very different implications!

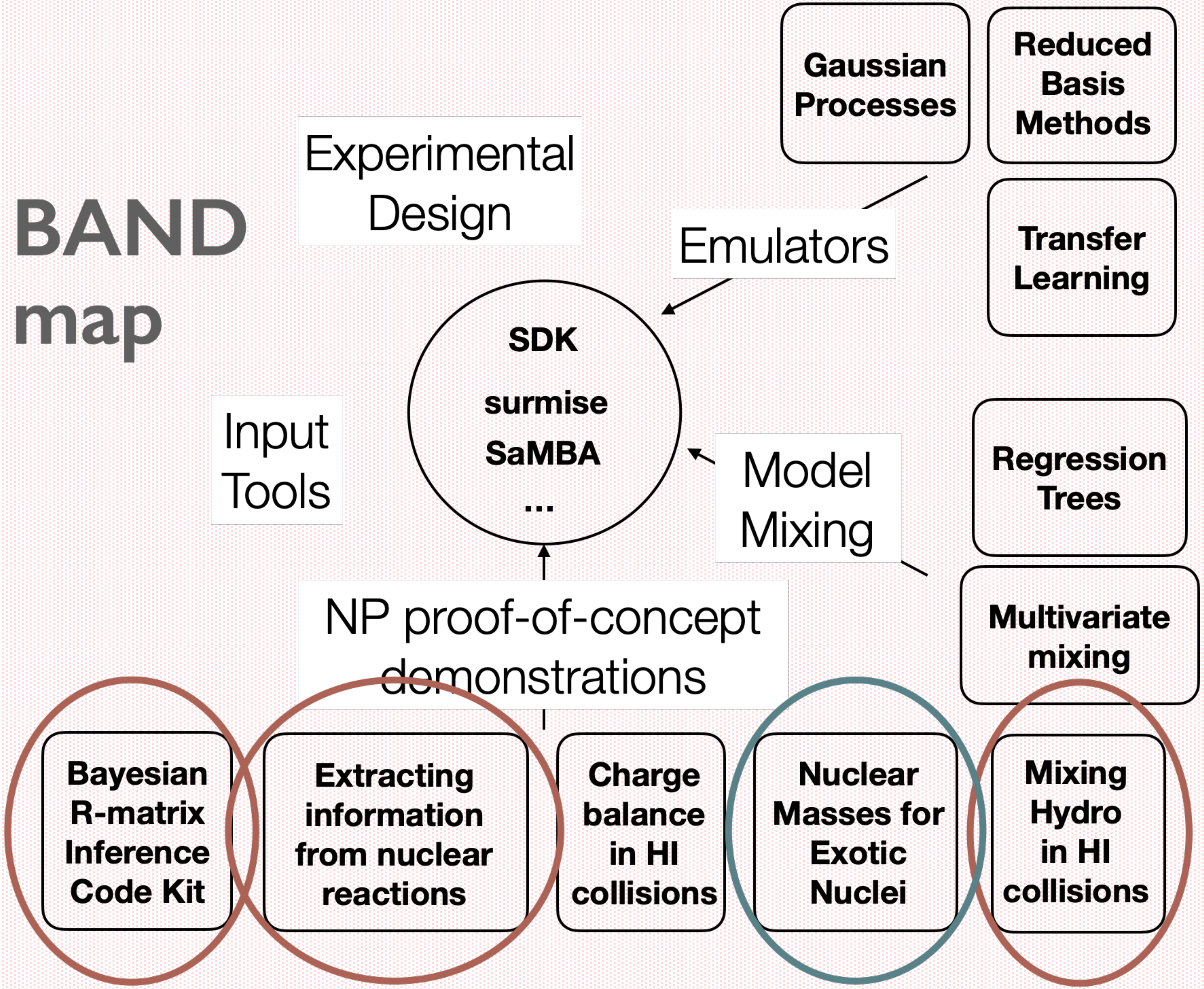
BAND (Bayesian Analysis of Nuclear Dynamics)

Outcome: *Physics discovery through statistics!*



An NSF CSSI Framework (5 years from 7/2020)

Look to https://bandframework.github.io/ for papers, talks, and software! v0.3 coming soon!


BAND map
Experimental Design
Emulators
Gaussian Processes
Reduced Basis Methods
Transfer Learning
SDK
surmise
SaMBA
...
Input Tools
Model Mixing
Regression Trees
Multivariate mixing
NP proof-of-concept demonstrations
Bayesian R-matrix Inference Code Kit
Extracting information from nuclear reactions
Charge balance in HI collisions
Nuclear Masses for Exotic Nuclei
Mixing Hydro in HI collisions

Github repo for BAND Framework

bandframework / software /

https://github.com/bandframework/bandframework

wildsm Update README.md 1ac26b7 · 8 months ago History

Name	Last commit message	Last commit date
..		
BRICK	Delete .DS_Store	8 months ago
Bfrescox	Update README.md	8 months ago
QGP_Bayes @ 4b3e236	updated the sdk policy for QGP_Bayes	8 months ago
SAMBA @ 0479b4d	updating the submodule SAMBA	8 months ago
surmise @ 9878d3b	updating surmise reference point	2 years ago

Current BAND Framework is v0.2

Coming soon: v0.3!

- ROSE
- Taweret
- parMOO
- BMEX
- ....

Tools:

- **surmise**: for model emulation via Gaussian Processes and calibration
- **SaMBA:** Sandbox for Mixing via Bayesian Analysis

Examples:

- **QGP_Bayes:** tutorial on Bayesian analysis of QGP simulations
- **BRICK:** Bayesian R-matrix Inference Code Kit
- **BFRESCOX:** Emulation and Bayesian model calibration of coupled-channels treatment of nuclear reactions

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
- 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 experimental-design capability and additional physics examples
- Summer 2025: Release of v1.0: full functionality

Thank you!

BAND
Bayesian Analysis of Nuclear Dynamics

Coming attraction:

2023: FRIB-TA Summer School on *Practical Uncertainty Quantification and Emulator Development in Nuclear Physics*, June 26-28, at FRIB.

Jupyter *book* (text plus notebooks) for physics applications:

Learning from Data (OSU course Physics 8820)

Extra slides

BMEX

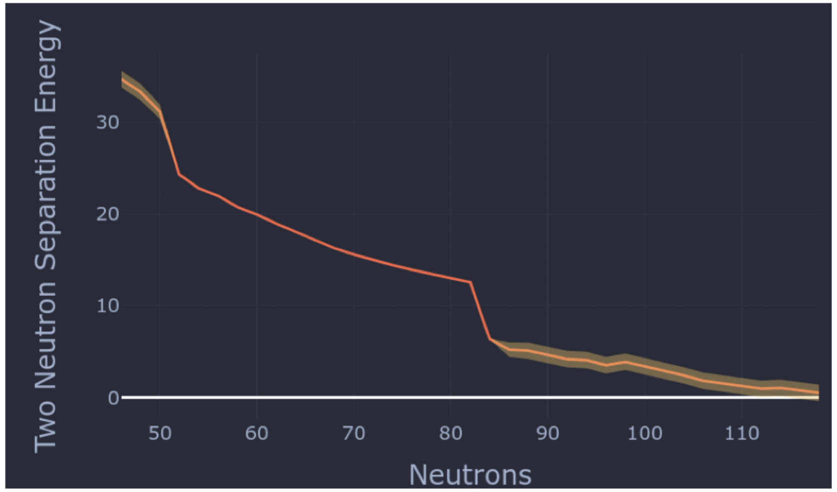
Godbey, Buskirk, Giuliani, Jain, Kejzlar, Nazarewicz, ….

- 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
- Ultimately want to mix different EDFs to get unified prediction, a la recent use of BMA to get best prediction for mass of ^{80}Zr

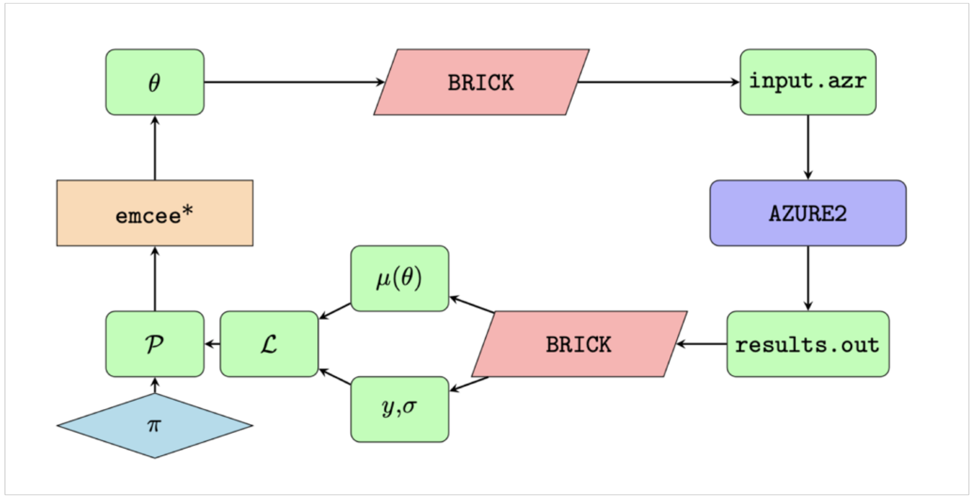
Tin isotopes

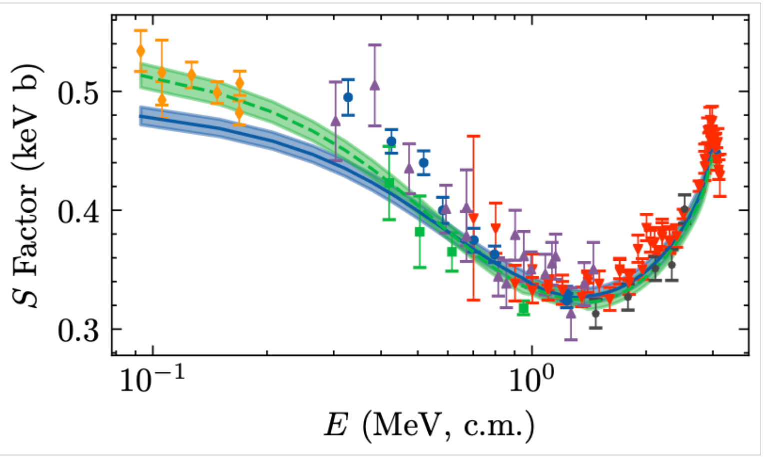


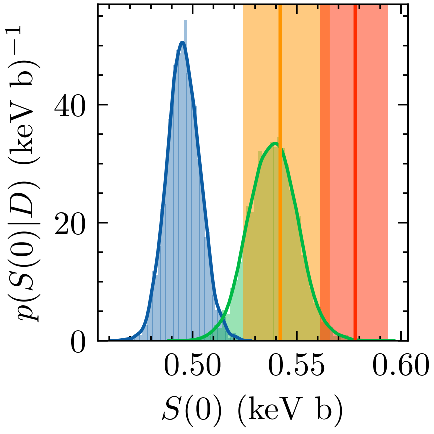
A. Hamaker, R. Jain, S. A. Giuliani, W. Nazarewicz, L. Neufcourt, et al., Nature Physics (2021)

BRICK

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



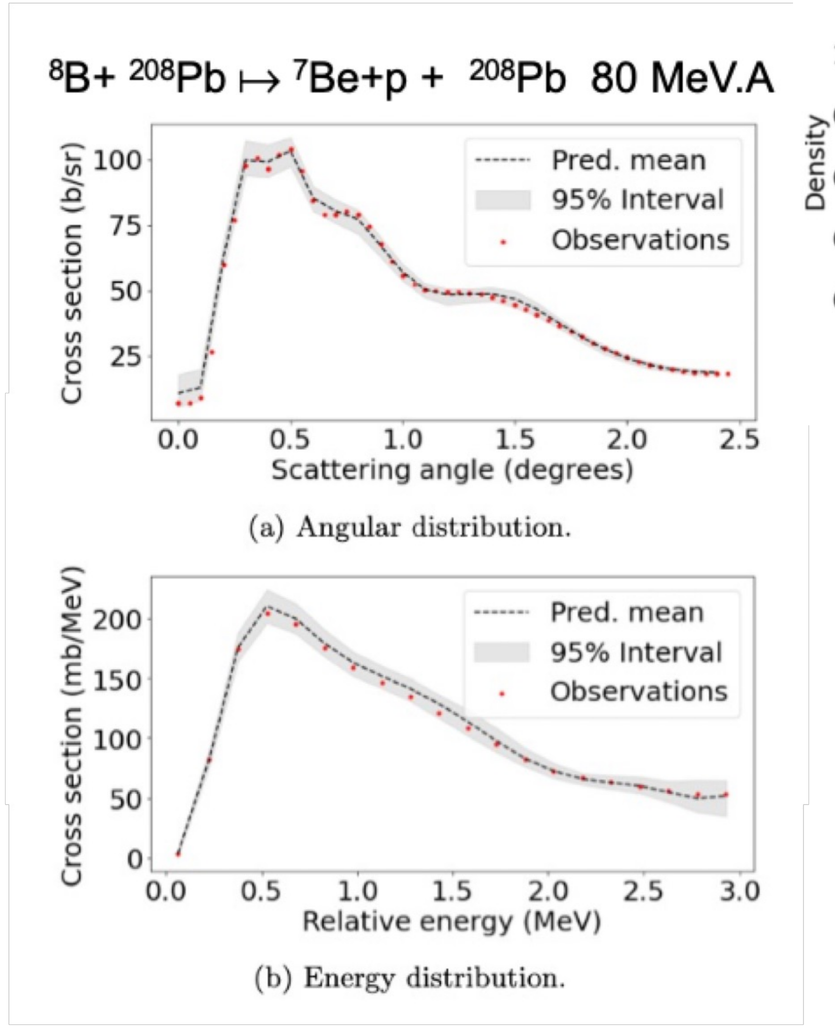




Odell, deBoer, Paneru, Brune, Phillips, Frontiers in Physics (2022)

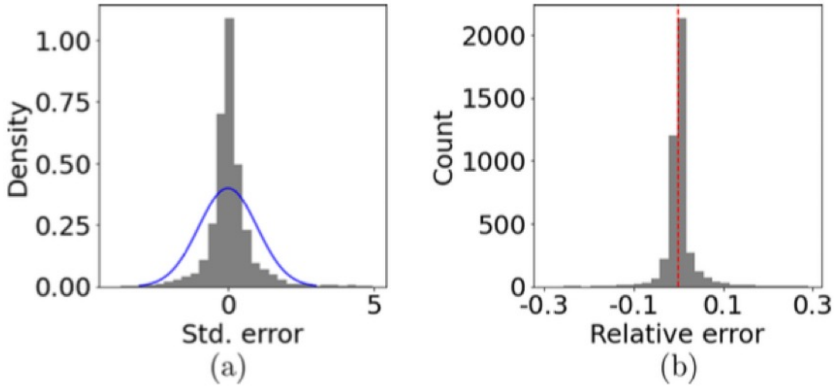
BFRESCOX

- 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

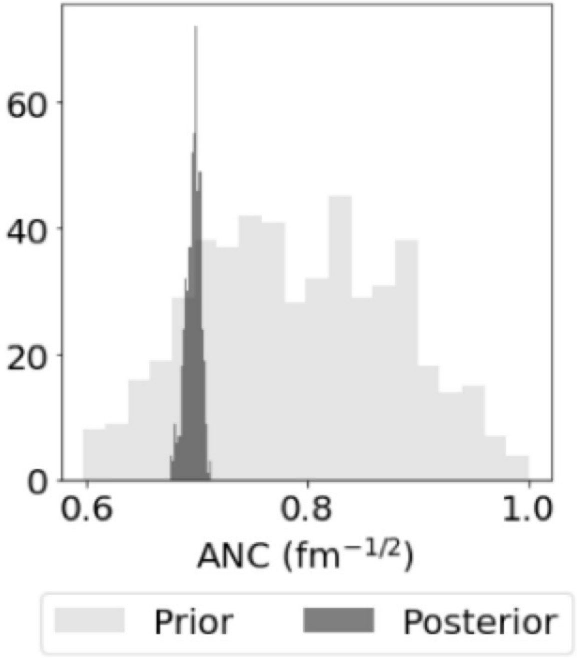


(a) Angular distribution.

(b) Energy distribution.



(a) (b)



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

Viscous Anisotropic Hydrodynamics: Parameter Estimation and Model Mixing

- Relativistic HIC simulated using a multi-stage model; each model calibrated separately
- Replace "Free Stream" & "MUSIC" by Viscous Anisotropic Hydrodynamics
- New models to be emulated then calibrated using RHIC & LHC data
- Preliminary emulators here
- Model mixing of particlization and perhaps hydro approach

Liyanage, Heinz, Plumlee, Surer, Wild