Simulation-based Inference

Inverting Simulators

Talk by Stefan Wezel

mlcolab @ Tübingen University Cluster of Excellence

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Overview

- The problem setting
- Traditional approaches and their issues
- Using Neural Nets to alleviate them
- A worked example
- Outlook

What and Why?

An Example

- Inverting simulators?
- What is a simulator?
  - Forward, generative model with parameters and stochasticity
  - Produces observations
  - In context of this talk computer program, but can be electrical circuit (Hodgkin–Huxley model)
- Used by scientists to model empirical observed data
- Used in particle physics, population genetics, epidemiology
- Encode knowledge about systems gathered over centuries

What and Why?

An Example

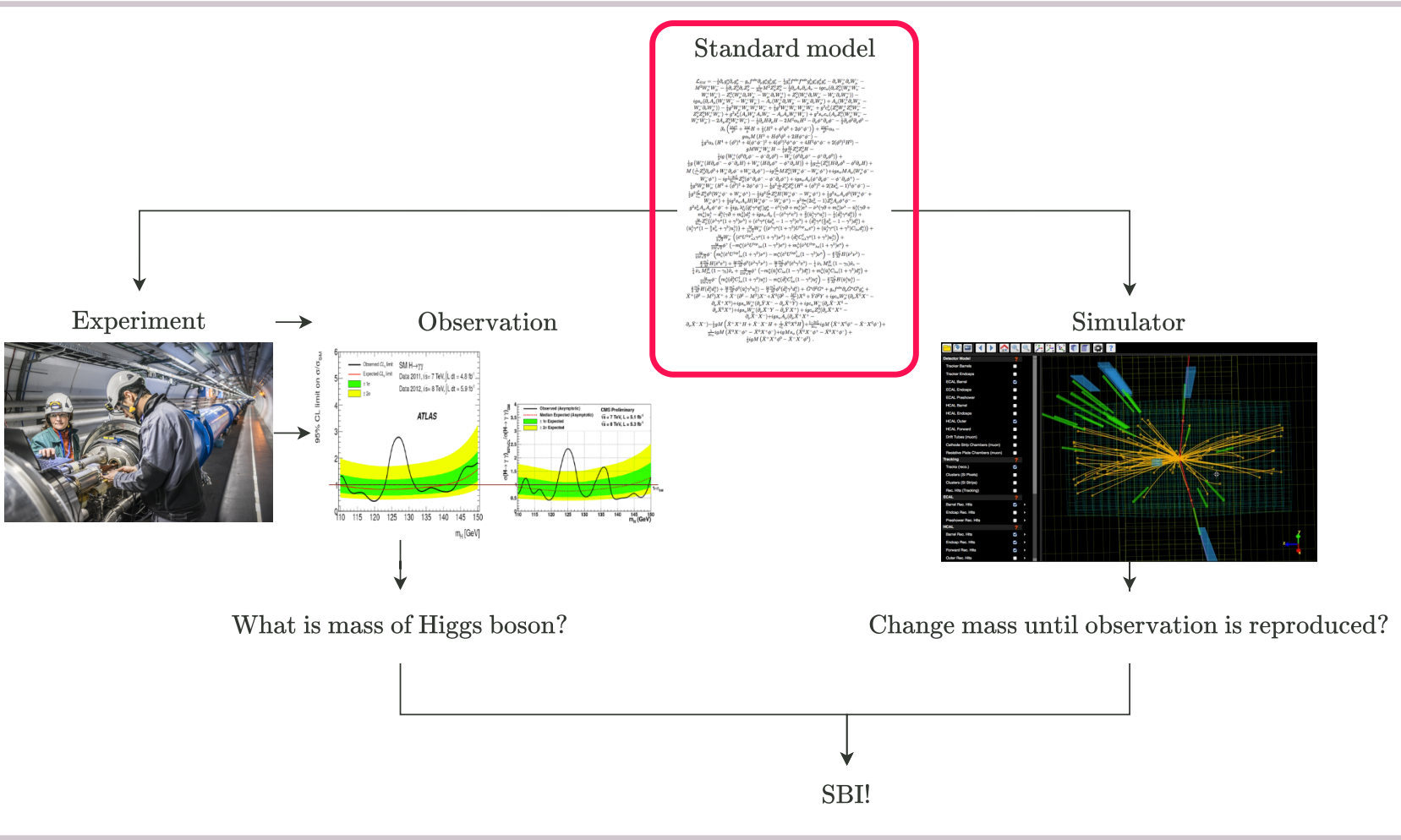

Figure derived from cern.ch, Achintya Rao and Tom McCauley, sciencealert.com

What and Why?

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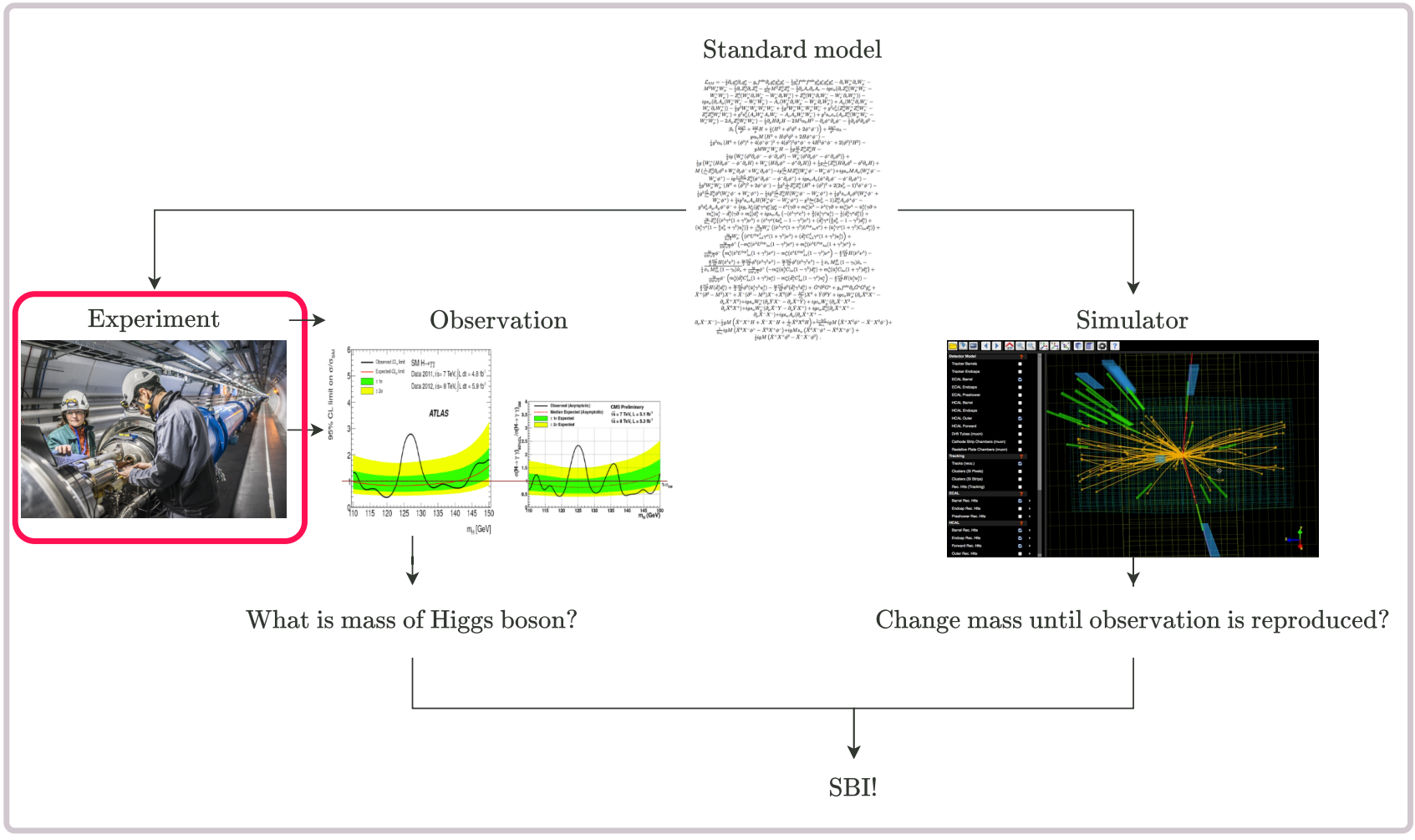

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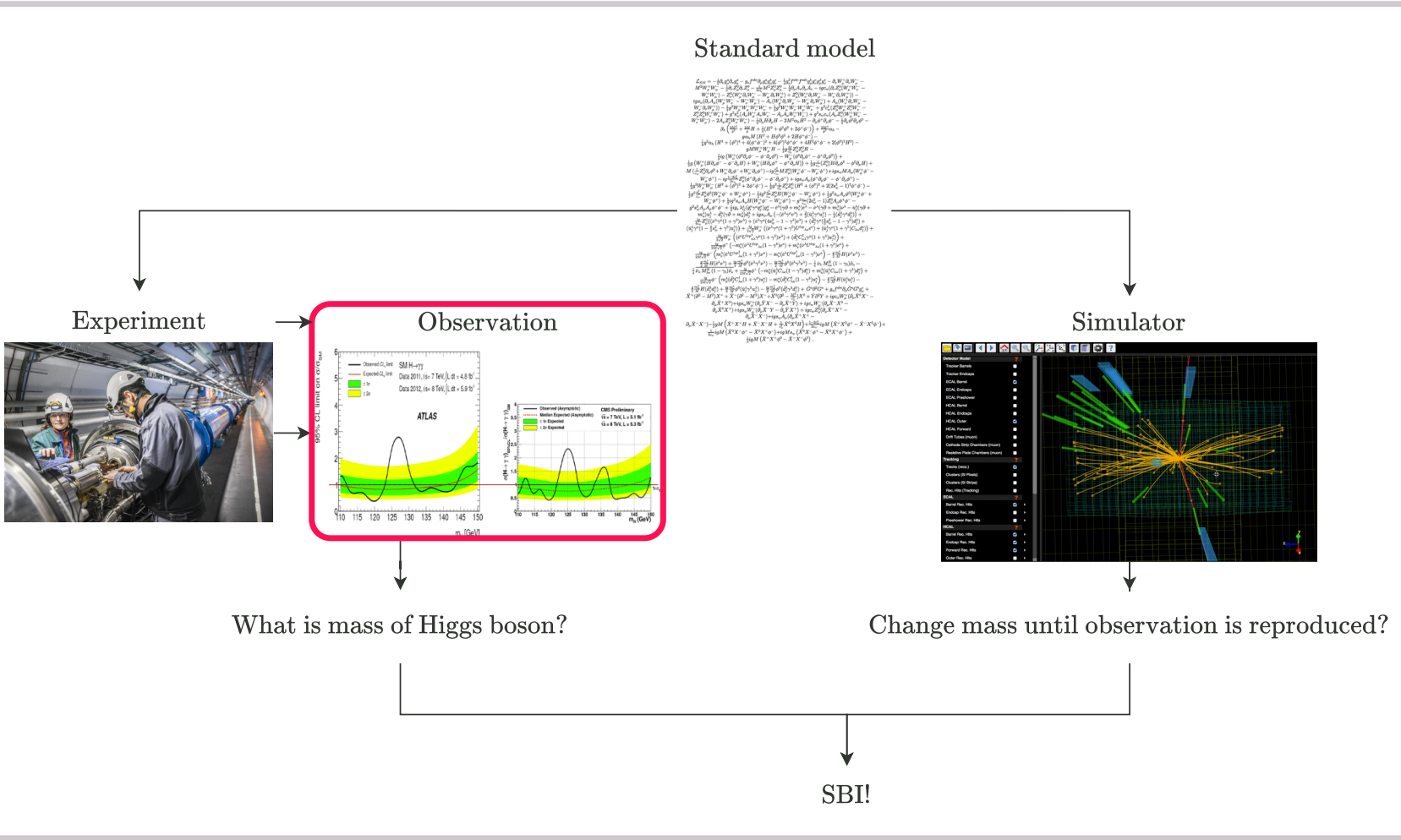

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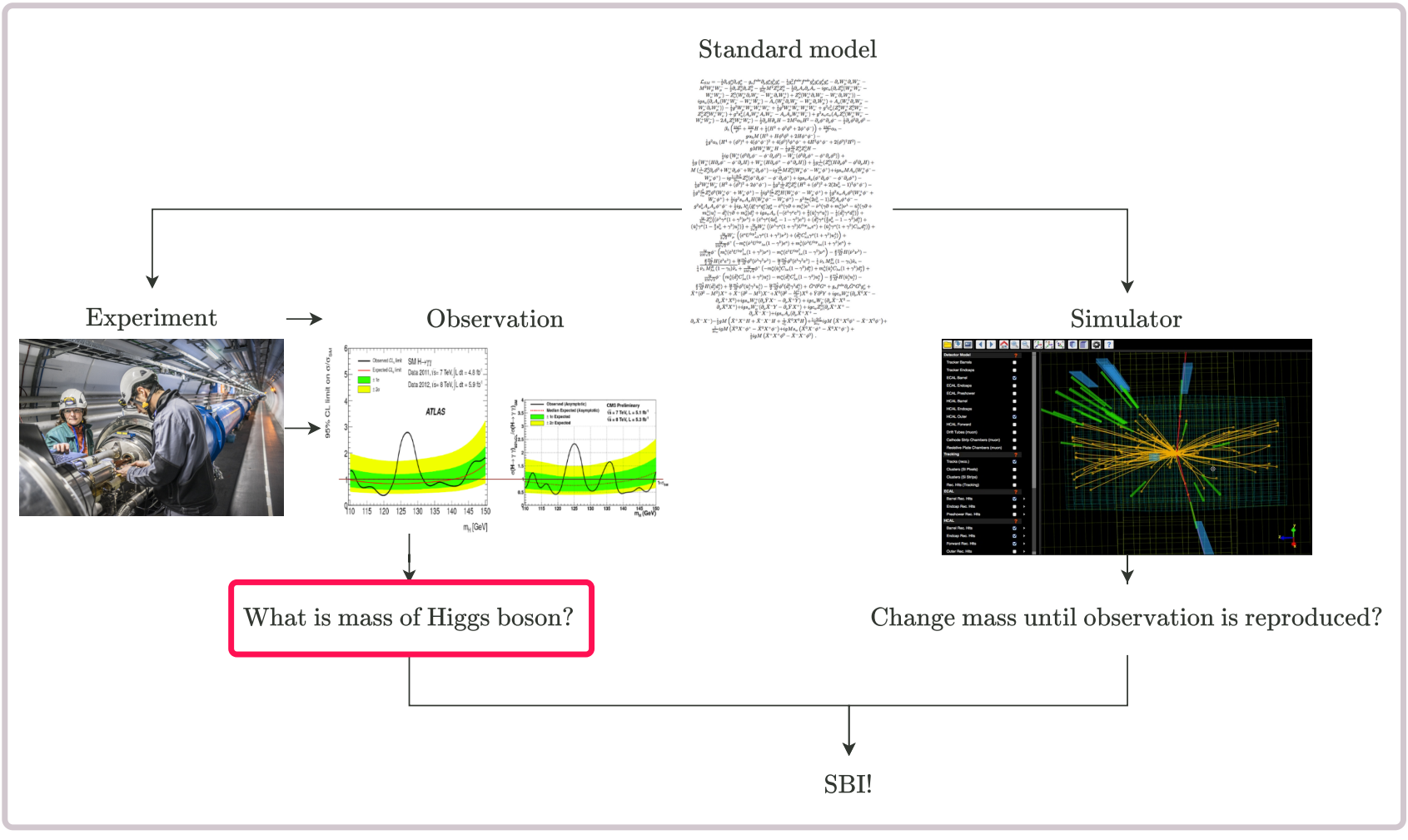

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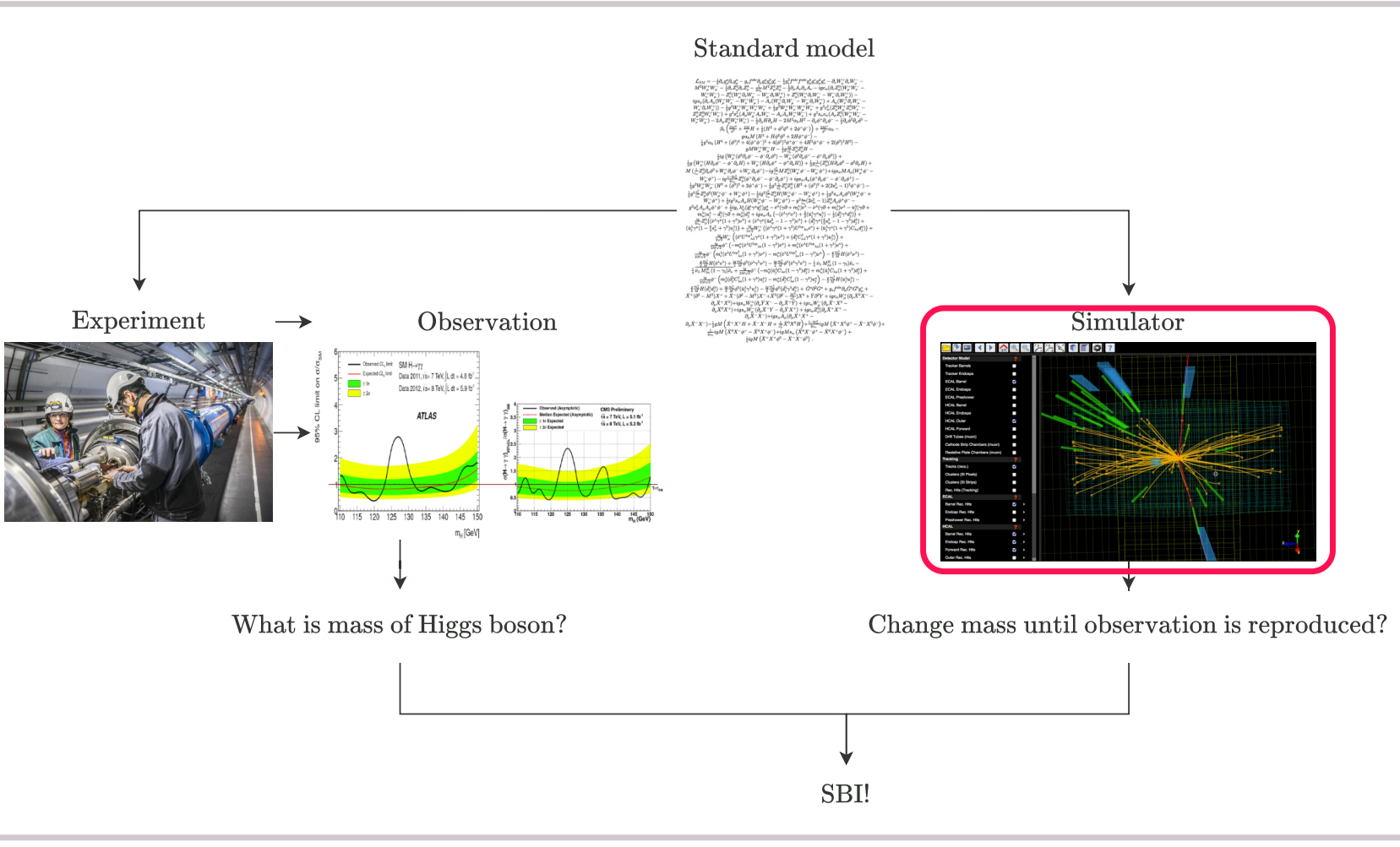

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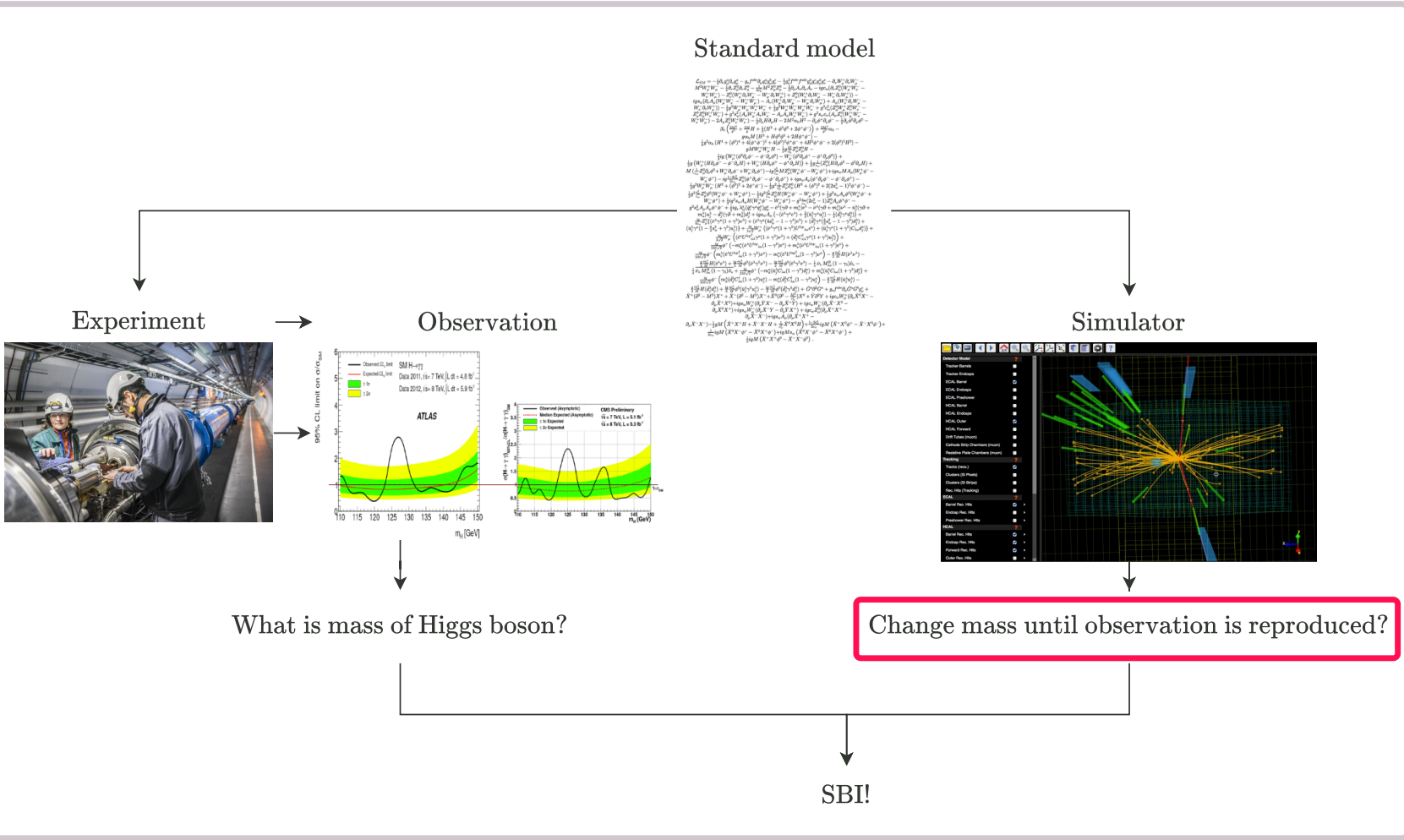

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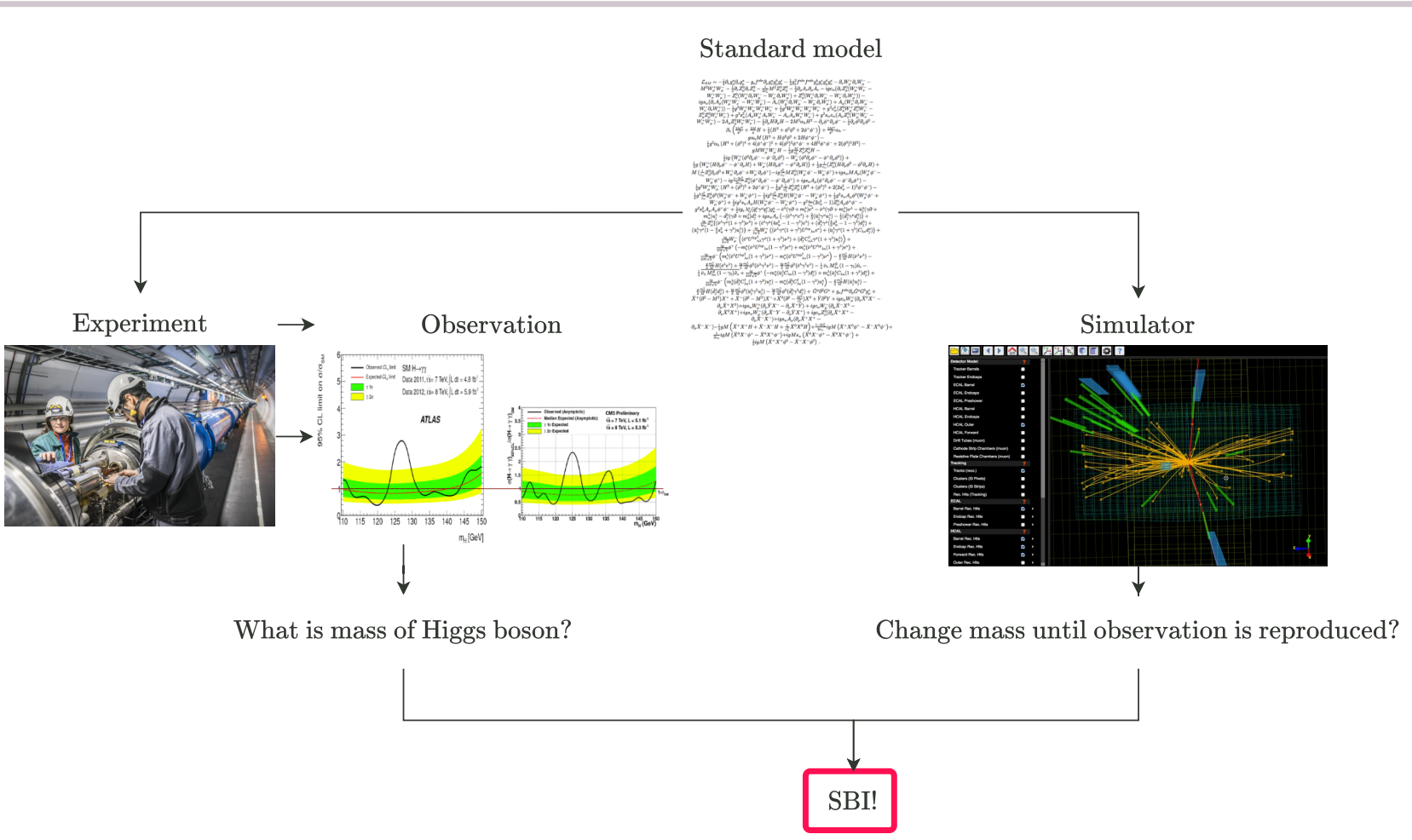

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- Before we go into SBI, let's take a minute to formalize our setting
- Simulator has parameters θ, nuisance parameter z and produces data $\hat{x}$
  - It implicitly defines $p(\hat{x}, z|\theta)$ (it yields samples from this distribution)
- Given a (real) observation x_0, we would be interested in the parameters that produced it

$$p(\theta|x = x_0) = \frac{p(x|\theta)p(\theta)}{p(x)} = \frac{\overbrace{\int p(x, z|\theta)dz}^{intractable}\, p(\theta)}{\underbrace{\int p(x|\theta)p(\theta)d\theta}_{intractable}}, \tag{1}$$

What and Why?

Simulation-based Inference to the rescue

- This is exactly a problem setting that scientists often deal with
  - They have a sophistic model (the simulator) that encapsulates a lot of prior knowledge
  - But inference in this setting often boils down to: What were parameters that produced this observation
- Simulation-based Inference inference tries to solve this problem
- by inverting the simulator

- Broader term: Approximate Bayesian Computation (ABC)
  - Rejection ABC
  - Sampling ABC (perturb initial parameters)
  - Sequential ABC (importance sampling)
- But gives only point estimates, not full posterior
- within ϵ
- [1] propose to use neural networks to parameterize GMM

// Create training set

for $n = 1..N$ do

  sample $\theta_n \sim \tilde{p}(\theta)$

  sample $x_n \sim p(x|\theta_n)$

end

// Find variational posterior over parameters

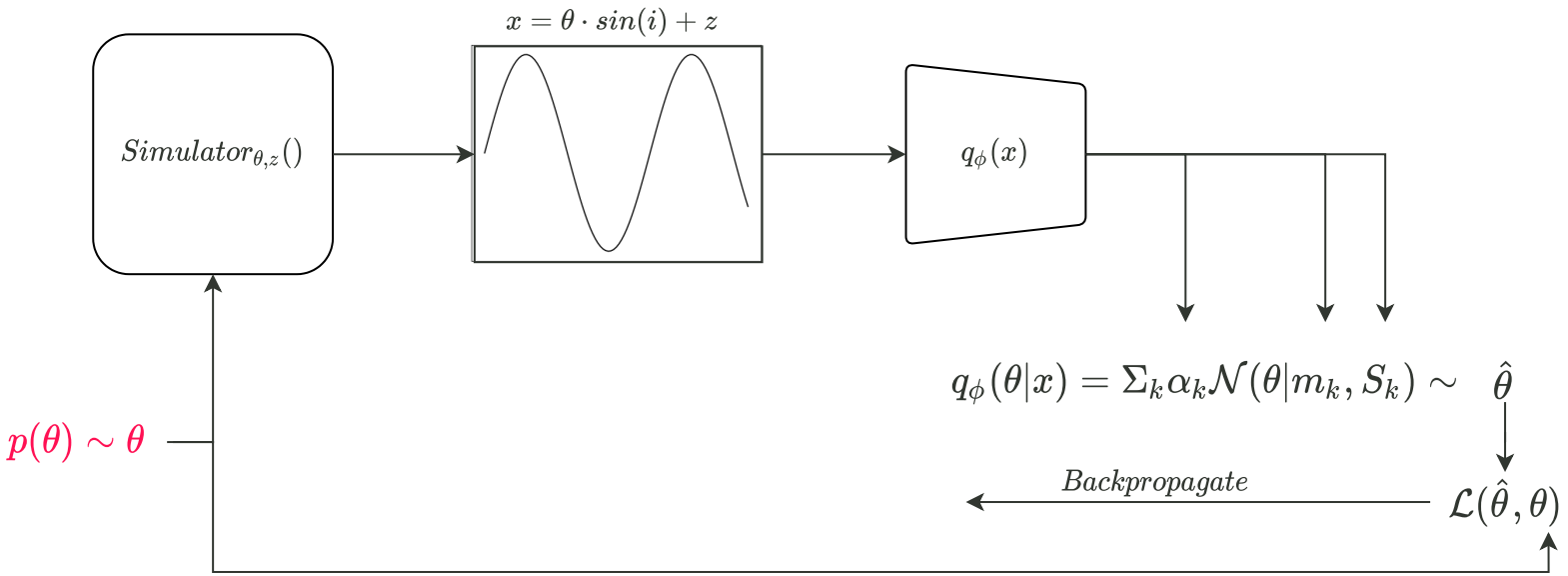
train $q_\phi(\theta|x)$ on $\{\theta_n, x_n\}$

// Find posterior over parameters for given observation

$\hat{p}(\theta|x = x_0) \leftarrow \frac{p(\theta)}{\tilde{p}(c)} q_\phi(\theta|x)$

Learning a Posterior

from Simulations



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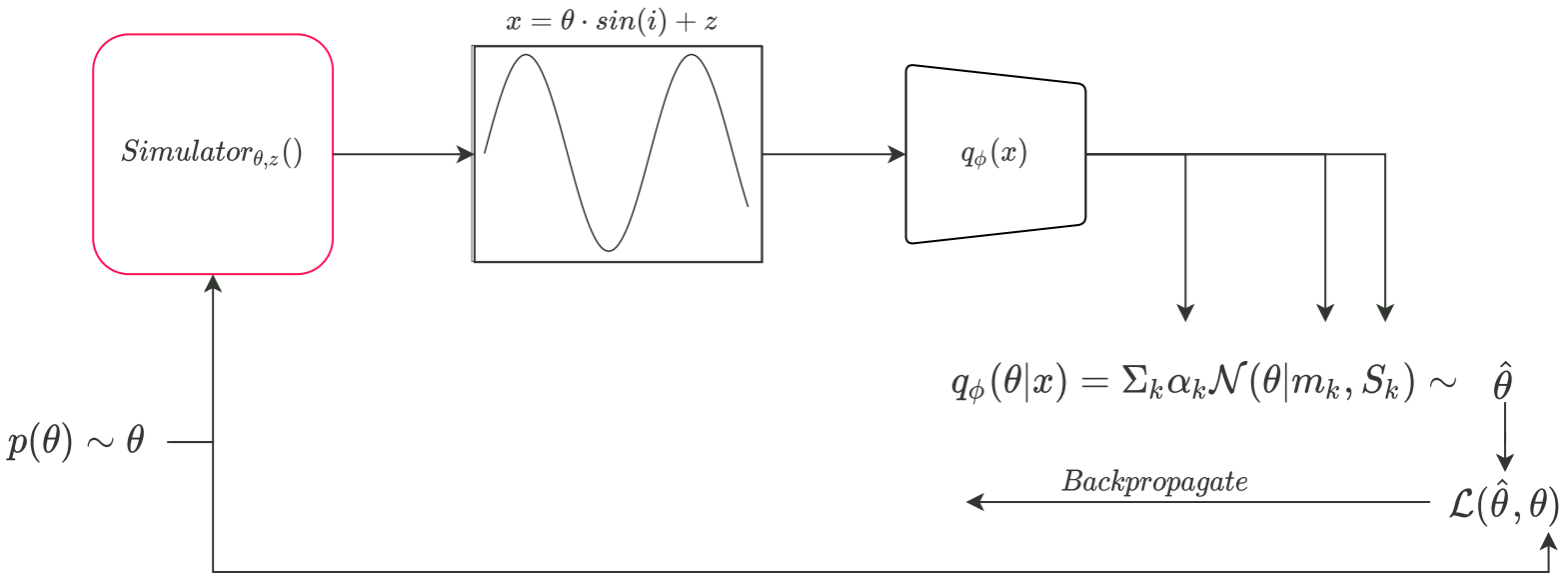

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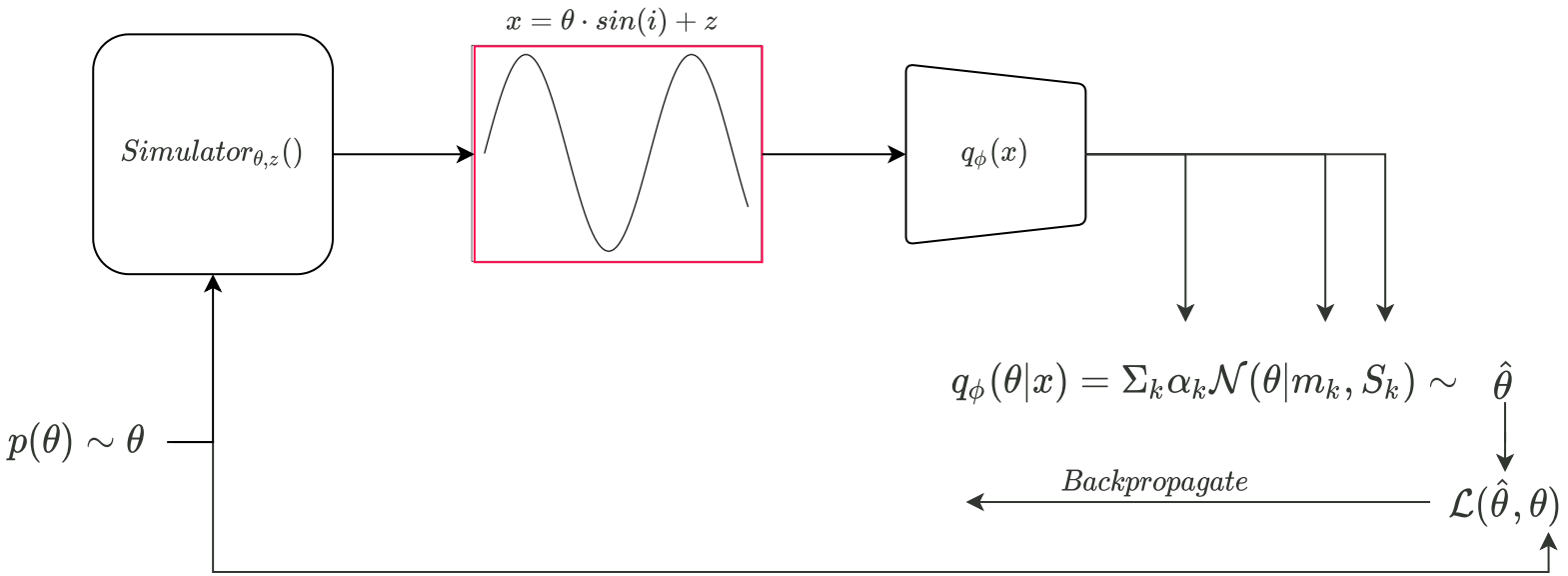

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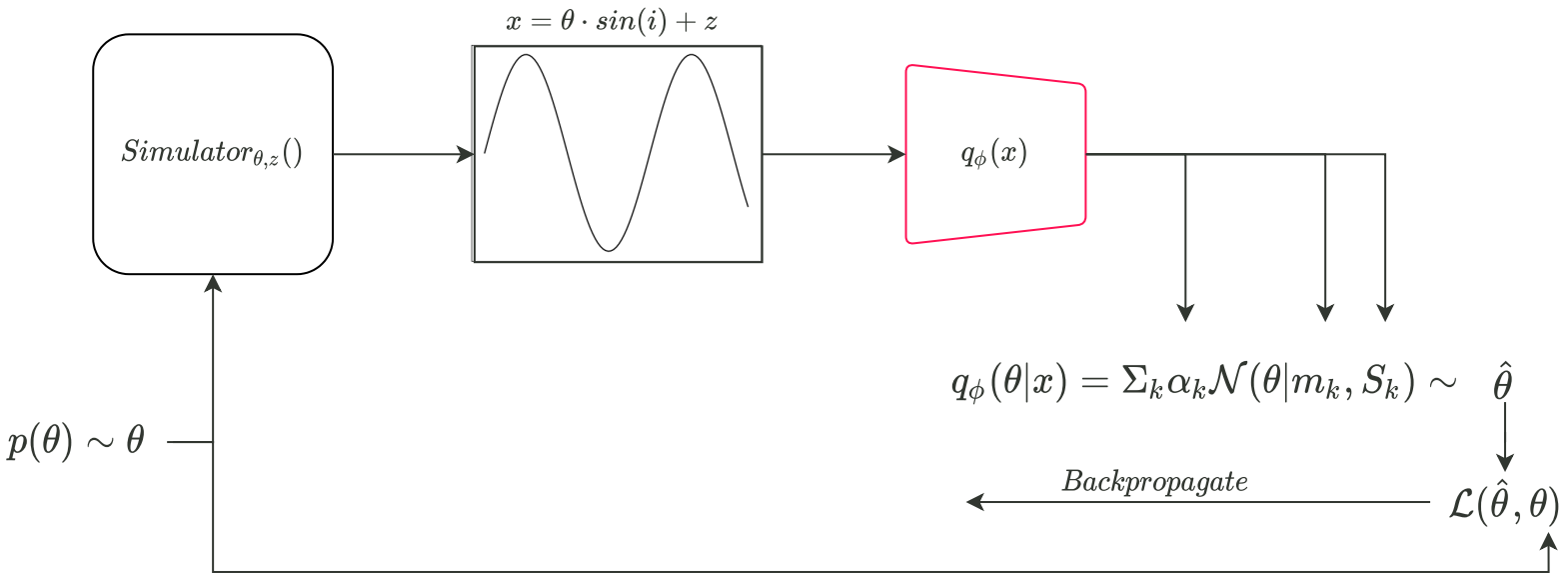

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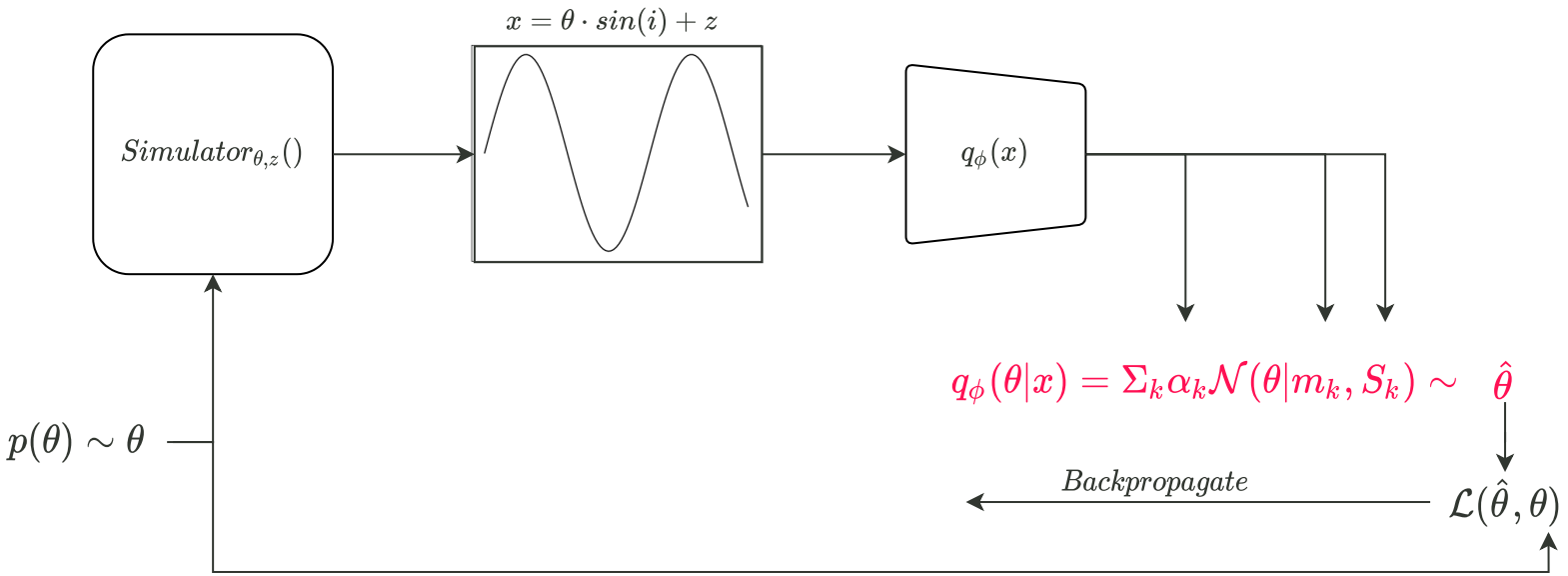

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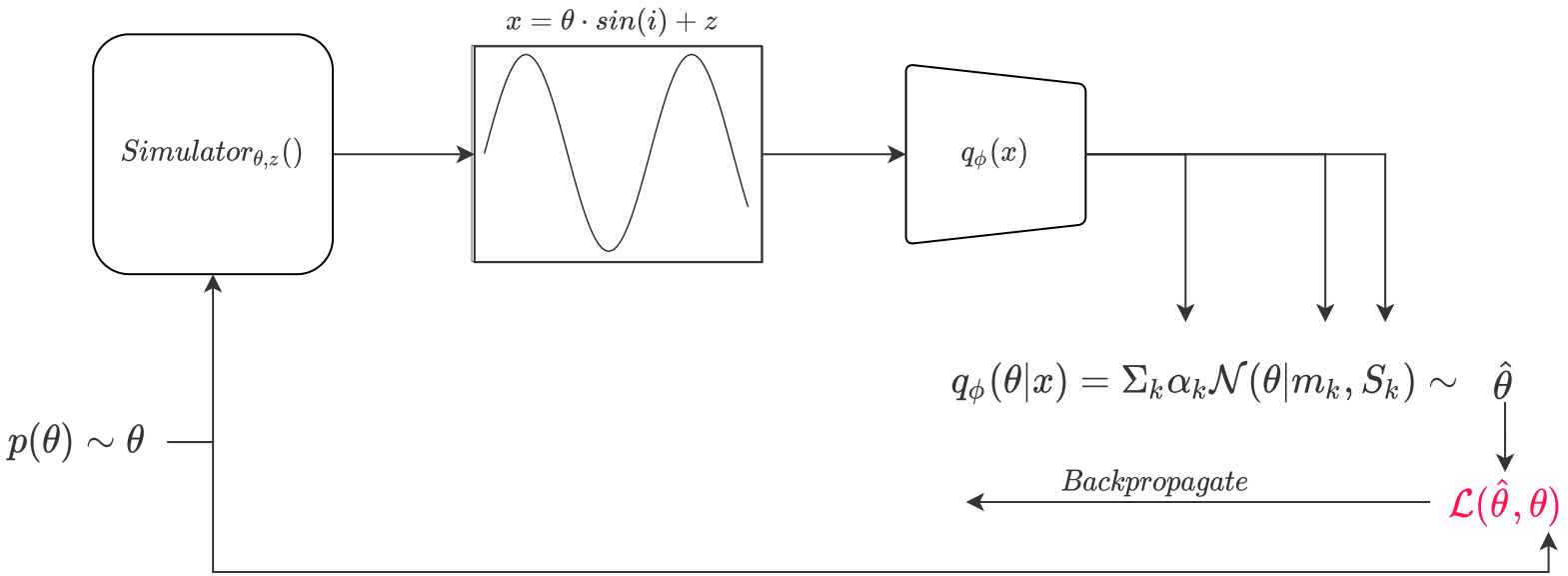

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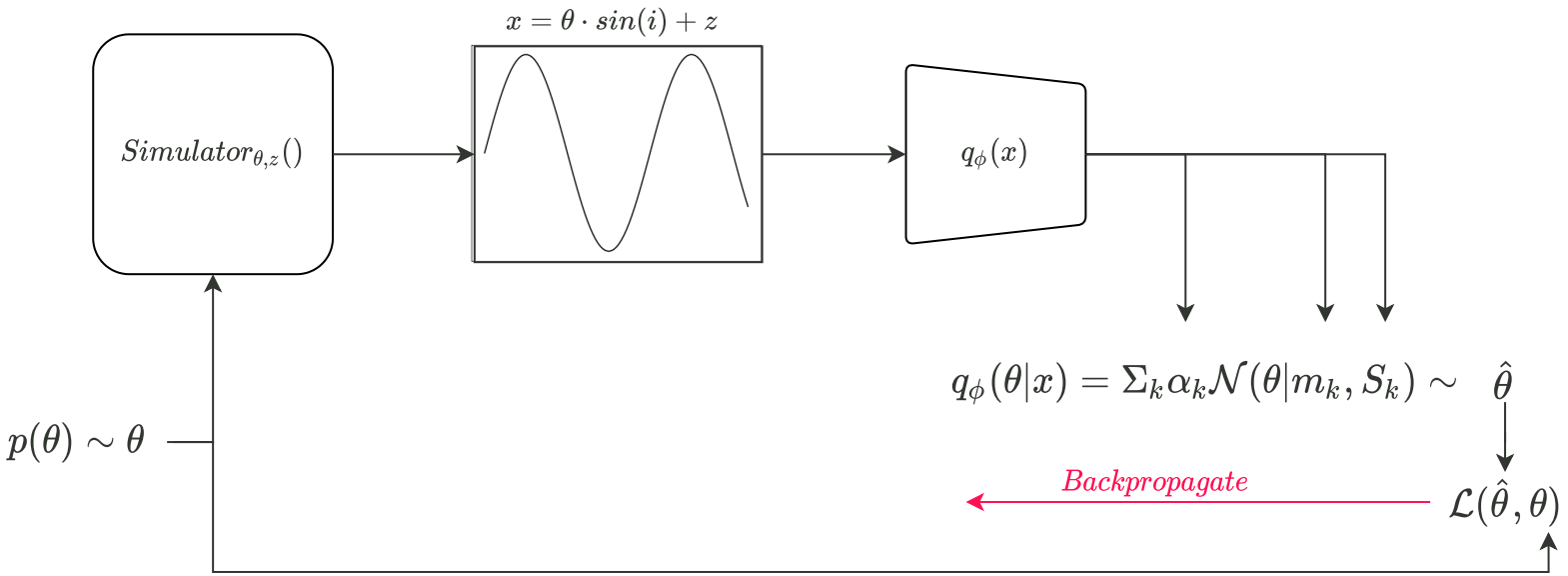

$\tilde{p}(\theta) \leftarrow p(\theta)$

repeat

  for $n = 1..N$ **do**

    sample $\theta_n \sim \tilde{p}(\theta)$

    sample $x_n \sim p(x|\theta_n)$

  end

  train $q_\phi(\theta|x)$ on $\{x_n, \theta_n\}$

  $\hat{p}(\theta|x = x_0) \leftarrow \frac{p(\theta)}{\tilde{p}(c)} q_\phi(\theta|x)$

until $\tilde{p}(\theta)$ has converged;

Pseudocode derived from [1]

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How to use SBI?

Some advertisement

- Now that you are pretty excited about SBI and its applications
- mlcolab and mackelab is developing a python (and eventually Julia) library (that I've used earlier)
- If you are interested: try it out and give us your feedback
- link to colab
- link to github

References

[1] G. Papamakarios and I. Murray. Fast epsilon-free inference of simulation models with bayesian conditional density estimation. arXiv preprint arXiv:1605.06376, 2016.

How

Approximate Bayesian Computation

- Finding parameters/posterior over parameters with
  - Rejection ABC
  - Markov Chain Monte Carlo ABC
  - Sequential Monte Carlo ABC
  - ...
- Problems
  -

What

is Simulation-based Inference?

- If we know generating factors, we can build a simulator
- But we want to constrain simulator output on observations from real world
- Thus we need realistic values for simulator parameters
- -> inverse problem
- SBI solvers this inverse problem using Bayesian inference

How

does Simulation-based Inference work?