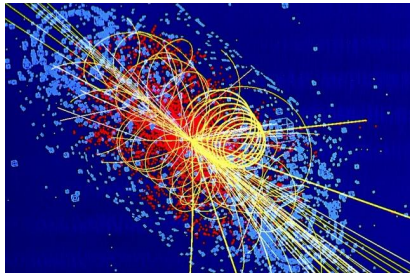
Probabilistic Inference in Simulators


Atılım Güneş Baydin, Lukas Heinrich, Wahid Bhimji,
Lei Shao, Saeid Naderiparizi, Andreas Munk,
Jialin Liu, Bradley Gram-Hansen, Gilles Louppe,
Lawrence Meadows, Philip Torr, Victor Lee, Prabhat,
Kyle Cranmer, Frank Wood

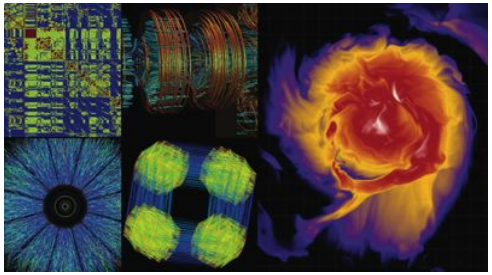
Applied Machine Learning Days, EPFL
28 Jan 2020

Simulation and physical sciences

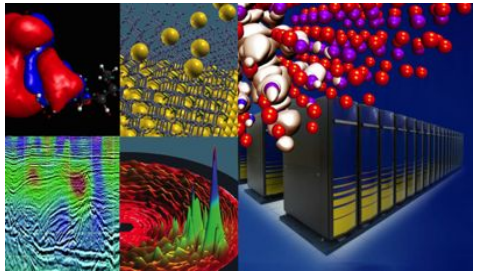
Computational models and simulation are key to scientific advance at all scales



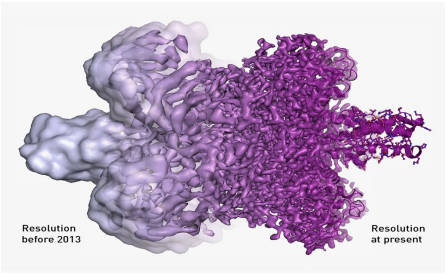
Particle physics



Nuclear physics

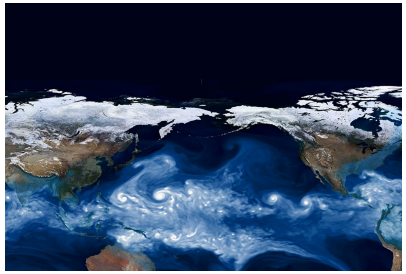


Material design

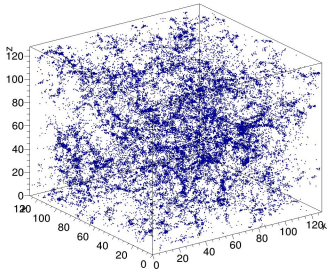


Drug discovery

Weather

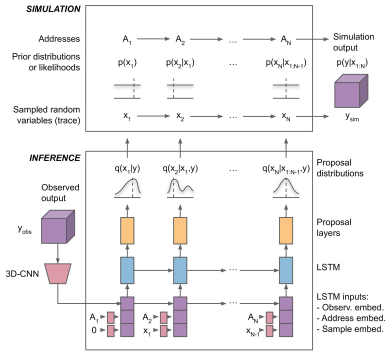


Climate science

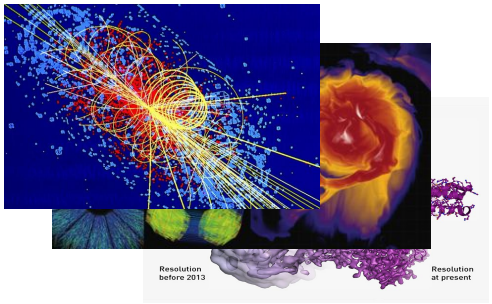


Cosmology

Introducing a new way to use existing simulators

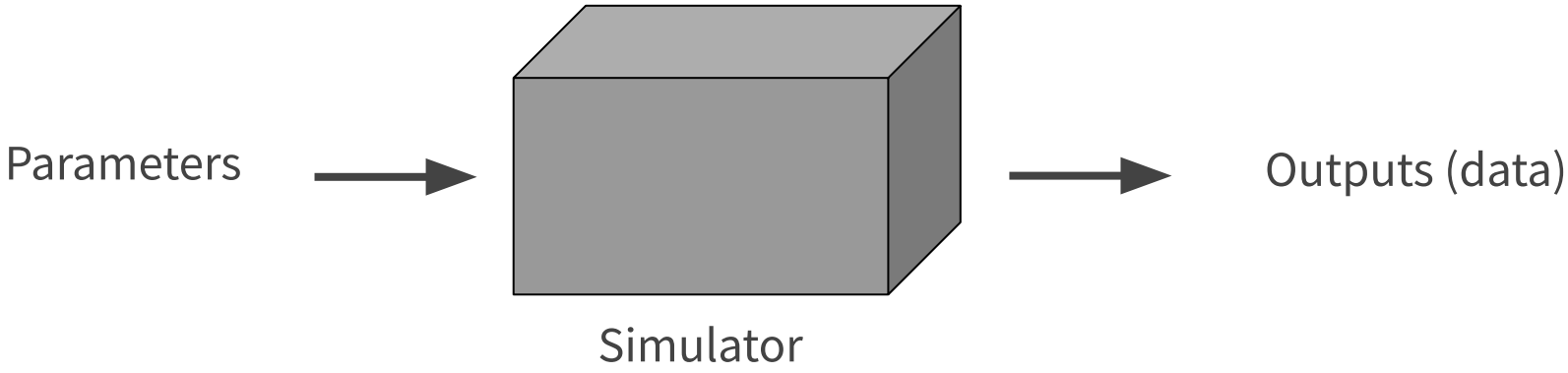


Probabilistic programming

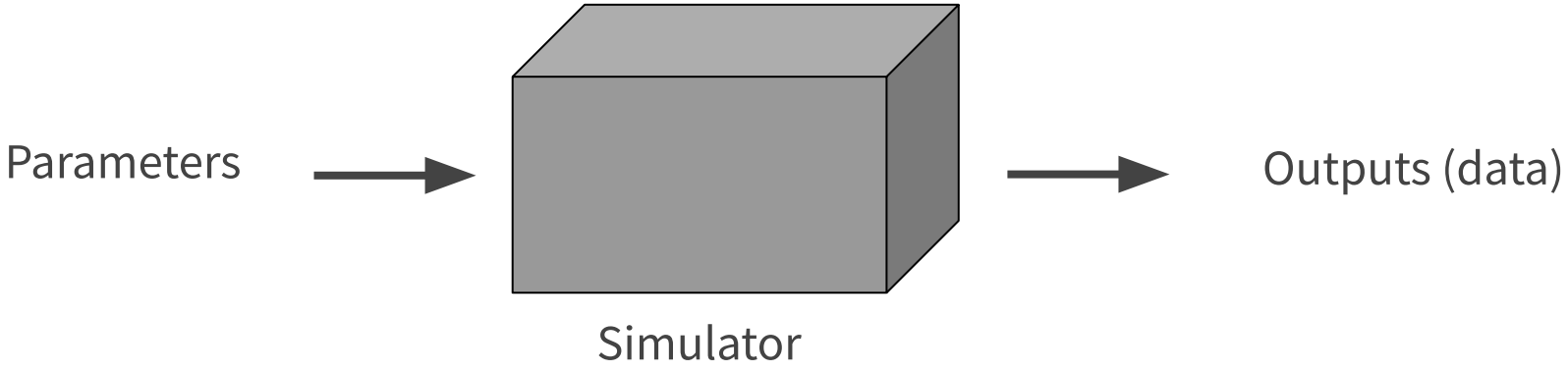


Simulation

Simulators



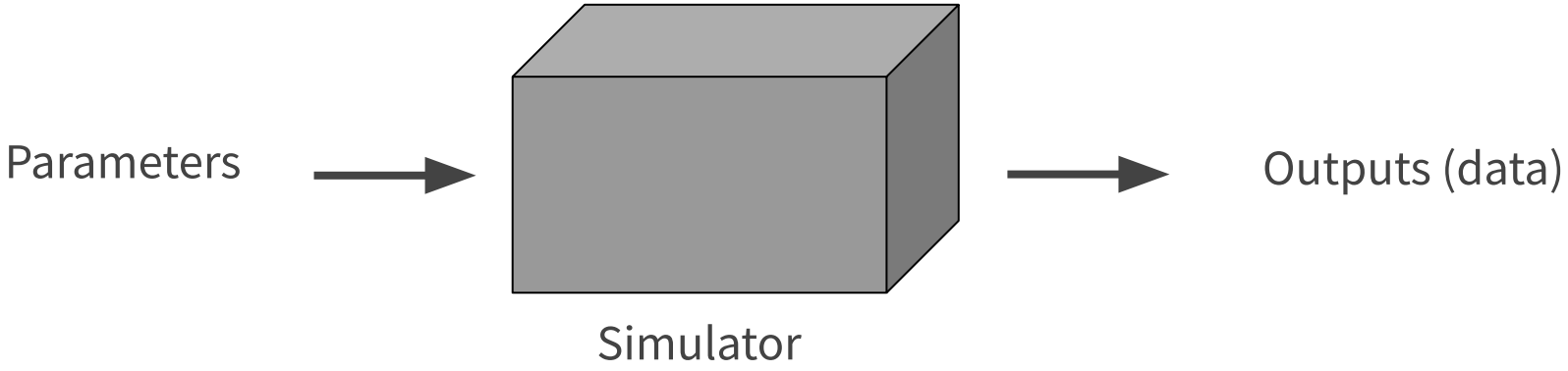
Simulators



Prediction:

- Simulate forward evolution of the system
- Generate samples of output

Simulators



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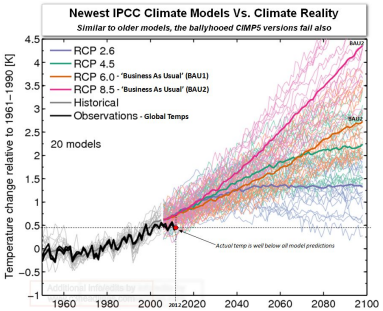
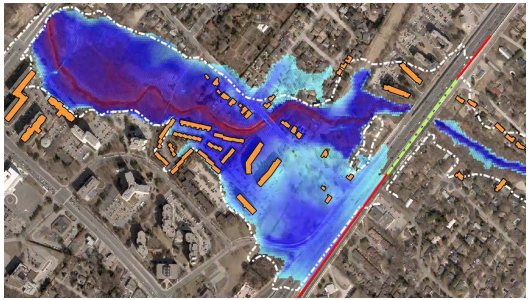
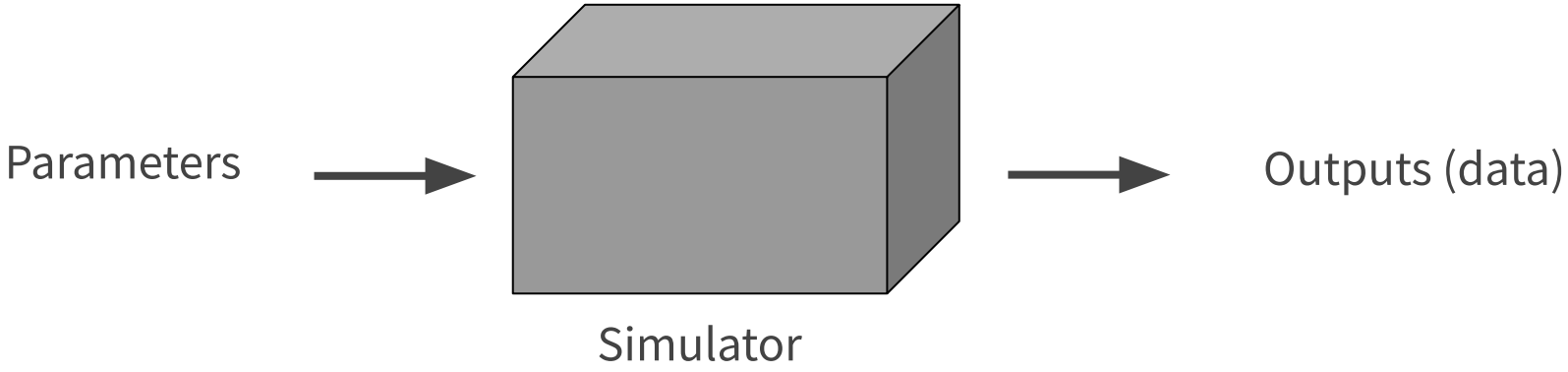




Simulators

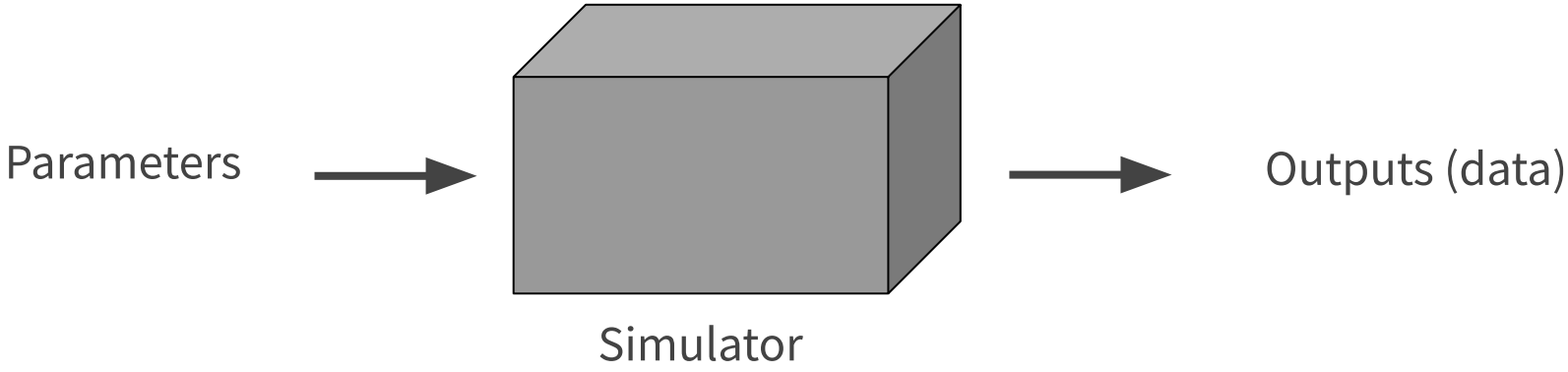


Prediction:

- Simulate forward evolution of the system
- Generate samples of output

WE NEED THE INVERSE!

Simulators



Prediction:

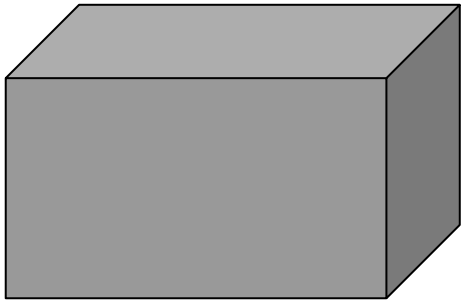
- Simulate forward evolution of the system
- Generate samples of output

Inference:

- Find parameters that can produce (explain) observed data
- Inverse problem
- Often a manual process

Simulators

Parameters



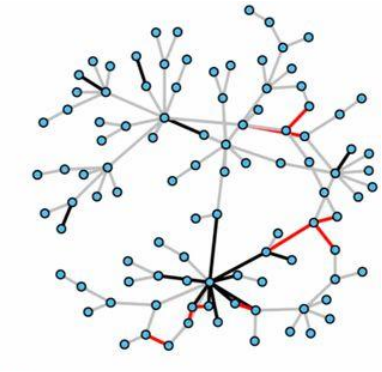
Outputs (data)

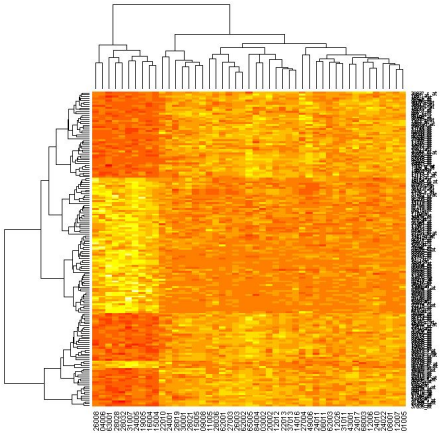
Simulator

Inferred parameters

Observed data

Gene network





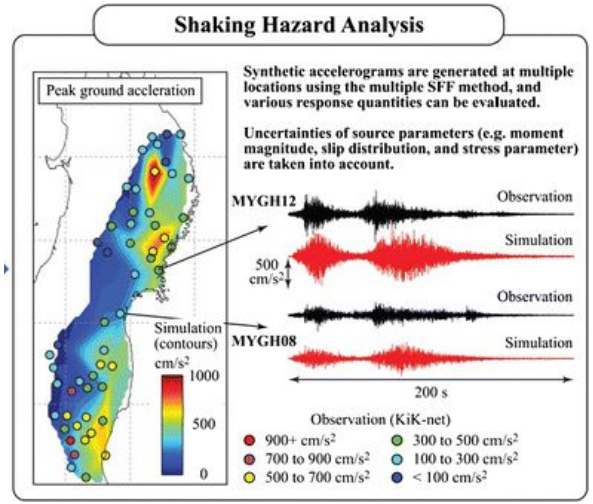
Gene expression

Simulators

Parameters → Simulator → Outputs (data)

Inferred parameters ← Simulator ← Observed data

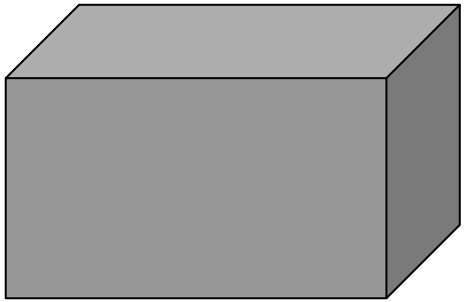
Earthquake location & characteristics



Seismometer readings

Simulators

Parameters



Outputs (data)

Simulator

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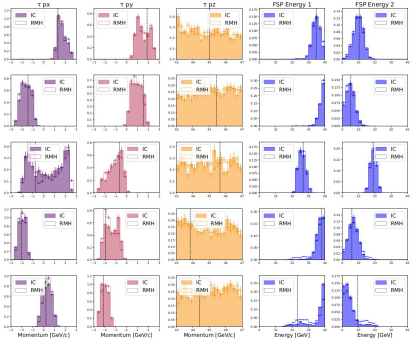
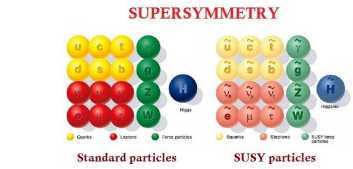
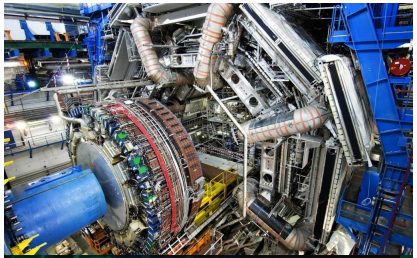
Observed data

Event analyses & new particle discoveries

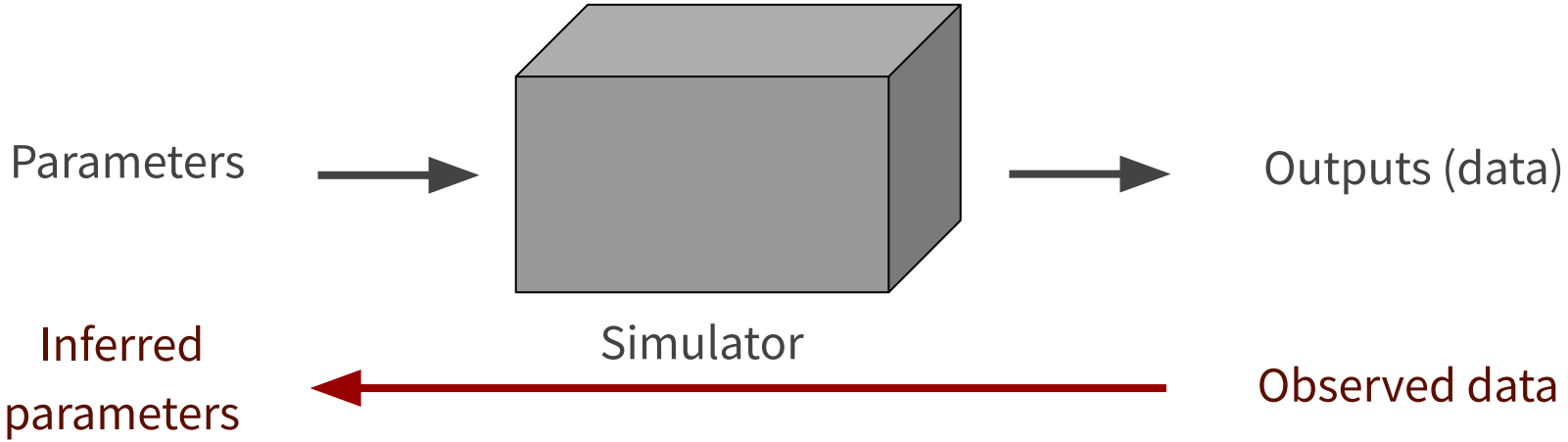






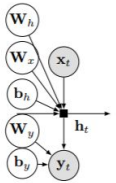
Particle detector readings

Inverting a simulator



Probabilistic programming is a machine learning framework allowing us to

- write ***programs that define probabilistic models***
- run automated Bayesian ***inference of parameters conditioned on observed outputs*** (data)



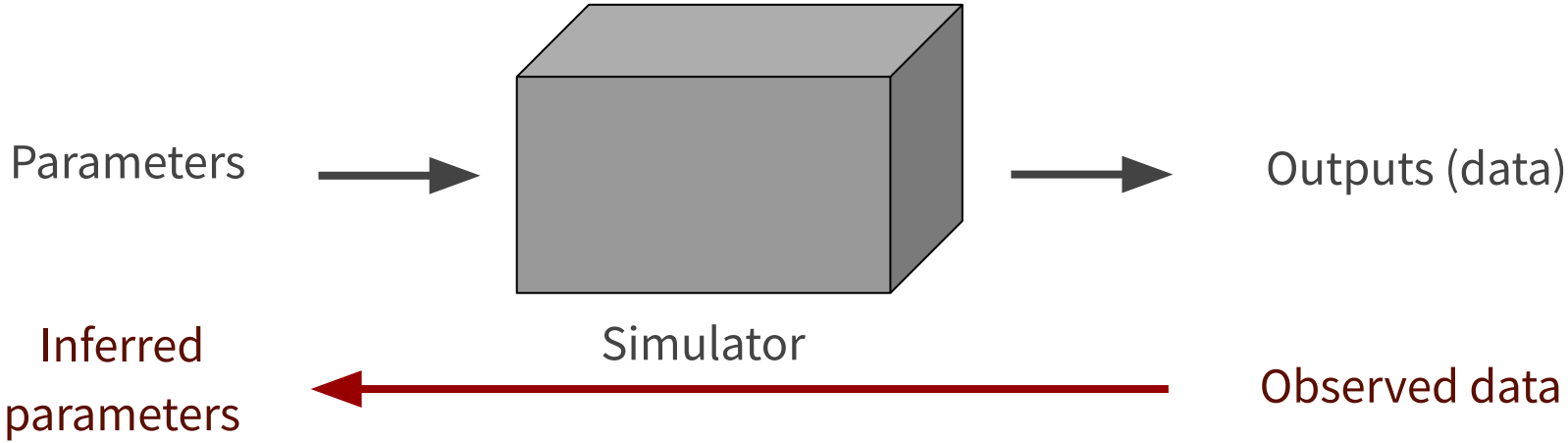

```
def rnn_cell(hprev, xt):
  return tf.tanh(tf.dot(hprev, Wh) + tf.dot(xt, Wx) + bh)

Wh = Normal(mu=tf.zeros([H, H]), sigma=tf.ones([H, H]))
Wx = Normal(mu=tf.zeros([D, H]), sigma=tf.ones([D, H]))
Wy = Normal(mu=tf.zeros([H, 1]), sigma=tf.ones([H, 1]))
bh = Normal(mu=tf.zeros(H), sigma=tf.ones(H))
by = Normal(mu=tf.zeros(1), sigma=tf.ones(1))

x = tf.placeholder(tf.float32, [None, D])
h = tf.scan(rnn_cell, x, initializer=tf.zeros(H))
y = Normal(mu=tf.matmul(h, Wy) + by, sigma=1.0)
```

Pyro Edward Stan

Inverting a simulator



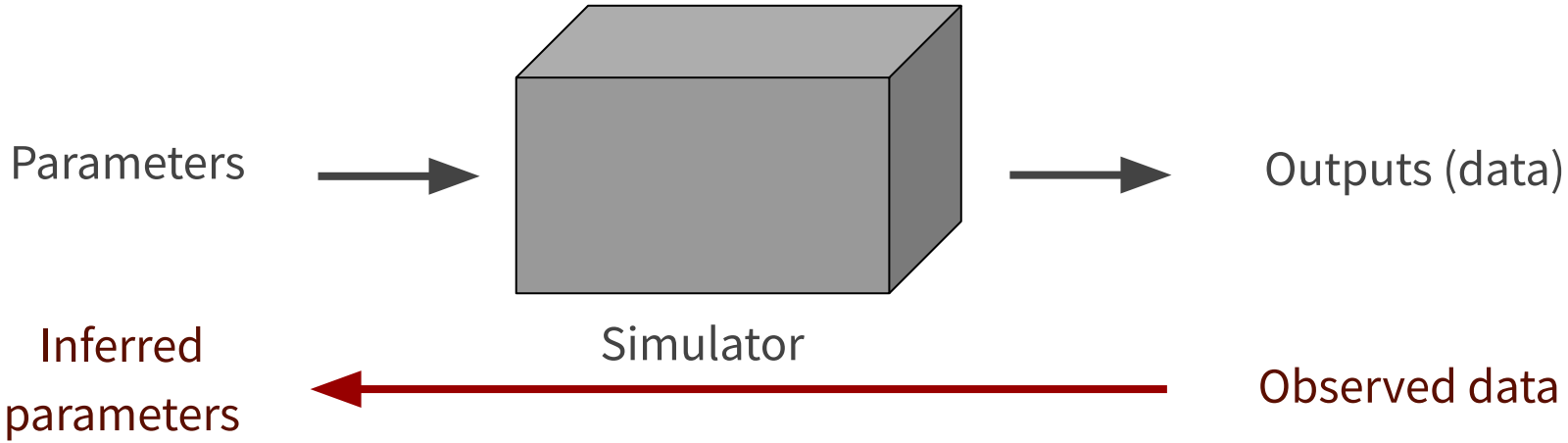
Probabilistic programming is a machine learning framework allowing us to

- writ
- run
  con

- Has been limited to **toy and small-scale problems**
- Normally requires one to **implement a probabilistic model from scratch** in the chosen language/system

Pyro Edward Stan

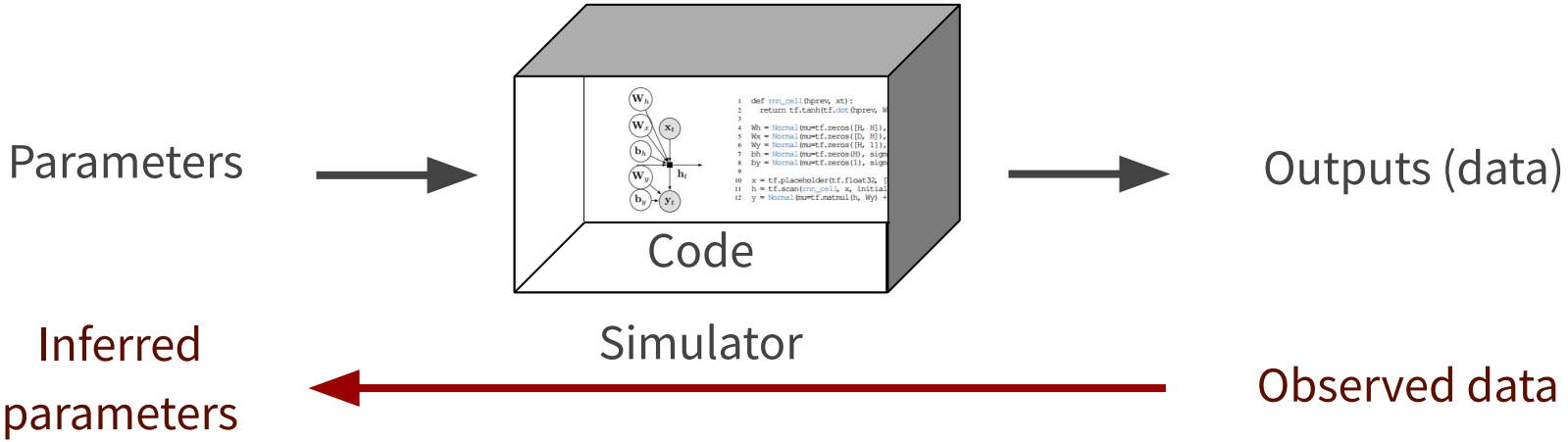
Inverting a simulator



Key idea:

Many simulators are stochastic and they define probabilistic models by sampling random numbers

Inverting a simulator



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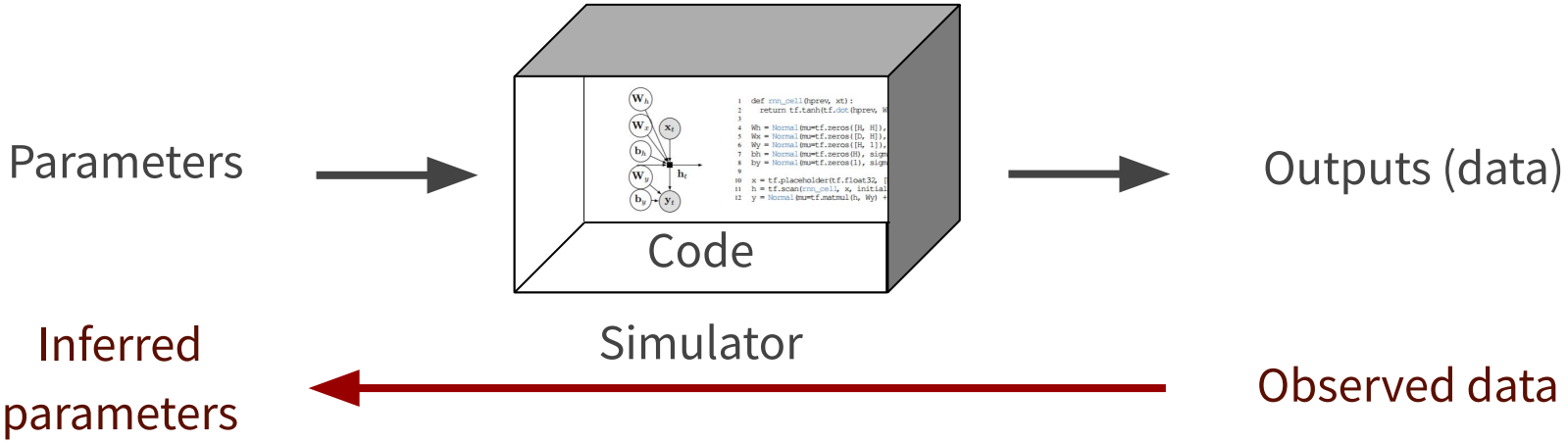
Simulators are probabilistic programs!

Inverting a simulator



Key idea:

Many simulators are stochastic and they define probabilistic models by sampling random numbers

Simulators are probabilistic programs!

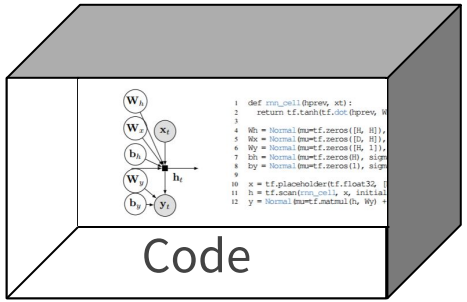
We "just" need an infrastructure to execute them as such

A new probabilistic programming system for existing simulators (in any language) based on PyTorch

Probabilistic execution

PyProb

Parameters



Outputs (data)

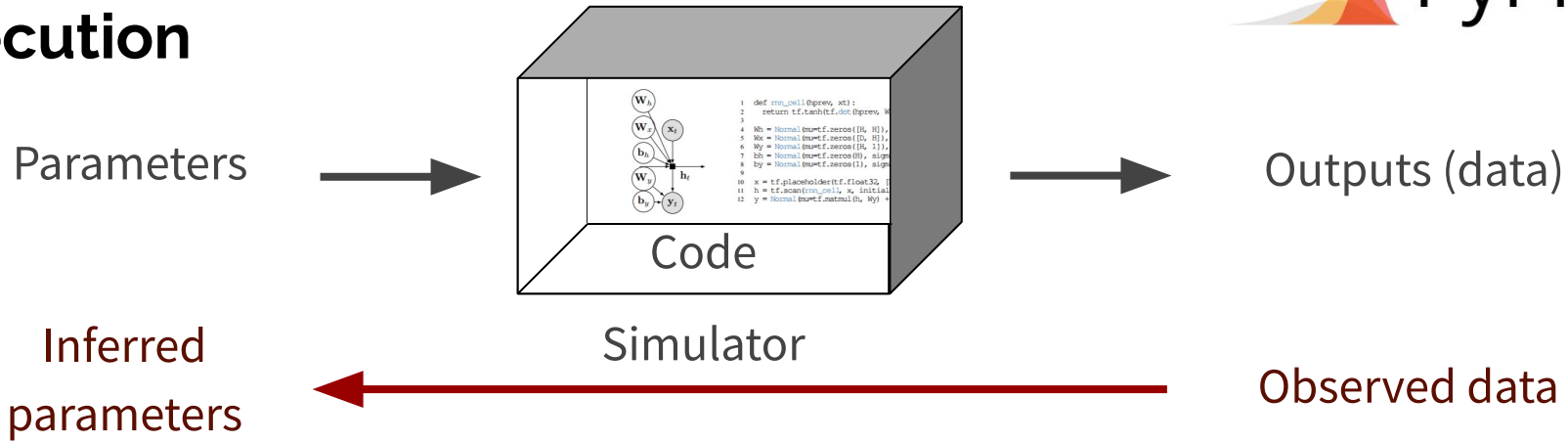
Inferred parameters

Simulator

Observed data

Probabilistic execution

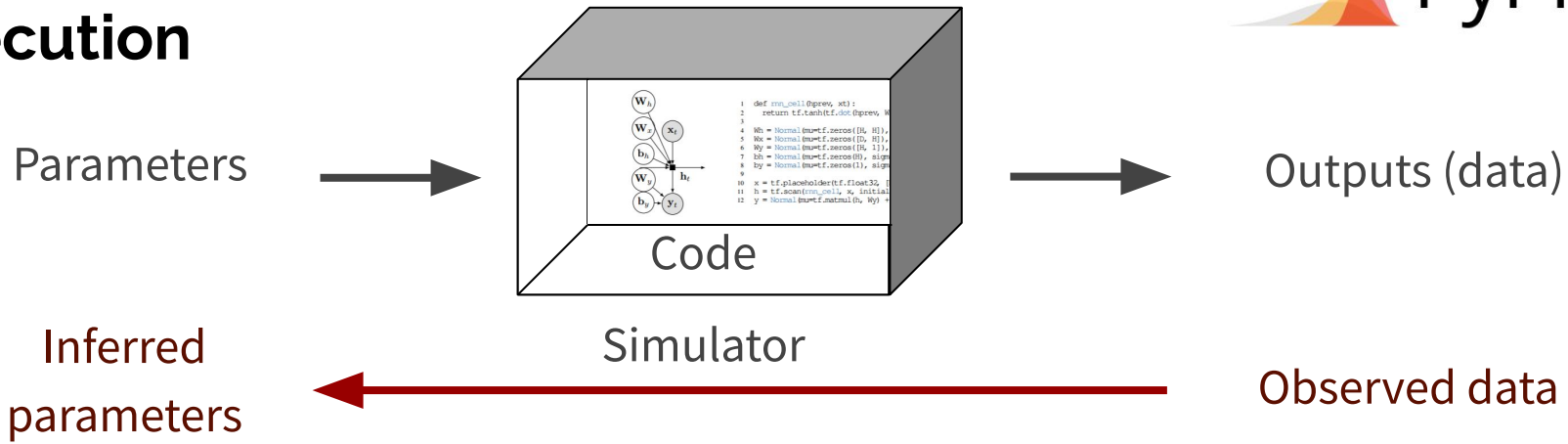
PyProb



- **Run forward & catch all random choices** (“hijack” all calls to RNG)
- Record an **execution trace**: a record of all parameters, random choices, outputs

Probabilistic execution

PyProb



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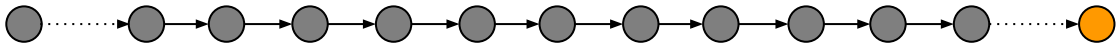
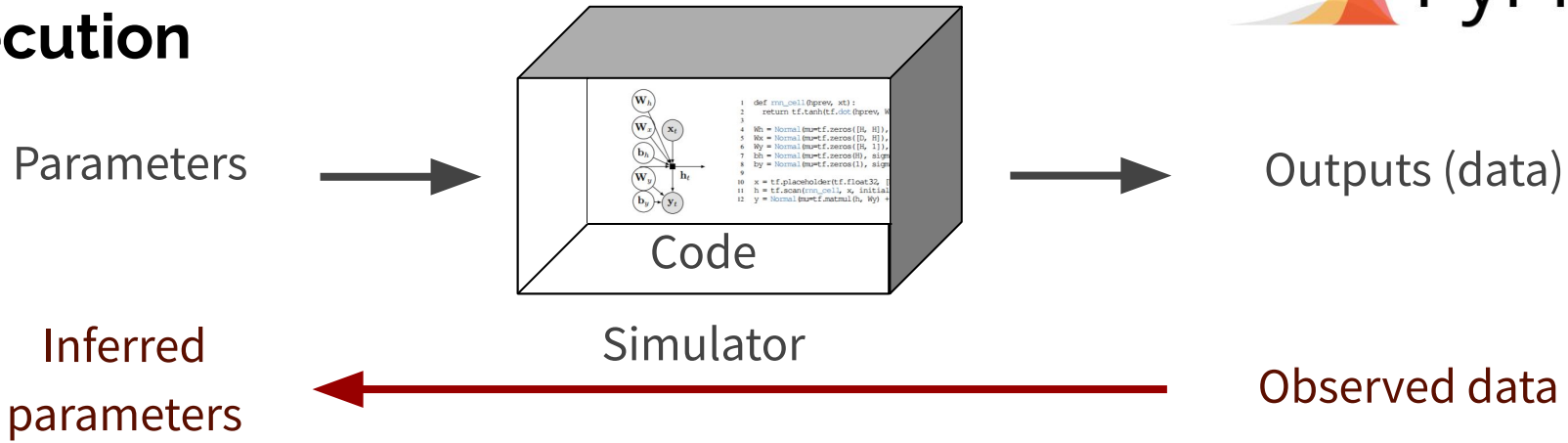


PPX

Probabilistic **P**rogramming e**X**ecution protocol
C++, C#, Dart, Go, Java, JavaScript, Lua, Python, Rust and others

Probabilistic execution

PyProb



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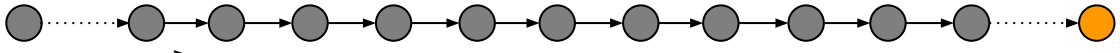
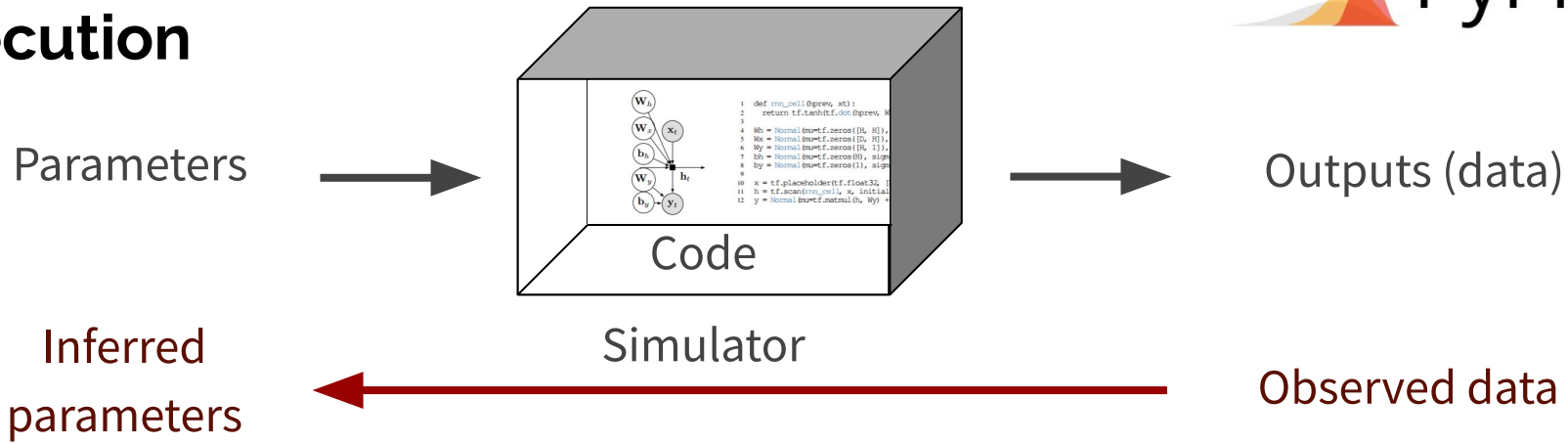


Uniquely label each choice at runtime by “addresses” of stack frames

[forward(xt:: xarray_container<xt:: uvector<double, std:: allocator<double> >, (xt:: layout_type)1, xt:: svector<unsigned long, 4ul, std:: allocator<unsigned long>, true>, xt:: xtensor_expression_tag>)+0x5f; SherpaGenerator:: Generate()+0x36; SHERPA:: Sherpa:: GenerateOneEvent(bool)+0x2fa; SHERPA:: Event_Handler:: GenerateEvent(SHERPA:: eventtype:: code)+0x44d; SHERPA:: Event_Handler:: GenerateHadronDecayEvent(SHERPA:: eventtype:: code&)+0x45f; ATOOLS:: Random:: Get(bool, bool)+0x1d5; probprog_RNG:: Get(bool, bool)+0xf9]_Uniform_1

Probabilistic execution

PyProb

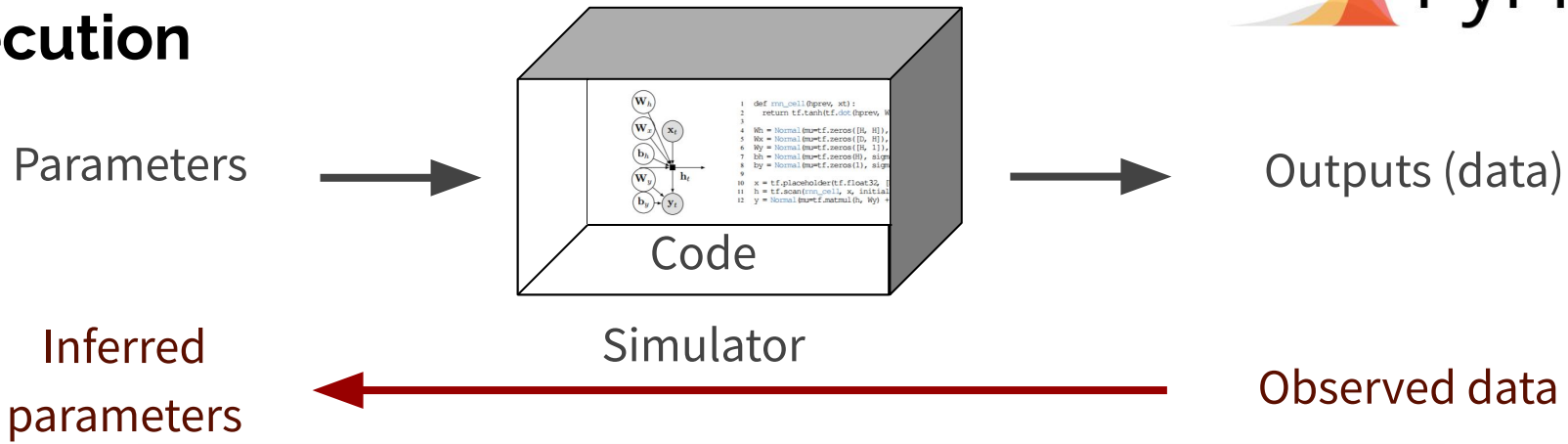


- **Run forward & catch all random choices** (“hijack” all calls to RNG)
- Record an **execution trace**: a record of all parameters, random choices, outputs

  - Conditioning: compare ***simulated output*** and ***observed data***
- **Approximate the distribution of parameters** that can produce (explain) observed data, using inference engines like Markov-chain Monte Carlo (MCMC)

Probabilistic execution

PyProb



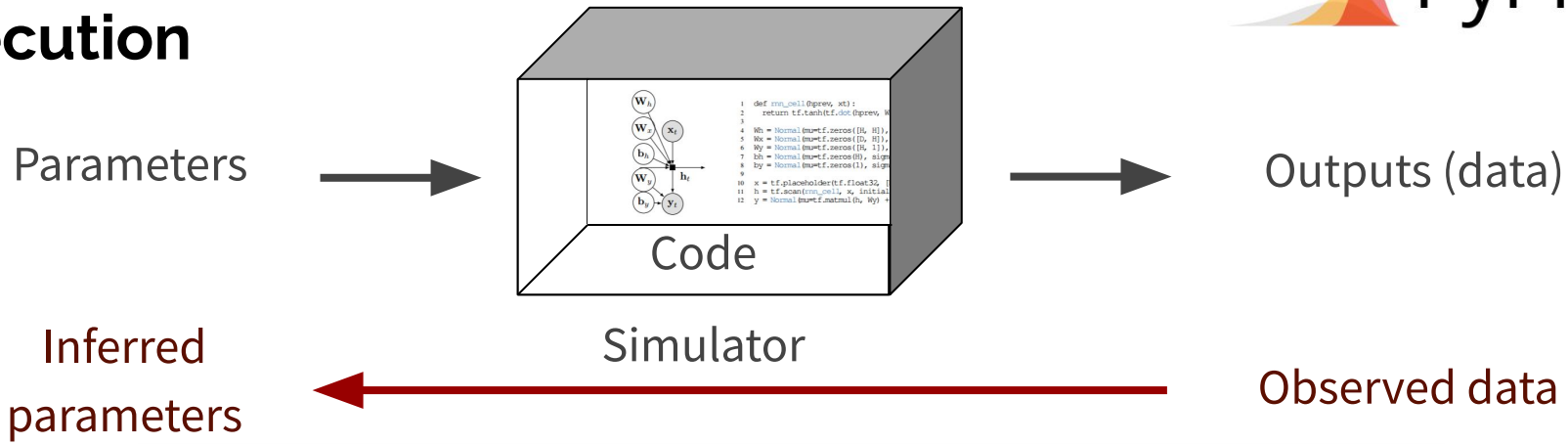
- **Ru**
- Re outputs
  - ○
- **Ap** n) ob MCMC)

Simulators = giant probability models so inference is hard and computationally costly

- Need to run simulator up to millions of times
- Simulator execution and MCMC inference are sequential
- MCMC has “burn-in period” and autocorrelation

Probabilistic execution

PyProb



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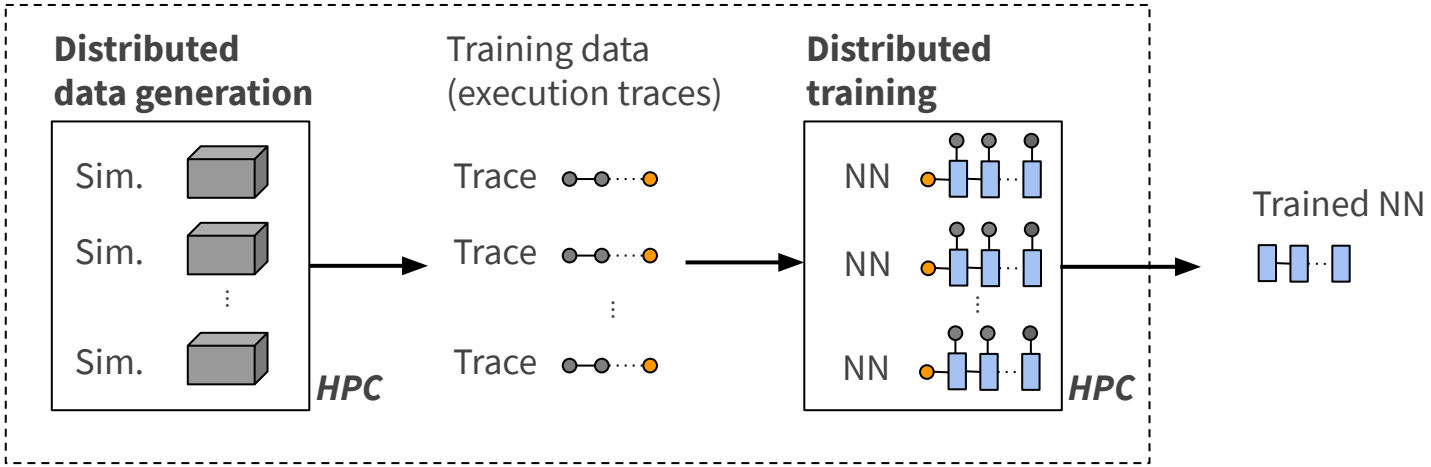
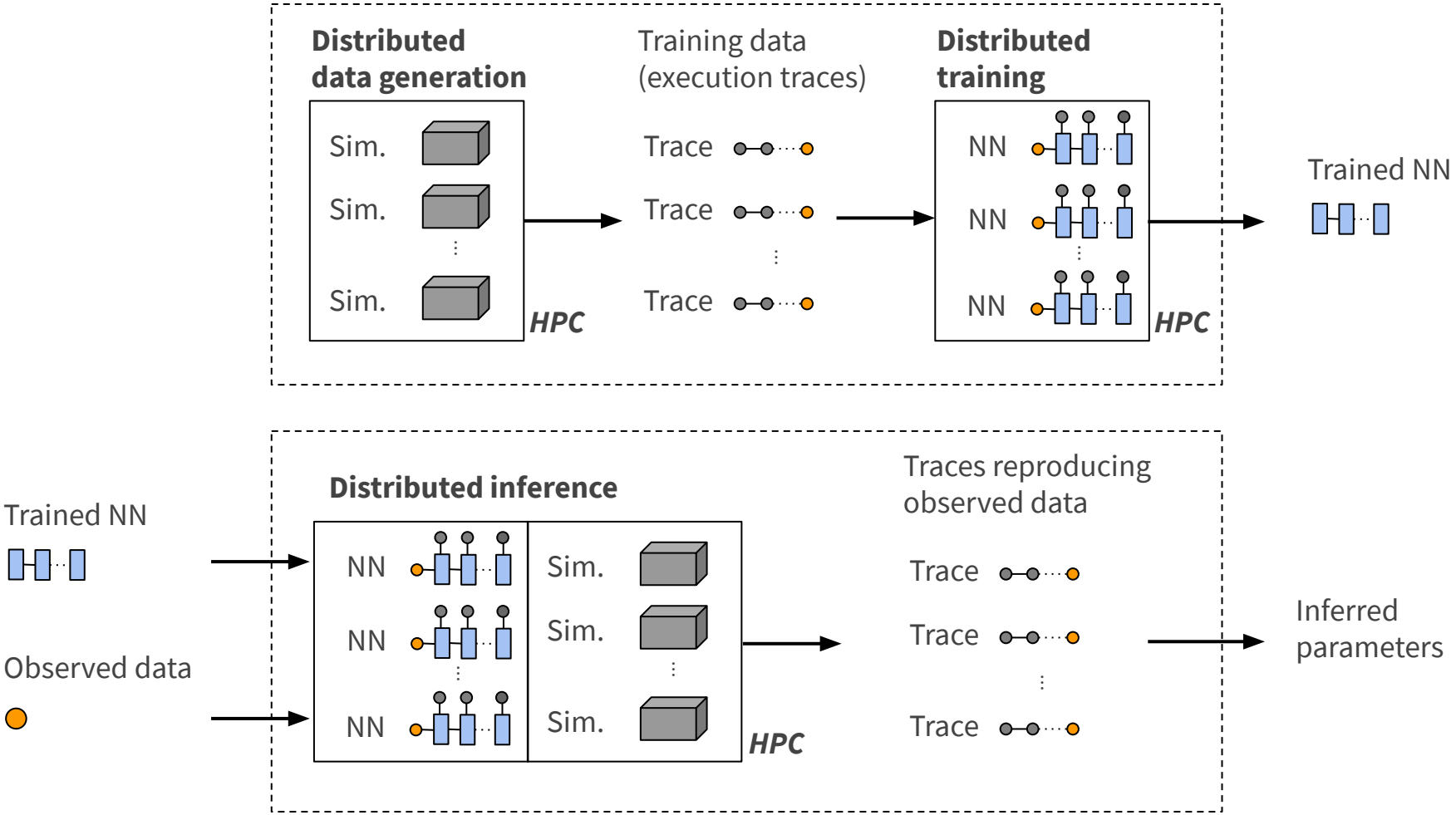
But we can amortize the cost of inference using deep learning



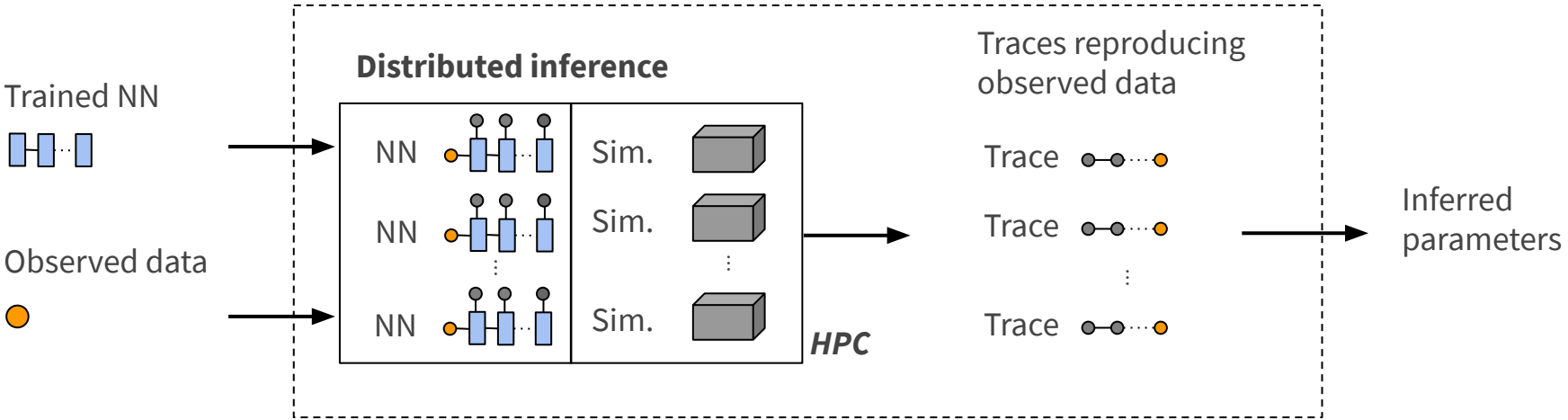
Training (recording simulator behavior)

- Deep recurrent neural network learns all random choices in simulator
- Dynamic NN: grows with simulator complexity
  - Layers get created as we learn more of the simulator
  - 100s of millions of parameters in particle physics simulation
- Costly, but amortized: we need to train only once per given model


Distributed
data generation
Sim.
Sim.
Sim.
HPC
Training data
(execution traces)
Trace
Trace
Trace
Distributed
training
NN
NN
NN
HPC
Trained NN
Trained NN
Observed data
Distributed inference
NN
NN
NN
Sim.
Sim.
Sim.
HPC
Traces reproducing
observed data
Trace
Trace
Trace
Inferred
parameters

Inference (controlling simulator behavior)

- Trained deep NN makes intelligent choices given data observation
- Embarrassingly parallel distributed inference
- No “burn in period”
- No autocorrelation: every sample is independent



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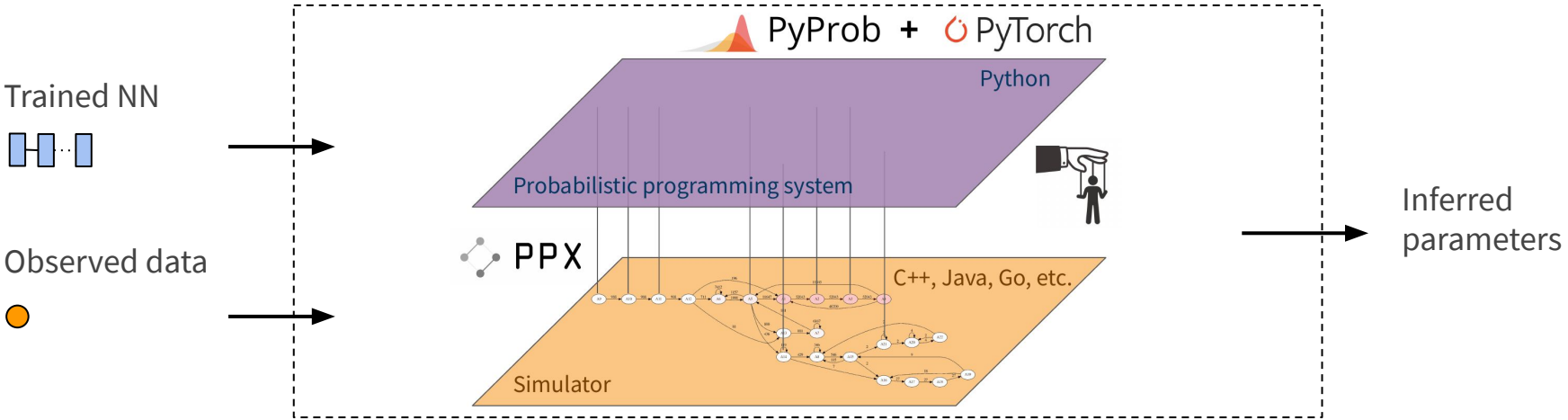


Probabilistic programming with simulators

https://github.com/pyprob/pyprob

- Probabilistic programming system for simulators and HPC, based on PyTorch
  Distributed training and inference, efficient support for multi-TB distribution files
  Optimized memory usage, parallel trace processing and combination

https://github.com/pyprob/ppx

- *P*robabilistic *P*rogramming e*X*ecution protocol
  Simulator and inference/NN executed in separate processes and machines across network
  Using Google flatbuffers to support C++, C#, Dart, Go, Java, JavaScript, Lua, Python, Rust and others
  Probabilistic programming analogue to Open Neural Network Exchange (ONNX) for deep learning

Pyprob_cpp, RNG front end for C++ simulators https://github.com/pyprob/pyprob_cpp

Containerized workflow
Develop locally, deploy to HPC on many nodes for experiments

etalumis → | ← simulate

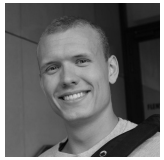

Atılım Güneş Baydin

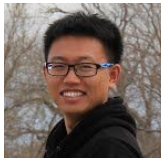

Lukas Heinrich


Wahid Bhimji


Lei Shao


Saeid Naderiparizi


Andreas Munk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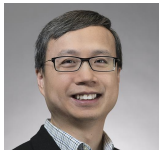
Lawrence Meadows


Phil Torr

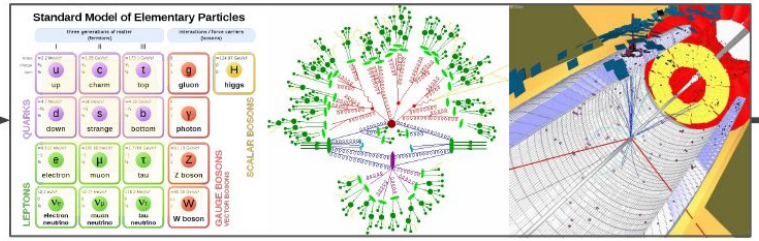

Victor Lee


Prabhat


Kyle Cranmer


Frank Wood

Inputs



Latents

$\mathbf{y}$

Simulated data
(detector response)

$$p(\mathbf{x}, \mathbf{y}) = p(\mathbf{y}|\mathbf{x})p(\mathbf{x})$$

Likelihood Prior

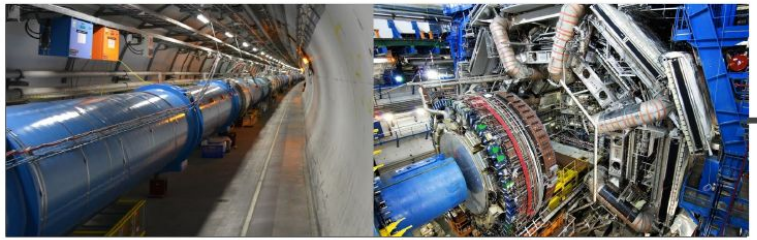
Inputs

Posterior $p(\mathbf{x}|\mathbf{y})$

$\text{observe}(p(\mathbf{y}|\mathbf{x}), \mathbf{y}_{\text{obs}})$

Generative model / simulator (e.g., Sherpa, Geant)

Real world system (e.g., Large Hadron Collider)



$\mathbf{y}_{\text{obs}}$

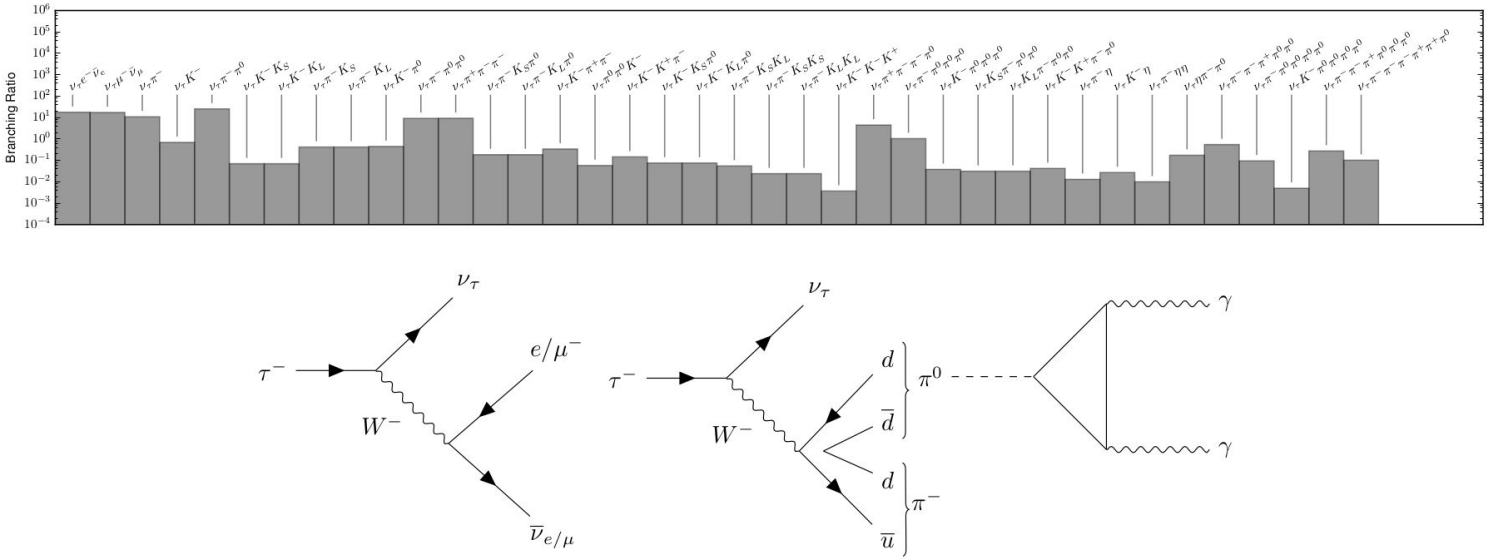
Observed data
(detector response)

Baydin, Heinrich, Bhimji, Shao, Naderiparizi, Munk, Liu, Gram-Hansen, Louppe, Meadows, Torr, Lee, Prabhat, Cranmer, Wood.
NeurIPS 2019

Tau lepton decay

We study tau lepton decay using the state-of-the-art Sherpa simulator (C++)

Coupled to a fast approximate calorimeter simulation in C++



Baydin, Heinrich, Bhimji, Shao, Naderiparizi, Munk, Liu, Gram-Hansen, Louppe, Meadows, Torr, Lee, Prabhat, Cranmer, Wood.
NeurIPS 2019

Latent variables in Sherpa

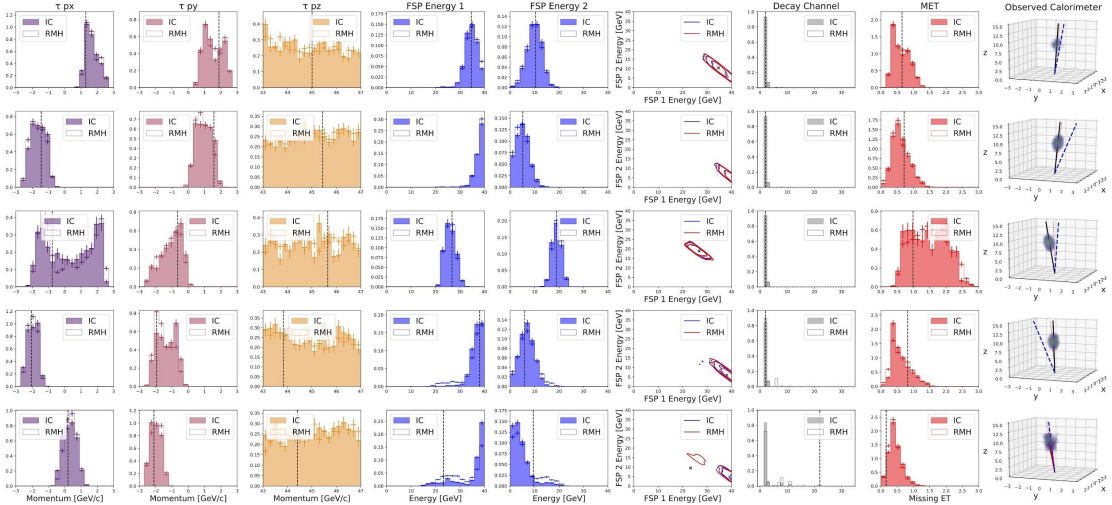
We found Sherpa to contain **at least 25k addresses (latent variables)**

Note: the **simulator defines an unlimited number of latents** due to Turing-complete host language and presence of sampling loops

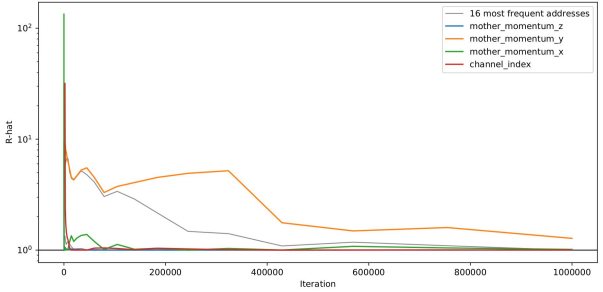
Address ID	Full address
A1	[forward(xt:: xarray_container<xt:: uvector<double, std:: allocator<double> >, (xt:: layout_type)1, xt:: svector<unsigned long, 4ul, std:: allocator<unsigned long>, true>, xt:: xtensor_expression_tag>)+0x5f; SherpaGenerator:: Generate()+0x36; SHERPA:: Sherpa:: GenerateOneEvent(bool)+0x2fa; SHERPA:: Event_Handler:: GenerateEvent(SHERPA:: eventtype:: code)+0x44d; SHERPA:: Event_Handler:: GenerateHadronDecayEvent(SHERPA:: eventtype:: code&)+0x45f; ATOOLS:: Random:: Get(bool, bool)+0x1d5; probprog_RNG:: Get(bool, bool)+0xf9]_Uniform_1
A6	[forward(xt:: xarray_container<xt:: uvector<double, std:: allocator<double> >, (xt:: layout_type)1, xt:: svector<unsigned long, 4ul, std:: allocator<unsigned long>, true>, xt:: xtensor_expression_tag>)+0x5f; SherpaGenerator:: Generate()+0x36; SHERPA:: Sherpa:: GenerateOneEvent(bool)+0x2fa; SHERPA:: Event_Handler:: GenerateEvent(SHERPA:: eventtype:: code)+0x44d; SHERPA:: Event_Handler:: GenerateHadronDecayEvent(SHERPA:: eventtype:: code&)+0x982; SHERPA:: Event_Handler:: IterateEventPhases(SHERPA:: eventtype:: code&, double&)+0x1d2; SHERPA:: Hadron_Decays:: Treat(ATOOLS:: Blob_List*, double&)+0x975; SHERPA:: Decay_Handler_Base:: TreatInitialBlob(ATOOLS:: Blob*, METOOLS:: Amplitude2_Tensor*, std:: vector<ATOOLS:: Particle*, std:: allocator<ATOOLS:: Particle*> > const&)+0x1ab1; SHERPA:: Hadron_Decay_Handler:: CreateDecayBlob(ATOOLS:: Particle*)+0x4cd; PHASIC:: Decay_Table:: Select() const+0x9d7; ATOOLS:: Random:: GetCategorical(std:: vector<double, std:: allocator<double> > const&, bool, bool)+0x1a5; probprog_RNG:: GetCategorical(std:: vector<double, std:: allocator<double> > const&, bool, bool)+0x111]_Categorical(length_categories:38)_1
...	

Inference results

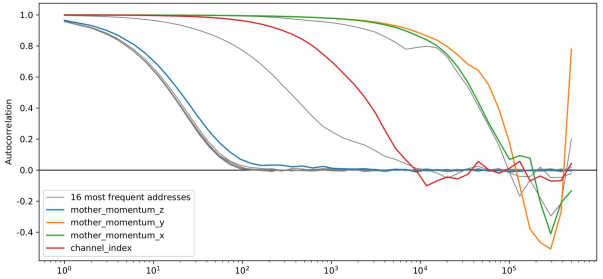
- Achieved MCMC (RMH) “ground truth”
- **First tractable Bayesian inference for LHC physics**
  - Posterior over full latent space (>25k latent variables)
  - Autocorrelation typically around 10^5
- Amortized inference (IC) closely matches MCMC (RMH)
  - No autocorrelation, embarrassingly parallel
  - MCMC: 115 hours, IC: 30 minutes



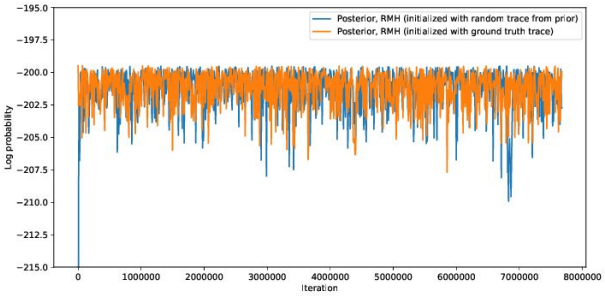
Gelman-Rubin convergence diagnostic

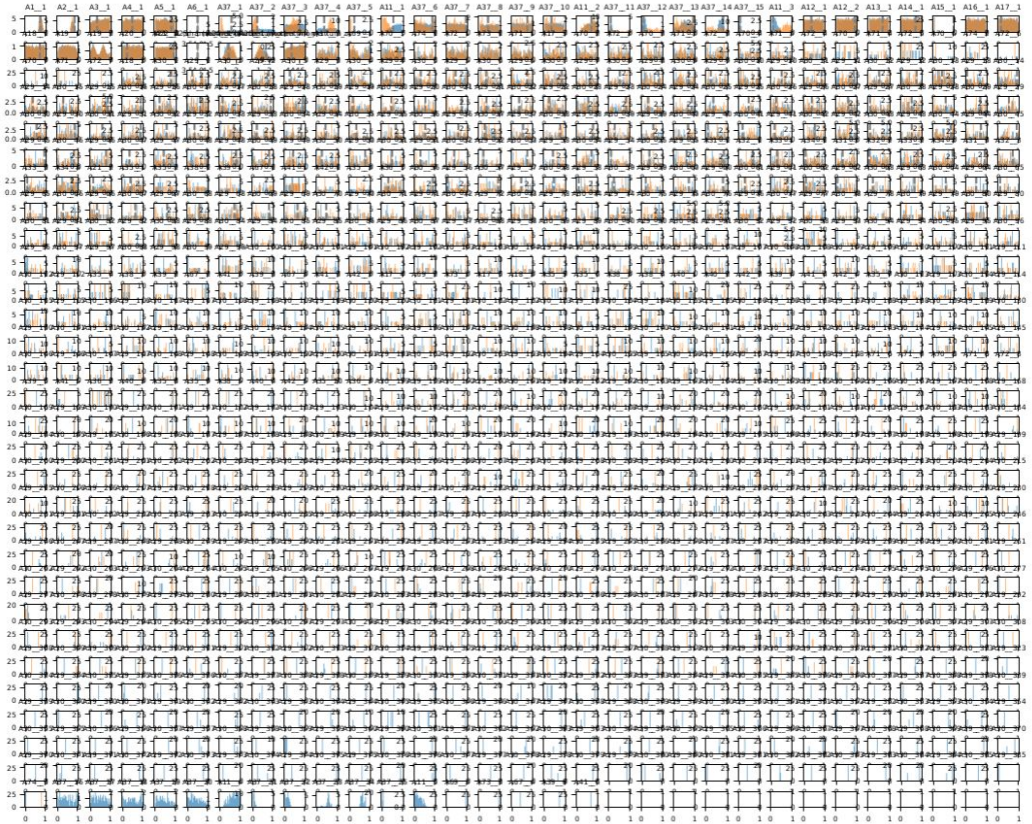


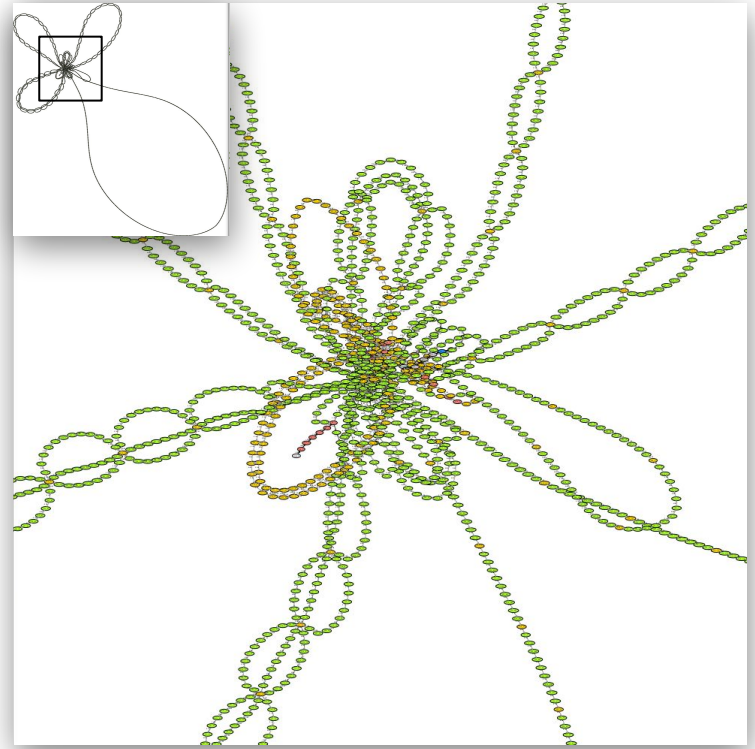
Autocorrelation



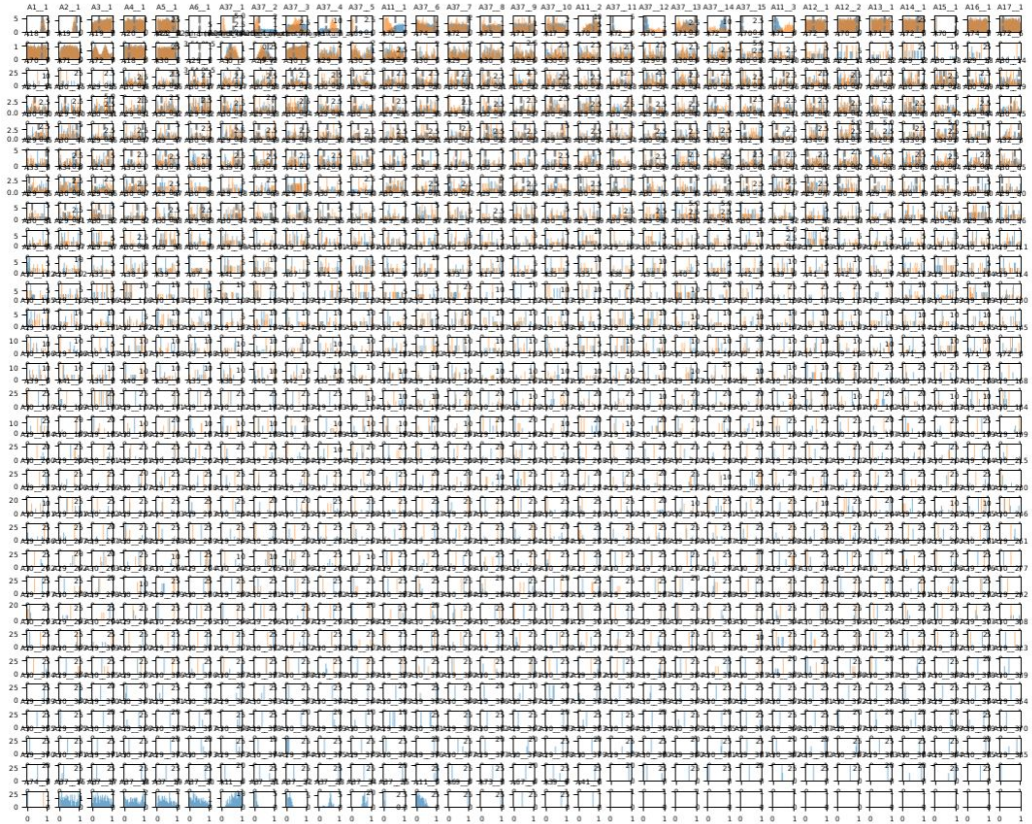
Trace log-probability



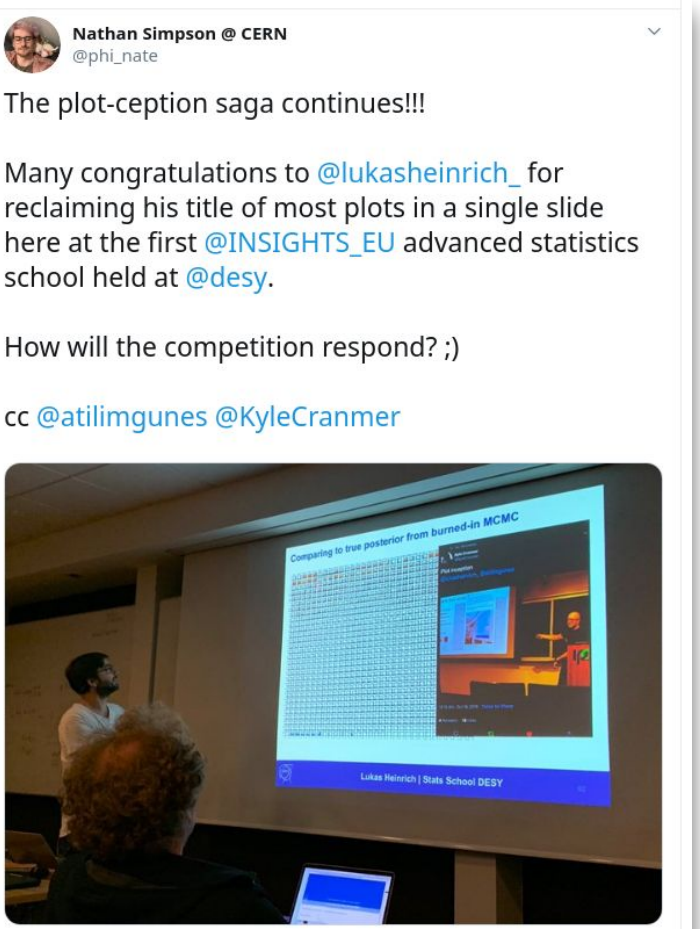




Etalumis gives access to all latent variables: allows answering *any* model-based question

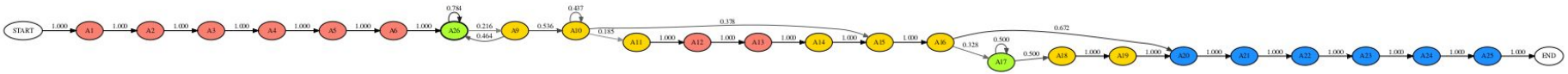


Etalumis gives access to all latent variab
any model-based question



Interpretability

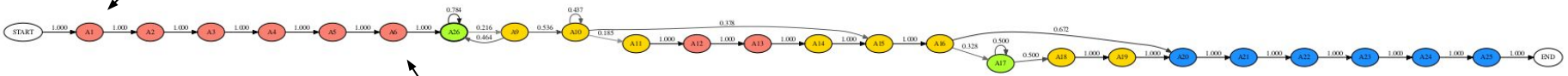
Latent probabilistic structure of **10** most frequent trace types



Interpretability

Latent probabilistic structure of **10** most frequent trace types

[forward(xt:: xarray_container<xt:: uvector<double, std:: allocator<double> >, (xt:: layout_type)1, xt:: svector<unsigned long, 4ul, std:: allocator<unsigned long>, true>, xt:: xtensor_expression_tag>)+0x5f; SherpaGenerator:: Generate()+0x36; SHERPA:: Sherpa:: GenerateOneEvent(bool)+0x2fa; SHERPA:: Event_Handler:: GenerateEvent(SHERPA:: eventtype:: code)+0x44d; SHERPA:: Event_Handler:: GenerateHadronDecayEvent(SHERPA:: eventtype:: code&)+0x45f; ATOOLS:: Random:: Get(bool, bool)+0x1d5; probprog_RNG:: Get(bool, bool)+0xf9]_Uniform_1



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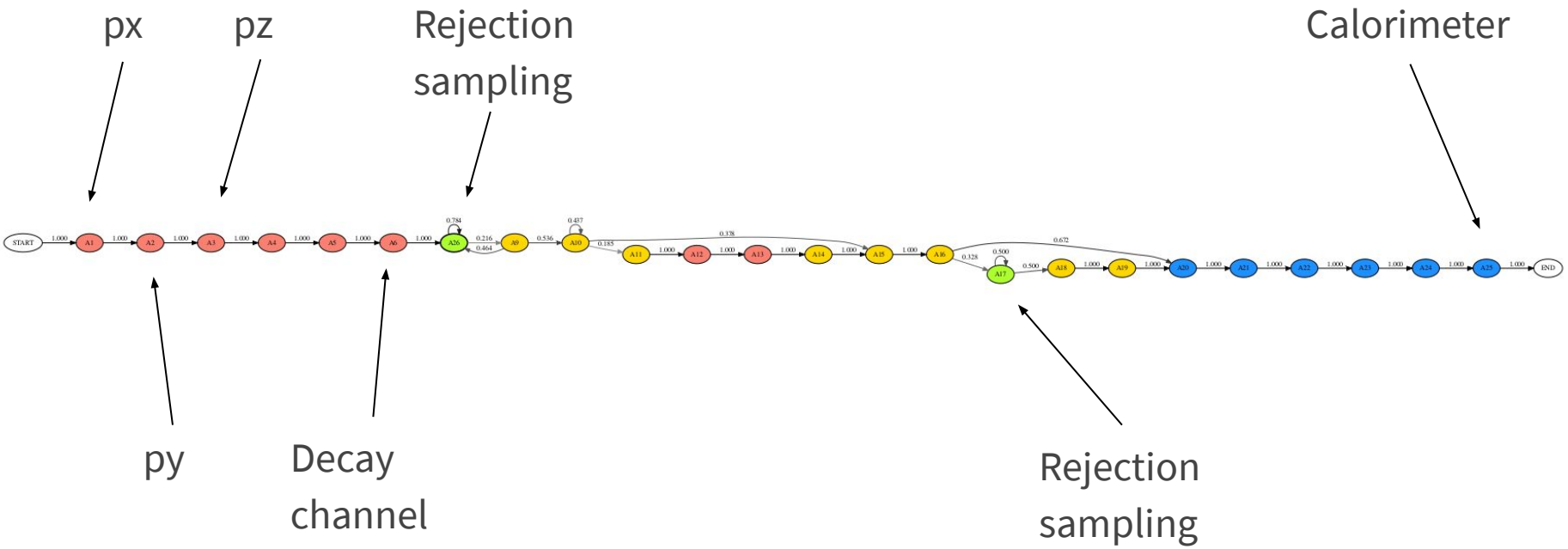
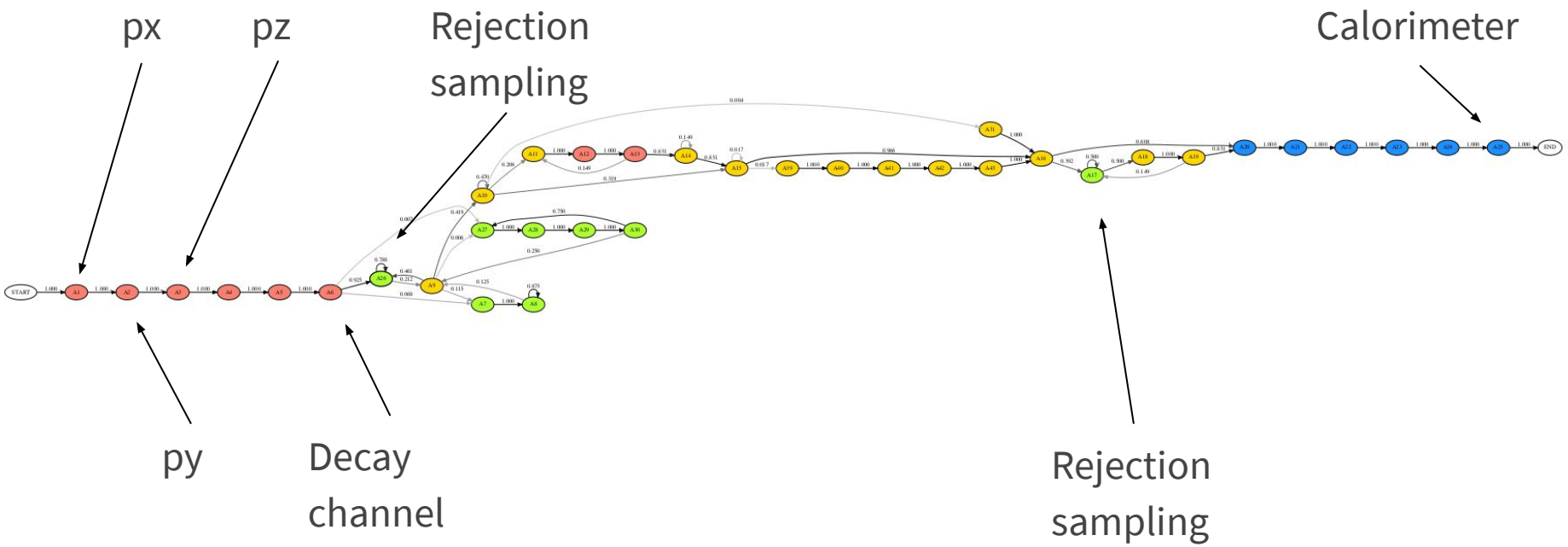
Interpretability

Latent probabilistic structure of **10** most frequent trace types



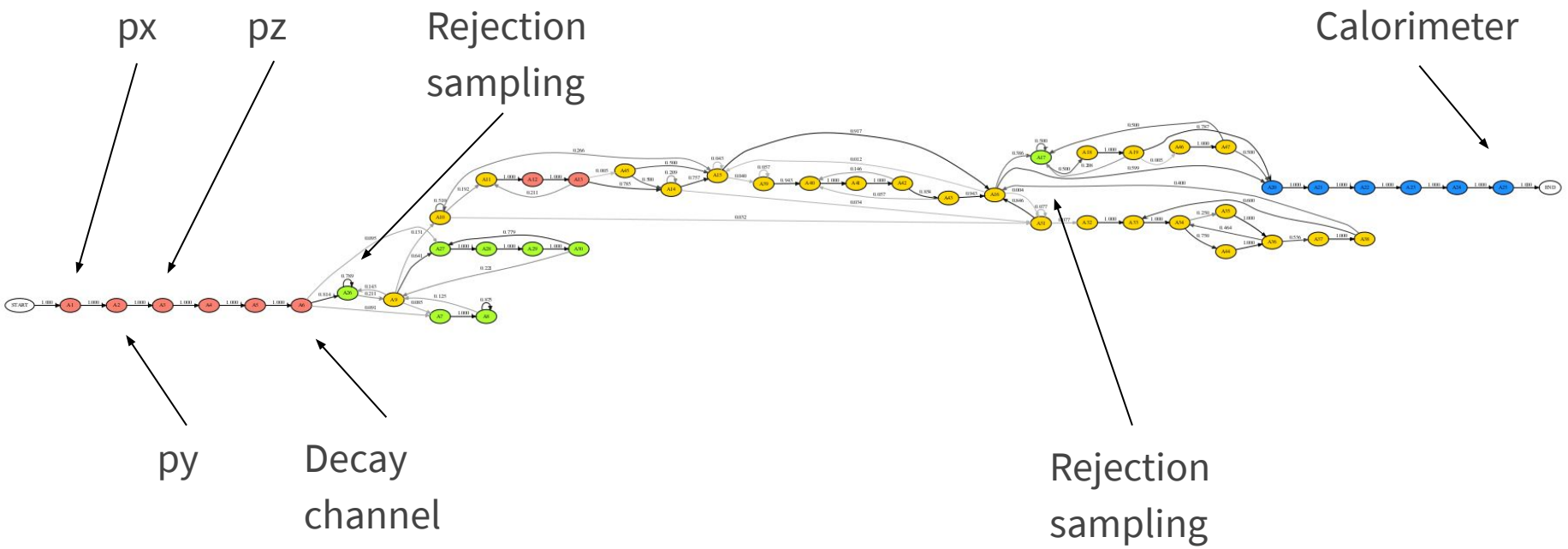
Interpretability

Latent probabilistic structure of **25** most frequent trace types



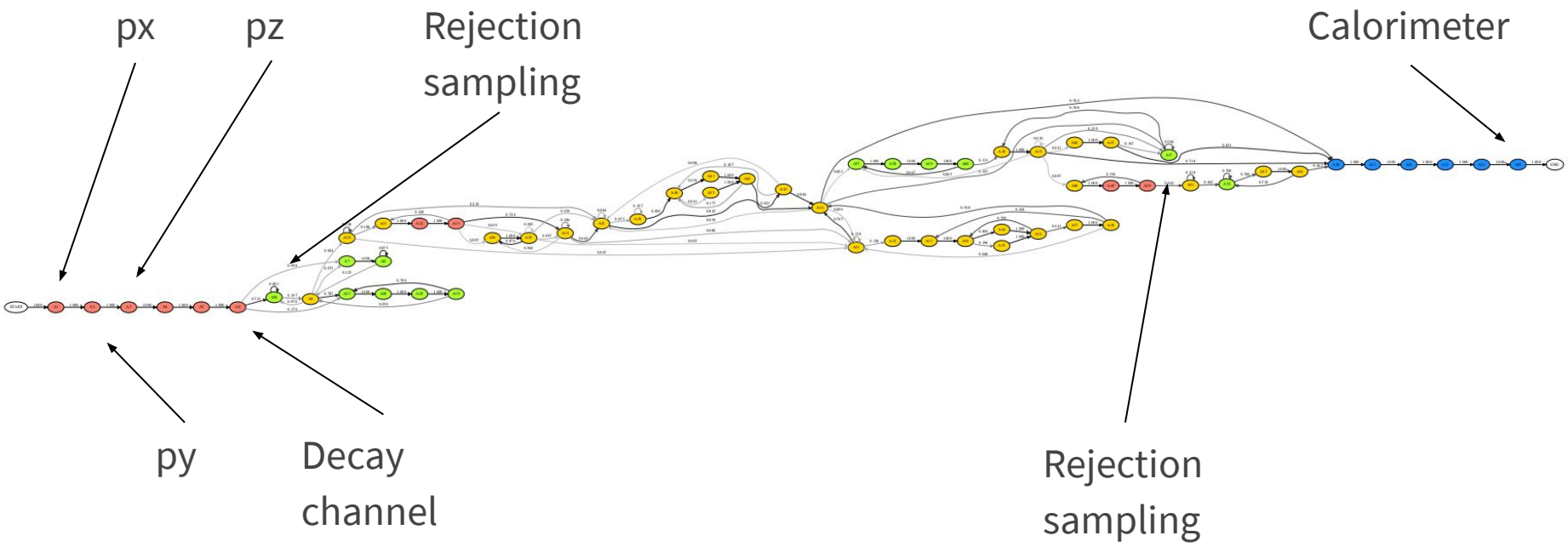
Interpretability

Latent probabilistic structure of **100** most frequent trace types



Interpretability

Latent probabilistic structure of **250** most frequent trace types



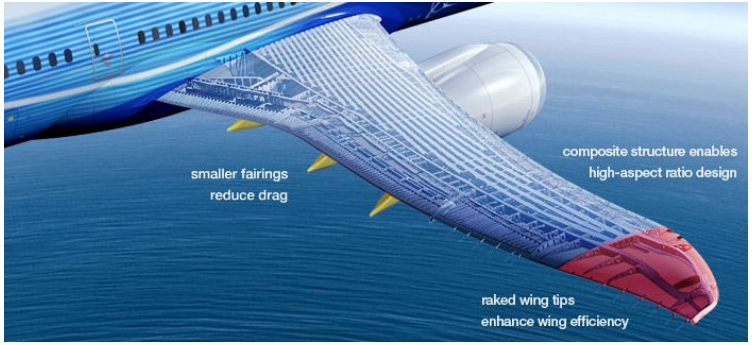
What’s next?

Current and upcoming work

- Autodiff through PPX protocol
- **Learning simulator surrogates** (approximate forward simulators)
- **Rejection sampling loops** (weighting schemes)
- Rare event simulation for compilation (“prior inflation”)
- Batching of open-ended traces for NN training
- Distributed training of dynamic networks
  - Recently ran on 32k CPU cores on Cori (largest-scale PyTorch MPI)
- User features: posterior code highlighting, etc.
- Other simulators: astrophysics, epidemiology, computer vision

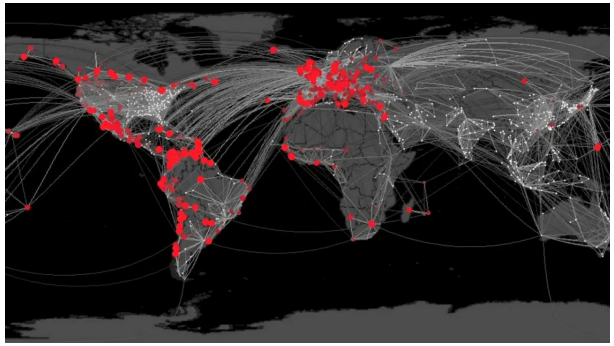
Probabilistic programming is for the first time practical for large-scale real-world science models

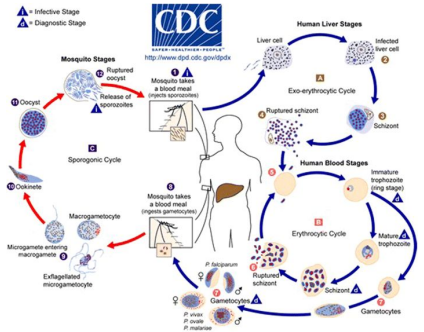
This is just the beginning ...



Simulation of composite materials

(Munk et al. 2019, in sub. arXiv:1910.11950)





Simulation of epidemics

(Gram-Hansen et al., 2019, in prep.)

Thank you for listening

Applied Machine Learning Days, EPFL
28 Jan 2020

References

Atılım Güneş Baydin, Lukas Heinrich, Wahid Bhimji, Lei Shao, Saeid Naderiparizi, Andreas Munk, Jialin Liu, Bradley Gram-Hansen, Gilles Louppe, Lawrence Meadows, Philip Torr, Victor Lee, Prabhat, Kyle Cranmer, Frank Wood. 2019. *"Efficient Probabilistic Inference in the Quest for Physics Beyond the Standard Model."* **NeurIPS 2019**

Atılım Güneş Baydin, Lei Shao, Wahid Bhimji, Lukas Heinrich, Lawrence F. Meadows, Jialin Liu, Andreas Munk, Saeid Naderiparizi, Bradley Gram-Hansen, Gilles Louppe, Mingfei Ma, Xiaohui Zhao, Philip Torr, Kyle Cranmer, Victor Lee, Prabhat, Frank Wood. 2019. *"Etalumis: Bringing Probabilistic Programming to Scientific Simulators at Scale."* International Conference for High Performance Computing, Networking, Storage, and Analysis - **SC19**

Extra slides

Calorimeter

For each particle in the final state coming from Sherpa:

1. Determine whether it interacts with the calorimeter at all (muons and neutrinos don't)
2. Calculate the total mean number and spatial distribution of energy depositions from the calorimeter shower (simulating combined effect of secondary particles)
3. Draw a number of actual depositions from the total mean and then draw that number of energy depositions according to the spatial distribution

Training objective and data for IC

- Minimize

$$\begin{aligned}\mathcal{L}(\phi) &= \mathbb{E}_{p(\mathbf{y})}\left[\mathrm{KL}(p(\mathbf{x}|\mathbf{y})||q(\mathbf{x}|\mathbf{y};\phi))\right] \\ &= \int_{\mathbf{y}} p(\mathbf{y}) \int_{\mathbf{x}} p(\mathbf{x}|\mathbf{y}) \log \frac{p(\mathbf{x}|\mathbf{y})}{q(\mathbf{x}|\mathbf{y};\phi)} \,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y} \\ &= -\mathbb{E}_{p(\mathbf{x},\mathbf{y})}\left[\log q(\mathbf{x}|\mathbf{y};\phi)\right] + \text{const.}\end{aligned}$$

- Using stochastic gradient descent with Adam
- Infinite stream of minibatches

$$\mathcal{D}_{\text{train}} = \left\{ \left(x_t^{(m)}, a_t^{(m)}, i_t^{(m)} \right)_{t=1}^{T^{(m)}}, \left(y_n^{(m)} \right)_{n=1}^{N} \right\}_{m=1}^{M}$$

sampled from the model $p(\mathbf{x}, \mathbf{y})$

Gelman-Rubin and autocorrelation formulae

Gelman-Rubin diagnostic ($\hat{R}$)

- Compute *m* independent Markov chains
- Compares variance of each chain to pooled variance
- If initial states (θ_{1j}) are overdispersed, then $\hat{R}$ approaches unity from above
- Provides estimate of how much variance could be reduced by running chains longer
- It is an *estimate!*

$$W = \frac{1}{m}\sum_{j=1}^{m} s_j^2 \qquad \bar{\bar{\theta}} = \frac{1}{m}\sum_{j=1}^{m} \bar{\theta}_j$$

$$B = \frac{n}{m-1}\sum_{j=1}^{m}(\bar{\theta}_j - \bar{\bar{\theta}})^2 \qquad s_j^2 = \frac{1}{n-1}\sum_{i=1}^{n}(\theta_{ij} - \bar{\theta}_j)^2$$

$$\hat{\mathrm{Var}}(\theta) = (1 - \frac{1}{n})W + \frac{1}{n}B \qquad \hat{R} = \sqrt{\frac{\hat{\mathrm{Var}}(\theta)}{W}}$$

From Eric B. Ford (Penn State): Bayesian Computing for Astronomical Data Analysis
http://astrostatistics.psu.edu/RLectures/diagnosticsMCMC.pdf

Gelman-Rubin and autocorrelation formulae

Check Autocorrelation of Markov chain

- Autocorrelation as a function of lag

$$\rho_{lag} = \frac{\sum_i^{N-lag}(\theta_i - \bar{\theta})(\theta_{i+lag} - \bar{\theta})}{\sum_i^N(\theta_i - \bar{\theta})^2}$$

- What is smallest lag to give an $\rho_{lag} \approx 0$?
- One of several methods for estimating how many iterations of Markov chain are needed for *effectively* independent samples

From Eric B. Ford (Penn State): Bayesian Computing for Astronomical Data Analysis
http://astrostatistics.psu.edu/RLectures/diagnosticsMCMC.pdf