# GRAND COMBINATIONS @ HL-LHC & FAIROS-HEP



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Data Science Institute
Physics, Computer Science, Statistics







# Combined fits for the Higgs discovery



 $\mathbf{f}_{tot}(\mathcal{D}_{sim}, \mathcal{G} | \boldsymbol{\alpha}) = \prod_{c \in channels} \left| \text{Pois}(n) \right|$ 

$$n_c | \nu_c(\boldsymbol{\alpha})) \prod_{e=1}^{n_c} f_c(x_{ce} | \boldsymbol{\alpha}) \left[ \cdot \prod_{p \in \mathbb{S}} f_p(a_p | \alpha_p) \right]$$

# Combined fits for EFTs





# Comments on Unfolding

• Fiducial and differential cross section measurements

- $\rightarrow$  minimise model dependence
- $\rightarrow$  re-interpretable outside experiment

Desirable to have results at particle level, and distributions (STXS or fiducial distr.)

Unfolding is deceptively attractive

- It seems very convenient and to address what we want to know, but
- unfolding is a can of worms statistically and pushes many problems down stream
  - Combinations, correlated systematics, artifacts and bias introduced by the unfolding. procedure. These will all turn into systematics in the final results.
- It is good for fast approximate answers, but
- I do not recommend it as a platform for the final "gold standard" results.



# Likelihood scans vs. full statistical models



for measurements that constrain EFT coefficients

- Lots of progress in publishing statistical models recently in BSM searches
- **Second Level Message:** There are a few ways to describe the dependence on EFT parameters. We can and should separate the specification and implementation.
- First define a **specification** for one or more of these choices that removes all ambiguity. This allows multiple groups to **implement** the specification.
- **Third Level Message:** In addition to publishing statistical models, RECAST-like infrastructure would allow us to consider new EFT operators and update / improve background modeling after publishing
- This infrastructure is being used in BSM searches already

# **Top Level Message**: We should publish the full statistical model (aka "likelihood")









# Likelihood Publishing + RECAST =





Message 1: Publishing Statistical Models

# The first PhyStat

## It was 24 years ago!

#### Massimo Corradi

It seems to me that there is a general consensus that what is really meaningful for an experiment is *likelihood*, and almost everybody would agree on the prescription that experiments should give their likelihood function for these kinds of results. Does everybody agree on this statement, to publish likelihoods?

#### Louis Lyons

Any disagreement ? Carried unanimously. That's actually quite an achievement for this Workshop.

https://cds.cern.ch/record/411537?ln=en

CERN 200 30 May 200

#### ORGANISATION EUROPÉENNE POUR LA RECHERCHE NUCLÉAIRE CERN EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

#### **WORKSHOP ON CONFIDENCE LIMITS**

CERN, Geneva, Switzerland 17–18 January 2000

CERN LIBRARIES, GENEVA



#### PROCEEDINGS

Editors: F. James, L. Lyons, Y. Perrin

GENEVA 2000



## Publishing statistical models: Getting the most out of particle physics experiments

Kyle Cranmer  $\mathbb{O}^{1^*}$ , Sabine Kraml  $\mathbb{O}^{2^{\ddagger}}$ , Harrison B. Prosper  $\mathbb{O}^{3^{\$}}$  (editors), Philip Bechtle  $\mathbb{O}^4$ , Florian U. Bernlochner  $\mathbb{O}^4$ , Itay M. Bloch  $\mathbb{O}^5$ , Enzo Canonero  $\mathbb{O}^6$ , Marcin Chrzaszcz  $\mathbb{D}^7$ , Andrea Coccaro  $\mathbb{D}^8$ , Jan Conrad  $\mathbb{D}^9$ , Glen Cowan <sup>10</sup>, Matthew Feickert  $\mathbb{D}^{11}$ , Nahuel Ferreiro Iachellini  $\mathbb{O}^{12,13}$  Andrew Fowlie  $\mathbb{O}^{14}$ , Lukas Heinrich  $\mathbb{O}^{15}$ , Alexander Held  $\mathbb{O}^{1}$ , Thomas Kuhr <sup>13,16</sup>, Anders Kvellestad <sup>17</sup>, Maeve Madigan <sup>18</sup>, Farvah Mahmoudi <sup>15,19</sup>, Knut Dundas Morå <sup>20</sup>, Mark S. Neubauer <sup>11</sup>, Maurizio Pierini <sup>15</sup>, Juan Rojo <sup>8</sup>, Sezen Sekmen  $\mathbb{O}^{22}$ , Luca Silvestrini  $\mathbb{O}^{23}$ , Veronica Sanz  $\mathbb{O}^{24,25}$ , Giordon Stark  $\mathbb{O}^{26}$ , Riccardo Torre  $\mathbb{O}^{8}$ , Robert Thorne  $\mathbb{O}^{27}$ , Wolfgang Waltenberger  $\mathbb{O}^{28}$ , Nicholas Wardle  $\mathbb{O}^{29}$ , Jonas Wittbrodt  $\mathbb{O}^{30}$ 



# Concepts

While it may seem overly technical, these subtle distinctions are very important.

We overcame decades of stagnation when we focused on declarative specification for **closed-world** models and moved to standard approaches to **serialization** (e.g. ROOT binary to JSON/ yaml)

• breakthrough with pyhf

### Glossary of terms

• Statistical model: This is a synonym for the probability model  $p(x, y | \mu, \theta)$  as in Eq. (7) that includes dependence on the data x and y, the parameters of interest  $\mu$  and nuisance parameters  $\theta$ , access to the individual terms and the ability to generate pseudo- (or synthetic-) data (i.e., "toy Monte Carlo").

• Likelihood: The value of the statistical model for a given *fixed* dataset as a function of the parameters, e.g.,  $L(\mu, \theta)$  in Eq. (7).

• **Constraint term**: A term in the full statistical model that relates auxiliary data y to a particular nuisance parameter  $\theta$ .

• Observed data the n, x, and y of Eq. (7) needed to construct the likelihood.

• **Open-world**: An approach to statistical modelling that allows users to define and implement custom components in the statistical model.

• **Closed-world**: An approach to statistical modelling that requires users to work with a finite set of modelling components.

• Declarative specification: An unambiguous specification (e.g., of a statistical model) that is independent of implementation. Often there exists a reference implementation of a specification, but in the declarative approach there may be multiple implementations that are conceptually and mathematically equivalent.

• Serialization: The process of writing a data structure (e.g., a statistical model) in memory to a file in a way that can be read back into memory. Loading the serialized object typically requires access to compatible software libraries present at the time of serialization.



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### ATLAS Public Results Page

s theme" gives access to specific additional keywords allowing to refine the selection.

TeV         5 TeV         2.36 TeV         2.76 GeV         900 GeV
6 TeV/NN
Higgs       BSM Searches       Heavy Ion       Upgrade Studies       Outreach       Statistical methods
/Etmiss Flavour tagging Physics Modelling
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2)

<u>1</u> + D

## It's a reality

analysis:rivet (Rivet analysis) analysis:MadAnalysis (MadAnalysis 5 analysis)



https://www.hepdata.net/search/?q=analysis:HistFactory

# Using published likelihoods

Just a few lines of code to download the statistical model, re-run fit, make diagnostic plots

```
1 import json
2 import cabinetry
3 import pyhf
4 from cabinetry.model_utils import prediction
5 from pyhf.contrib.utils import download
7 # download the ATLAS bottom-squarks analysis probability models from HEPData
8 download("https://www.hepdata.net/record/resource/1935437?view=true", "bottom-squarks")
9
10 # construct a workspace from a background-only model and a signal hypothesis
11 bkg_only_workspace = pyhf.Workspace(json.load(open("bottom-squarks/RegionC/BkgOnly.json")))
12 patchset = pyhf.PatchSet(json.load(open("bottom-squarks/RegionC/patchset.json")))
13 workspace = patchset.apply(bkg_only_workspace, "sbottom_600_280_150")
14
15 # construct the probability model and observations
16 model, data = cabinetry.model_utils.model_and_data(workspace)
17
18 # produce visualizations of the pre-fit model and observed data
19 prefit_model = prediction(model)
20 cabinetry.visualize.data_mc(prefit_model, data)
21
22 # fit the model to the observed data
23 fit_results = cabinetry.fit.fit(model, data)
24
25 # produce visualizations of the post-fit model and observed data
26 postfit_model = prediction(model, fit_results=fit_results)
27 cabinetry.visualize.data_mc(postfit_model, data)
```



Figure 3: Pre-fit (left) and post-fit (right) visualizations of a selected signal hypothesis for four signal regions of the ATLAS search [41] of a bottom-squark of mass 600 GeV with a secondlightest neutralino of mass 280 GeV and lightest supersymmetric particle of mass 150 GeV generated from the full statistical models published in Ref. [20] using code from Ref. [40]







# Browse and interact with published statistical models

## http://hepexplorer.net. Built by FAIROS-HEP

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# The HS3 Effort

There is now an effort to create a common serialization standard for pyhf, RooFit, BAT, zfit, etc. models

• Key idea: separate **specification** from **implementation** 

 $HS^3$ 

### **High Energy Physics**

### Statistics Serialization Standard

### Carsten Burgard

Tomas Dado, Jonas Eschle, Matthew Feickert, Cornelius Grunwald, Alexander Held, Robin Pelkner, Jonas Rembser, Oliver Schulz

technische universität dortmund

Aug 30, 2023

Talk at Reinterpretation Forum [<u>link]</u> https://indico.cern.ch/event/1264371/contributions/5338176/ https://videos.cern.ch/record/2296062 https://github.com/hep-statistics-serialization-standard

### **RooWorkspace ≠ JSON/YAM**

#### **Carsten Burgard**

huge thanks to Nicolas Morange and Jonas Rembser for their help with getting this together! special thanks also to the whole pyhf team as well as Jonas Eschle for valuable input

for the ROOT Users Workshop 2022

HELMHOLTZ

Disclaimer: This talk has an ATLAS bias! Disclaimer: This talk draws some inspiration from pyhf

#### HS<sup>3</sup> - HEP Statistics Serialization Standard technische universität dortmund

idea: provide standardized format for statistical models:

- human-readable, in JSON format
- machine-readable for direct implementation of statistical models
- software-independent
- generic, mathematical definitions
- full compatibility with respect to RooWorkspace and pyhf

https://github.com/hep-statistics-serialization-standarg

HS<sup>3</sup> - Overview of supported types and components

16. February 2023

#### 1 Introduction

sorely lacking. With the release of ROOT 6.26/00 [1] and the is document sets out to document the syntax and features of the HEP 2 dard (HS<sup>3</sup>) for likelihoods, as to be adopted by any HS<sup>3</sup>-co ease note that this document as well as the HS<sup>3</sup> standard are still in development and can s

de such a component is referred to as a component. If not explicitly stated onents mentioned are mandatory



Robin Pelkner (TU Dortmund)

HS<sup>3</sup> - HEP Statistics Serialization Standard



Message 2: EFT-Specific Model Specification

#### The HistFactory specification Also applies to Combine's binned-templates

The HistFactory specification is pure math with two main implementations (original C++ version in ROOT/RooFit and newer python version pyhf)

Widely used and has almost everything needed for EFT

## **HistFactory Template: at a glance**

 $f (\text{data}|\text{parameters}) = f (\vec{n}, \vec{a}|\vec{\eta}, \vec{\chi}) =$ 

 $\vec{n}$ : events,  $\vec{a}$ : auxiliary data,  $\vec{a}$ 



multiplicative

**Use:** Multiple disjoint channels (or regions) of binned distributions with multiple samples contributing to each with additional (possibly shared) systematics between sample estimates

#### Main pieces:

- Main Poisson p.d.f. for simultaneous measurement of multiple channels
- Event rates  $\nu_{cb}(\vec{\eta}, \vec{\chi})$  (nominal rate  $\nu_{scb}^0$  with rate modifiers)

• encode systematic uncertainties (e.g. normalization, shape)

• Constraint p.d.f. (+ data) for "auxiliary measurements"

$$= \prod_{c \in \text{channels}} \prod_{b \in \text{bins}_c} \text{Pois}\left(n_{cb} | \nu_{cb}\left(\vec{\eta}, \vec{\chi}\right)\right) \prod_{\chi \in \vec{\chi}} c_{\chi}\left(a_{\chi} | \chi\right)$$
  
 $\vec{\eta}$ : unconstrained pars,  $\vec{\chi}$ : constrained pars

$$(\vec{\eta}, \vec{\chi}) \left( 
u_{scb}^0(\vec{\eta}, \vec{\chi}) + \sum_{\Delta \in \vec{\Delta}} \Delta_{scb}(\vec{\eta}, \vec{\chi}) \right)$$





#### The HistFactory specification Also applies to Combine's binned-templates

... but the HistFactory specification is not natural for describing interference effects encountered in EFTs.

## **HistFactory Template: at a glance**

 $f (\text{data}|\text{parameters}) = f (\vec{n}, \vec{a}|\vec{\eta}, \vec{\chi}) =$ 

 $\vec{n}$ : events,  $\vec{a}$ : auxiliary data,  $\vec{\eta}$ : unconstrained pars,  $\vec{\chi}$ : constrained pars



multiplicativ

**Use:** Multiple disjoint channels (or regions) of binned distributions with multiple samples contributing to each with additional (possibly shared) systematics between sample estimates

#### Main pieces:

- Main Poisson p.d.f. for simultaneous measurement of multiple channels
- Event rates  $\nu_{cb}(\vec{\eta}, \vec{\chi})$  (nominal rate  $\nu_{scb}^0$  with rate modifiers)

• encode systematic uncertainties (e.g. normalization, shape)

• Constraint p.d.f. (+ data) for "auxiliary measurements"

## • We can create / extend the specification to handle EFT parameter dependence

$$=\prod_{c\,\in\, ext{channels}}\prod_{b\,\in\, ext{bins}_c} ext{Pois}\left(n_{cb}ig|
u_{cb}\left(ec{\eta},ec{\chi}
ight)
ight)\prod_{\chi\,\in\,ec{\chi}}c_{\chi}\left(a_{\chi}ig|\chi
ight)$$

$$(\vec{\eta}, \vec{\chi}) \left( 
u_{scb}^{0}(\vec{\eta}, \vec{\chi}) + \sum_{\Delta \in \vec{\Delta}} \Delta_{scb}(\vec{\eta}, \vec{\chi}) \right)$$









# EFT "morphing" trick

As one changes the parameters of the EFT, the distributions  $p(x \mid \alpha)$  change due to interference. But there is a trick:

Simple example:

 $|g_1 M_{SM} + g_2 M_{BSM}|^2 = g_1^2 |M_{SM}|^2 + 2g_1 g_2 Re \left[M_{SM}^* M_{BSM}\right] + g_2^2 |M_{BSM}|^2$ 





## EFT "morphing" trick

$$d\sigma \propto \left| \begin{pmatrix} production \\ \mathcal{M}_{SM}^{p} + \sum_{i} \frac{f_{i}}{\Lambda^{2}} \mathcal{M}_{i}^{p} \end{pmatrix} \begin{pmatrix} decay \\ \mathcal{M}_{SM}^{d} + \sum_{j} \frac{f_{j}}{\Lambda^{2}} \mathcal{M}_{j}^{d} \end{pmatrix} \right|^{2}$$
Express EFT as a mixture:  

$$p(x \mid \alpha) = \sum_{c} w_{c}(\alpha) p_{c}(x)$$
Fully difference of the provided equation of the provided

 $w_c(\alpha)$  are polynomials,  $p_c(x)$  are physical distributions! Can truncate to  $\mathcal{O}(\Lambda^{-n})$  if desired

Process	Number of components for <i>n</i> operators					
1100000	$\mathcal{O}(\Lambda^0)$	$\mathcal{O}(\Lambda^{-2})$	$\mathcal{O}ig(\Lambda^{-4}ig)$	$\mathcal{O}(\Lambda^{-6})$	$\mathcal{O}(\Lambda^{-8})$	Σ
<i>hV</i> / WBF production	1	п	$\frac{n(n+1)}{2}$			$\frac{(n+1)(n+2)}{2}$
$h \rightarrow VV$ decay	1	п	$\frac{n(n+1)}{2}$			$\frac{(n+1)(n+2)}{2}$
Production + decay	1	п	$\frac{n(n+1)}{2}$	$\binom{n+2}{3}$	$\binom{n+3}{4}$	$\begin{pmatrix} n+4\\ 4 \end{pmatrix}$

Table 1: Number of components *c* as given in Eq. (6) for different processes, sorted by their suppression by the EFT cutoff scale  $\Lambda$ .

For 2 BSM operators affecting VBF Higgs production and decay, we need a 15-D vector space For 5 BSM operators we need 126-D vector space This is implemented in MadMiner

## rerential ection



Figure 13: Morphing weights  $w_i(\theta)$  for basis points distributed over the full relevant parameter space.



# Other descriptions

Same idea, different in details

Here are two concrete examples for describing how the (truthlevel) fiducial cross section in phase space region k' depends on the EFT coefficients  $\alpha = \{c_i\}$ 

- Can extend to fully differential cross-section  $\frac{d\sigma(\alpha)}{dz}\Big|_{z_i}$  where  $z_i$  is the truth-level kinematics
- Used in MadMiner for Simulation-based inference



# Extending template specifications for EFT fits



### Summary

- **Challenge**: Neutrino-induced experimental complexities in  $B^+ \to K^+ \nu \bar{\nu}$  lead to model-dependent results due to kinematic assumptions and hadronic matrix element description.
- Solution: A model-independent likelihood function enables maximum likelihood fits for any given (B)SM signal prediction, using the supplied information about the  $q^2$ distribution.
- Tool integration:
  - Extend pyhf and interface it with EOS for run-time template updating.
  - Method fully applicable to other decay channels and results.
- Benefits:
  - Exploration of exclusions in BSM parameter space.
  - Individual model studies with provided decay rate predictions.
- Significance: Publishing such likelihoods is crucial for a full exploitation of experimental results.



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RIF 2023

30.08.2023 18 / 18

https://conference.ippp.dur.ac.uk/event/1178/contributions/6443/ https://indico.cern.ch/event/1296757/timetable/#3-area-4-a-practical-framework



This was done by Belle II





30.08.2023 14 / 18

• Subject of my talk at LHC EFT WG, with some more details about "on-the-fly" reweighting

## Focus of LHC EFT effort should be to converge on the specification(s).

A PRACTICAL FRAMEWORK OF EFT FITS WITH PUBLISHED LIKELIHOODS



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Message 3: Extensible EFT reinterpretation with RECAST infrastructure

# Extending the EFT reinterpretation

This morning, Sergio covered motivations and strategies for incorporating changes at a lower level (new EFT operators, changes to sig/bkg models, etc.) keeping the analysis strategy (event selection, observables, etc.) fixed

#### Why would we want to incorporate changes?

Expand the interpretation

CERN

- Analyses are performed for a fixed set of WCs (typically one sector, say, "top physics")
- (Global) combinations may be interested in a superset of those
- "Promote" backgrounds to signals
- Consider EFT effects on the background
- · Updated signal/background models More precise calculations will necessarily appear
- Inside the collaborations it is often possible to assess these problems
- Predictions can only be updated by running the analysis code
- Communication among theorists and experimentalists is of utmost importance!!



#### **Post-generation reweighting**

- Samples can be reweighted after the generation
- Conceptually the same to what reco-level analyses typically do already
- Reweighting needs to be carefully validated
- Phase space is not guaranteed to be fully covered
- These validations are "standard" when designing the analysis  $\rightarrow$  generation point can be tuned
- Not guaranteed when adding new operators
- In practice, helicity-ignorant reweighing works better for many use-cases (see next slide)
- Procedure straightforward for EFT effects  $\rightarrow$  those are evaluated at parton level

## In BSM context, this is often referred to as "recasting" and we have built infrastructure to do this

Sergio Sánchez Cruz's talk earlier today: https://indico.cern.ch/event/1378665/timetable/?view=standard#b-562259-reconstruction-level

Update signal / background components & export a new statistical model





# Preservation & Reinterpretation

First results using the RECAST reinterpretation framework and publishing full statistical likelihoods (using pyhf) in 2019

• Recent pMSSM effort uses 10 searches, 19 parameter pMSSM, and 20,000 parameter points





ATLAS PUB Note ATL-PHYS-PUB-2019-029 5th August 2019



**Reproducing searches for new physics with the** ATLAS experiment through publication of full statistical likelihoods

The ATLAS Collaboration

The ATLAS Collaboration is starting to publicly provide likelihoods associated with statistical fits used in searches for new physics on HEPData. These likelihoods adhere to a specification first defined by the HistFactory p.d.f. template. This note introduces a JSON schema that fully describes the HistFactory statistical model and is sufficient to reproduce key results from published ATLAS analyses. This is per-se independent of its implementation in ROOT and it can be used to run statistical analysis outside of the ROOT and RooStats/RooFit framework. The first of these likelihoods published on HEPData is from a search for bottom-squark pair production. Using two independent implementations of the model, one in ROOT and one in pure Python, the limits on the bottom-squark mass are reproduced, underscoring the implementation independence and long-term viability of the archived data.

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AT 12

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**ATLAS PUB Note** ATL-PHYS-PUB-2019-032 11th August 2019

#### **RECAST** framework reinterpretation of an ATLAS **Dark Matter Search constraining a model of a dark** Higgs boson decaying to two *b*-quarks

The ATLAS Collaboration

The reinterpretation of a search for dark matter produced in association with a Higgs boson decaying to *b*-quarks performed with RECAST, a software framework designed to facilitate the reinterpretation of existing searches for new physics, is presented. Reinterpretation using RECAST is enabled through the sustainable preservation of the original data analysis as re-executable declarative workflows using modern cloud technologies and integrated with the wider CERN Analysis Preservation efforts. The reinterpretation targets a model predicting dark matter production in association with a hypothetical dark Higgs boson decaying into *b*-quarks where the mass of the dark Higgs boson  $m_s$  is a free parameter, necessitating a faithful reinterpretation of the analysis. The dataset has an integrated luminosity of  $79.8 \text{ fb}^{-1}$ and was recorded with the ATLAS detector at the Large Hadron Collider at a centre-of-mass energy of  $\sqrt{s} = 13$  TeV. Constraints on the parameter space of the dark Higgs model for a fixed choice of dark matter mass  $m_v = 200 \text{ GeV}$  exclude model configurations with a mediator mass up to 3.2 TeV.

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# **ENERGY FRONTIERS**

#### Reports from the Large Hadron Collider experiments ATLAS **Electroweak SUSY after LHC Run 2**

Supersymmetry (SUSY) provides elegant solutions to many of the problems of the Standard Model (SM) by introducing new boson/fermion partners for each SM fermion/boson, and by extending the Higgs sector. If SUSY is realised in nature at the TeV scale, it would accommodate a light Higgs boson without excessive fine-tuning. It could furthermore provide a viable dark-matter candidate, and be a key ingredient to the unification of the electroweak and strong forces at high energy. The SUSY partners of the SM bosons can mix to form what are called charginos and neutralinos, collectively referred to as electroweakinos.

Electroweakinos would be produced only through the electroweak interaction, where their production cross sections in proton-proton collisions are orders of magnitude smaller than strongly produced squarks and gluinos (the supersymmetric partners of quarks and gluons). Therefore, while extensive searches using the Run 1 (7-8 TeV) and Run 2 (13 TeV) LHC datasets have turned up null results, the corresponding chargino/neutralino exclusion limits remain substantially weaker than those for strongly interacting SUSY particles.

The ATLAS collaboration has recently released a comprehensive analysis of the electroweak SUSY landscape based on its Run 2 searches. Each individual search targeted specific chargino/ neutralino production mechanisms and subsequent decay modes. The analyses were originally interpreted in so-called "simplified models", where only one production mechanism is considered, and only one possible decay. However, if SUSY is realised in nature, its particles will have many possible production and the SUSY parameters. The new ATLAS upper limits from the LZ experiment. analysis brings these pieces together by reinterpreting 10 searches in the remain to be explored.



Fig. 1. The fraction of pMSSM models excluded by ATLAS in the plane of the lightest chargino mass (x-axis) versus the lightest neutralino mass (y-axis). The dashed line shows the exclusion of simplified SUSY models reported by individual searches in this mass plane.



Fig. 2. The fraction of pMSSM models excluded by ATLAS in the plane of the lightest neutralino (i.e. the dark-matter candidate) mass (x-axis) versus the spin-independent WIMP-nucleon decay modes, with rates depending on scattering cross-section (y-axis). The dashed line shows the

phenomenological Minimal Super- The 19-dimensional pMSSM paramesymmetric Standard Model (pMSSM), ter space was randomly sampled to prowhich includes a range of SUSY parti- duce a set of 20,000 SUSY model points. cles, production mechanisms and decay The 10 selected ATLAS searches were modes governed by 19 SUSY parameters. then performed on each model point The results provide a global picture of to determine whether it is excluded ATLAS's sensitivity to electroweak SUSY with at least 95% confidence level. This and, importantly, reveals the gaps that involved simulating datasets for each SUSY model, and re-running the corresponding analyses and statistical fits. An extensive suite of reinterpretation tools was employed to achieve this, including preserved likelihoods and RECAST a framework for preserving analysis workflows and re-applying them to new signal models.

The results show that, while electroweakino masses have been excluded up to 1TeV in simplified models, the coverage with regard to the pMSSM is not exhaustive. Numerous scenarios remain viable, including mass regions nominally covered by previous searches (inside the dashed line in figure 1). The pMSSM models may evade detection due to smaller production cross-sections and decay probabilities compared to simplified models. Scenarios with small mass-splittings between the lightest and next-to-lightest neutralino can reproduce the dark-matter relic density, but are particularly elusive at the LHC. The decays in these models produce challenging event features with low-momentum particles that are difficult to reconstruct and separate from SM events.

Beyond ATLAS, experiments such as LZ aim at detecting relic dark-matter particles through their scattering by target nuclei. This provides a complementary probe to ATLAS searches for dark matter produced in the LHC collisions. Figure 2 shows the LZ sensitivity to the pMSSM models considered by ATLAS, compared to the sensitivity of its SUSY searches. ATLAS is particularly sensitive to the region where the dark-matter candidate is around half the Z/Higgs-boson mass, causing enhanced dark-matter annihilation that could have reduced the otherwise overabundant dark-matter relic density to the observed value.

The new ATLAS results demonstrate the breadth and depth of its search programme for supersymmetry, while uncovering its gaps. Supersymmetry may still be hiding in the data, and several scenarios have been identified that will be targeted, benefiting from the incoming Run 3 data.

Further reading

ATLAS Collab. 2024 arXiv:2402.01392.

# A RECAST-like service for EFTs

Consider the case where ATLAS and CMS publish statistical models parametrized for some subset of operators in a specified EFT basis.

• Sometime later one wants to reinterpret the analysis for a different set of operators keeping the same event selection, breakdown of signal and control regions, observables, binning, etc.

RECAST is a framework for reinterpretations like this for BSM searches

• In general, this requires running new signal through the full MC simulation + reco + analysis chain. ATLAS is actually doing this with preserved analysis workflows!

In most cases for EFTs we can simply reweight the existing fully simulated SM events (doesn't require running more simulation, reconstruction, etc.)

• The service could calculate the coefficients for the mini-database based on truth-level kinematics and export a new statistical model that implements the specification as describe above.







# FAIROS-HEP

## What is FAIROS-HEP?

Network project titled "FAIROS-HEP".

around data and publications in HEP.

- By focusing on FAIR data practices and how data and software can be linked to physics results, we hope to build a network of researchers thinking about how we can create a "living publication" to preserve and extend physics results.
- The project includes some funding for building infrastructure as well as future workshops connecting groups.







## Recently, the US National Science Foundation funded a new Research Coordination

- FAIROS = Findable. Accessible. Interoperable. Reusable. Open Science.
  - The FAIROS-HEP project aims to connect groups of researchers thinking about FAIR data in HEP and other experts in this field to envision a more cohesive infrastructure













# FAIROS-HEP Continues a Legacy of Contributions

### DASPOS (2012-2016)

- https://daspos.crc.nd.edu/
- Contributions to **RECAST** led to **REANA** as a spinoff project now led by CERN
- Supported REANA Common Workflow Language
- DIANA-HEP (2015-2021)
  - <u>https://diana-hep.org/</u>
  - Learning for reinterpretation
  - Supported GitHub -> Zenodo DOI minting

IRIS-HEP (2018-?)

- <u>https://iris-hep.org/</u>
- Major contributions to likelihood publishing, HEPData integration, SCAILFIN (2018-2021)
  - <u>https://scailfin.github.io/</u>

FAIROS-HEP (2022-2025)

- https://fairos-hep.org/
- Continue the legacy of contributions, help coordinate the ecosystem

• Contributions to **REANA**, **RECAST**, launched **pyhf likelihood publishing**, early work in **simulation-based inference**, Active

• Contributions to REANA (Slurm and HPC backends, applications built on top of REANA), Active Learning for reinterpretation





## Conclusion

**Top Level Message**: We should publish the full statistical model (aka "likelihood") for measurements that constrain EFT coefficients

• Lots of progress in publishing statistical models recently in BSM searches

We can and should separate the specification and implementation.

• First define a **specification** for one or more of these choices that removes all ambiguity. This allows multiple groups to **implement** the specification.

publishing

• This infrastructure is being used in BSM searches already

design of this infrastructure.

**Second Level Message:** There are a few ways to describe the dependence on EFT parameters.

**Third Level Message:** In addition to publishing statistical models, RECAST-like infrastructure would allow us to consider new EFT operators and update / improve background modeling after

**Bonus:** The FAIROS-HEP project has funds to support (travel to) workshops to coordinate the







# PhyStat workshop on SBI in Munich

### PHYSTAT-SBI 2024 - Simulation Based Inference in Fundamental Physics

15-17 May 2024 Max Planck Institute for Physics Europe/Zurich timezone

#### Overview

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Fueled by the recent advances of Machine Learning in the last decade, a new breed of techniques have been developed to tackle statistical inference problems for "likelihood-free" cases, where it is possible to sample from the data-generating process (i.e. via stochastic simulators) but a closed form evaluation of the density is intractable.

This group of methods is known as "simulation-based inference" (SBI) or "likelihood-free inference" (LFI) and will be the dedicated topic of this PHYSTAT Workshop taking place from May 15th - May 17th 2024 at the Max-Planck Institute for Physics (MPP) in Garching near Munich.

PHYSTAT https://phystat.github.io/Website/) is a long-running workshop series that brings together statisticians, machine learning researchers and physicists to discuss shared topics and foster collaboration among the research communities.

**Confirmed Speakers:** 

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- Ann Lee (Carnegie Mellon)
- Julia Linhart (INRIA)
- Noemi Montel (U of Amsterdam)
- Jakub Tomczak (Eindhoven)
- Christoph Weniger (GRAPPA)
- Alexander Held (U Wisconsin-Madison)

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## https://indico.cern.ch/event/1355601/overview



# Backup & Referees

## Related talks

# Talk at Higgs 2020

- <u>https://indico.cern.ch/event/900384/contributions/3796227/</u>
- Unfolding vs. simplified likelihoods vs. full statistical models
- STXS vs. Fully differential
- Simulation-based inference

Talk at LHC EFT WG in 2023

- https://indico.cern.ch/event/1296757/
- Full statistical models and on-the-fly reweighting



## A brief idea

Journal of Brief Ideas Home New idea Trending ideas All ideas

### **Recasting through reweighting**

#### By Kyle Cranmer, Lukas Heinrich

reinterpretation lhc physics

Recasting refers to reinterpreting the results of searches for new particles or standard model measurements in the context of different theoretical models [1]. The fundamental task is to replace the original hypothesis  $p_0(x)$  with a new hypothesis  $p_1(x)$ , where x is some observed quantity. The effect of the detector response and analysis cuts can be encoded in a folding operator  $\int W(x|z)dz$  acting on the truth-level distribution p(z). By keeping the analysis fixed, W(x|z) does not change, thus recasting amounts to:

$$p_0(x) = \int p_0(z)W(x|z)dz \implies p_1(x) = \int p_1(z)dz$$

There are two primary approaches:

- folding: Samples from  $p_1(z)$  are run through a detector simulation and analysis chain to estimate  $p_1(x)$  [2]. This is common when z is high-dimensional,  $p_0(z)$  and  $p_1(z)$  are very different, or W(x|z) is sensitive to experimental details.
- **unfolding**: An alternate theory  $p_1(z)$  is compared directly to an unfolded distribution p(z) obtained from applying an approximate inverse operation to the observed data. Typically, unfolding is restricted to low-dimensional x, z and Gaussian uncertainties.

We point out a third option

• reweighting: Reweight pre-folded events  $(x_i, z_i) \sim p_0(x, z)$  by the factor  $r(z_i)$ 

$$p_1(x) = \int p_1(z)W(x|z)dz = \int p_0(z) \underbrace{\frac{p_1(z)}{p_0(z)}}_{\text{reweighting}} W(z)dz = \int p_1(z) \underbrace{\frac{p_1(z)}{p_0(z)}}_{\text{reweighting}} W(z)dz$$

This approach does not require simulating new events or the approximations used in unfolding. Note, sample variance becomes a problem if  $r(z_i) \gg 1$ .

### https://beta.briefideas.org/ideas/8106c030eba22dd3a8d268940d5e42d8

(x|z)W(x|z)dz

$$p_{i} = p_{1}(z_{i})/p_{0}(z_{i})$$
, as in

W(x|z)dz





Exceprts from Simulation-Based Inference

# Conclusion

Likelihood fits in the data space are the gold standard for statistical inference

- RECAST and likelihood publishing are technical solutions that address model dependence and the theory-experiment interface
- STXS a good step, but more differential information can lead to large gain in sensitivity

Properties we want

- Ability to be fully differential
- Exploit highest fidelity simulation (QCD, detector simulation) without approximations that introduce additional systematic errors
- Clear statistical motivation and compatibility with traditional combined analyses.
- Scalability in terms of channels and parameters

The approach I presented (implemented in MadMiner) achieves these goals





### High-dimensional event data

[CMS]





## Precision constraints on new physics

Parameterization e.g. in Effective Field Theory:

systematic expansion of new physics around **Standard Model** 

$$\mathcal{L}_{\mathrm{EFT}} = \mathcal{L}_{\mathrm{SM}} + \sum rac{J_i}{\Lambda^2}$$

10s to 100s "universal" parameters to measure



# Benchmarking STXS in WH

• Simplified Template Cross-Sections (STXS) define observable bins that are supposed to capture as much information on NP as possible

[N. Berger et al. 1906.02754; HXSWG YR4]



Let's check! How much information on

$$\begin{split} \tilde{\mathcal{O}}_{HD} &= \mathcal{O}_{H\Box} - \frac{\mathcal{O}_{HD}}{4} = (\phi^{\dagger}\phi)\Box(\phi^{\dagger}\phi) - \frac{1}{4}(\phi^{\dagger}D^{\mu}\phi)^{*}(\phi^{\dagger}D_{\mu}\phi) \\ \mathcal{O}_{HW} &= \phi^{\dagger}\phi W^{a}_{\mu\nu}W^{\mu\nu a} \\ \mathcal{O}^{(3)}_{Hq} &= (\phi^{\dagger}i\overleftrightarrow{D}^{a}_{\mu}\phi)(\overline{Q}_{L}\sigma^{a}\gamma^{\mu}Q_{L}) , \end{split}$$

can we extract from  $pp \rightarrow WH \rightarrow \ell \nu \ b\bar{b}$  ?

• Results: STXS are indeed sensitive to operators, adding a few more bins improve them, but a multivariate analysis is still stronger





## An incomplete wrap-up of simulation-based inference methods

### Method

Summary statistics:

Likelihood for summary stats (standard histograms)

Approximate Bayesian Computation

### Matrix elements:

Matrix Element Method Optimal Observables

### Neural networks:

Neural likelihood

- Neural posterior
- Neural likelihood ratio

#### Neural networks + matrix elements:

Neural likelihood (ratio) + gold mining (RASCAL etc) Neural optimal observables (SALLY)

Approximations	Upfront cost	Eva
Reduction to summary stats	Fast	Fast
Reduction to summary stats	Depends	Dep
Transfer fns	Fast	Slov
Transfer fns, optimal only locally	Fast	Slov
NN	Needs many samples	Fast
NN	Needs many samples	Fast
NN	Needs many samples	Fast
NN	Needs less samples	Fast
NN, optimal only locally	Needs less samples	Fast

#### bends

N

N

#### **Opinionated review**

K. Cranmer, JB, G. Louppe: "The frontier of simulation-based inference" [1911.01429]

### **Do It Yourself (for LHC physics)**

JB, F. Kling, I. Espejo, K. Cranmer: "MadMiner: Machine learning—based inference for particle physics" [CSBS, 1907.10621, https://github.com/diana-hep/madminer]

#### LHC HXSWG YR4 STXS

JB, S. Dawson, S. Homiller, F. Kling, T. Plehn: "Benchmarking simplified template cross sections in WH production" [JHEP, 1908.06980]

#### **Use in Astro: Strong lensing**

JB, S. Mishra-Sharma, J. Hermans, G. Louppe, K. Cranmer "Mining for Dark Matter Substructure: Inferring subhalo population properties from strong lenses with machine learning" [ApJ, 1909.02005]

### **Original works**

JB, K. Cranmer, G. Louppe, J. Pavez: "A guide to constraining Effective Field Theories with machine learning" [PRD, 1805.00020] JB, G. Louppe, J. Pavez, K. Cranmer:

"Mining gold from implicit models to improve likelihood-free inference" [PNAS, 1805.12244]

#### Follow-up with incremental improvements

M. Stoye, JB, K. Cranmer, G. Louppe, J. Pavez: "Likelihood-free inference with an improved cross-entropy estimator" [NeurIPS workshop, 1808.00973]

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## https://indico.cern.ch/event/1355601/overview

# On-the-fly Event-by-Event Reweighting

Excerpts from https://indico.cern.ch/event/1296757/

# Abstract

Recently there has been rapid increase in the number of full statistical models (or "likelihoods") published by the experiments.

- Most are based on the HistFactory (pyhf) format and published in HEPData.
- This allows theorists and others to reproduce and combine measurements with the same gold standard as the internal experimental results.
- However, these are mainly from SUSY and exotics searches and
- working with EFTs is more complicated because quantum interference effects lead to changes in the signal template (via the dependence of the differential cross-sections and phase-space dependent selection efficiency on the EFT parameters).

In this talk I will propose a simple, lightweight framework that would extend current the same level of detail as the internal experimental fits and combinations).

- likelihood publishing to overcome these challenges and enable 'exact' EFT fits (i.e. with
  - https://indico.cern.ch/event/1296757/timetable/



## Scope of this talk

The focus of this talk is about a practical statistical framework for doing EFT fits

- Emphasis is on statistical correctness, not optimality of observables, etc.
- Fit distributions in the data space (no unfolding)
  - Focusing on binned template fits with full systematic uncertainty treatment
- With some user-defined observables x (probably 1-D or 2-D)
  - This talk is **not** about what is a good observable
- Independent of which EFT operators, which basis, how many parameters, etc.

outside experiments can re-do fits, perform combinations, etc.

• So it addresses many of the motivations for unfolding, but its cleaner statistically

The framework lends itself well to publishing the full statistical model so that groups



# Morphing histograms vs. event-by-event reweighting

- Statistical fluctuations for bin probability (or fiducial cross-section) can lead to unphysical negative probabilities when morphing to a new value of  $\alpha$
- Efficiency and acceptance aren't constant for all events in a given bin of the observable x, so there is some (mild) approximation

when applicable in Sections 3 and ATLAS CONF Note **ATLAS** EXPERIMENT ATLAS-CONF-2023-052

Morphing histograms (or fiducial cross-sections estimated with MC) has some subtle issues:

The acceptance factors  $\epsilon_{\text{STXS}}$  and  $\epsilon_{\text{diff.}}$ , as well as the signal shape factors  $f_s$ , are derived under the assumption of SM Higgs boson kinematics. For interpretations of the measurements in physics models that significantly alter kinematic distributions, additional correction factors may be needed to account for changes in the acceptance and signal shape as a function of BSM model parameters. These are discussed













# Morphing histograms vs. event-by-event reweighting

- Statistical fluctuations for bin probability (or fiducial cross-section) can lead to unphysical negative probabilities when morphing to a new value of  $\alpha$
- Efficiency and acceptance aren't constant for all events in a given bin of the observable x, so there is some (mild) approximation

However, event-by-event reweighing based on morphing avoids these issues

- The event weights are always positive
- The weights are for a specific event (that either passes or fails selection criteria), so there is no approximation due to averaging efficiencies / acceptances for different types of events.

Morphing histograms (or fiducial cross-sections estimated with MC) has some subtle issues:







# Idea 1: a model that builds histograms on-the-fly

For any fully simulated event with observable  $x_i$  and MC truth record  $z_i$  that was generated from EFT with parameters  $\alpha_0$  (e.g. the SM), we can reweight to a new EFT parameter point  $\alpha$ with

- Similar to what we do with PDF reweighing.
- reconstructed quantities on event-by-event basis.
- equations or closely related approaches

**Idea:** For each value of  $\alpha$  fill a signal histogram with set of weighted events  $\{x_i, w_i(\alpha)\}$ 

- Can do this on-the-fly while doing the fit.
- It captures the  $\alpha$ -dependence of efficiency and acceptance

 $w_i(\alpha) = \frac{d\sigma(\alpha)/dz}{d\sigma(\alpha_0)/dz}\Big|_{z}$ 

• Kinematics don't change! Efficiency and acceptance are already included by selection on

• The  $\alpha$ -dependence of differential cross-sections can be computed using "morphing"







# **Details**: how to build histograms on-the-fly

- **Idea:** For each value of  $\alpha$  fill a signal histogram with set of weighted events  $\{x_i, w_i(\alpha)\}$ • Can do this on-the-fly while doing the fit
- It captures the  $\alpha$ -dependence of efficiency and acceptance

includes information for a set of simulated events:

- Store  $x_i$  (observed value of observable) and the coefficients needed to reweight event to a new point  $\alpha$ . For example:
  - The differential cross-section (at truth-level) for set of basis points as implemented in MadMiner
- The fully differential versions of the coefficients  $A_i^{i,k'}$  in ATLAS-CONF-2023-052 It may be a bit slow, but its very flexible and avoids the problems mentioned above.

**Details:** To do this, the statistical model would need to maintain a **tiny database** that





# Idea 2: RECAST-like service for EFTs

Consider the case where ATLAS and CMS publish statistical models parametrized for some subset of operators in a specified EFT basis.

• Sometime later one wants to reinterpret the analysis for a different set of operators keeping the same event selection, breakdown of signal and control regions, observables, binning, etc.

RECAST is a framework for reinterpretations like this for BSM searches

• In general, this requires running new signal through the full MC simulation + reco + analysis chain. ATLAS is actually doing this with preserved analysis workflows!

require running more simulation, reconstruction, etc.)

• The service could calculate the coefficients for the mini-database based on truth-level kinematics and export a new statistical model that implements the statistical model for those operators as describe above.

But for EFTs we can simply to reweight the existing fully simulated SM events (doesn't







# Conclusion

Recently there has been rapid increase in the number of full statistical models (or "likelihoods") published by the experiments — mainly for BSM searches and their reinterpretation.

- Ironically, it's not being used much for EFTs. This should change!
- standard as the internal experimental results.

We will need to define new **specifications** for components of statistical models that describe the details for how distributions of observables depend on EFT parameters including interference effects

- them in public tools
- some nice properties and should be explored

Finally, we have all the ingredients needed to create a **RECAST-like service for EFTs** that would allow us to reweight fully simulated samples of events to new EFT scenarios at some point in the future

• It would allow theorists and others to reproduce and combine measurements with the same gold

• This is already very mature, but we should make the specifications concrete and then **implement** 

• Approaches based on event-by-event reweighting and on-the-fly creation of histograms have











