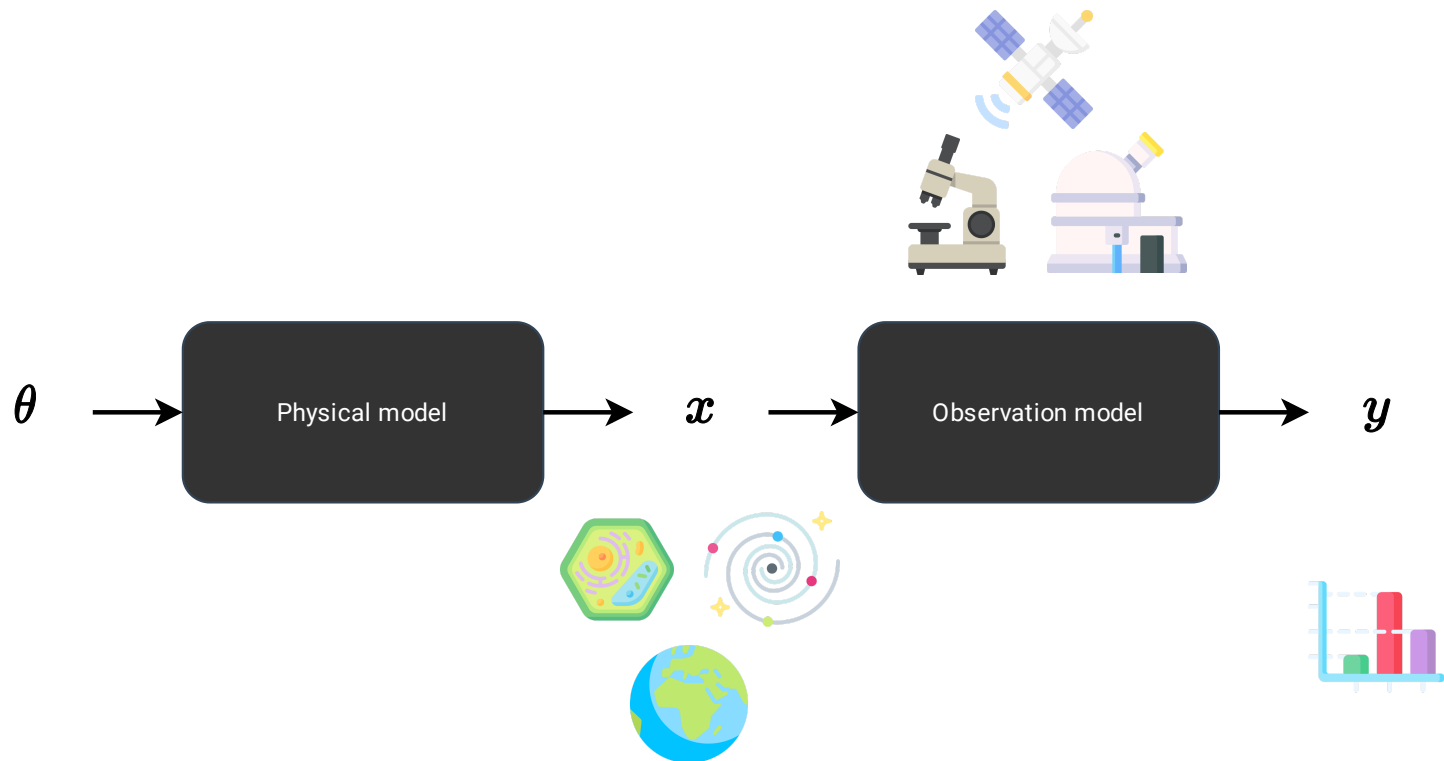
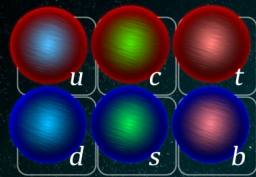


# Neural simulation-based inference for LHC analysis

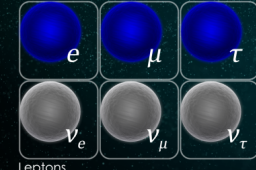
Gilles Louppe  
[g.louppe@uliege.be](mailto:g.louppe@uliege.be)  
December 6, 2024



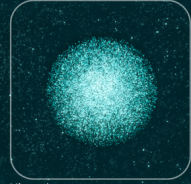
$$\begin{aligned}
\mathcal{L}_{SM} = & -\frac{1}{4} \partial_\mu \partial_\nu \partial_\rho \partial_\sigma - g_1 f^{abc} \partial_\mu \partial_\nu \partial_\rho \partial_\sigma - \frac{1}{2} g_2 f^{abc} f^{def} \partial_\mu \partial_\nu \partial_\rho \partial_\sigma - \partial_\mu W_\nu^\alpha W_\rho^\beta - \\
& M^2 W_\mu^\alpha W_\nu^\beta - \frac{1}{4} \partial_\mu \partial_\nu \partial_\rho \partial_\sigma - \frac{1}{2} M^2 \partial_\mu \partial_\nu \partial_\rho \partial_\sigma - \frac{1}{2} \partial_\mu A_\nu \partial_\rho A_\sigma - 19 \alpha_s (G_\mu^\alpha G_\nu^\beta W_\rho^\gamma W_\sigma^\delta - \\
& W_\mu^\alpha W_\nu^\beta - \mathcal{L}_2(W_\mu^\alpha W_\nu^\beta - W_\mu^\beta W_\nu^\alpha) + \mathcal{L}_2(W_\mu^\alpha W_\nu^\beta - W_\mu^\beta W_\nu^\alpha) - \\
& 19 \alpha_s (\partial_\mu A_\nu W_\rho^\alpha W_\sigma^\beta - W_\mu^\alpha W_\nu^\beta - \partial_\mu W_\nu^\alpha W_\rho^\beta + A_\mu (W_\nu^\alpha W_\rho^\beta - W_\nu^\beta W_\rho^\alpha) + A_\nu (W_\mu^\alpha W_\rho^\beta - \\
& W_\mu^\beta W_\rho^\alpha) - \frac{1}{2} g_2^2 W_\mu^\alpha W_\nu^\beta W_\rho^\gamma W_\sigma^\delta + \frac{1}{2} g_2^2 W_\mu^\alpha W_\nu^\beta W_\rho^\gamma W_\sigma^\delta - g_2^2 \mathcal{L}_2(W_\mu^\alpha W_\nu^\beta - \\
& W_\mu^\beta W_\nu^\alpha) + g_2^2 \mathcal{L}_2(A_\mu W_\nu^\alpha W_\rho^\beta - A_\nu W_\mu^\alpha W_\rho^\beta) + g_2^2 \alpha_s (A_\mu W_\nu^\alpha W_\rho^\beta - \\
& W_\mu^\alpha W_\nu^\beta) - 2A_\mu \mathcal{L}_2(W_\nu^\alpha W_\rho^\beta) - \frac{1}{2} \partial_\mu H \partial_\nu H - 2M^2 \alpha_s H \partial_\mu \phi^\alpha \partial_\nu \phi^\beta - \frac{1}{2} \partial_\mu \phi^\alpha \partial_\nu \phi^\beta - \\
& A_\mu \left( \frac{1}{2} H^2 + \frac{1}{2} H \phi^\alpha \phi^\beta + 2\phi^\alpha \phi^\beta \right) + \frac{1}{2} H^2 \alpha_s - \\
& \frac{1}{2} g_2 \alpha_s (H^2 + (\phi^\alpha)^2 + 4(\phi^\alpha \phi^\beta)^2 + 4(\phi^\alpha)^2 \phi^\beta \phi^\gamma + 4H^2 \phi^\alpha \phi^\beta + 2(\phi^\alpha)^2 H^2) - \\
& g M W_\mu^\alpha W_\nu^\beta H - \frac{1}{2} g_2^2 \mathcal{L}_2(H) - \\
& \frac{1}{2} i g (W_\mu^\alpha (\partial^\mu \phi^\beta \phi^\gamma - \phi^\beta \partial_\mu \phi^\gamma) - W_\nu^\beta (\partial^\nu \phi^\alpha \phi^\gamma - \phi^\alpha \partial_\nu \phi^\gamma)) + \\
& \frac{1}{2} i g (W_\mu^\alpha (H \partial_\nu \phi^\beta - \phi^\beta \partial_\nu H) + W_\nu^\beta (H \partial_\mu \phi^\alpha - \phi^\alpha \partial_\mu H)) + \frac{1}{2} i g \mathcal{L}_2(H \partial_\mu \phi^\alpha - \phi^\alpha \partial_\mu H) + \\
& M \left( \frac{1}{2} \mathcal{L}_2 \partial_\mu \phi^\alpha + W_\mu^\alpha \partial_\nu \phi^\beta + W_\nu^\beta \partial_\mu \phi^\alpha \right) - i g_2^2 M \mathcal{L}_2(W_\mu^\alpha \phi^\beta - W_\nu^\beta \phi^\alpha) + i g_2 M A_\mu (W_\nu^\alpha \phi^\beta - \\
& W_\nu^\beta \phi^\alpha) - i g \frac{1}{2} \mathcal{L}_2(\partial^\mu \partial_\nu \phi^\alpha - \phi^\alpha \partial_\mu \partial_\nu) + i g_2 M A_\mu (\partial^\mu \partial_\nu \phi^\alpha - \phi^\alpha \partial_\mu \partial_\nu) - \\
& \frac{1}{2} g_2^2 W_\mu^\alpha W_\nu^\beta (H^2 + 2\phi^\alpha \phi^\beta) - \frac{1}{2} g_2^2 \mathcal{L}_2(H^2 + (\phi^\alpha)^2 + 2(2\phi^\alpha - 1)\phi^\beta \phi^\gamma) - \\
& \frac{1}{2} g_2^2 \mathcal{L}_2(W_\mu^\alpha W_\nu^\beta + W_\nu^\beta W_\mu^\alpha) - \frac{1}{2} g_2^2 \mathcal{L}_2(H W_\mu^\alpha \phi^\beta - W_\nu^\beta \phi^\alpha) + \frac{1}{2} g_2 M A_\mu \partial^\mu W_\nu^\alpha \phi^\beta + \\
& W_\nu^\beta \phi^\alpha) + \frac{1}{2} i g_2^2 A_\mu H (W_\nu^\alpha \phi^\beta - W_\nu^\beta \phi^\alpha) - g_2^2 \alpha_s (2\phi^\alpha - 1) \mathcal{L}_2 A_\mu \phi^\beta \phi^\gamma - \\
& g_2^2 A_\mu A_\nu \phi^\alpha \phi^\beta + \frac{1}{2} i g_2 \mathcal{L}_2(\partial^\mu \gamma^\nu \partial_\rho \phi^\alpha - \partial^\nu \gamma^\mu \partial_\rho \phi^\alpha) - \partial^\mu (\gamma^\nu \partial_\rho + \\
& m_\mu^2 \delta_\mu^\nu - \partial^\mu \gamma^\nu \partial_\rho + m_\mu^2 \delta_\mu^\nu) + i g_2 M A_\mu (-\partial^\mu \gamma^\nu \partial_\rho + \frac{1}{2} (\partial^\mu \gamma^\nu \partial_\rho)) + \\
& \frac{1}{2} \mathcal{L}_2((\partial^\mu \gamma^\nu (1 + \gamma^\mu) \partial_\rho) + (\partial^\mu \gamma^\nu (4\phi^\alpha - 1 - \gamma^\mu) \partial_\rho) + (\partial^\mu \gamma^\nu (\frac{1}{2} \phi^\alpha - 1 - \gamma^\mu) \partial_\rho)) + \\
& (\partial^\mu \gamma^\nu (1 - \frac{1}{2} \phi^\alpha + \gamma^\mu) \partial_\rho)) + \frac{1}{2} g_2 W_\mu^\alpha (\partial^\mu \gamma^\nu (1 + \gamma^\mu) \partial_\rho) + (\partial^\mu \gamma^\nu (1 + \gamma^\mu) \partial_\rho \phi^\alpha) + \\
& \frac{1}{2} g_2 W_\nu^\beta (\partial^\mu \gamma^\nu (1 + \gamma^\mu) \partial_\rho) + (\partial^\mu \gamma^\nu (1 + \gamma^\mu) \partial_\rho) + \\
& \frac{1}{2} \mathcal{L}_2 \phi^\alpha \left( -m_\mu^2 (\partial^\mu \gamma^\nu \partial_\rho) (1 + \gamma^\mu) \partial_\rho \right) + m_\mu^2 (\partial^\mu \gamma^\nu \partial_\rho) (1 + \gamma^\mu) \partial_\rho + \\
& \frac{1}{2} \mathcal{L}_2 H (\partial^\mu \gamma^\nu) + \frac{1}{2} \mathcal{L}_2 \phi^\alpha (\partial^\mu \gamma^\nu \partial_\rho) - \frac{1}{2} \mathcal{L}_2 \phi^\alpha (\partial^\mu \gamma^\nu \partial_\rho) - \frac{1}{2} \mathcal{L}_2 H (\partial^\mu \gamma^\nu) - \\
& \frac{1}{2} \mathcal{L}_2 M_\mu^2 (1 - \gamma^\mu) \partial_\rho + \frac{1}{2} \mathcal{L}_2 \phi^\alpha (-m_\mu^2 (\partial^\mu \gamma^\nu \partial_\rho) (1 - \gamma^\mu) \partial_\rho) + m_\mu^2 (\partial^\mu \gamma^\nu \partial_\rho) (1 + \gamma^\mu) \partial_\rho + \\
& \frac{1}{2} \mathcal{L}_2 \phi^\alpha \left( m_\mu^2 (\partial^\mu \gamma^\nu \partial_\rho) (1 + \gamma^\mu) \partial_\rho \right) - m_\mu^2 (\partial^\mu \gamma^\nu \partial_\rho) (1 - \gamma^\mu) \partial_\rho - \frac{1}{2} \mathcal{L}_2 H (\partial^\mu \gamma^\nu) - \\
& \frac{1}{2} \mathcal{L}_2 H (\partial^\mu \gamma^\nu) + \frac{1}{2} \mathcal{L}_2 \phi^\alpha (\partial^\mu \gamma^\nu \partial_\rho) - \frac{1}{2} \mathcal{L}_2 \phi^\alpha (\partial^\mu \gamma^\nu \partial_\rho) + \mathcal{L}_2 \partial^\mu \phi^\alpha \partial_\nu \phi^\beta + g_1 f^{abc} \partial_\mu \phi^\alpha \partial_\nu \phi^\beta + \\
& X^\alpha (\partial^\mu - M^\alpha) X^\beta + X^\gamma (\partial^\mu - M^\alpha) X^\delta + X^\epsilon (\partial^\mu - \frac{2}{3}) X^\zeta + Y \partial^\mu Y + i g_2 W_\mu^\alpha W_\nu^\beta (\partial_\mu X^\alpha X^\beta - \\
& \partial_\nu X^\alpha X^\beta) + i g_2 W_\mu^\alpha W_\nu^\beta (\partial_\mu X^\alpha X^\beta - \partial_\nu X^\alpha X^\beta) + i g_2 W_\mu^\alpha W_\nu^\beta (\partial_\mu X^\alpha X^\beta - \\
& \partial_\nu X^\alpha X^\beta) + i g_2 W_\mu^\alpha W_\nu^\beta (\partial_\mu X^\alpha X^\beta - \partial_\nu X^\alpha X^\beta) + i g_2 W_\mu^\alpha W_\nu^\beta (\partial_\mu X^\alpha X^\beta - \\
& \partial_\nu X^\alpha X^\beta) + i g_2 W_\mu^\alpha W_\nu^\beta (\partial_\mu X^\alpha X^\beta - \partial_\nu X^\alpha X^\beta) + \\
& \partial_\mu X^\alpha X^\beta + i g_2 W_\mu^\alpha W_\nu^\beta (\partial_\mu X^\alpha X^\beta - \partial_\nu X^\alpha X^\beta) + \\
& \partial_\mu X^\alpha X^\beta - \frac{1}{2} i g M (X^\alpha X^\beta H + X^\alpha X^\beta H + \frac{1}{2} X^\alpha X^\beta H) - \frac{1}{2} i g M (X^\alpha X^\beta \phi^\alpha - X^\alpha X^\beta \phi^\beta) + \\
& \frac{1}{2} i g M (X^\alpha X^\beta \phi^\alpha - X^\alpha X^\beta \phi^\beta) + i g M A_\mu (X^\alpha X^\beta \phi^\alpha - X^\alpha X^\beta \phi^\beta) + \\
& \frac{1}{2} i g M (X^\alpha X^\beta \phi^\alpha - X^\alpha X^\beta \phi^\beta).
\end{aligned}$$



Quarks



Leptons

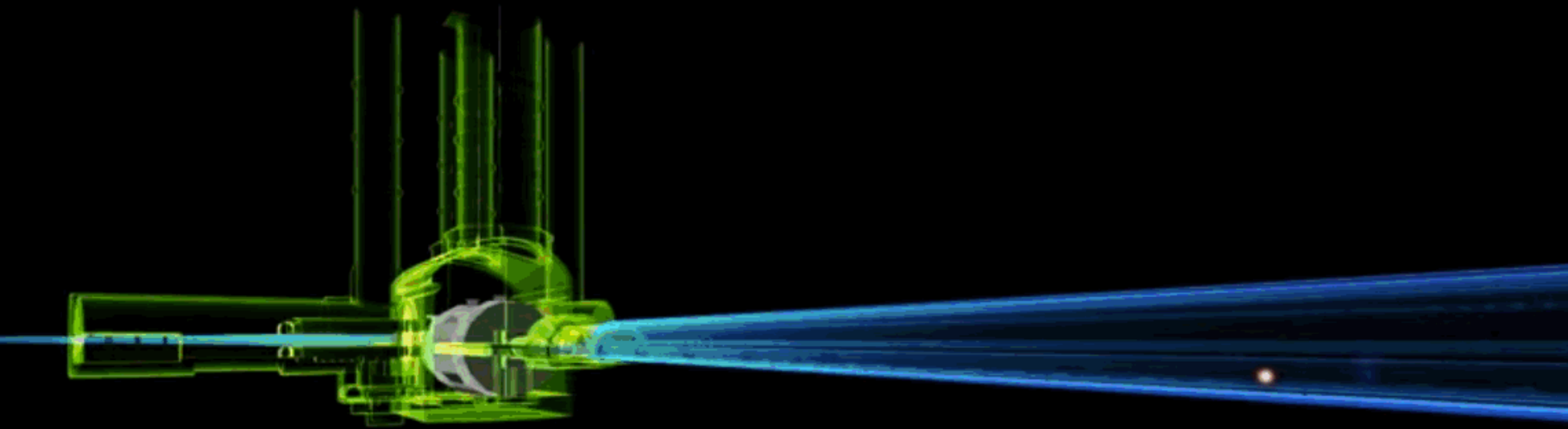


Higgs boson

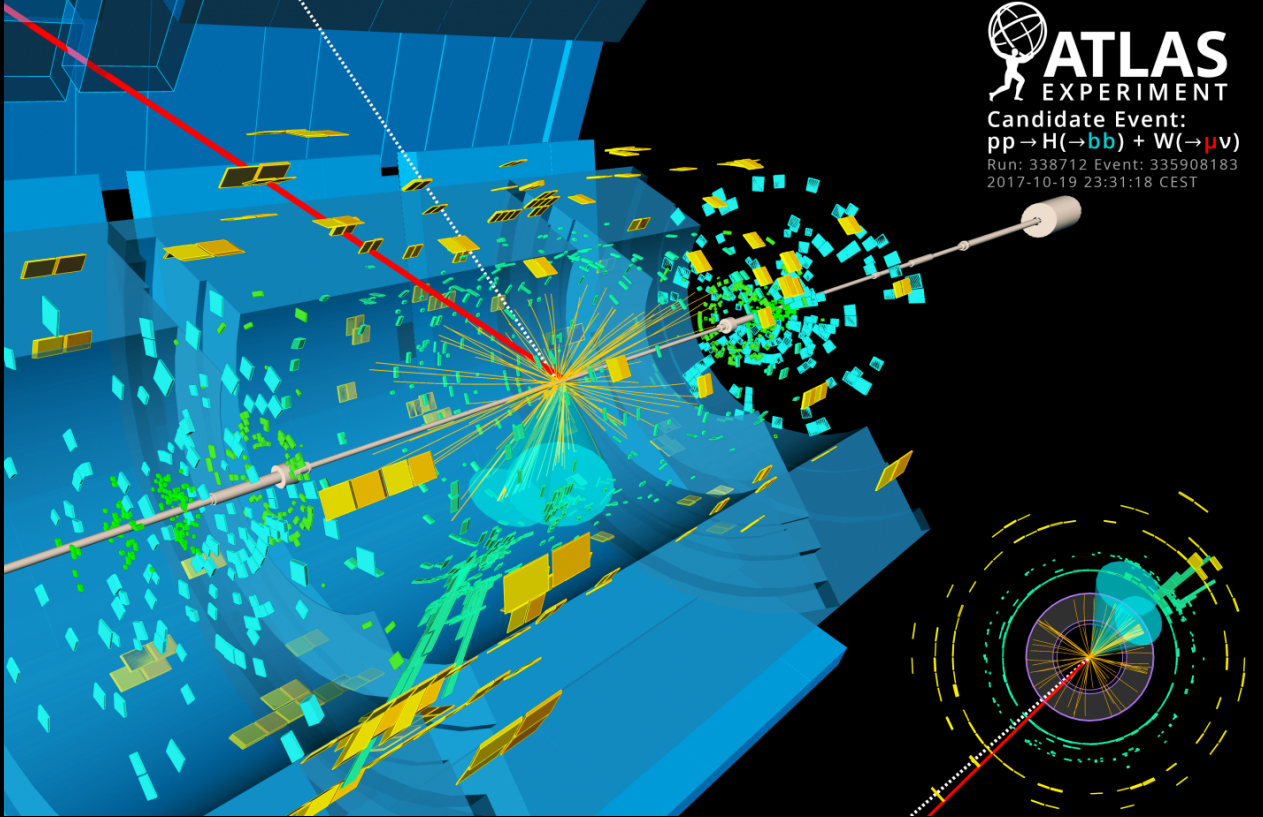


Forces

$$\theta = \{m_e, m_\mu, m_\tau, \dots\}$$



$$x, y \sim p(x|\theta)p(y|x)$$



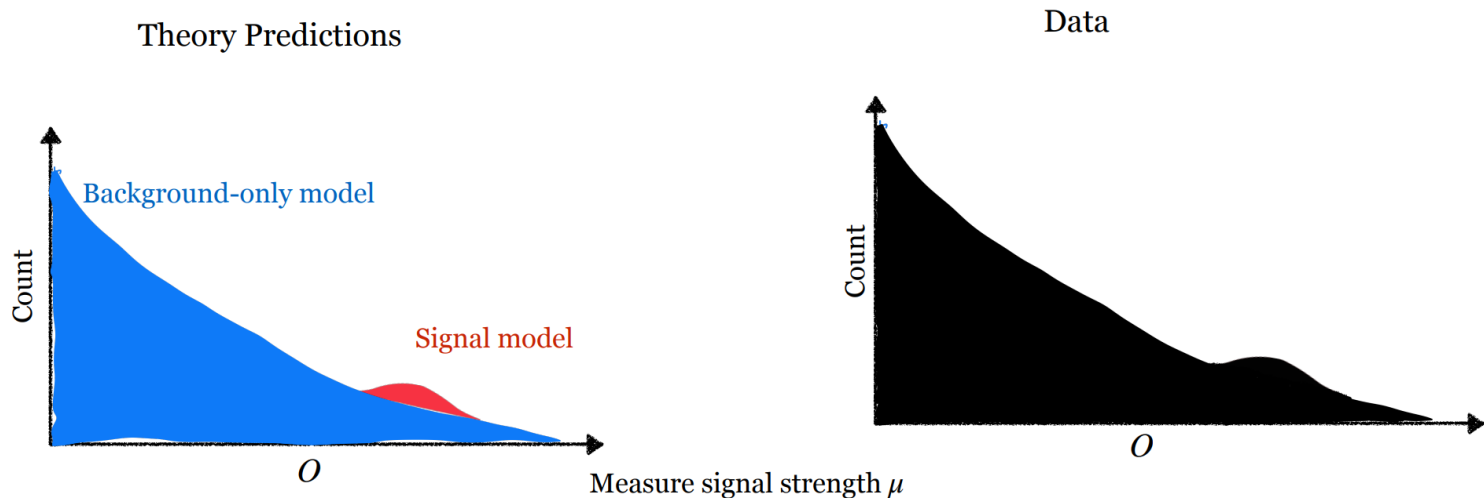
 **ATLAS**  
EXPERIMENT  
Candidate Event:  
 $pp \rightarrow H(\rightarrow bb) + W(\rightarrow \mu\nu)$   
Run: 338712 Event: 335908183  
2017-10-19 23:31:18 CEST

# Bump hunting at the LHC

Assuming a background+signal model

$$p(x|\mu) = \frac{\mu\nu_S p_S(x) + \nu_B p_B(x)}{\mu\nu_S + \nu_B},$$

the discovery of a signal can be formulated as a statistical hypothesis test of the null hypothesis  $\mu = 0$  against the alternative hypothesis  $\mu > 0$ .



Because of Neyman-Pearson's lemma, the likelihood ratio

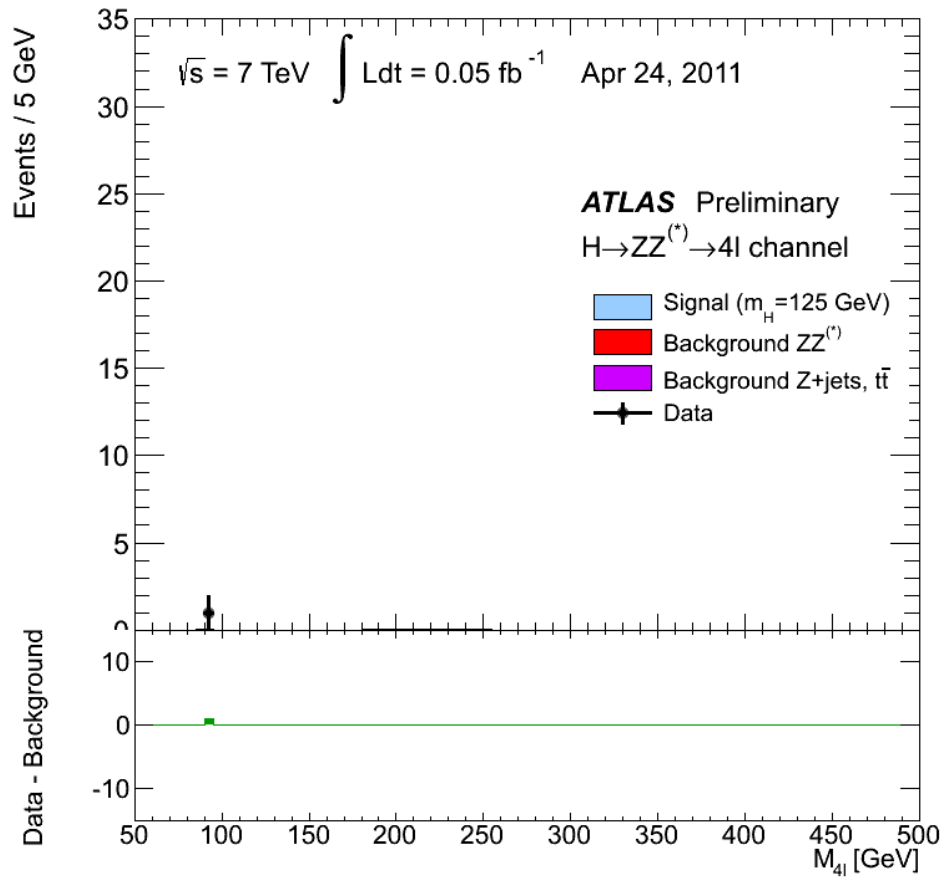
$$\frac{p(x|\mu)}{p(x|\mu=0)} = \frac{1}{\mu\nu_S + \nu_B} \left( \mu\nu_S \frac{p_S(x)}{p_B(x)} + \nu_B \right)$$

is the most powerful test statistic.

For a well-chosen summary statistic  $s(x)$ , the signal-to-background ratio can be approximated as

$$\frac{p_S(x)}{p_B(x)} \approx \frac{p_S(s(x))}{p_B(s(x))}$$

by filling histograms of  $s(x)$  for signal and background events.





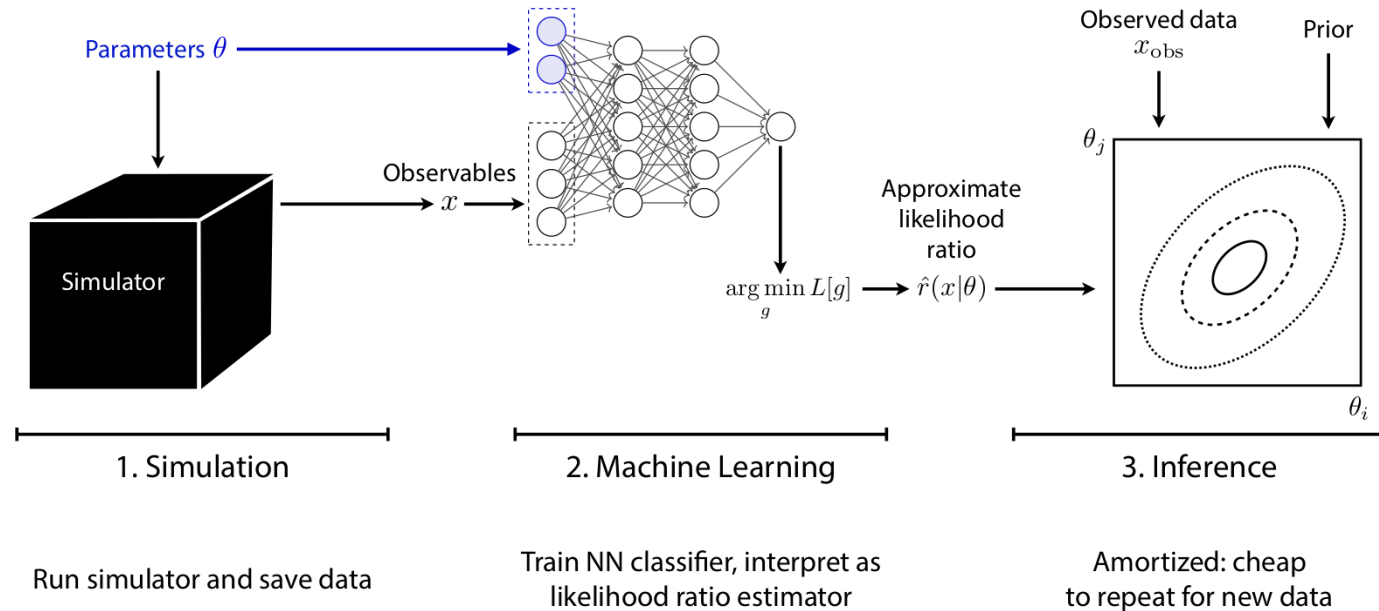


Wait a minute...

- How do we pick the right summary statistic  $s$ ?
- Don't we lose in statistical power by binning the data?



# Neural simulation-based inference



Learn the statistic  $s(\cdot)$  with a neural network approximating the per-event likelihood ratio  $r(x|\mu) = \frac{p(x|\mu)}{p(x|\mu=0)}$  itself!

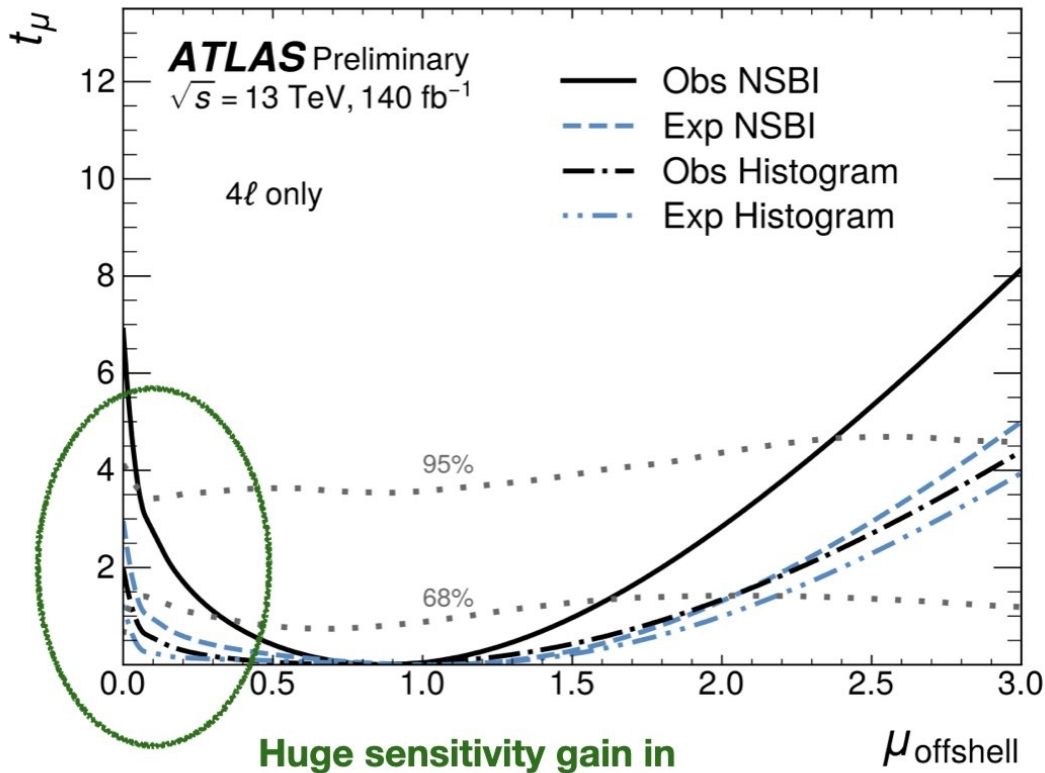


## From a prototype to a full ATLAS analysis

Measurement of the off-shell Higgs boson production in the  $H^* \rightarrow ZZ \rightarrow 4\ell$  decay channel, while

- accounting for quantum interference effects,
- accounting for systematic uncertainties,
- extending the Neyman construction for unbinned analysis,
- validating, validating, validating to convince the collaboration.





**Huge sensitivity gain in interference rich regions**  
 $\sqrt{\mu} \cdot p_I(x) \gg \mu \cdot p_S(x)$

**ATLAS CONF Note**  
 ATLAS-CONF-2024-016  
 November 4, 2024

**Measurement of off-shell Higgs boson production in the  $H^* \rightarrow ZZ \rightarrow 4l$  decay channel using a neural simulation-based inference technique with the ATLAS detector at  $\sqrt{s} = 13 \text{ TeV}$**

The ATLAS Collaboration

A measurement of off-shell Higgs boson production in the  $H^* \rightarrow ZZ \rightarrow 4l$  decay channel is presented. The measurement uses the  $140 \text{ fb}^{-1}$  of integrated luminosity collected by the ATLAS detector during the Run 2 proton-proton collisions at the Large Hadron Collider at  $\sqrt{s} = 13 \text{ TeV}$  and supersedes our previous result in this decay channel using the same dataset. The data analysis is performed using a neural simulation-based inference method, which handles per-event likelihood ratios using neural networks. The observed (expected) off-shell Higgs boson production signal strength in the  $ZZ \rightarrow 4l$  decay channel is  $0.87_{-0.24}^{+0.25}$  ( $1.00_{-0.25}^{+0.26}$ ) at 68% CL. The process result was not able to achieve expected sensitivity to span a one-sided interval at this CL. The expected plus-side uncertainty is reduced by 10%. The evidence for off-shell Higgs boson production has an observed (expected) significance of  $2.56$  ( $1.79$ ) using the  $ZZ \rightarrow 4l$  decay channel only. The expected significance score is 2.6 times that of our previous result using the same dataset. When combined with our most recent measurement in  $ZZ \rightarrow 2l2\gamma$  decay channel, the evidence for off-shell Higgs boson production has an observed (expected) significance of  $3.7$  ( $2.6$ ). The off-shell measurements are combined with the measurement of on-shell Higgs boson production to obtain constraints on the Higgs boson total width. The observed (expected) value of the Higgs boson width is  $4.27_{-0.14}^{+0.15}$  ( $4.1_{-0.14}^{+0.15}$ ) MeV at 68% CL.

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**ATLAS CONF Note**  
 ATLAS-CONF-2024-015  
 28th October 2024

**An implementation of Neural Simulation-Based Inference for Parameter Estimation in ATLAS**

The ATLAS Collaboration

Neural Simulation-Based Inference (NSBI) is a powerful class of machine learning (ML)-based methods for statistical inference that naturally handles high-dimensional parameter estimation without the need to bin data into low-dimensional summary histograms. Such methods are promising for a range of measurements, including at the Large Hadron Collider (LHC), where no single observable may be optimal to scan over the entire theoretical phase space under consideration, or where binning data into histograms could result in a loss of sensitivity. This work develops an NSBI framework for statistical inference, using neural networks to estimate probability density ratios, which enables the application of NSBI to a full scale LHC analysis. It incorporates a large number of systematic uncertainties, quantifies the uncertainty coming from finite training statistics, develops a method to construct confidence intervals, and demonstrates a series of intermediate diagnostic checks that can be performed to validate the robustness of the method. As an example, the power and feasibility of the method are demonstrated on simulated data for a simplified version of an off-shell Higgs boson coupling measurement in the four-lepton final states. This NSBI framework is an extension of the standard statistical framework used by LHC experiments and can benefit a large number of physics analyses.

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The off-shell Higgs boson production signal strength is  $\mu = 0.87_{-0.54}^{+0.75}$ .

## **Next steps**

- The ATLAS NSBI analysis is the first of hopefully many.
- Methodological and computational challenges remain for its wider adoption.

