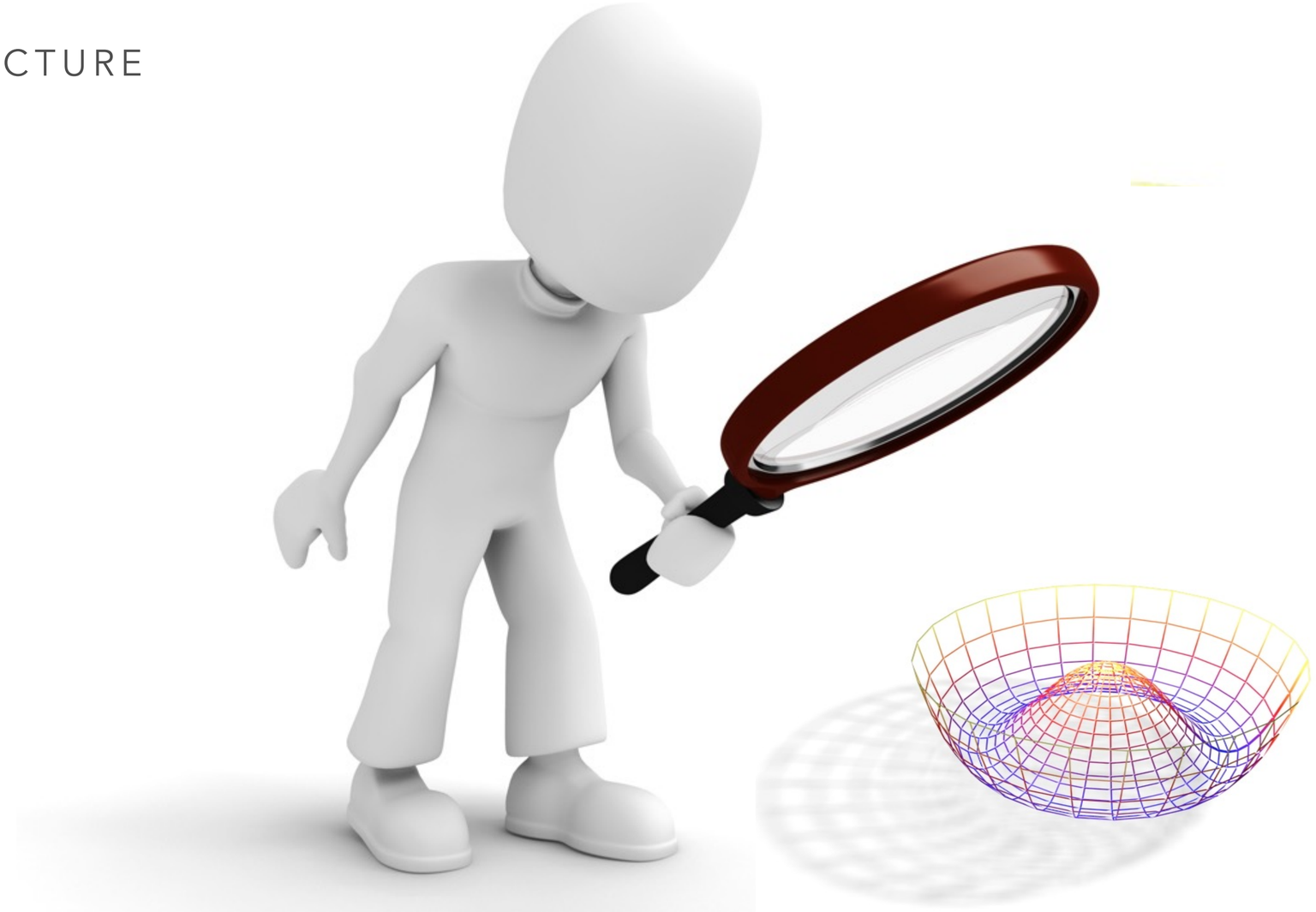
NYU Center for Data Science

Center for Cosmology and Particle Physics

MADMINER TUTORIAL

+ TOOLS & INFRASTRUCTURE



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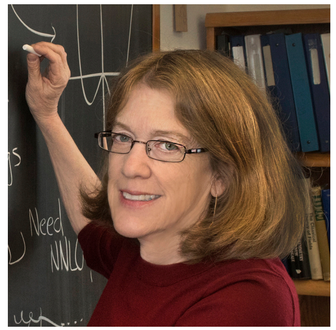

Sally Dawson


Sam Homiller


Giordon Stark


Matthew Feickert


Lukas Heinrich

NYU

MSDSE
Moore - Sloan
Data Science Environments

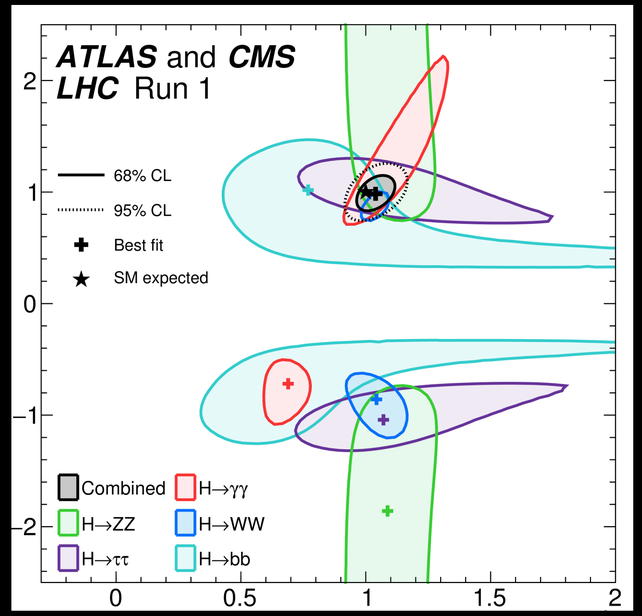
diana hep

iris hep
Institute for Research and Innovation
in Software for High Energy Physics

The SCAILFIN Project
scailfin.github.io

High-dimensional event data

[CMS]

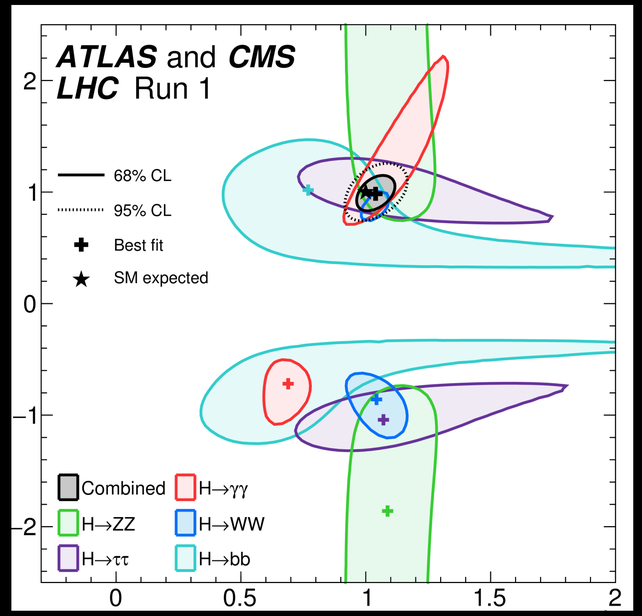


[ATLAS, CMS 1606.02266]

Precision constraints on new physics

High-dimensional event data

[CMS]



[ATLAS, CMS 1606.02266]

Precision constraints on new physics

Parameterization e.g. in Effective Field Theory:

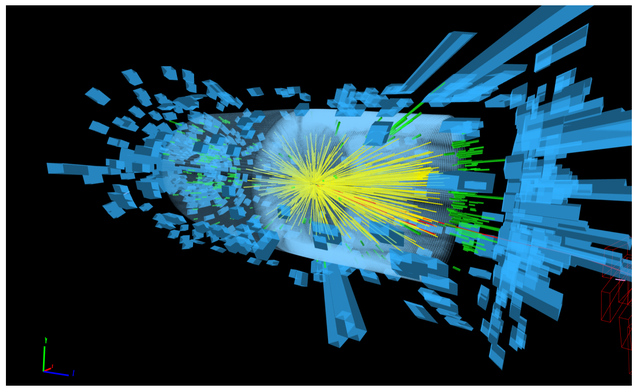
$$\mathcal{L}_{\mathrm{EFT}} = \mathcal{L}_{\mathrm{SM}} + \sum_i \frac{f_i}{\Lambda^2} \mathcal{O}_i + \dots$$

systematic expansion of new physics around Standard Model

10s to 100s "universal" parameters to measure

The likelihood is a key object

Let θ denote the coefficients of higher dimensional operators in the Lagrangian, x be high-dimensional data associated to an event, and $p(x \mid \theta) = \dfrac{1}{\sigma(\theta)} \dfrac{d\sigma}{d\theta}$ be the distribution for the data

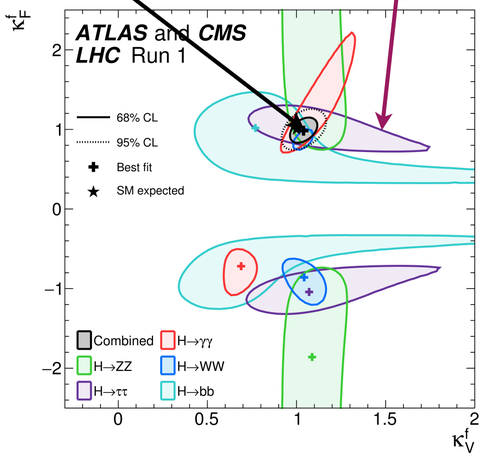


High-dimensional event data x

Likelihood function
$p(x|\theta)$

Maximum-likelihood estimator

Confidence limits based on likelihood ratio tests



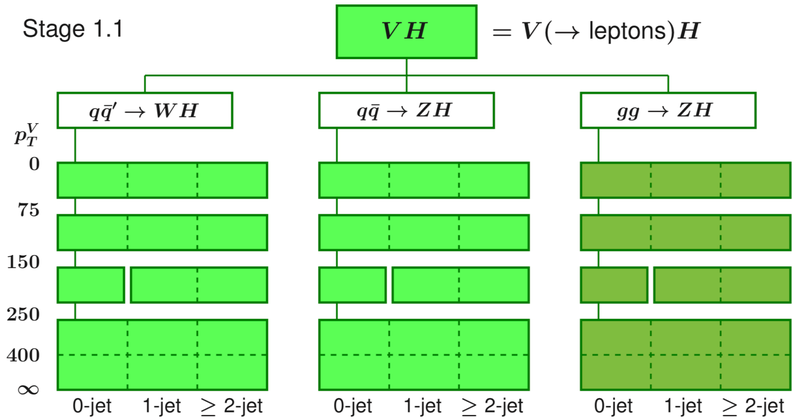
Constraints on parameters θ

Benchmarking STXS in fully differential in WH

[JB, S. Dawson, S. Homiller, F. Kling, T. Plehn 1908.06980]

- 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

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

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

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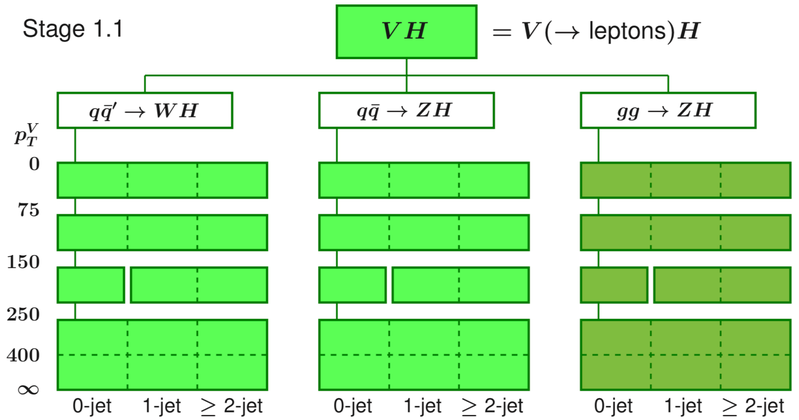

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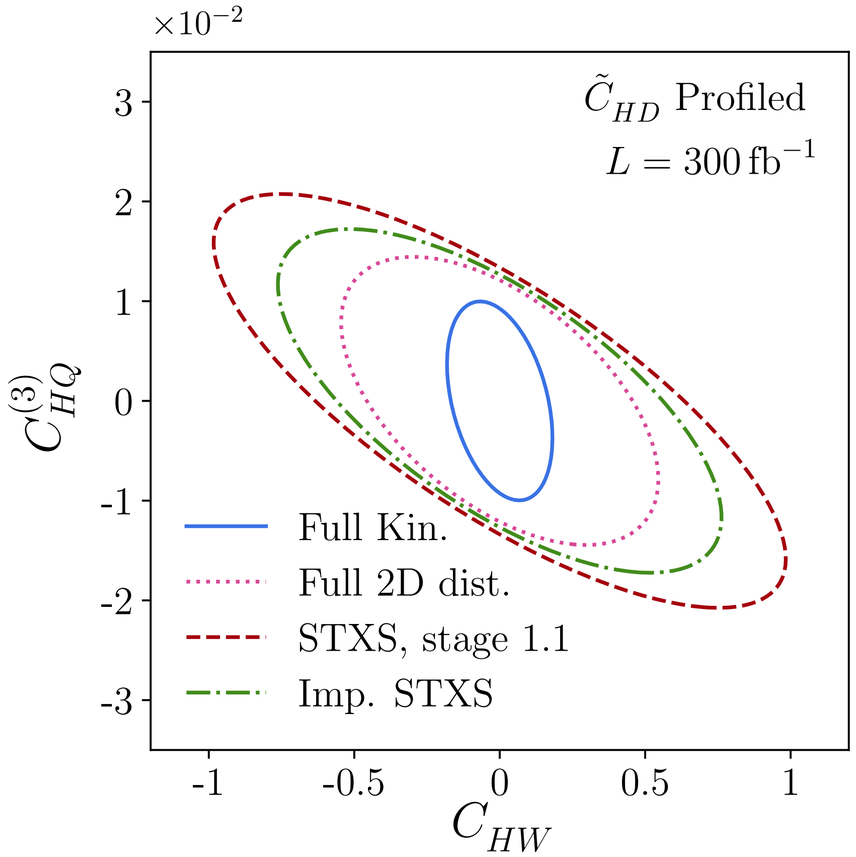
- Results: STXS are indeed sensitive to operators, adding a few more bins improve them, but a multivariate analysis is *much* stronger



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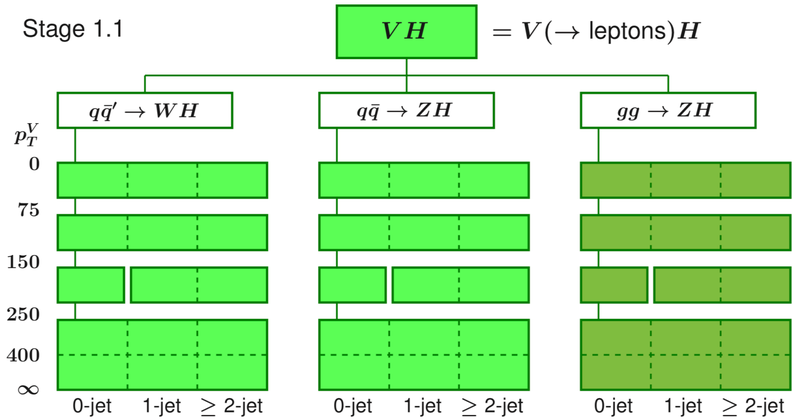

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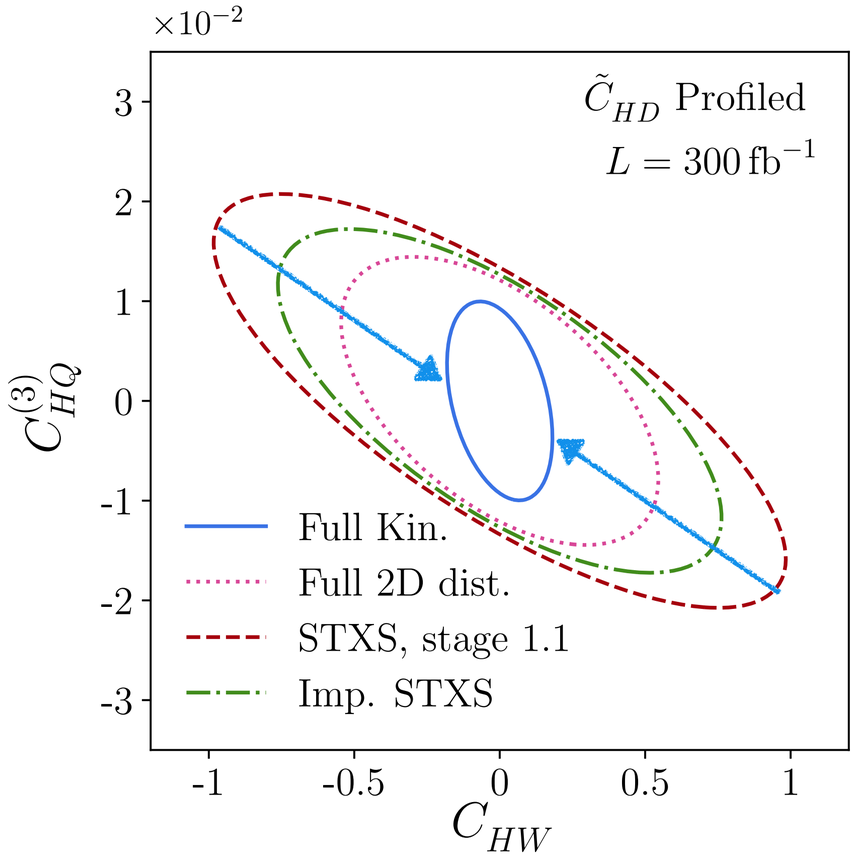
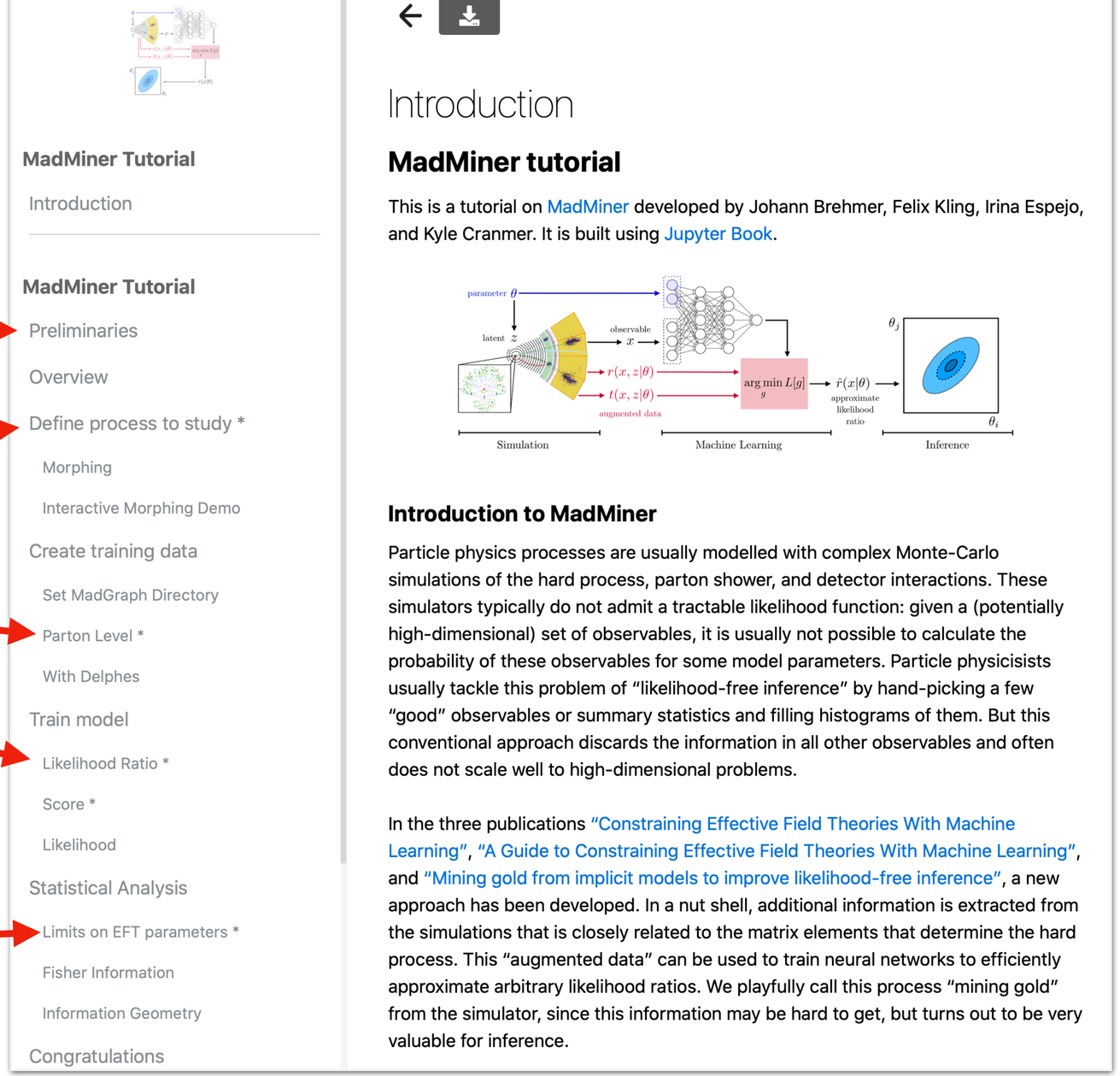


https://cranmer.github.io/madminer-tutorial/

Hands-on Tutorial

- Step-by-step instructions
- Do Preliminaries
  - Need to install Docker
  - And then start Jupyter
- Step 1 is fast
- Step 2 takes ~25 min
- Step 3 takes ~20 min
- While they are running I will lecture
- Then we will finish with results



The MadMiner for REANA

- Designed to scale to a cluster
  - Here six jobs for event generation and DELPHES simulation
  - Uses pre-built docker containers

reana

Home Examples Get Started Documentation News Roadmap Contact Blog

reana

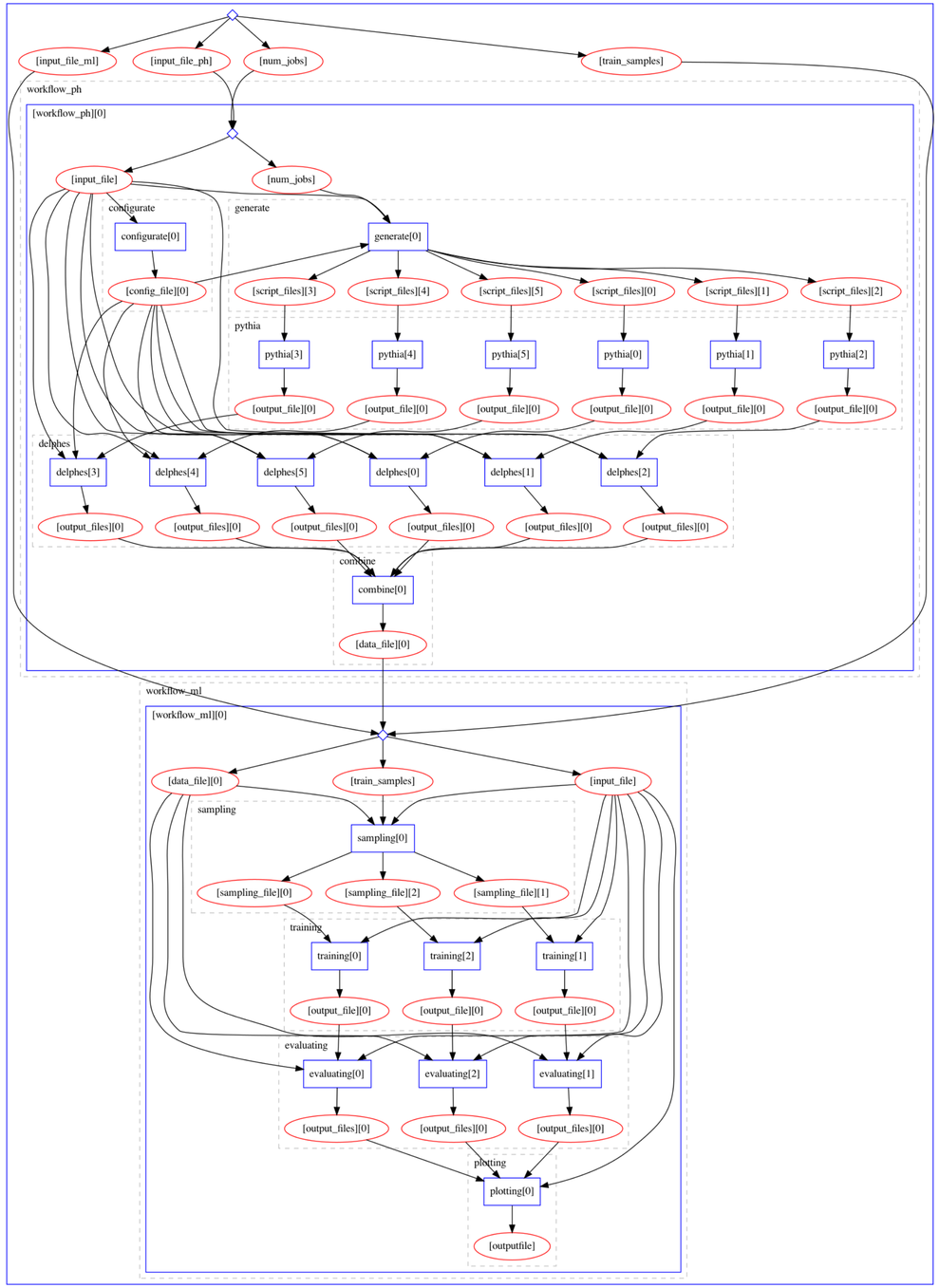
Reproducible research data analysis platform

Flexible	Scalable	Reusable	Free
Run many computational workflow engines.	Support for remote compute clouds.	Containerise once, reuse elsewhere. Cloud-native.	Free Software. MIT licence. Made with ❤ at CERN.

COMMON WORKFLOW LANGUAGE

kubernetes

CERN



Now for some bad news….

Particle physics processes do not have a tractable likelihood function.

Modeling particle physics processes

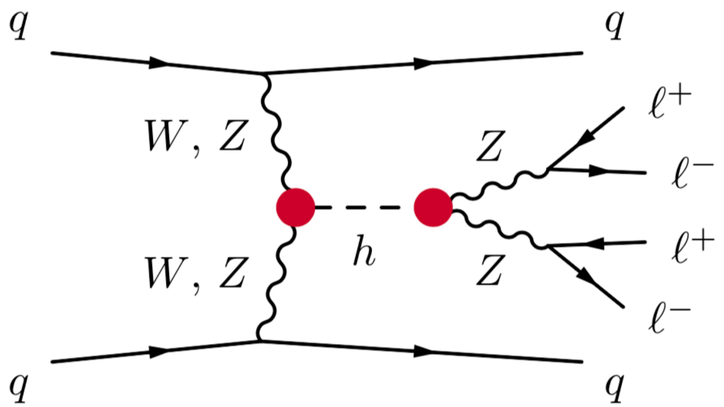
Theory
parameters
θ

Evolution

Modeling particle physics processes

Latent variables

Parton-level momenta z_p ← Theory parameters θ



Evolution

Modeling particle physics processes

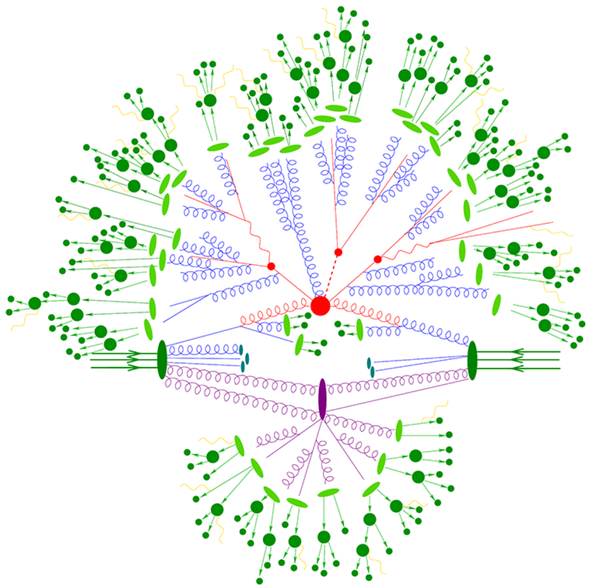
Latent variables

Shower splittings

Parton-level momenta

Theory parameters

z_s ← z_p ← θ



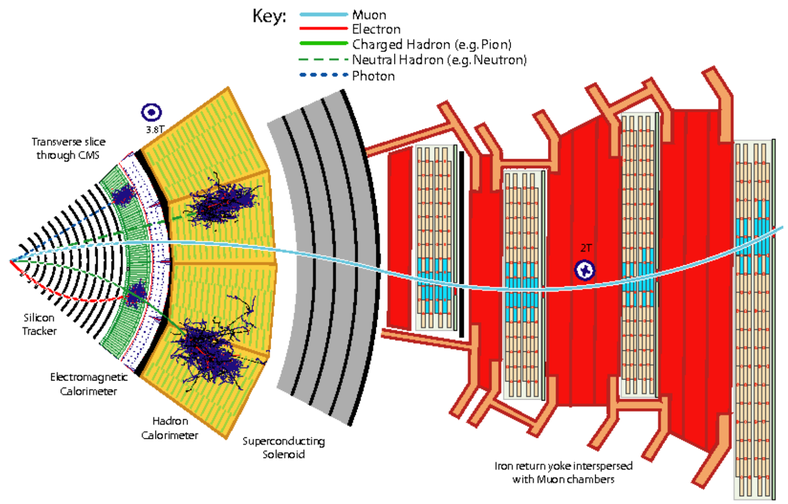
[F. Krauss]

Evolution

Modeling particle physics processes

Latent variables

Detector interactions	Shower splittings	Parton-level momenta	Theory parameters
z_d	z_s	z_p	θ



[CMS]

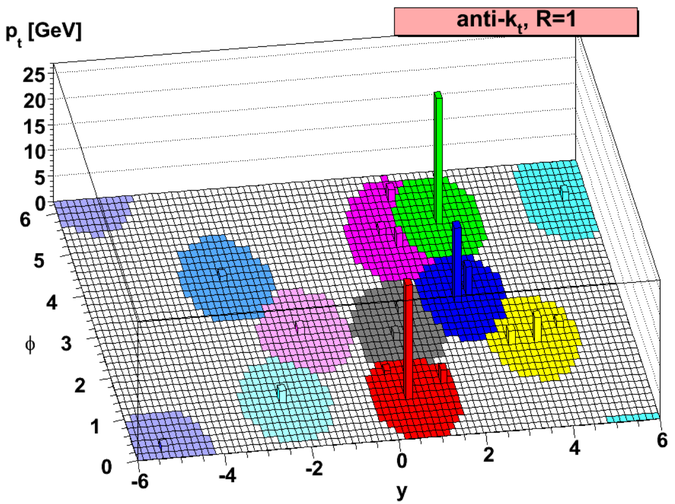
Evolution

Modeling particle physics processes

Latent variables

Observables | Detector interactions | Shower splittings | Parton-level momenta | Theory parameters

$x \leftarrow z_d \leftarrow z_s \leftarrow z_p \leftarrow \theta$



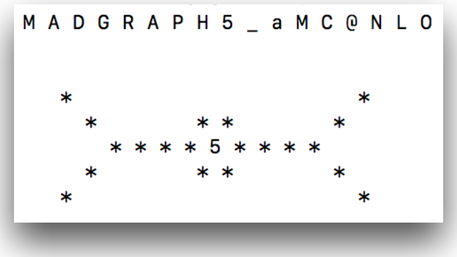
[M. Cacciari, G. Salam, G. Soyez 0802.1189]

Evolution

Modeling particle physics processes

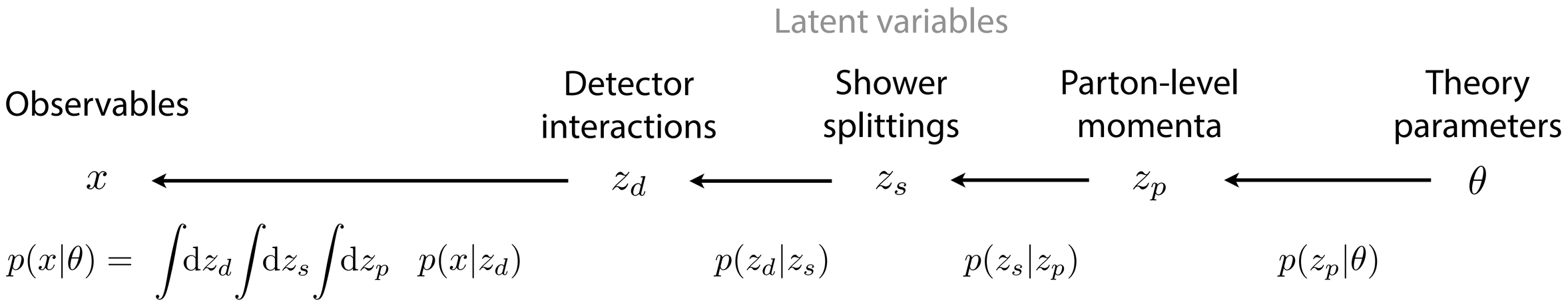
Latent variables

Observables	Detector interactions	Shower splittings	Parton-level momenta	Theory parameters
x	z_d	z_s	z_p	θ
Sample from	$p(x\|z_d)$	$p(z_d\|z_s)$	$p(z_s\|z_p)$	$p(z_p\|\theta)$



Prediction (simulation)

Modeling particle physics processes



Inference

Modeling particle physics processes

Latent variables

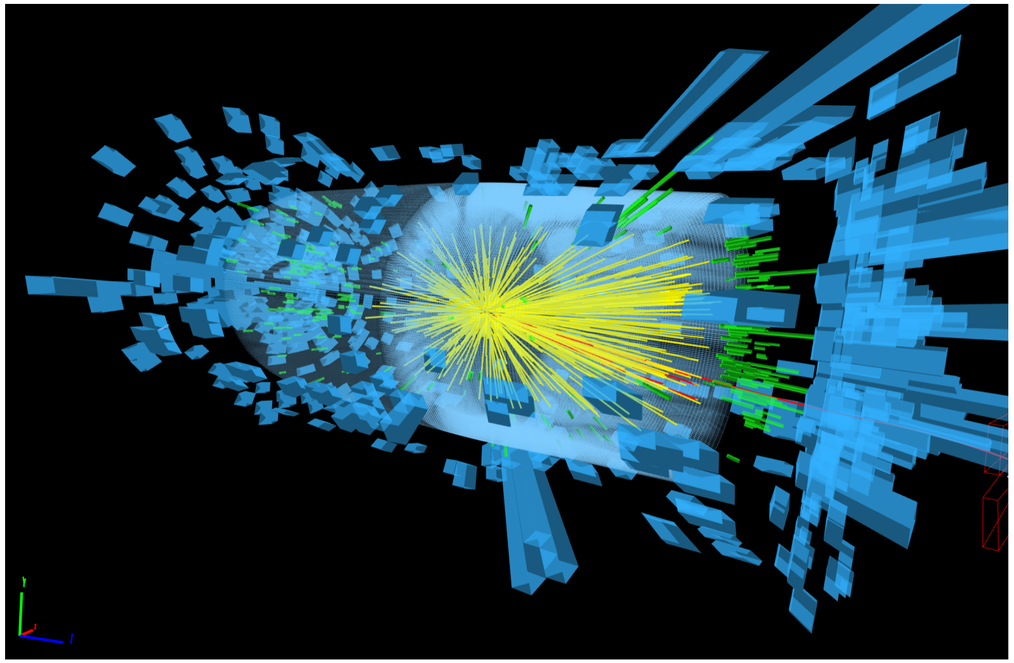
Observables	Detector interactions	Shower splittings	Parton-level momenta	Theory parameters
x	z_d	z_s	z_p	θ

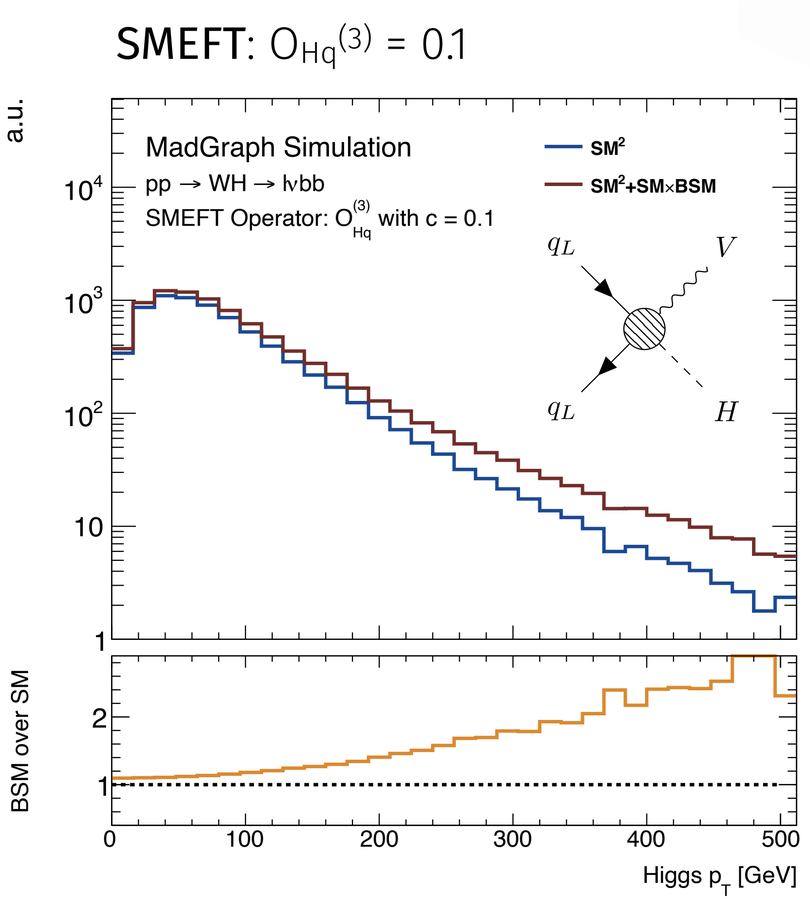
$$p(x|\theta) = \int \mathrm{d}z_d \int \mathrm{d}z_s \int \mathrm{d}z_p \; p(x|z_d) \quad p(z_d|z_s) \quad p(z_s|z_p) \quad p(z_p|\theta)$$

It's infeasible to calculate the integral over this enormous space!

Inference

What we usually do: number counting or singly differential

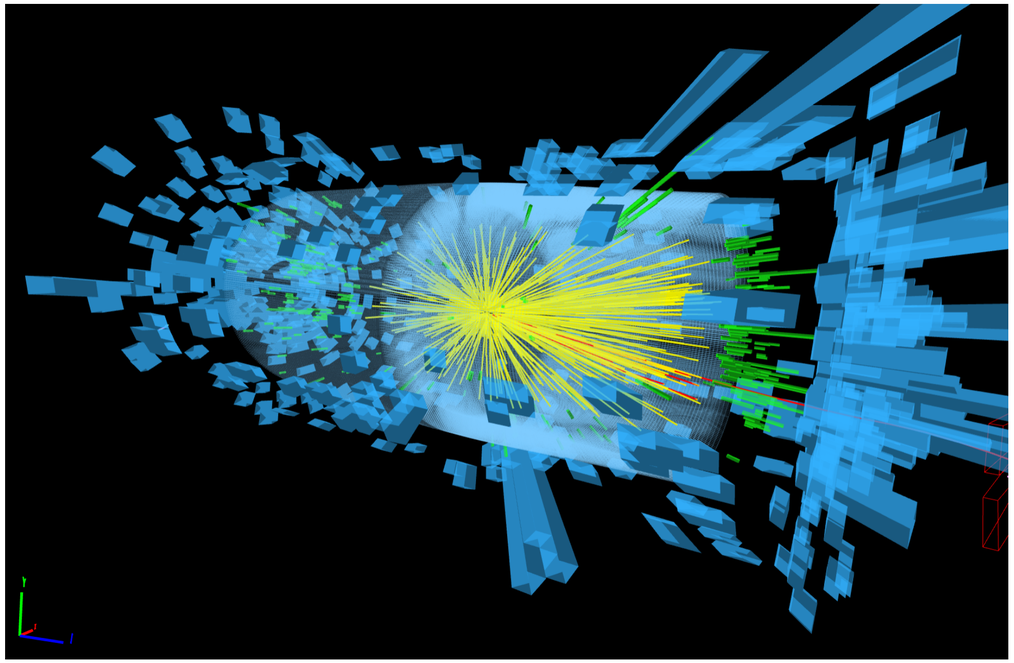


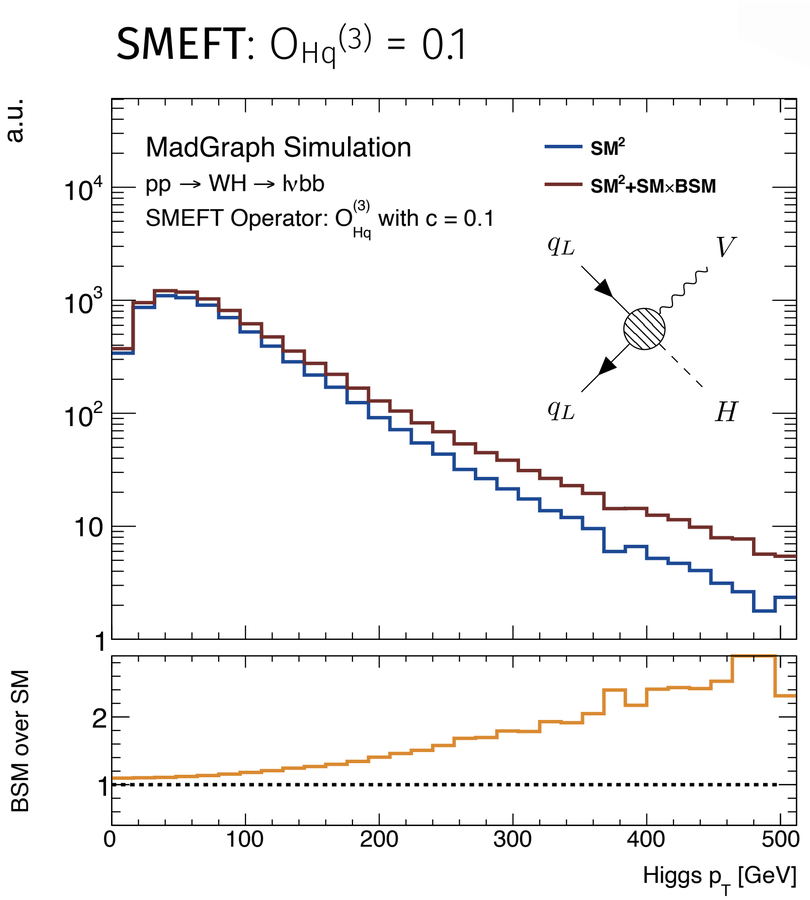


High-dimensional event data x

$p(x|\theta)$ cannot be calculated

What we usually do: number counting or singly differential





High-dimensional event data x

$p(x|\theta)$ cannot be calculated

One or two summary statistics x'

$p(x'|\theta)$ can be estimated with histograms

n.b. "summary statistic" = a sensitive observable

What if we could estimate the likelihood...

- for high-dimensional observables, including correlations?

  like MEM: no need to pick summary statistics

- including state-of-the-art shower and detector models?

  allowing for extra radiation, no need for transfer functions

- in microseconds?

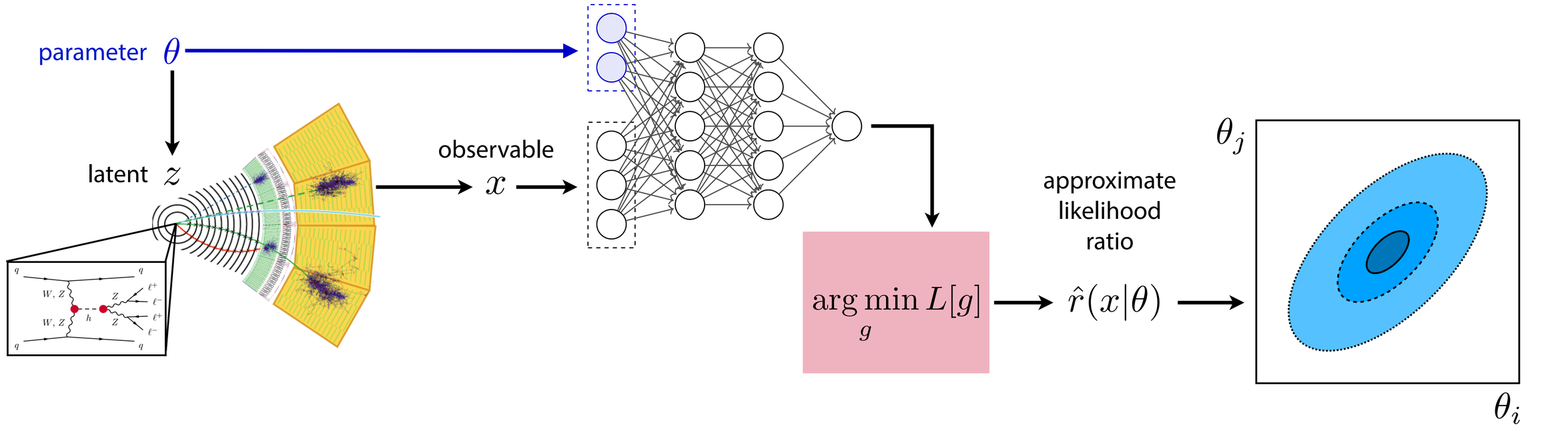
  amortized inference: train once, then always evaluate fast

- requiring less training examples than established machine learning methods?

  using matrix element information: “ML version of MEM”

Learning with Simulated Data

arXiv:1805.12244
PRL, arXiv:1805.00013
PRD, arXiv:1805.00020
physics.aps.org/articles/v11/90



Simulation

"Mining gold": Extract additional information from simulator

Machine Learning

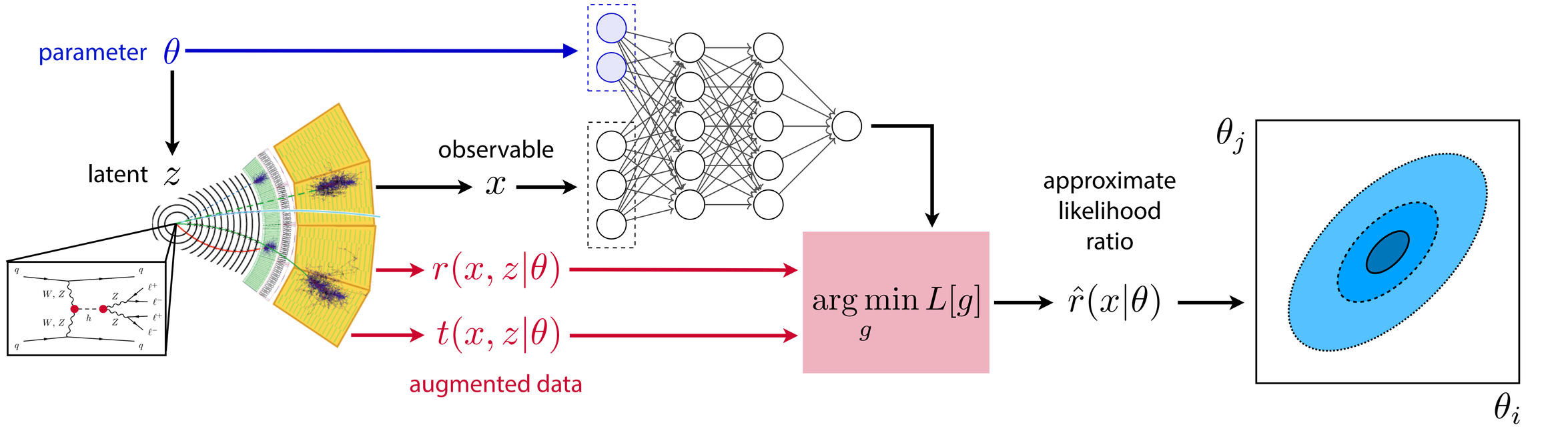
Use this information to train estimator for likelihood ratio

Inference

Limit setting with standard hypothesis tests

Learning with Augmented Data

arXiv:1805.12244
PRL, arXiv:1805.00013
PRD, arXiv:1805.00020
physics.aps.org/articles/v11/90



Simulation

"Mining gold": Extract additional information from simulator

Machine Learning

Use this information to train estimator for likelihood ratio

Inference

Limit setting with standard hypothesis tests

EFT Decomposition

$$\mathrm{d}\sigma \propto \left| \left(\mathcal{M}^{p}_{\mathrm{SM}} + \sum_i \frac{f_i}{\Lambda^2} \mathcal{M}^{p}_{i} \right) \right|^2 \left(\mathcal{M}^{d}_{\mathrm{SM}} + \sum_j \frac{f_j}{\Lambda^2} \mathcal{M}^{d}_{j} \right)$$

production

decay

Express EFT as a mixture:

$$p(x|\theta) = \sum_c w_c(\theta) p_c(x)$$

$w_c(\theta)$ are polynomials

$\nabla_\theta \log p(x|\theta)$ is now possible!

Process	Number of components for n operators					
	$\mathcal{O}(\Lambda^0)$	$\mathcal{O}(\Lambda^{-2})$	$\mathcal{O}(\Lambda^{-4})$	$\mathcal{O}(\Lambda^{-6})$	$\mathcal{O}(\Lambda^{-8})$	$\sum$
hV / WBF production	1	n	$\frac{n(n+1)}{2}$			$\frac{(n+1)(n+2)}{2}$
$h \to VV$ decay	1	n	$\frac{n(n+1)}{2}$			$\frac{(n+1)(n+2)}{2}$
Production + decay	1	n	$\frac{n(n+1)}{2}$	$\binom{n+2}{3}$	$\binom{n+3}{4}$	$\binom{n+4}{4}$

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

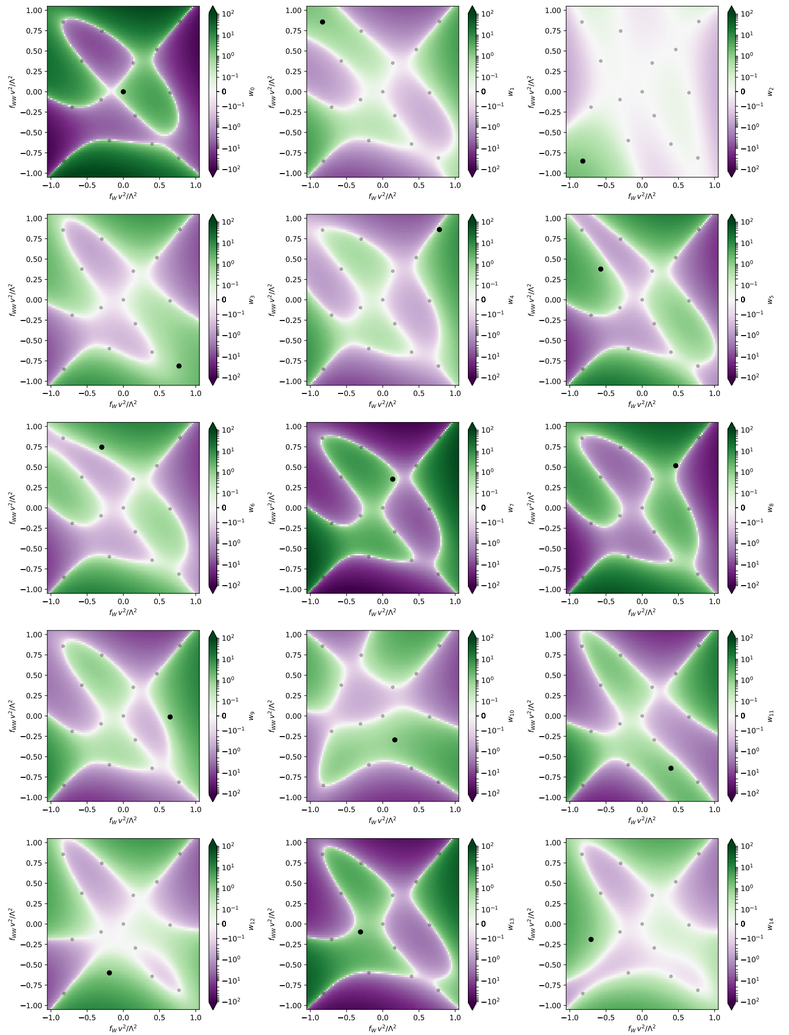
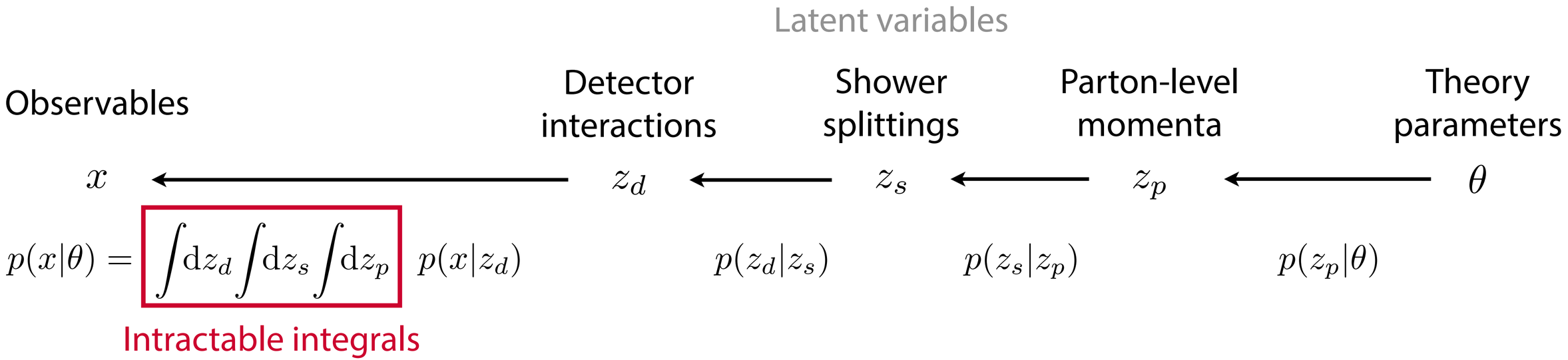


Figure 13: Morphing weights $w_i(\boldsymbol{\theta})$ for basis points distributed over the full relevant parameter space.

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

Mining gold from the simulator



Mining gold from the simulator

Latent variables

Observables	Detector interactions	Shower splittings	Parton-level momenta	Theory parameters
x	z_d	z_s	z_p	θ

$$p(x|\theta) = \int \mathrm{d}z_d \int \mathrm{d}z_s \int \mathrm{d}z_p \quad p(x|z_d) \qquad p(z_d|z_s) \qquad p(z_s|z_p) \qquad \boxed{p(z_p|\theta)}$$

Parton-level likelihood is given by matrix element and can be evaluated!

⇒ For each simulated event, we can calculate the joint likelihood ratio which depends on the specific evolution of the simulation:

$$r(x, z|\theta_0, \theta_1) \equiv \frac{p(x, z_d, z_s, z_p|\theta_0)}{p(x, z_d, z_s, z_p|\theta_1)} = \frac{p(x|z_d)}{p(x|z_d)} \frac{p(z_d|z_s)}{p(z_d|z_s)} \frac{p(z_s|z_p)}{p(z_s|z_p)} \quad \boxed{\frac{p(z_p|\theta_0)}{p(z_p|\theta_1)} \sim \frac{|\mathcal{M}(z_p|\theta_0)|^2}{|\mathcal{M}(z_p|\theta_1)|^2}}$$

The value of gold

We can calculate the joint likelihood ratio

$$r(x, z|\theta_0, \theta_1) \equiv \frac{p(x, z_d, z_s, z_p|\theta_0)}{p(x, z_d, z_s, z_p|\theta_1)}$$

("How much more likely is this simulated event, including all intermediate states, for θ_0 compared to θ_1?")

We want the likelihood ratio function

$$r(x|\theta_0, \theta_1) \equiv \frac{p(x|\theta_0)}{p(x|\theta_1)}$$

("How much more likely is the observation x for θ_0 compared to θ_1?")

The value of gold

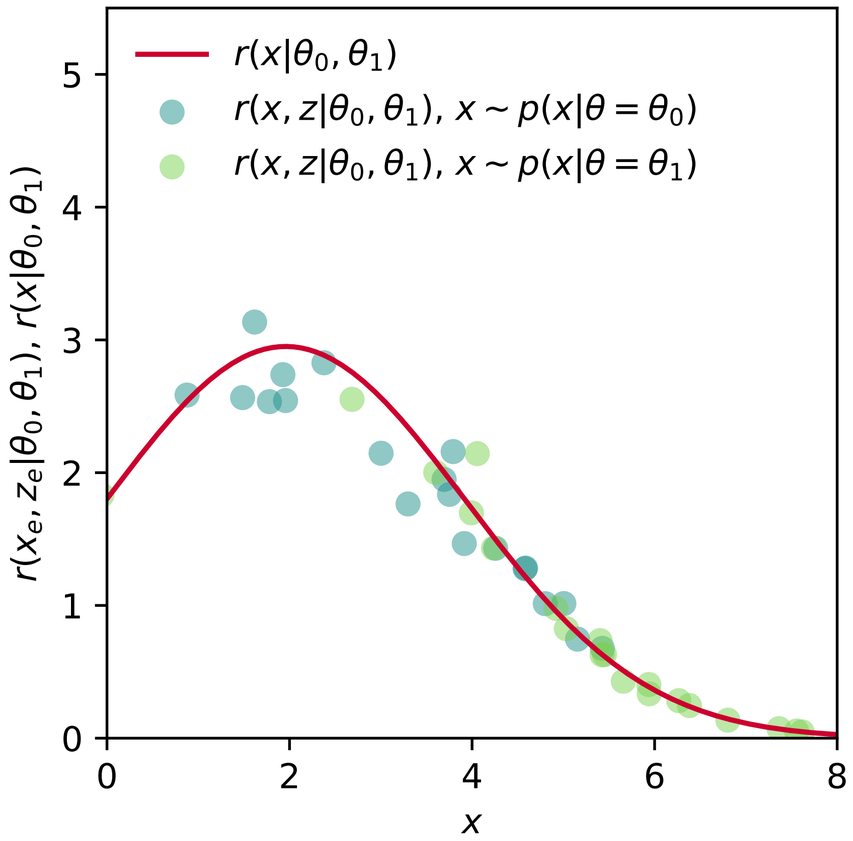
We can calculate the joint likelihood ratio

$$r(x, z|\theta_0, \theta_1) \equiv \frac{p(x, z_d, z_s, z_p|\theta_0)}{p(x, z_d, z_s, z_p|\theta_1)}$$

$r(x, z|\theta_0, \theta_1)$ are scattered around $r(x|\theta_0, \theta_1)$

We want the likelihood ratio function

$$r(x|\theta_0, \theta_1) \equiv \frac{p(x|\theta_0)}{p(x|\theta_1)}$$



The value of gold

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We want the likelihood ratio function

$$r(x|\theta_0, \theta_1) \equiv \frac{p(x|\theta_0)}{p(x|\theta_1)}$$

With $r(x, z|\theta_0, \theta_1)$, we define a functional like

$$L_r[\hat{r}(x|\theta_0, \theta_1)] = \int \mathrm{d}x \int \mathrm{d}z \; p(x, z|\theta_1) \left[(\hat{r}(x|\theta_0, \theta_1) - r(x, z|\theta_0, \theta_1))^2\right]$$

It is minimized by

$$\mathbb{E}_{z\sim p(z|x,\theta_1)}\left[r(x, z|\theta_0, \theta_1)\right] = \underset{\hat{r}(x|\theta_0,\theta_1)}{\arg\min}\; L_r[\hat{r}(x|\theta_0, \theta_1)]!$$

(And we can sample from $p(x, z|\theta)$ by running the simulator.)

The value of gold

We can calculate the joint likelihood ratio

$$r(x, z|\theta_0, \theta_1) \equiv \frac{p(x, z_d, z_s, z_p|\theta_0)}{p(x, z_d, z_s, z_p|\theta_1)}$$

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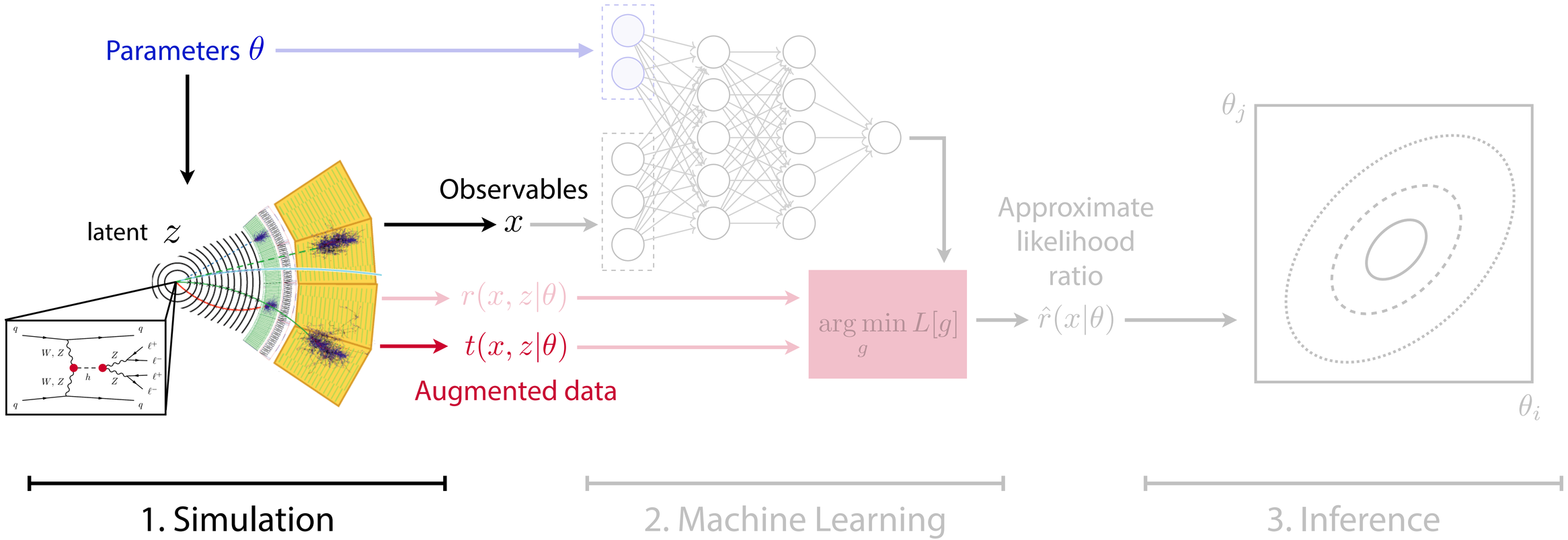
(And we can sample from $p(x, z|\theta)$ by running the simulator.)

.... and then magic ...

$$\begin{aligned}\mathbb{E}_{z\sim p(z|x,\theta_1)}\left[r(x, z|\theta_0, \theta_1)\right] &= \int \mathrm{d}z\, p(z|x, \theta_1)\, \frac{p(x, z|\theta_0)}{p(x, z|\theta_1)} \\ &= \int \mathrm{d}z\, \frac{p(x, z|\theta_1)}{p(x|\theta_1)}\, \frac{p(x, z|\theta_0)}{p(x, z|\theta_1)} \\ &= r(x|\theta_0, \theta_1)\ \textbf{!}\end{aligned}$$

Learning with Augmented Data



Learning the score (related to optimal observables)

Similar to the joint likelihood ratio, from the simulator we can extract the joint score

$$t(x, z|\theta_0) \equiv \nabla_\theta \log p(x, z_d, z_s, z_p|\theta)\Big|_{\theta_0}$$

We want the score

$$t(x|\theta_0) \equiv \nabla_\theta \log p(x|\theta)\Big|_{\theta_0}$$

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We want the score

$$t(x|\theta_0) \equiv \nabla_\theta \log p(x|\theta)\Big|_{\theta_0}$$

Given $t(x, z|\theta_0)$,
we define the functional

$$L_t[\hat{t}(x|\theta_0)] = \int \mathrm{d}x \int \mathrm{d}z \;\; p(x, z|\theta_0) \;\; \Big[\big(\hat{t}(x|\theta_0) - t(x, z|\theta_0)\big)^2\Big].$$

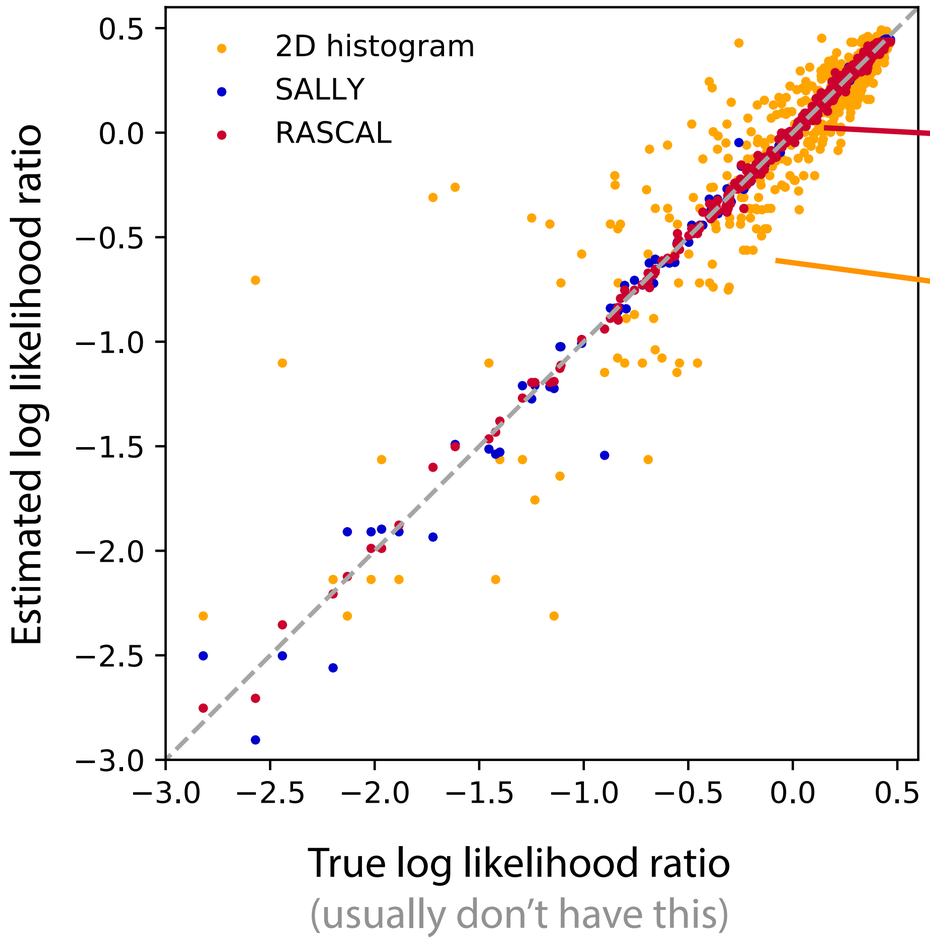
One can show it is minimized by

$$t(x|\theta_0) = \arg\min_{\hat{t}(x|\theta_0)} L_t[\hat{t}(x|\theta_0)]\,.$$

Again, we implement this minimization
through machine learning.

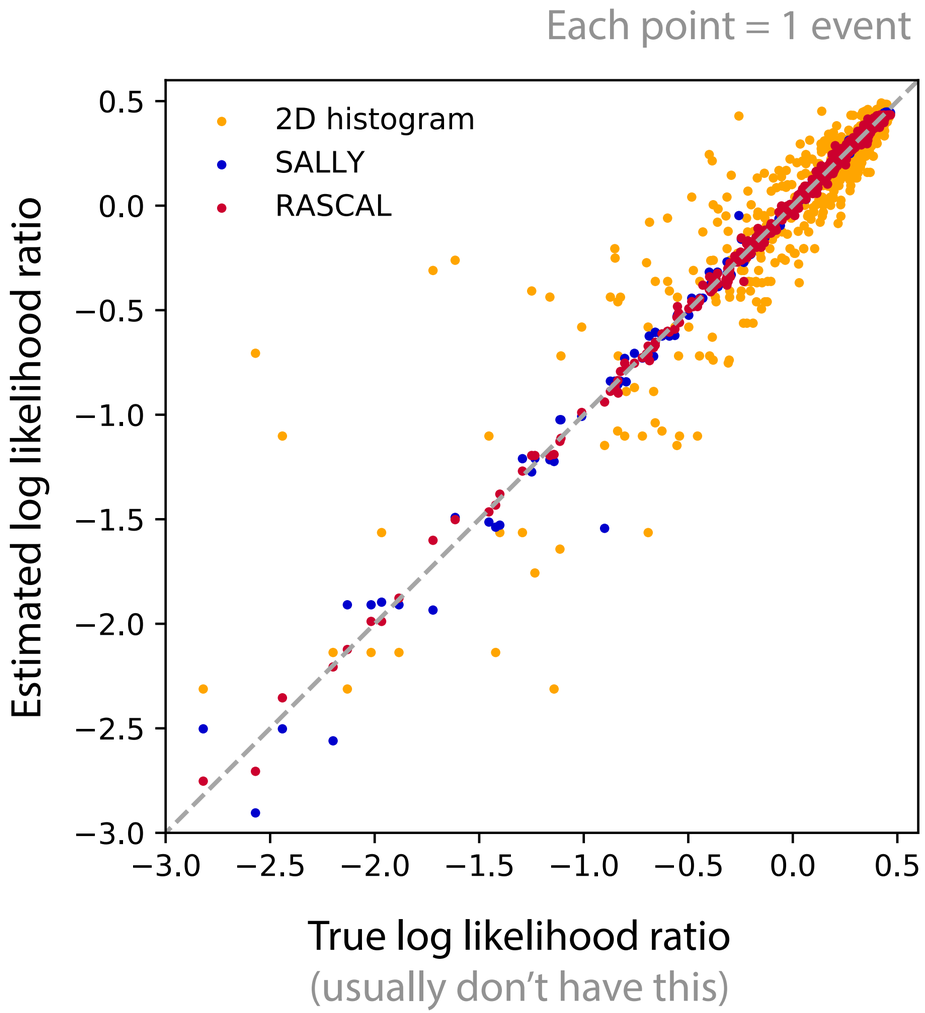
More precise likelihood ratio estimates with less training data

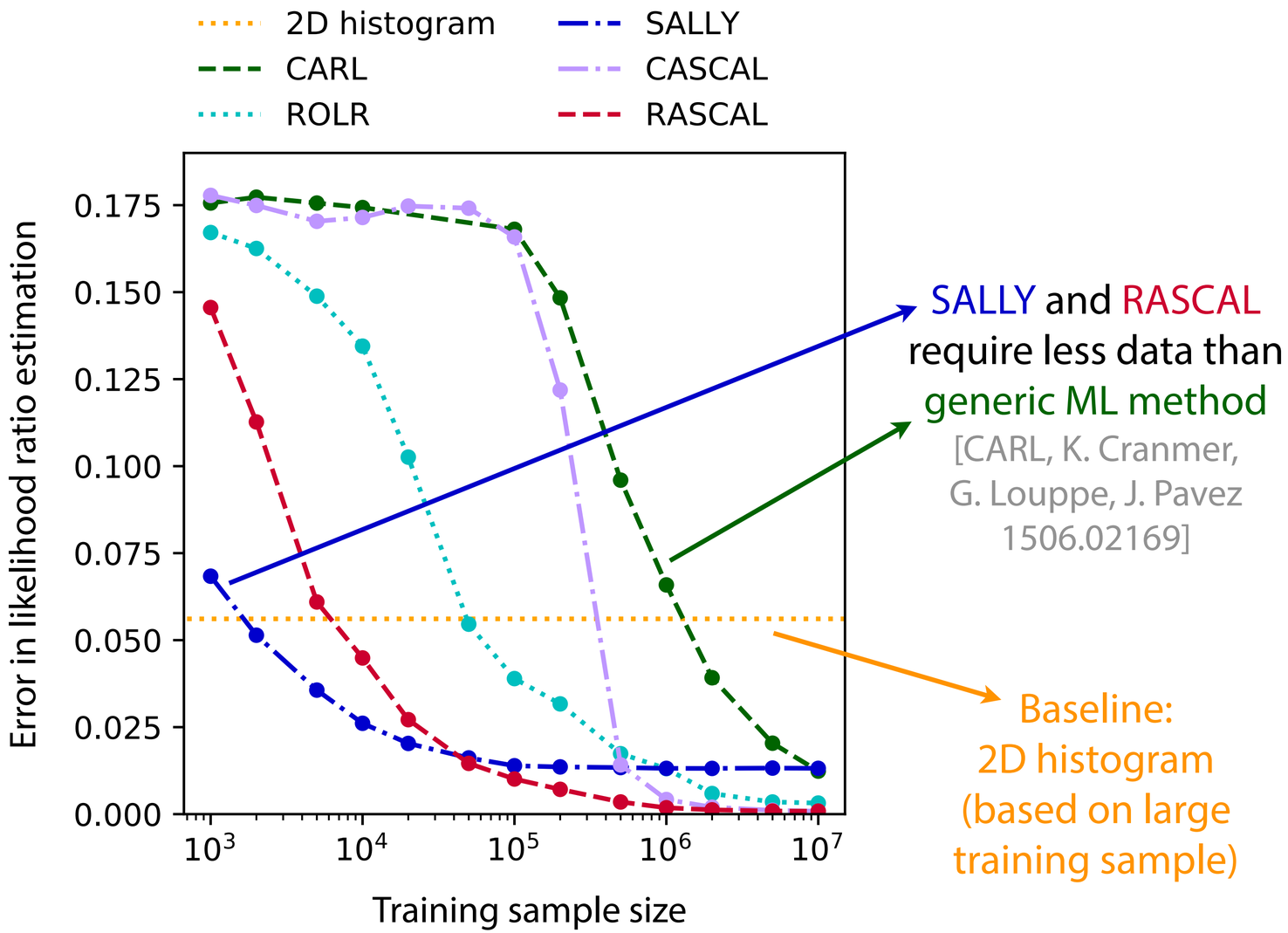
Each point = 1 event



RASCAL
gives more precise likelihood ratio estimates than the
2D histogram

More precise likelihood ratio estimates with less training data





MadMiner automates all of these methods.

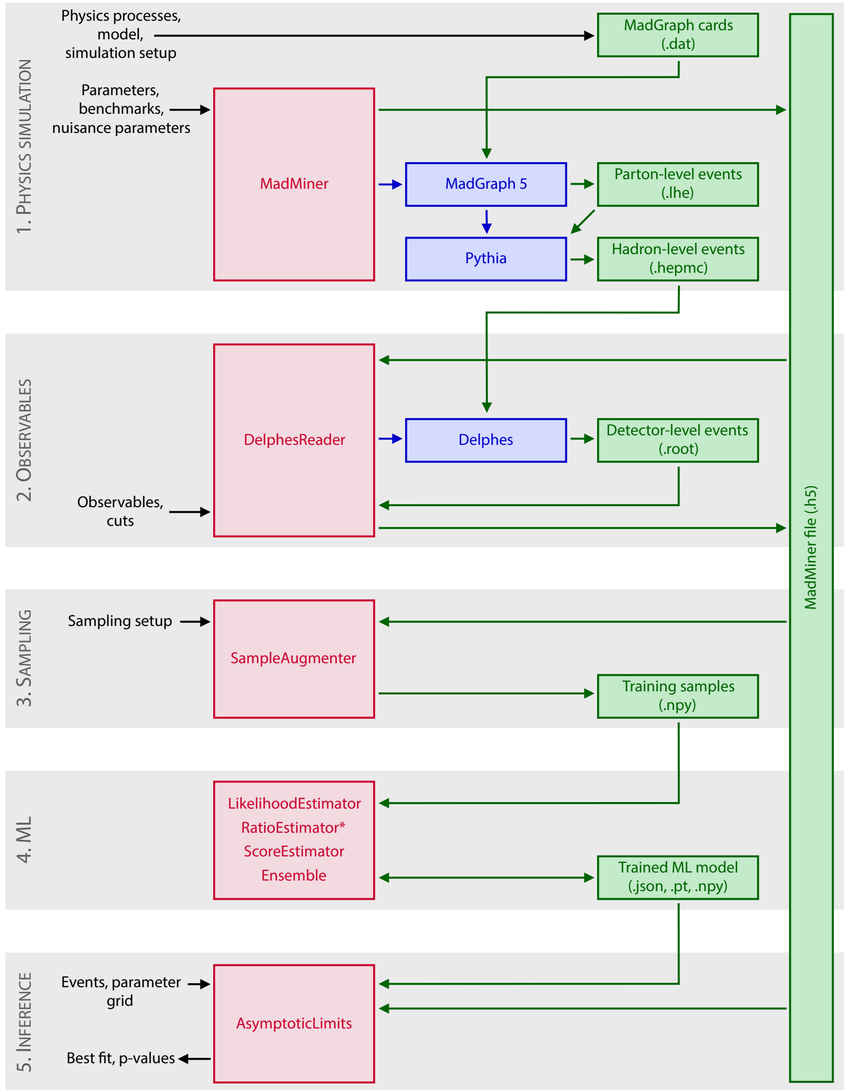
[JB, F. Kling, I. Espejo, K. Cranmer 1907.10621]

MadMiner

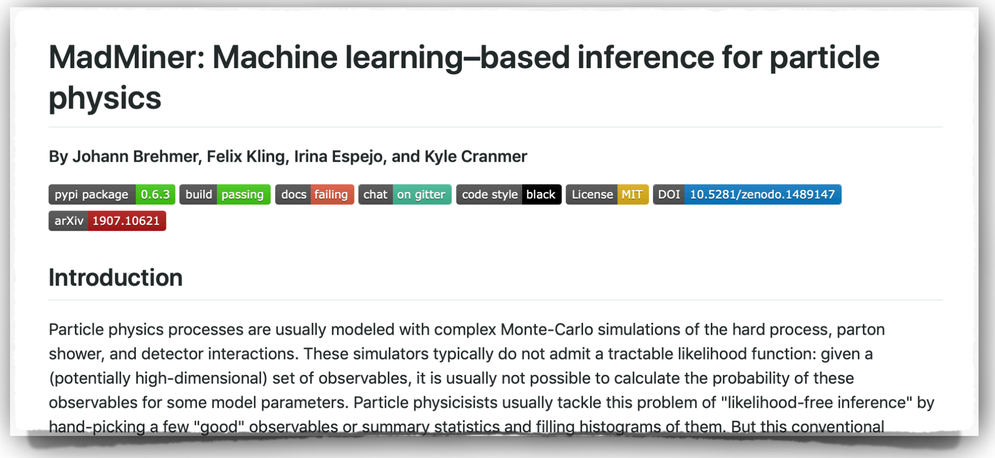
[JB, F. Kling, I. Espejo, K. Cranmer 1907.10621]

New Python package MadMiner makes it straightforward to apply the new techniques to LHC problems

- Out of the box: Pheno-level analyses
  - MadGraph, Pythia, Delphes, (could be GEANT4)
  - Systematic uncertainties from PDF / scale variation
- Scalable to state-of-the-art experimental tools
  - Mostly requires bookkeeping of fully differential cross sections
- Modular interface
  - Extensive documentation
  - Embedded into Python / ML ecosystem



MadMiner resources



MadMiner: Machine learning–based inference for particle physics

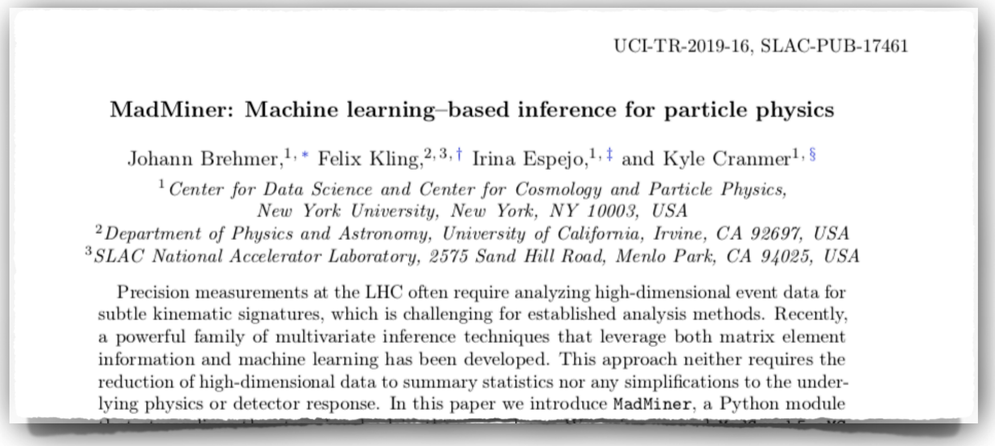
By Johann Brehmer, Felix Kling, Irina Espejo, and Kyle Cranmer

pypi package 0.6.3 | build passing | docs failing | chat on gitter | code style black | License MIT | DOI 10.5281/zenodo.1489147 | arXiv 1907.10621

Introduction

Particle physics processes are usually modeled with complex Monte-Carlo simulations of the hard process, parton shower, and detector interactions. These simulators typically do not admit a tractable likelihood function: given a (potentially high-dimensional) set of observables, it is usually not possible to calculate the probability of these observables for some model parameters. Particle physicisists usually tackle this problem of "likelihood-free inference" by hand-picking a few "good" observables or summary statistics and filling histograms of them. But this conventional

Repository and tutorials:
github.com/johannbrehmer/madminer



UCI-TR-2019-16, SLAC-PUB-17461

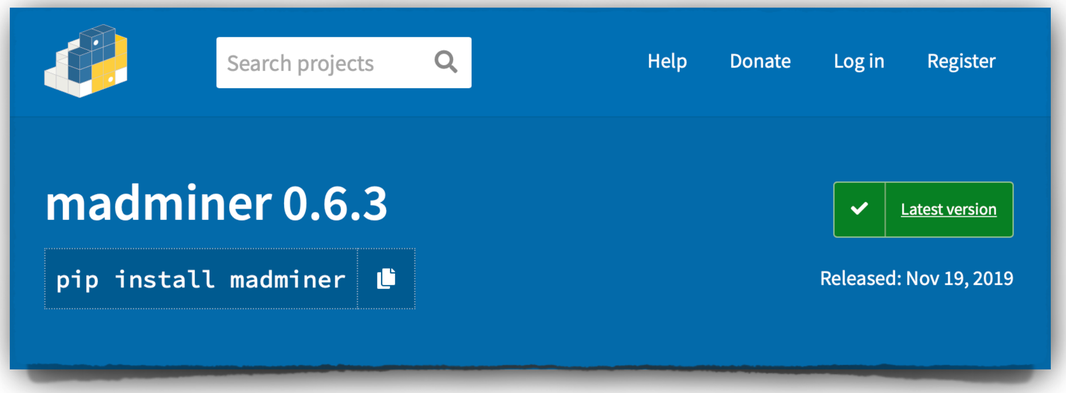
MadMiner: Machine learning–based inference for particle physics

Johann Brehmer,[1,*] Felix Kling,[2,3,†] Irina Espejo,[1,‡] and Kyle Cranmer[1,§]

[1] *Center for Data Science and Center for Cosmology and Particle Physics, New York University, New York, NY 10003, USA*
[2] *Department of Physics and Astronomy, University of California, Irvine, CA 92697, USA*
[3] *SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA*

Precision measurements at the LHC often require analyzing high-dimensional event data for subtle kinematic signatures, which is challenging for established analysis methods. Recently, a powerful family of multivariate inference techniques that leverage both matrix element information and machine learning has been developed. This approach neither requires the reduction of high-dimensional data to summary statistics nor any simplifications to the underlying physics or detector response. In this paper we introduce `MadMiner`, a Python module

Paper with detailed explanations:
1907.10621



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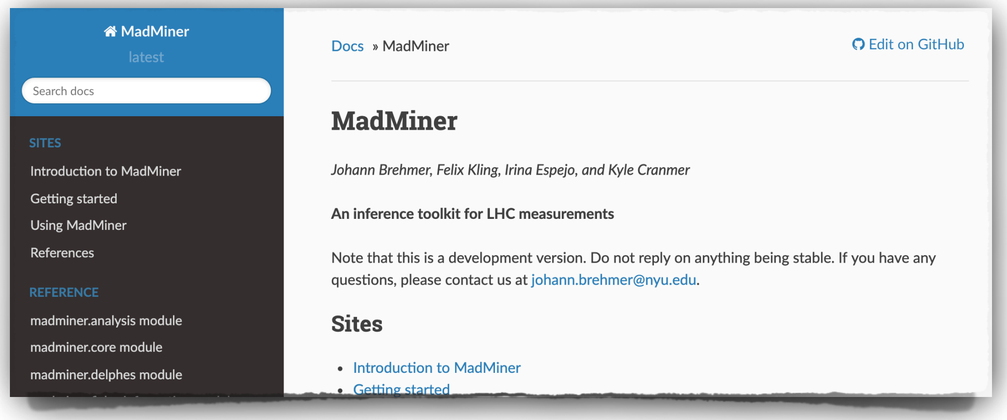
madminer 0.6.3

Latest version

pip install madminer

Released: Nov 19, 2019

Installation:
`pip install madminer`



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References

REFERENCE
madminer.analysis module
madminer.core module
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Docs » MadMiner

Edit on GitHub

MadMiner

Johann Brehmer, Felix Kling, Irina Espejo, and Kyle Cranmer

An inference toolkit for LHC measurements

Note that this is a development version. Do not reply on anything being stable. If you have any questions, please contact us at johann.brehmer@nyu.edu.

Sites

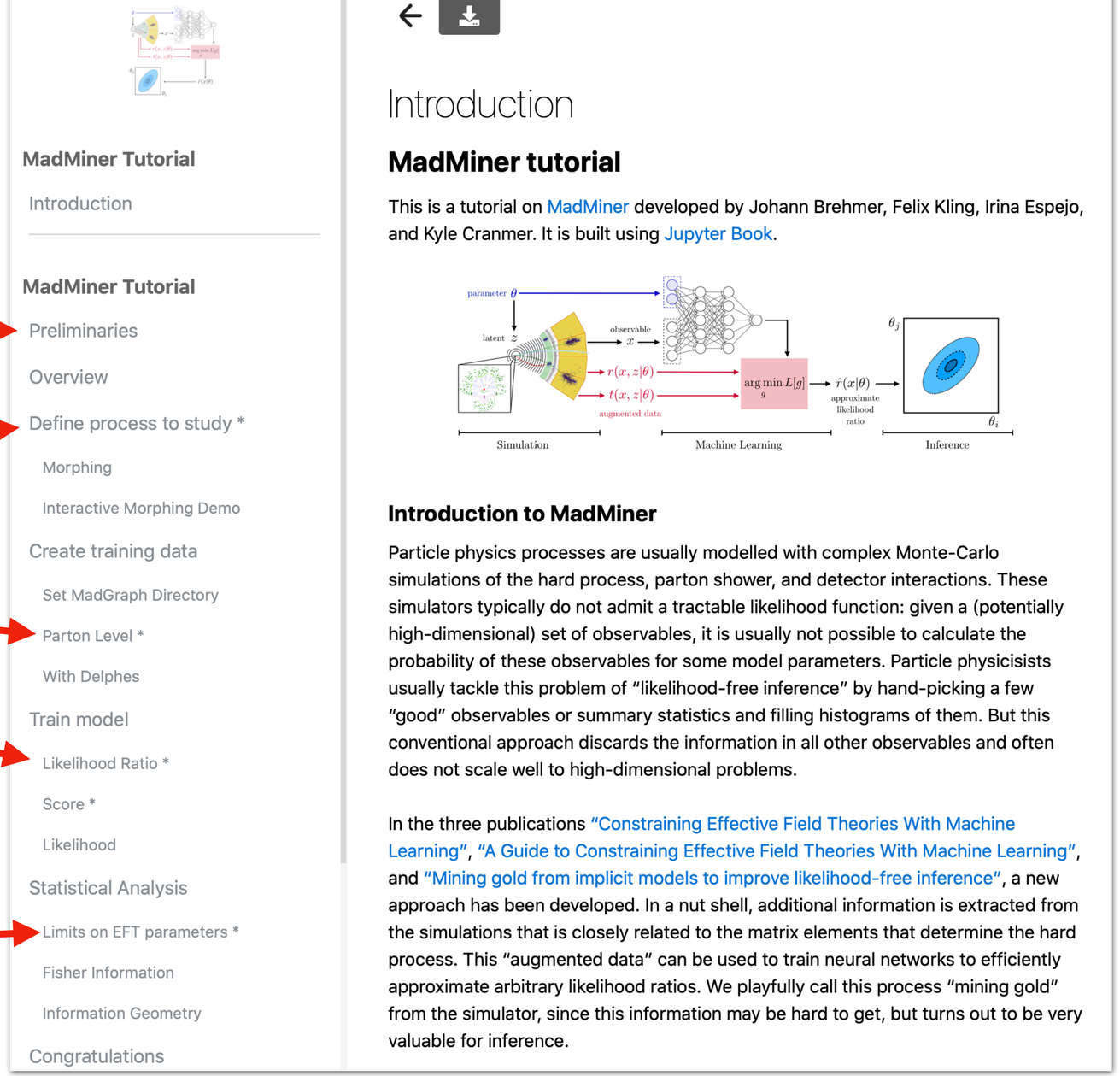
- Introduction to MadMiner
- Getting started

API documentation:
madminer.readthedocs.io

https://cranmer.github.io/madminer-tutorial/

Hands-on Tutorial

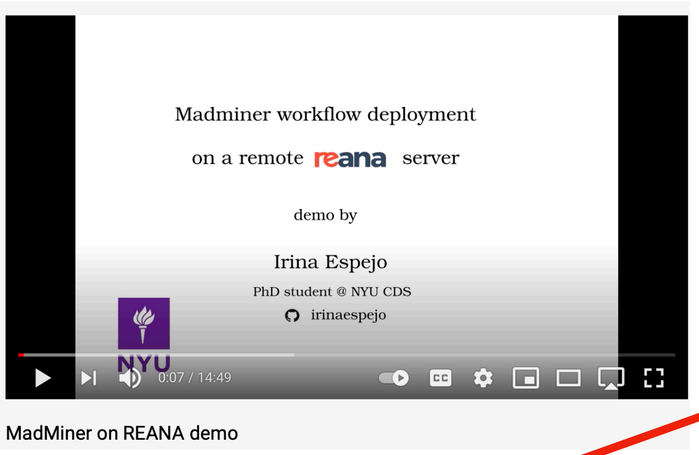
- Step-by-step instructions
- Do Preliminaries
  - Need to install Docker
  - And then start Jupyter
- Step 1 is fast
- Step 2 takes ~25 min
- Step 3 takes ~20 min
- While they are running I will lecture
- Then we will finish with results



https://cranmer.github.io/madminer-tutorial/

New: MadMiner on REANA

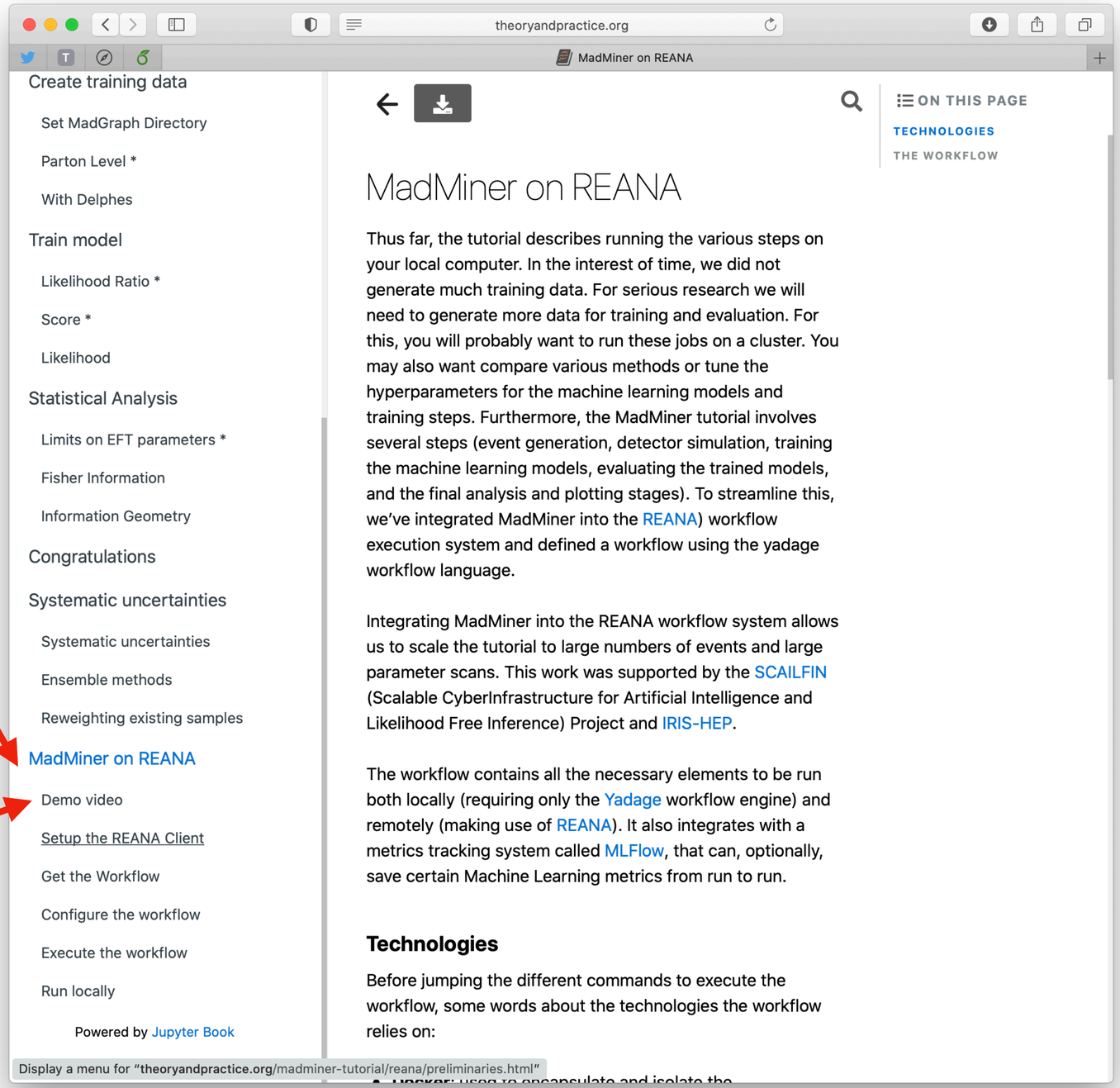
- Step-by-step instructions
- Do Preliminaries
  - Setup REANA Client
  - Get the workflow
  - Run on REANA
  - Run locally



MadMiner on REANA demo

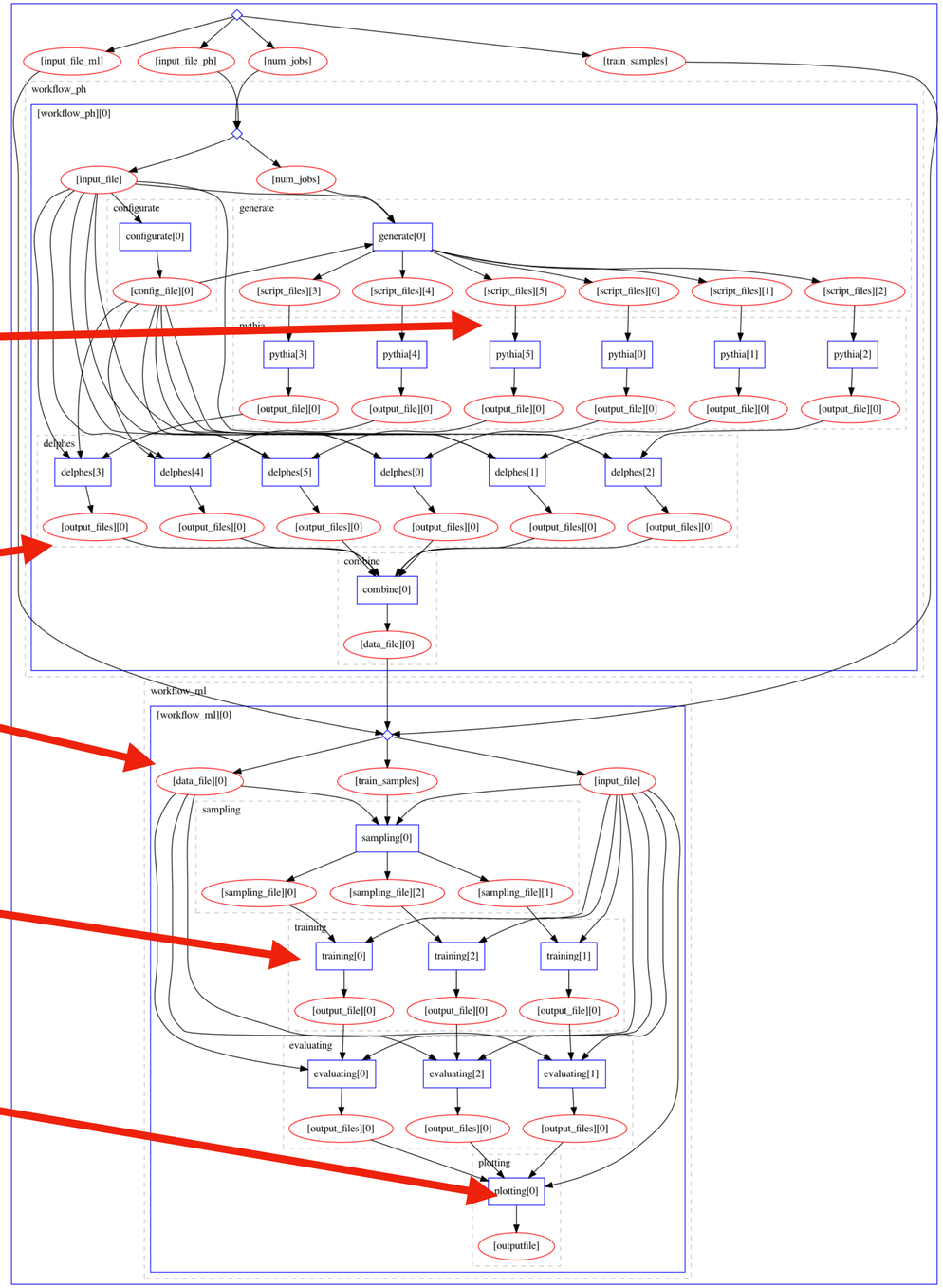
- There's also a video

https://www.youtube.com/watch?v=jzU5i-FKy6g



The MadMiner for REANA

- Designed to scale to a cluster
  - Here six jobs for event generation and DELPHES simulation
  - Uses pre-built docker containers
- Combines data generation and machine learning sub-workflows
- ML / inference workflow is configurable
  - Here 3 methods (SALLY, ALICE, ALICES) are being trained and evaluated
  - Followed by plots
- Launch the entire workflow with a single command:
  - make run-reana (remote)
  - make run-yadage (locally)



Configuring the workflow

- You can get the workflow from GitHub
  - Has top-level combined workflow as well as
  - madminer-ph sub-workflow
  - madminer-ml sub-workflow
  - Uses pre-built docker containers
- See madminer-*/workflow/input.yml for configuration

```
madminer-workflow$ git clone --recurse-submodules https://github.com/scailfin/madminer-workflow
madminer-workflow$ cd madminer-workflow/
madminer-workflow$ l
total 32
-rw-r--r--  1 cranmer  staff   1.1K Feb 11 16:11 LICENSE
-rw-r--r--  1 cranmer  staff   1.4K Feb 11 16:11 Makefile
-rw-r--r--  1 cranmer  staff   4.9K Feb 11 16:11 README.md
drwxr-xr-x  3 cranmer  staff    96B Feb 11 16:11 docs
drwxr-xr-x  4 cranmer  staff   128B Feb 11 16:11 modules
drwxr-xr-x  6 cranmer  staff   192B Feb 11 16:14 reana
madminer-workflow$ l modules/
total 0
drwxr-xr-x  17 cranmer  staff   544B Feb 11 16:11 madminer-workflow-ml
drwxr-xr-x  15 cranmer  staff   480B Feb 11 16:11 madminer-workflow-ph
madminer-workflow$ l modules/madminer-workflow-ph/workflow/input.yml
-rw-r--r--  1 cranmer  staff   1.4K Feb 11 16:11 modules/madminer-workflow-ph/workflow/input.yml
madminer-workflow$ l modules/madminer-workflow-ml/workflow/input.yml
-rw-r--r--  1 cranmer  staff   2.4K Feb 11 16:11 modules/madminer-workflow-ml/workflow/input.yml
```

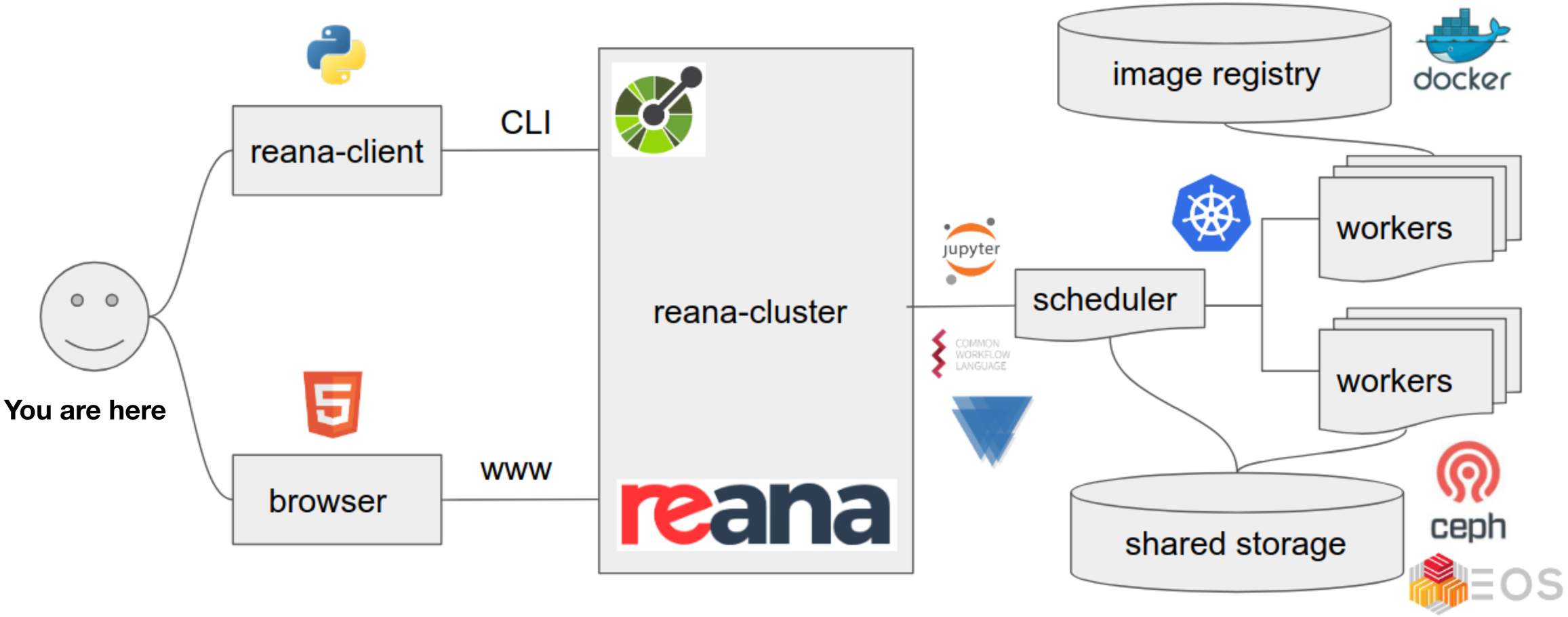
These configuration options mirror the options you see in the python notebooks

- See madminer-*/workflow/input.yml for configuration

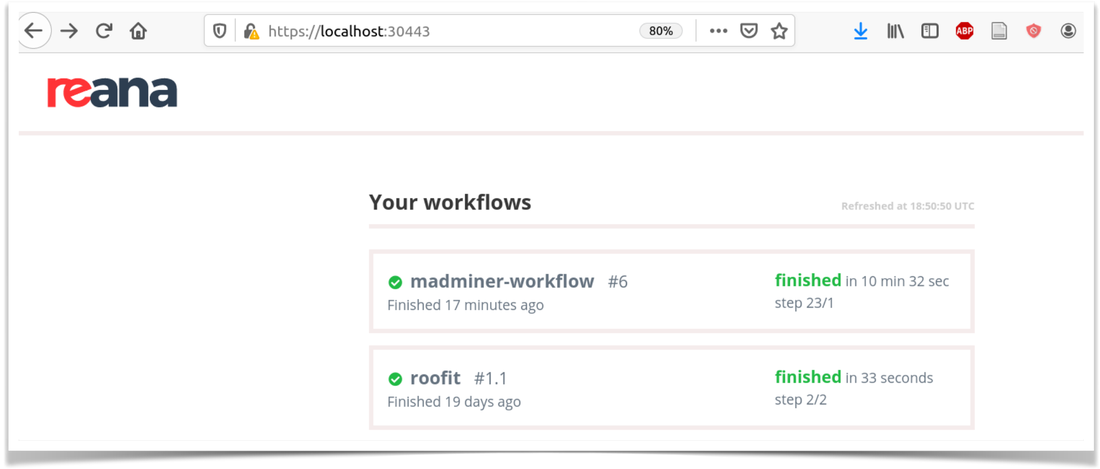
```yaml
parameters:
  - parameter_name: 'CWL2'
    lha_block: 'dim6'
    lha_id: 2
    morphing_max_power: 2
    param_card_transform: '16.52*theta'
    parameter_range: (-10.0,10.0)

  - parameter_name: 'CPWL2'
    lha_block: 'dim6'
    lha_id: 5
    morphing_max_power: 2
    param_card_transform: '16.52*theta'
    parameter_range: (-10.0,10.0)

# The number of benchmark params must match the number of parameters above
benchmarks:
  - benchmark: 1
    name: 'sm'
    parameter_name_1: 'CWL2'
    value_1: 0.0
    parameter_name_2: 'CPWL2'
    value_2: 0.0

  - benchmark: 2
    name: 'w'
    parameter_name_1: 'CWL2'
    value_1: 10.0
    parameter_name_2: 'CPWL2'
    value_2: 0.0
```

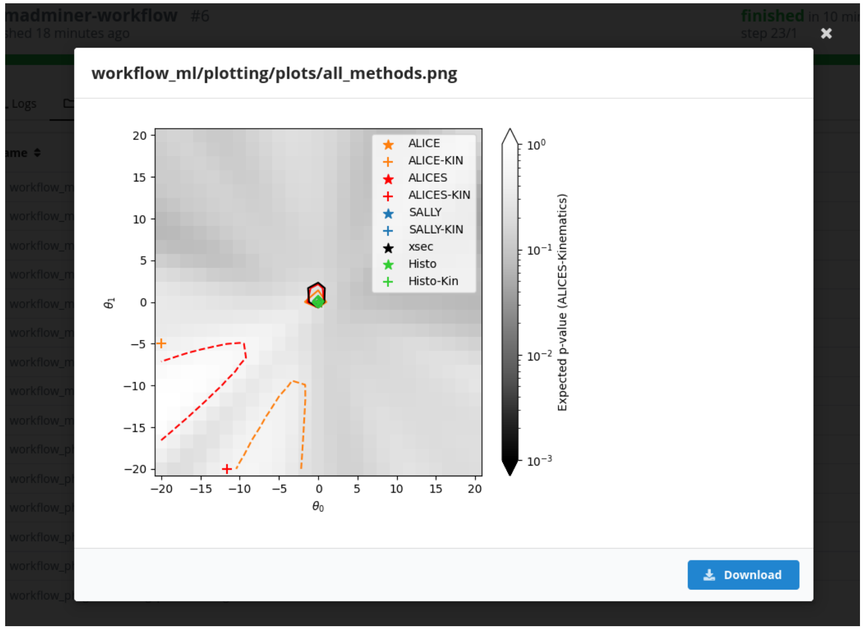
```yaml
##########################
### SHARED AMONG STEPS ####
##########################

estimator: 'parameterized'
methods: ['alice', 'alices', 'sally']

# Region of theory we want to test
asymptotic_limits:
  region:
    theta_0:
      min: -20.0
      max: 20.0
    theta_1:
      min: -20.0
      max: 20.0
  resolutions: [25, 25]
  theta_true: [0.0 ,0.0]

##########################
###### STEP: SAMPLING #####
##########################
alice:
  # When selecting random_morphing points as sampling method, the number of prior parameters
  # must be equal to the parameters specified in the Physics workflow 'input.yml' file
  # Ref: https://github.com/scailfin/madminer-workflow-ph/blob/master/workflow/input.yml#L5
  theta_0:
    sampling_method: 'random_morphing_points'
    sampling_number: 20
    prior:
      - parameter_0:
          prior_shape: 'gaussian'
          prior_param_0: 0.0
          prior_param_1: 1.0
```

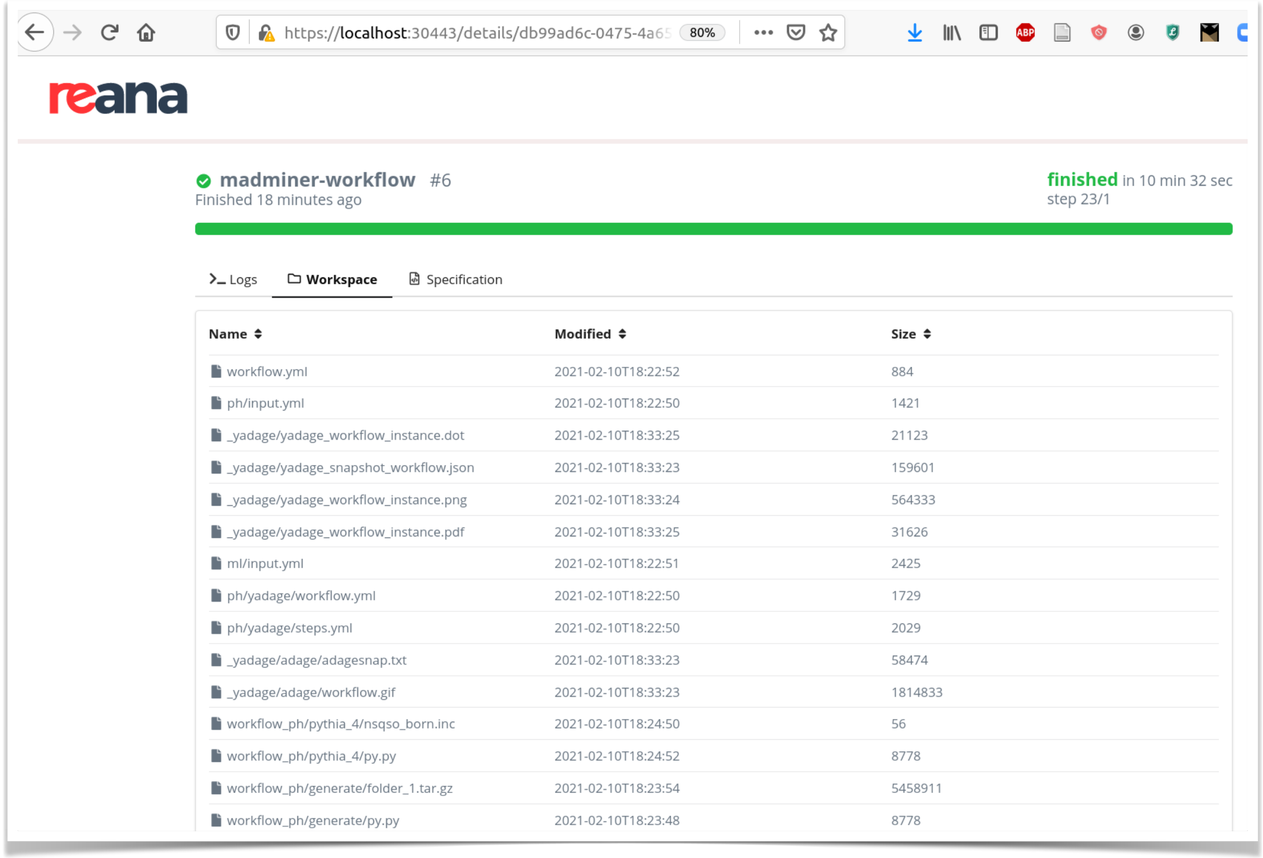
Schematic for REANA



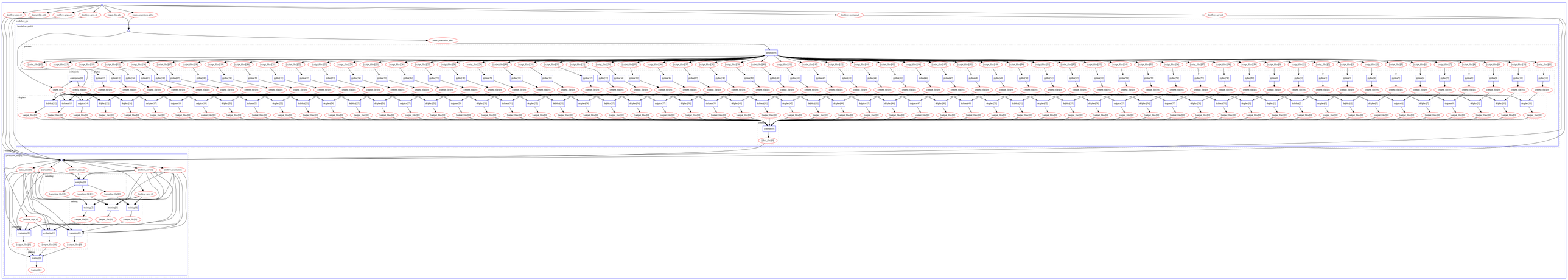
REANA Monitor







REANA Monitor



Workflow #1: 6 generation jobs for the various benchmark points
Workflow #2: 60 generation jobs for 10x at each of the points

Note: both took ~17 min to run.

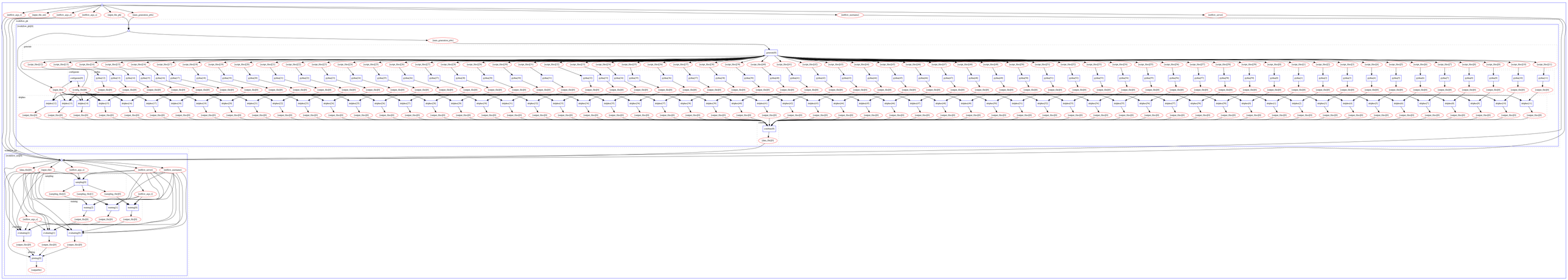
Your workflows

Refreshed at 12:25:15 UTC

madminer-workflow #2
Finished 9 hours ago
finished in 17 min 14 sec
step 131/1

madminer-workflow #1
Finished 9 hours ago
finished in 16 min 37 sec
step 23/1

REANA Monitor



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step 131/1

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