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
- Applying SBI

- 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

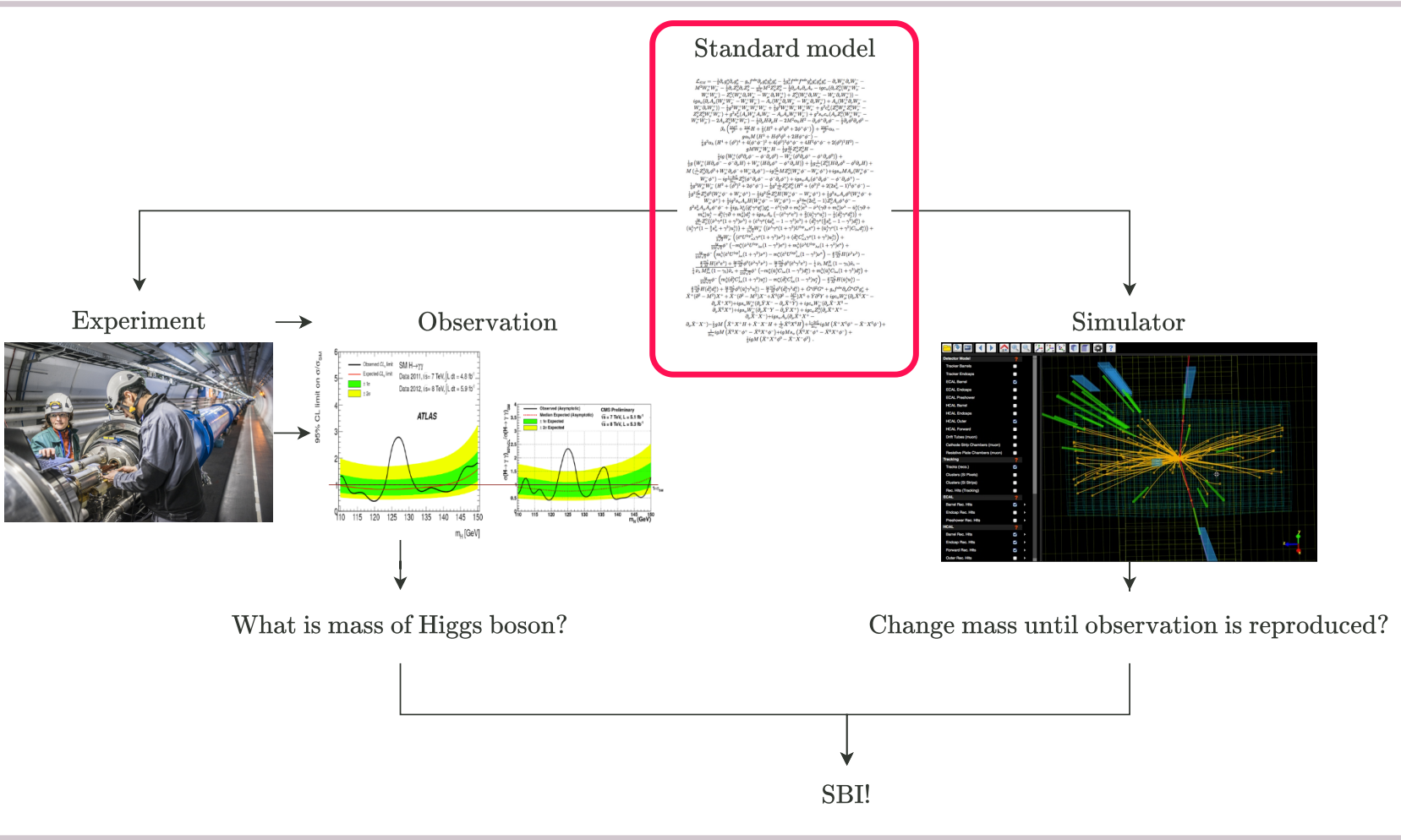

Figure derived from cern.ch, Achintya Rao and Tom McCauley, sciencealert.com

What and Why?

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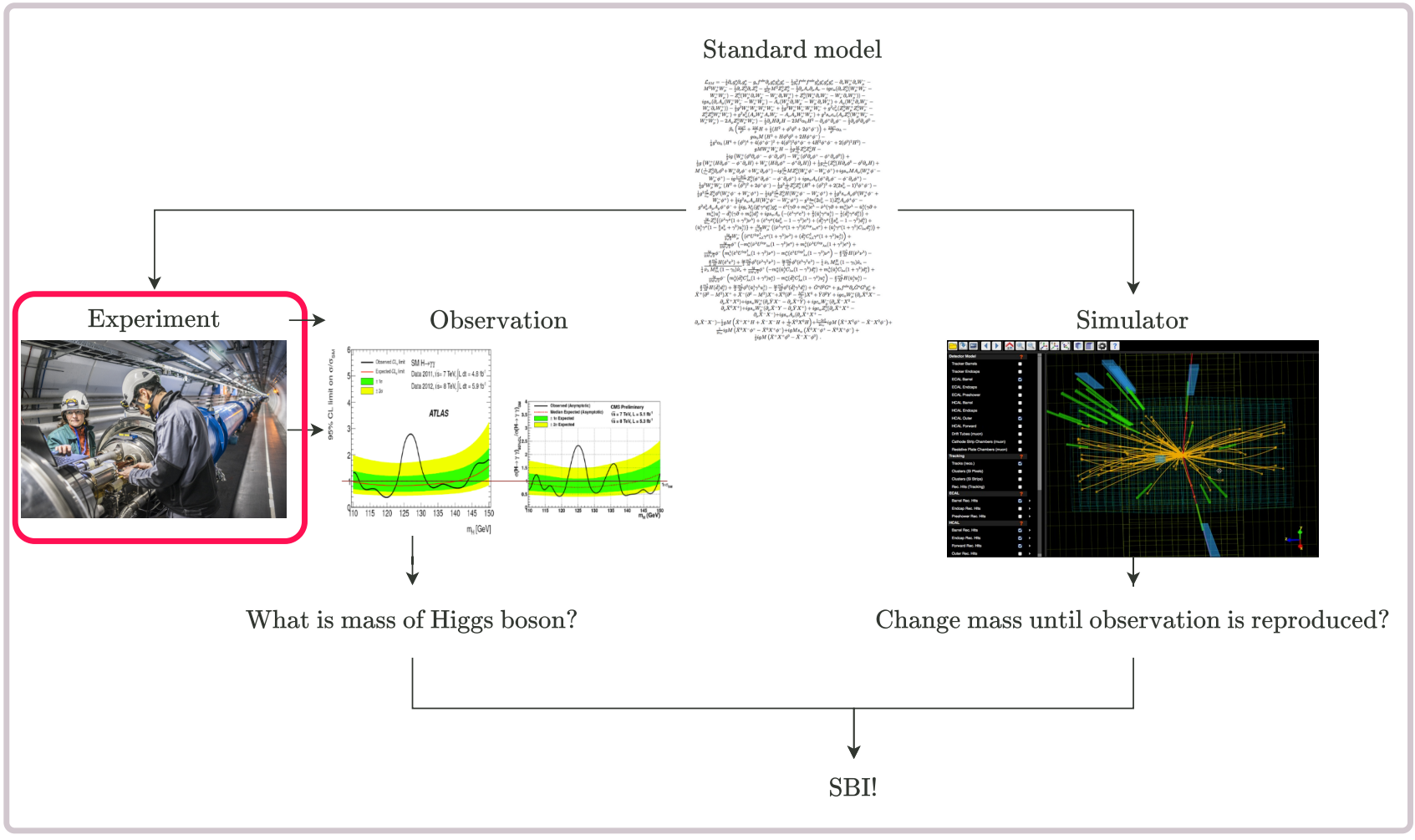

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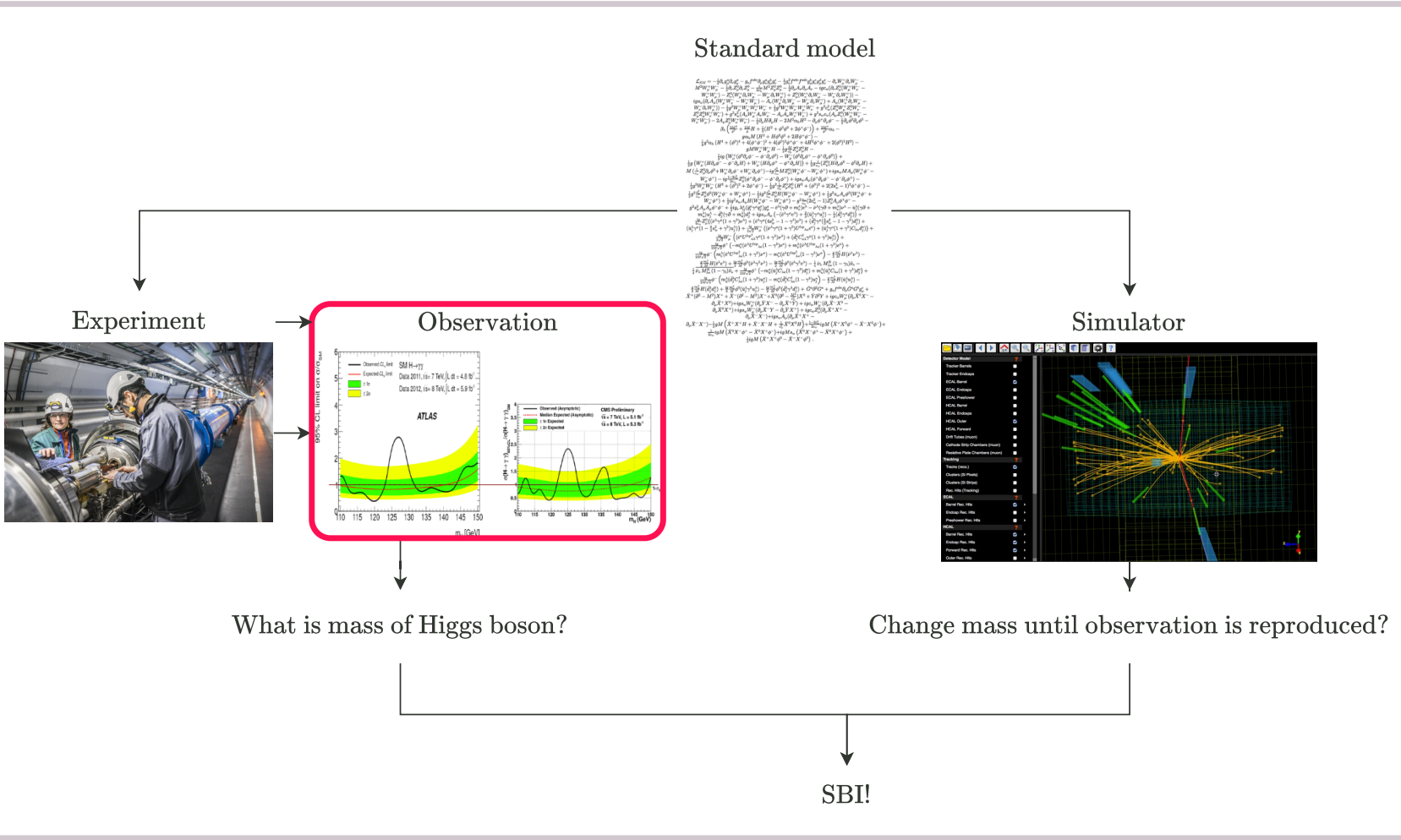

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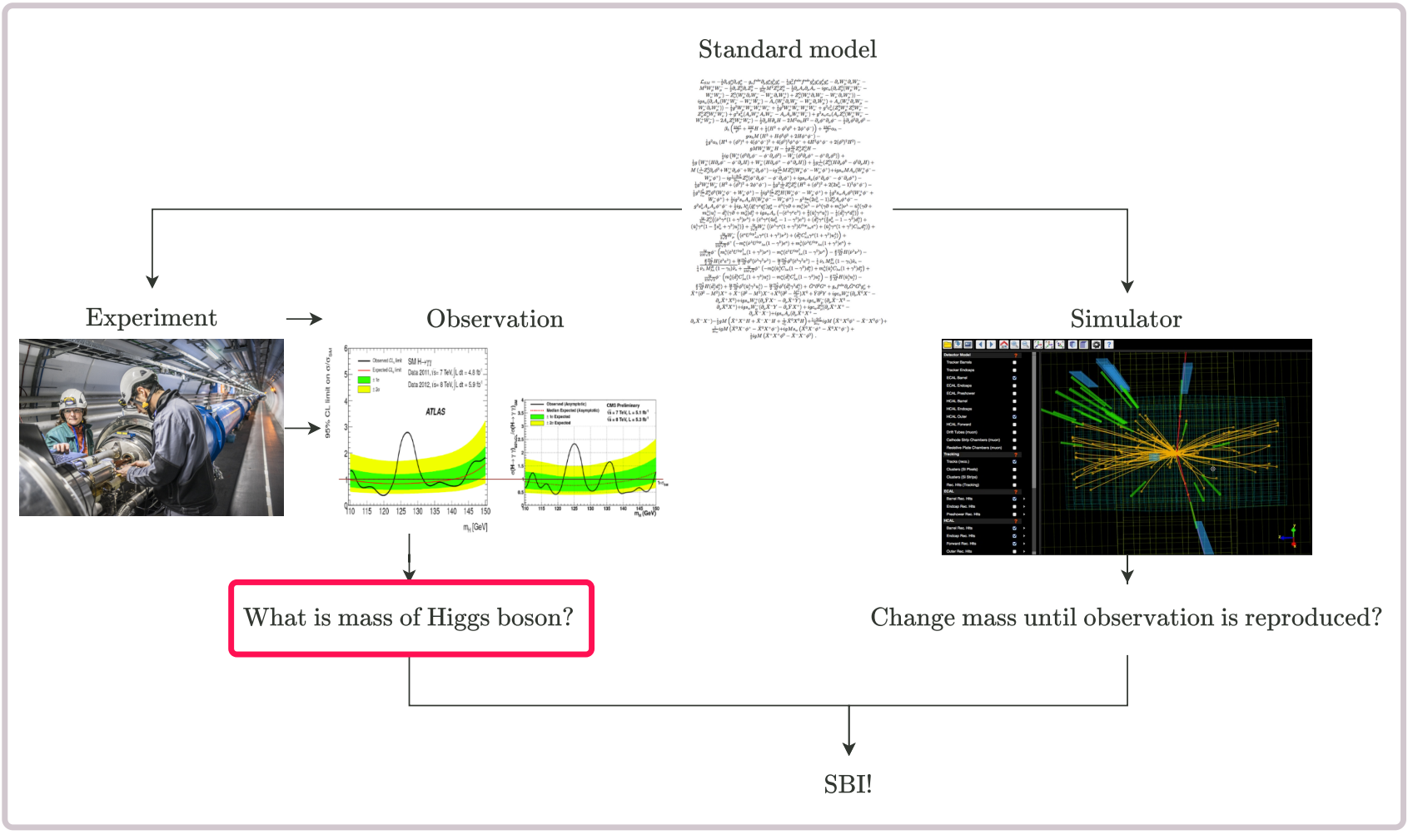

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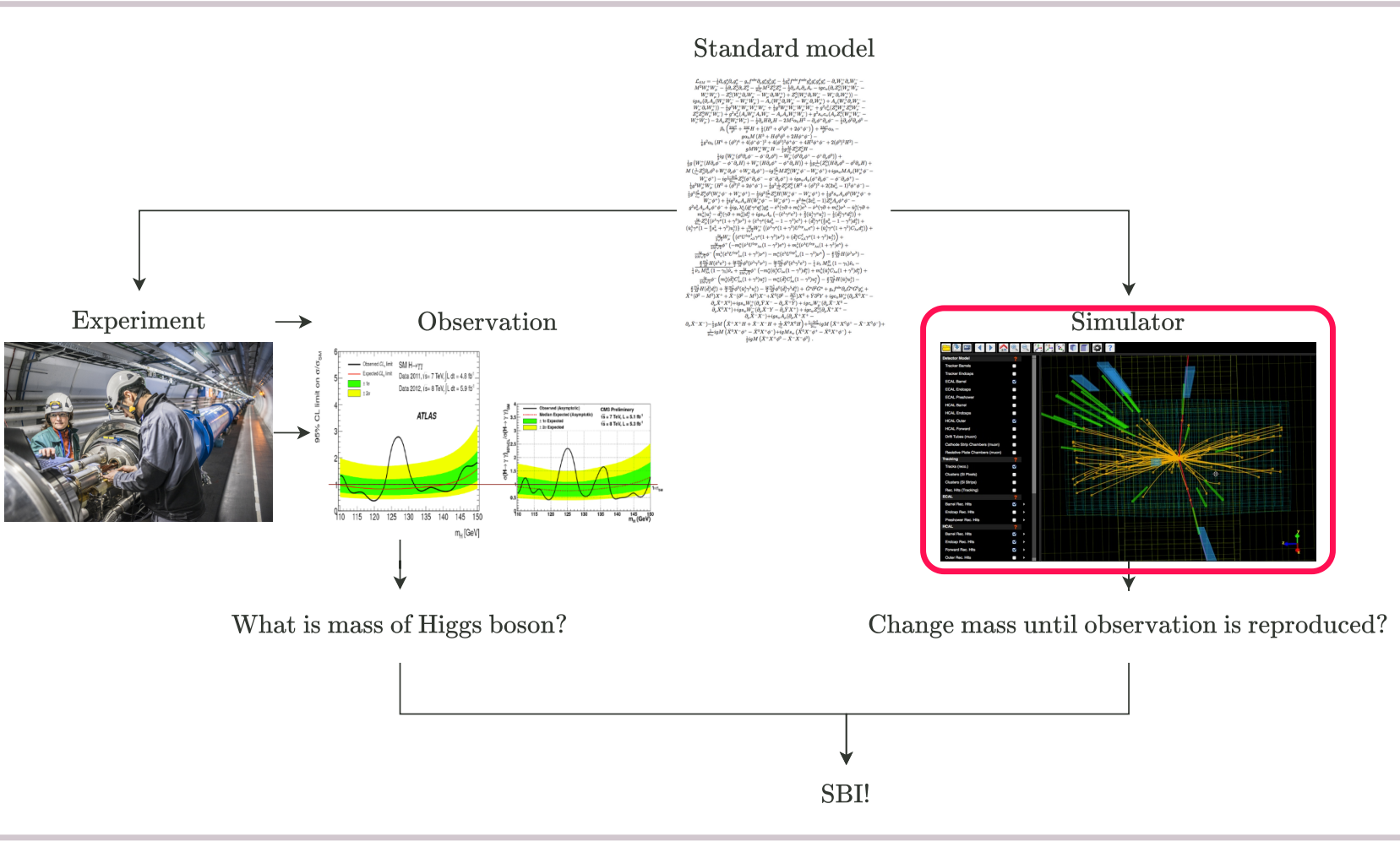

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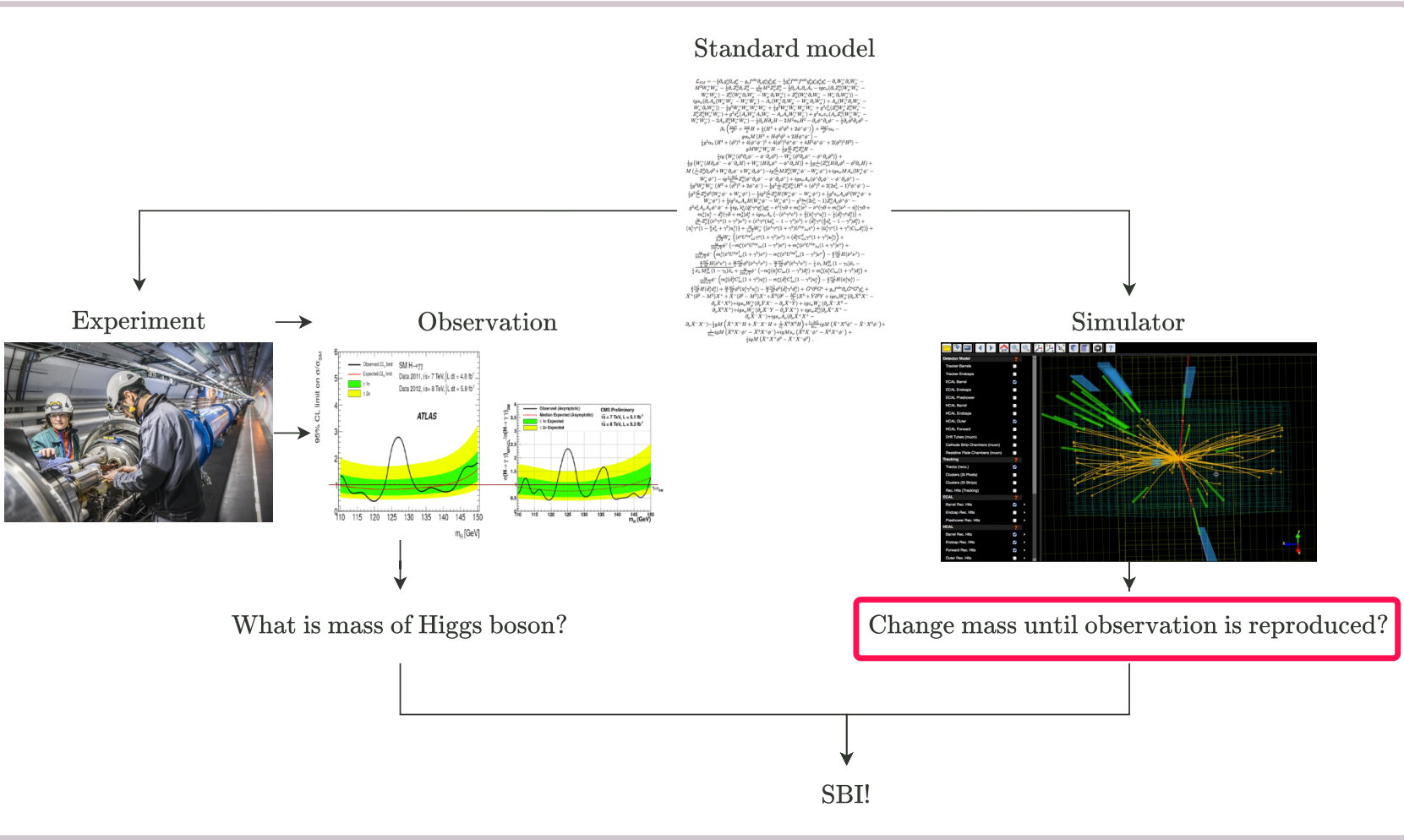

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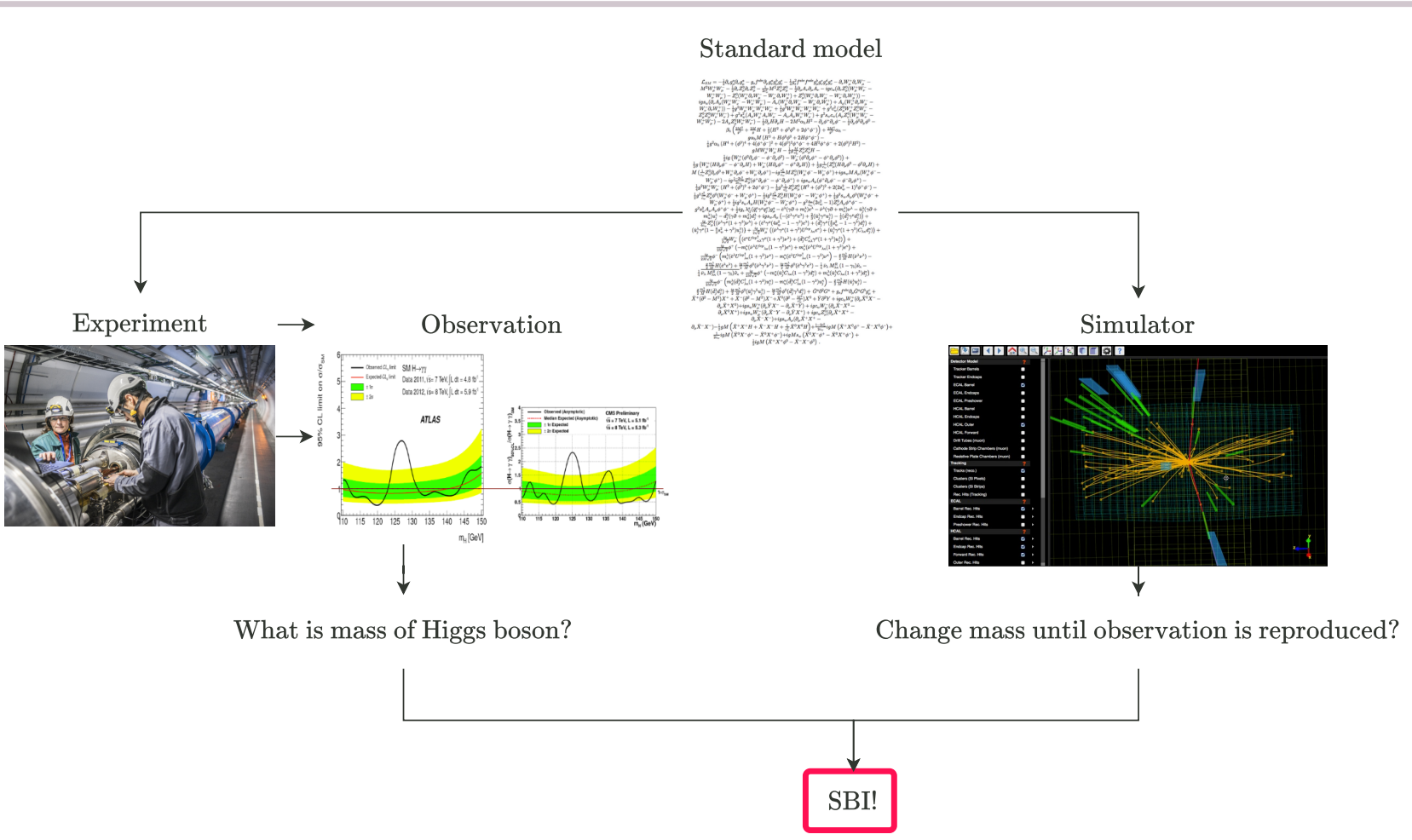

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- Before we go into SBI, let's take a minute to formalize our setting
- Simulator has parameters θ, nuisance parameter z and produces data $\hat{x}$
  - It implicitly defines $p(\hat{x}, z|\theta)$ (it yields samples from this distribution)
- Given 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
  - Change θ until something ϵ-close to x_0 is produced
  - Approximates $p(\theta|\ ||\ x - x_0\ ||< \epsilon)$
  - Inefficient for small ϵ
  - No actual posterior but only point estimate
- Some improvements
  - Sampling ABC (perturb matched parameters) [6]
  - Sequential ABC (simulate sequence of slowly-changing distribution with importance sampling) [1, 2]
- Point-estimate to posterior over parameters for ϵ-ball around observation

- Papamakarios and Murray [7] learn approximation to actual posterior
- Use simulator to create training set
  - $\{x_j, \theta_j\}_{j \in N}$
- Train neural network to predict parameters of posterior over θs

Simulation-based Inference

Predicting Parameter Posterior

for $n = 1..N$ **do**
  sample $\theta_n \sim p(\theta)$
  sample $x_n \sim p(x|\theta_n)$
end
train $q_\phi(\theta|x)$ on $\{x_n, \theta_n\}$
sample $\theta \sim q(\theta|x = x_0)$

Pseudocode derived from [7]

for $n = 1..N$ **do**
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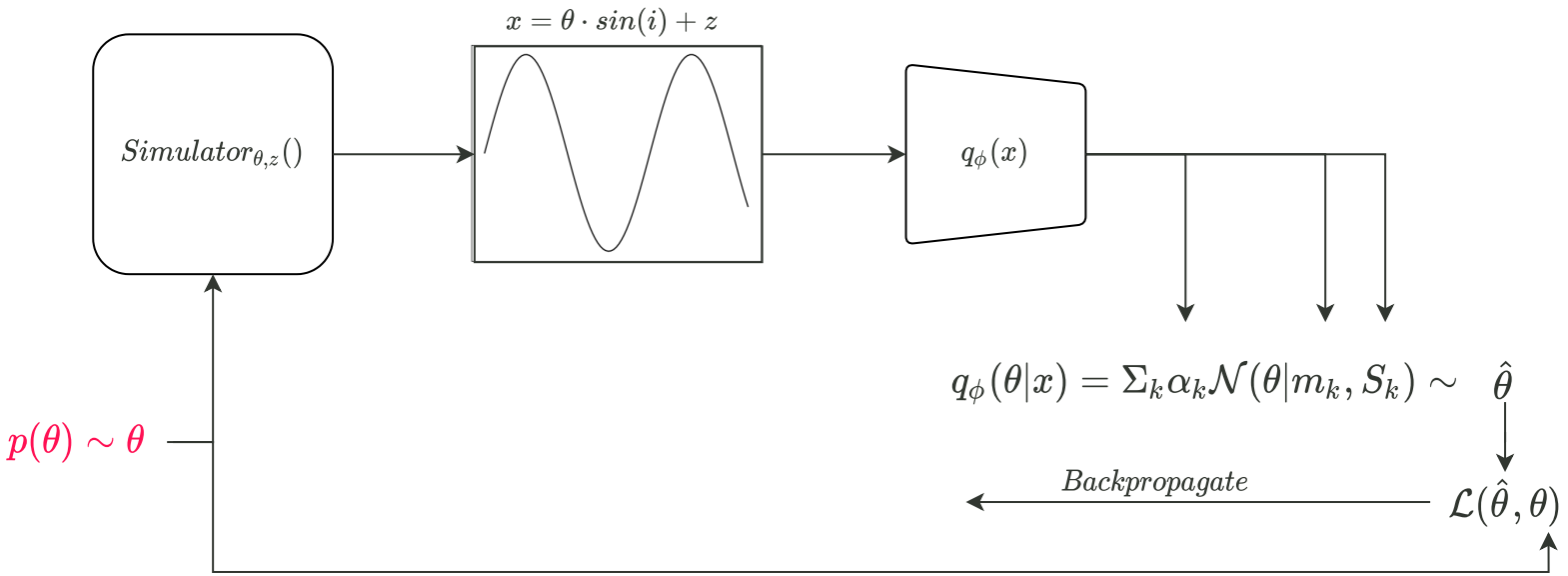
Learning a Posterior

from Simulations



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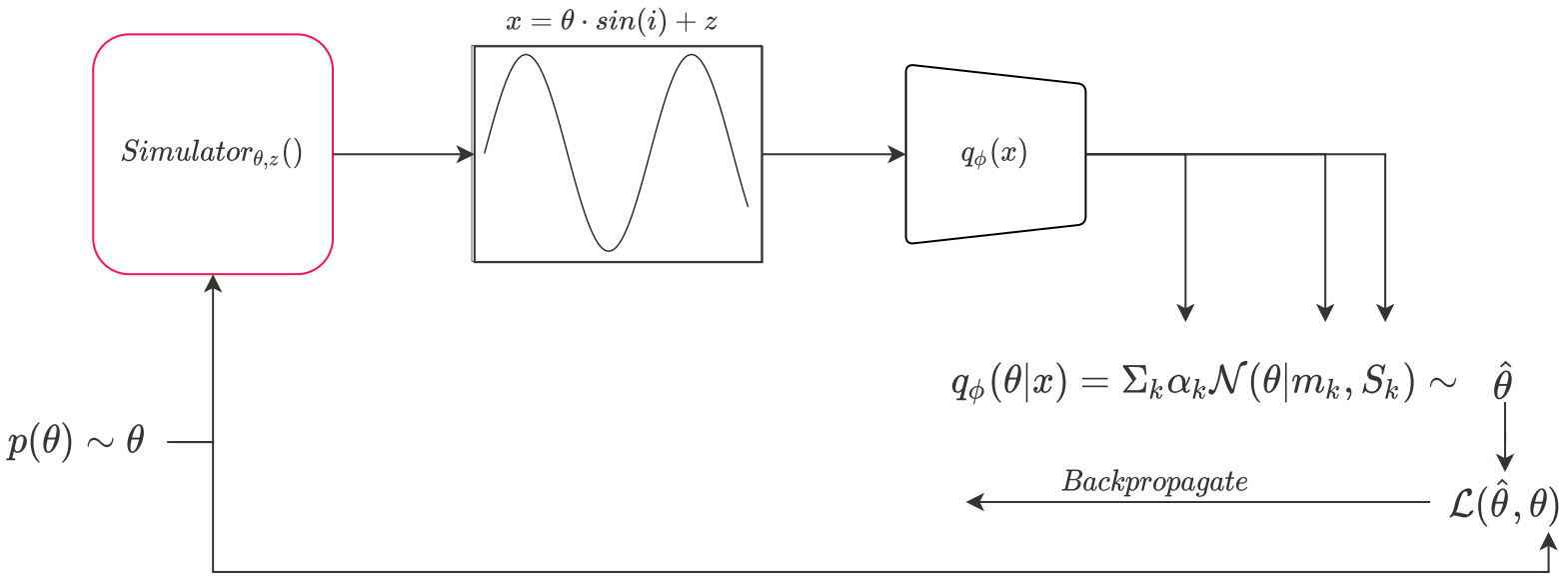

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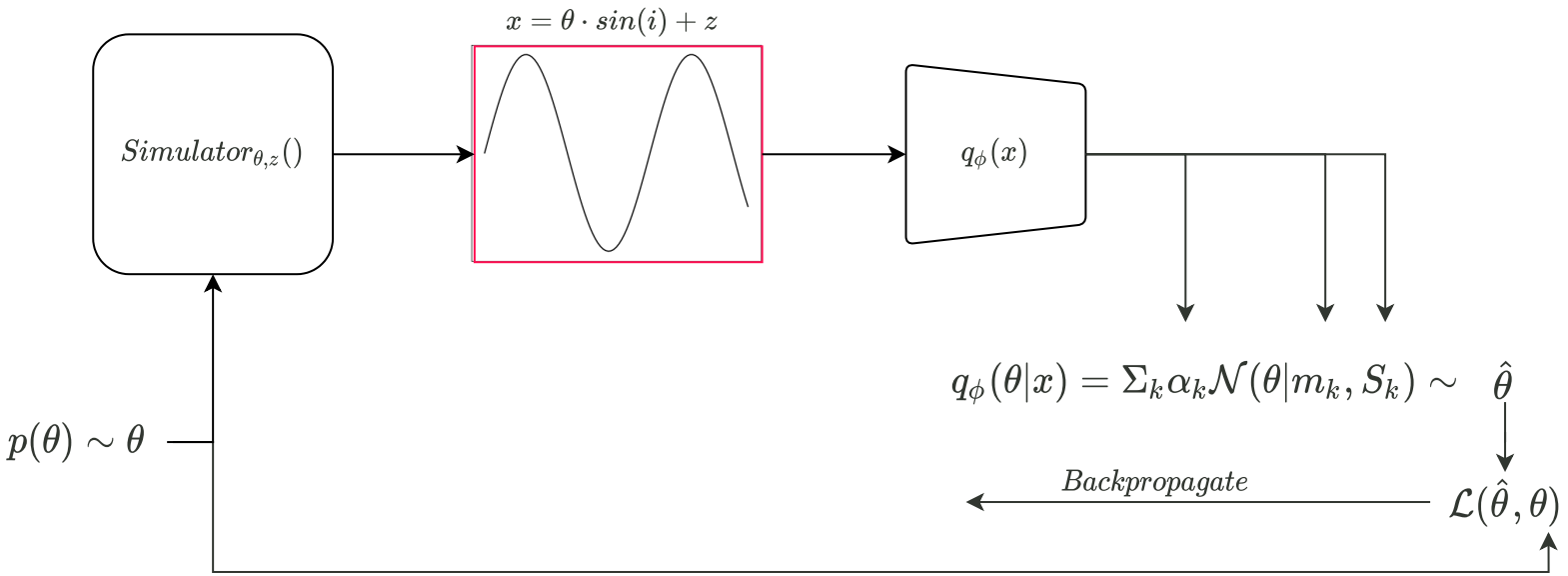

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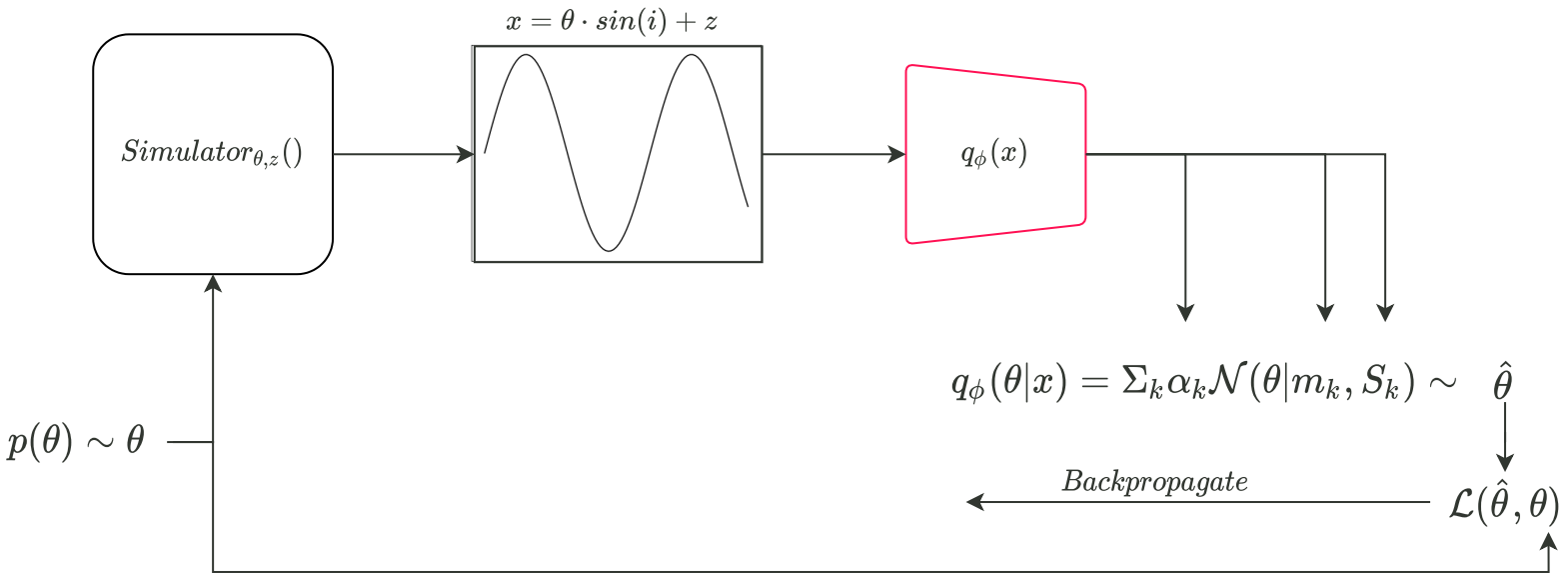

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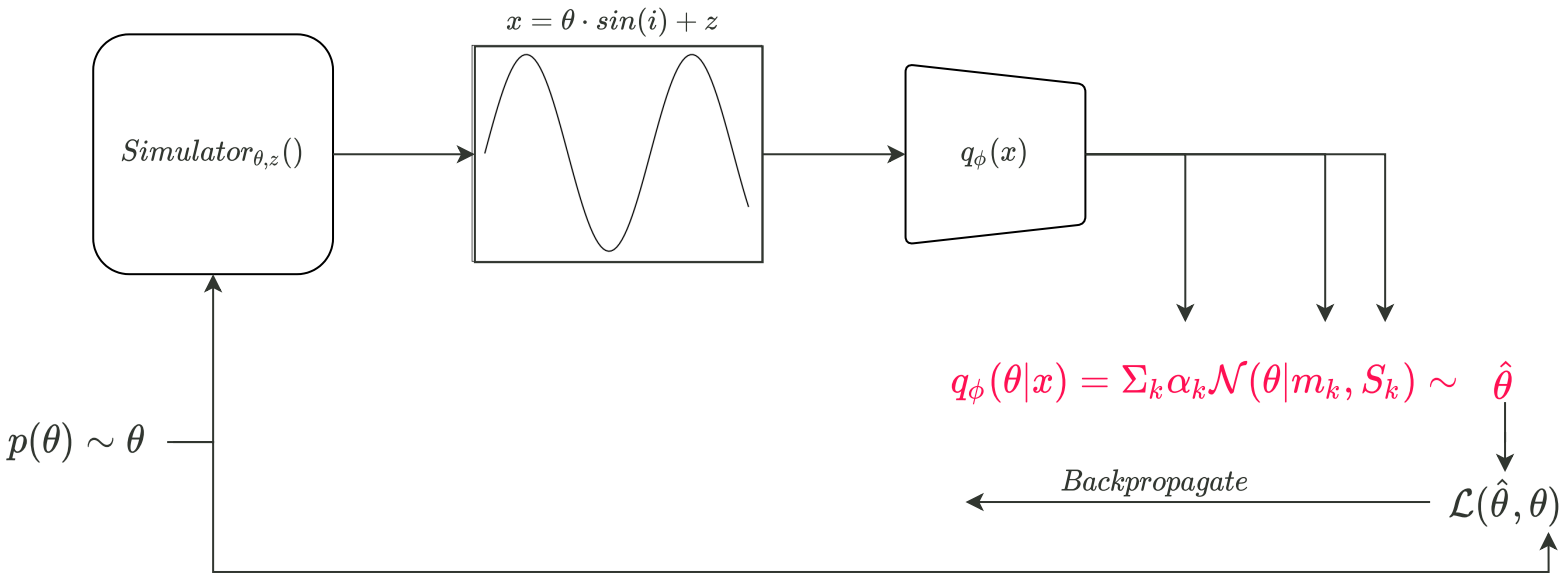

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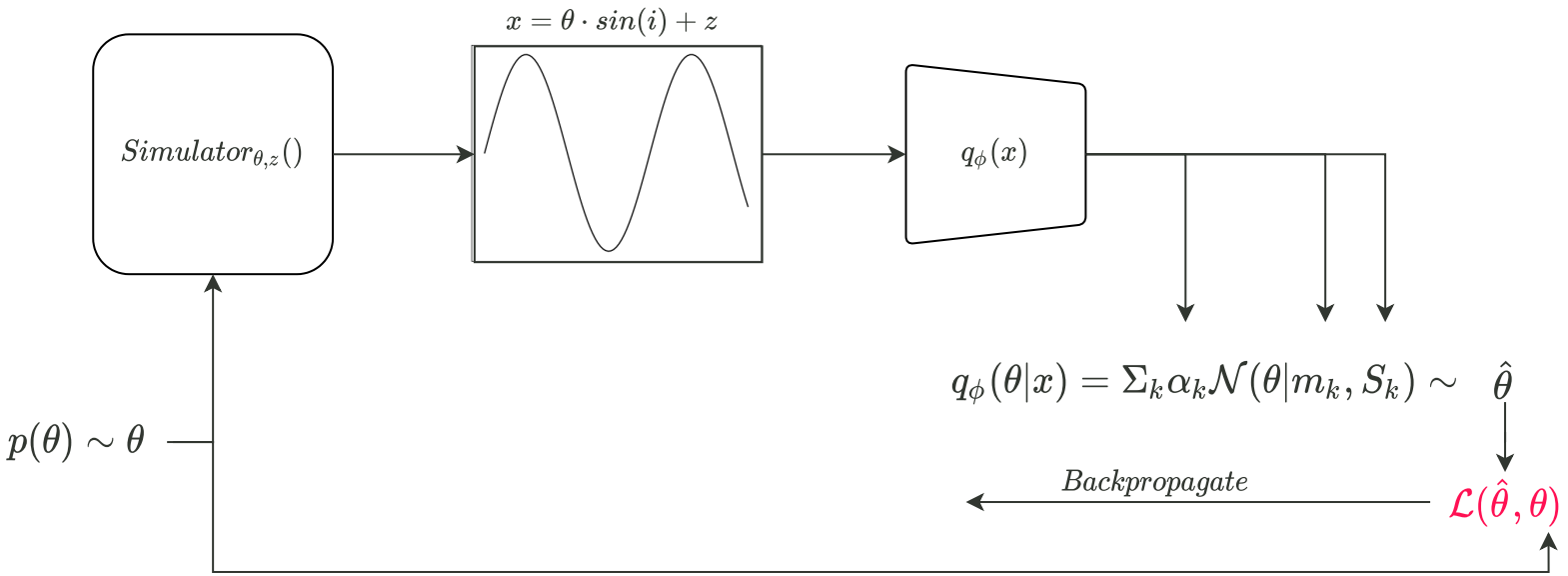

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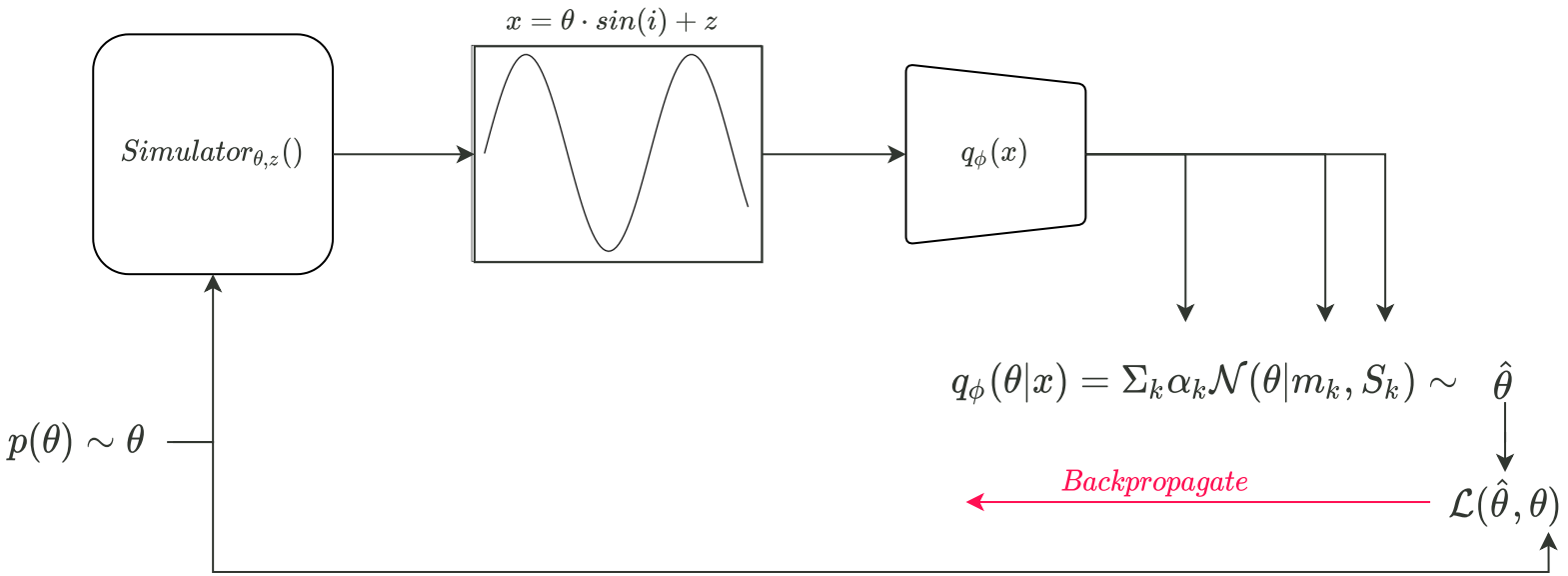
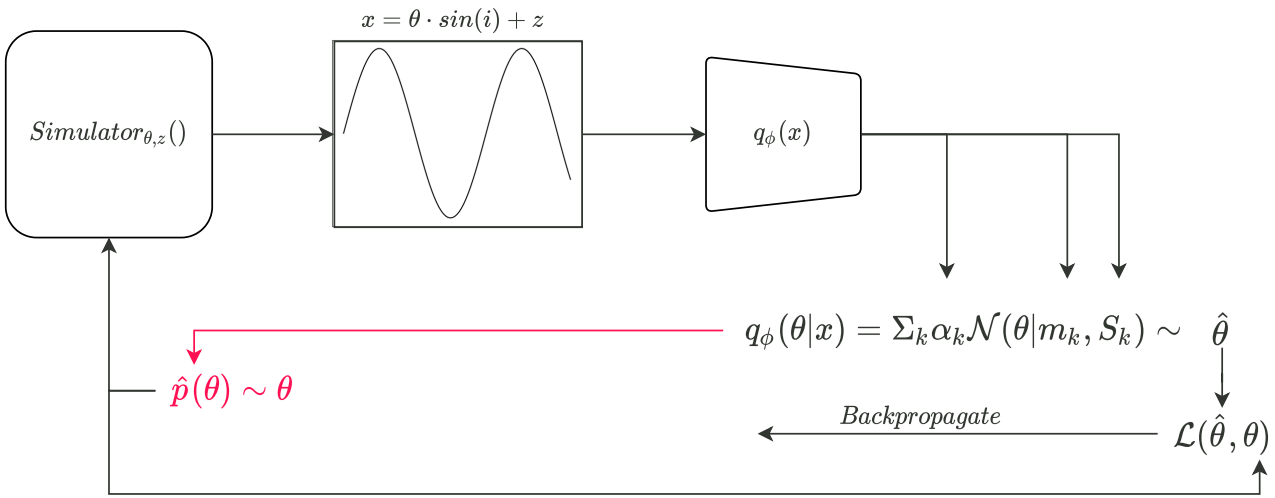


Updating the Prior

With the Posterior

- What if we only care about single observation?
- Iteratively replace prior with posterior
- Improves convergence speed



Updating the Prior

With the Posterior

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

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 $\{x_n, \theta_n\}$

  $\tilde{p}(\theta) \leftarrow q_\phi(\theta|x)$

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

Pseudocode derived from [7]

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Applying SBI

to Hodgkin–Huxley

- Lueckmann et al. [5] apply SBI to neuro-science setting
  - Diverging simulations
  - Corrupt data
  - Summary statistics challenging
- They propose
  - Posterior over network weights
  - Train classifier to predict whether parameters fail
  - Extract Features with RNN
- Apply Hodgkin-Huxley model [4]
  - Dynamics of neuron's membrane
  - Parameters (concentration of sodium, potassium, ...)
  - Numerical simulators available (NEURON software [3])

Applying SBI

Results

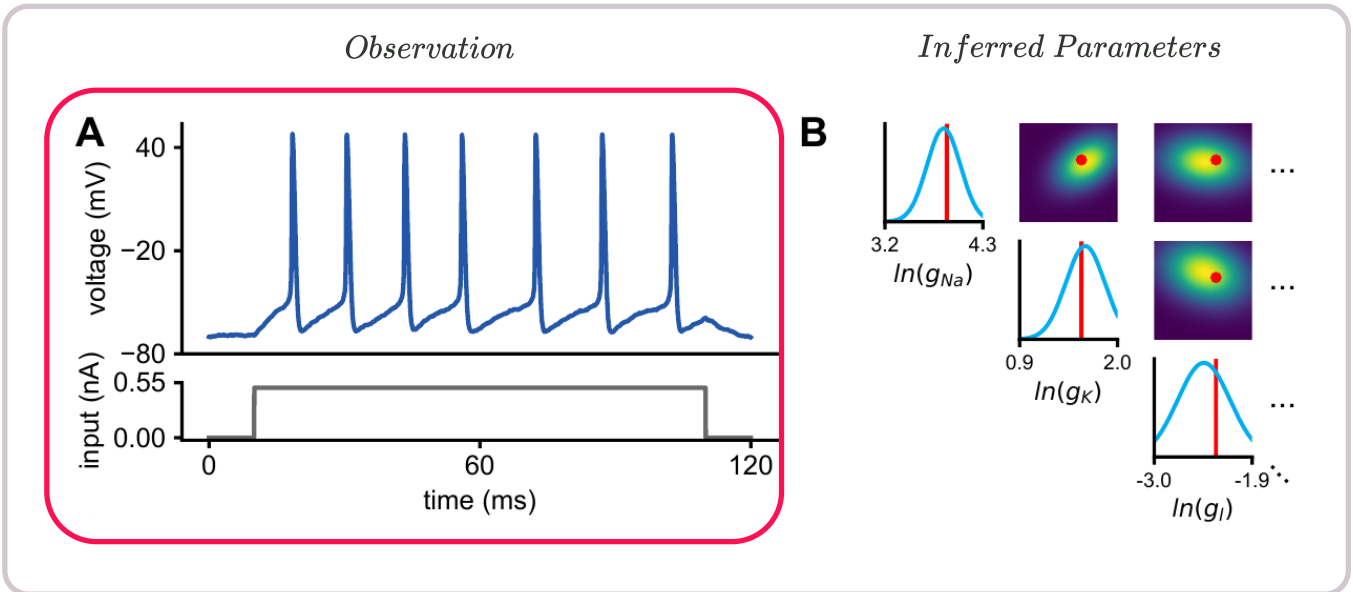


Figure derived from [5]

Applying SBI

Results

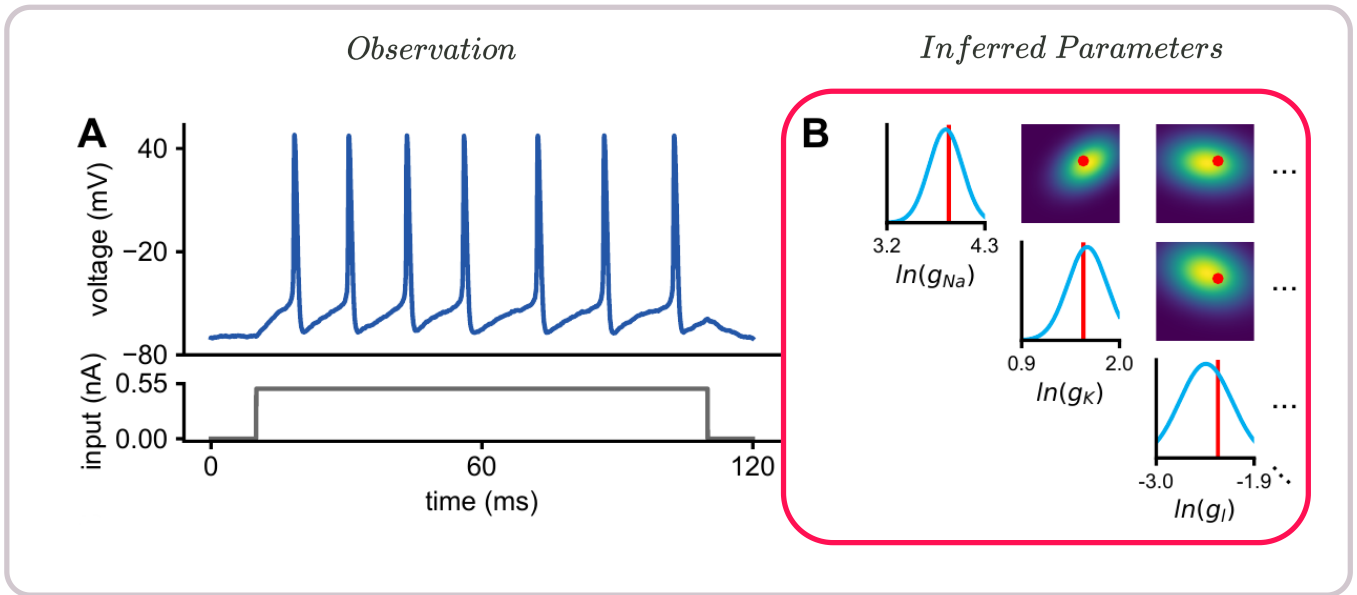


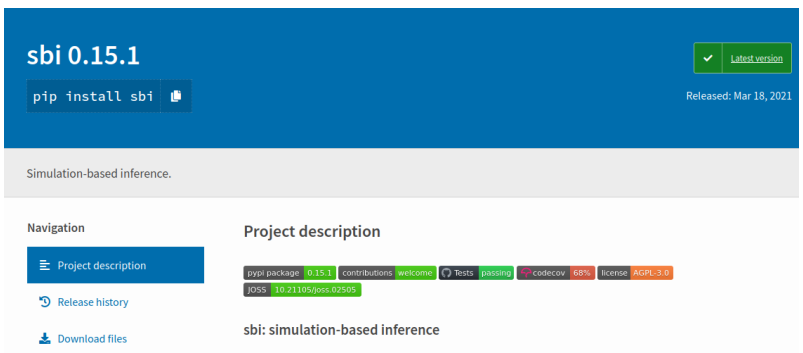
Figure derived from [5]

- Example

How to use SBI?

Some advertisement

- mlcolab and mackelab is developing a sbi python library
- If you are interested: try it out and give us your feedback
- `colab.research.google.com/drive/1L1T45hruoScyu3hN4WkDW6f0De4UemjI?usp=sharing`
- `github.com/mackelab/sbi`
- `pip install sbi`



References

[1] M. A. Beaumont, J.-M. Cornuet, J.-M. Marin, and C. P. Robert. Adaptive approximate bayesian computation. Biometrika, 96(4):983–990, 2009.

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[3] N. T. Carnevale and M. L. Hines. The NEURON book. Cambridge University Press, 2006.

[4] A. L. Hodgkin and A. F. Huxley. A quantitative description of membrane current and its application to conduction and excitation in nerve. The Journal of physiology, 117(4):500–544, 1952.

[5] J.-M. Lueckmann, P. J. Goncalves, G. Bassetto, K. Öcal, M. Nonnenmacher, and J. H. Macke. Flexible statistical inference for mechanistic models of neural dynamics. arXiv preprint arXiv:1711.01861, 2017.

[6] P. Marjoram, J. Molitor, V. Plagnol, and S. Tavaré. Markov chain monte carlo without likelihoods. Proceedings of the National Academy of Sciences, 100(26):15324–15328, 2003.

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