Simulation-based inference

— of bridging the gap between theory and experiment with neural networks —

Peter Steinbach[1], Ankush Checkervarty, Tim Burghardt, and many others at HZDR

[1] *Helmholtz-Zentrum Dresden-Rossendorf, Core Facility for Digital Infrastructure and Computing, mailto:p.steinbach@hzdr.de, https://www.hzdr.de*

MT Annual Meeting 2025, November 3, 2025

Outline of talk

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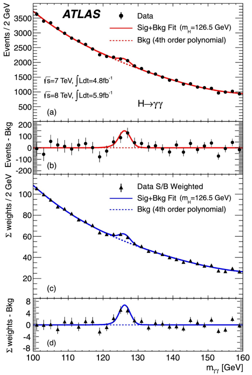
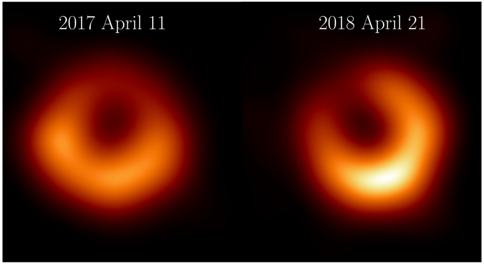
What do these discoveries have in common?



Discovery of the Higgs Boson 2012

[Aad et al., 2012]



Persistent View of a Supermassive Black Hole in M87*

[Event Horizon Telescope Collaboration et al., 2019] and [Akiyama et al., 2024]

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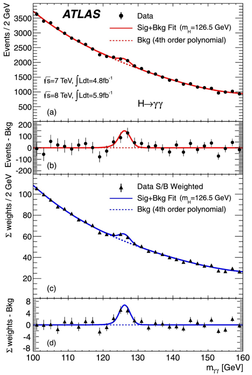

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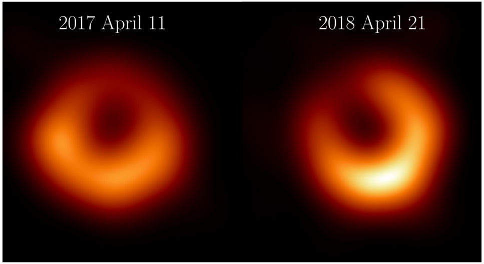


Persistent View of a Supermassive Black Hole in M87*

[Event Horizon Telescope Collaboration et al., 2019] and [Akiyama et al., 2024]

Correct, **they were only possible with simulations**!

HELMHOLTZAI DRESDEN concept HZDR

Invert Simulation to Infer Nature

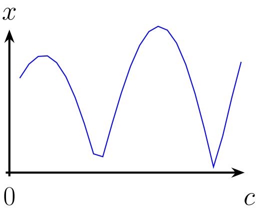
$$\vec{\vartheta} = \begin{pmatrix} 42. \\ 12. \\ 1. \\ -0.8 \\ 2. \\ 320 \end{pmatrix}$$

simulation

$$\vec{x} = f_{sim}(\vec{\vartheta})$$

inversion?

$$\hat{\vec{\vartheta}}$$



$$\begin{pmatrix} .50 \\ .60 \\ .67 \\ \cdots \\ \cdots \\ \cdots \\ .40 \\ .58 \\ .75 \end{pmatrix} = \vec{x}$$

- encapsulate mechanistic understanding of nature in simulator
- sample parameters ϑ

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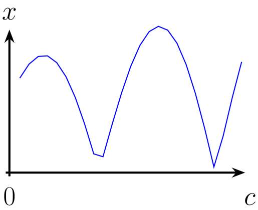

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- encapsulate mechanistic understanding of nature in simulator
- sample parameters ϑ
- simulate data x as close to observations as possible
- once new data x_o is recorded
- invert simulation to assess the corresponding parameters

Bayes Law

$$p(\vartheta|x) = \frac{p(x|\vartheta) \cdot p(\vartheta)}{\int p(x|\vartheta)p(\vartheta)d\vartheta}$$

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Goal: Estimate posterior to the best of our abilities!

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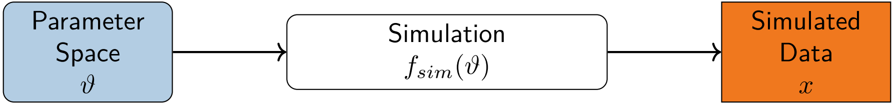
Simulation-Based Inference Core Pipeline



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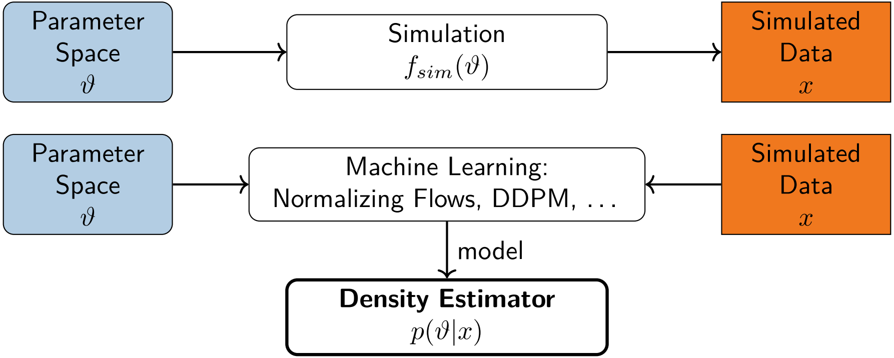

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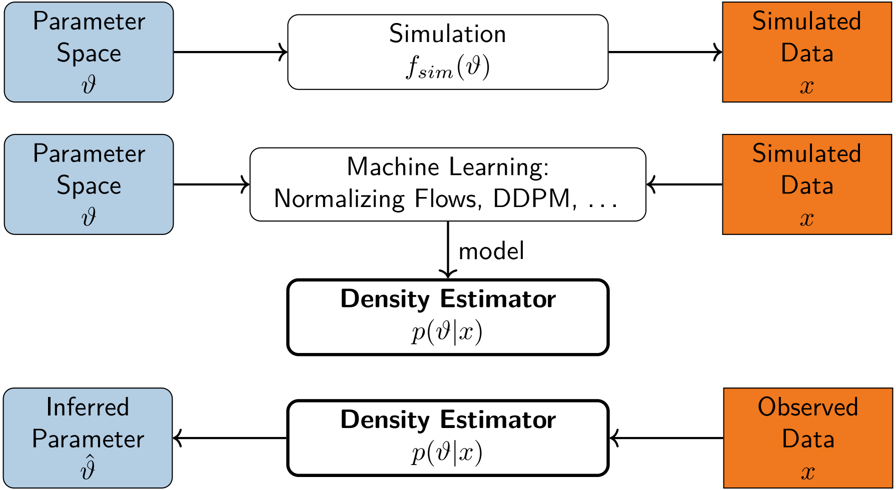
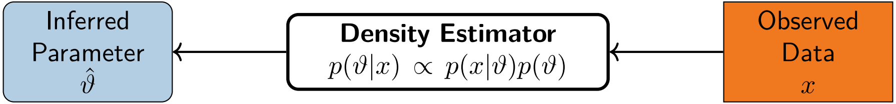


Neural Posterior Estimation (NPE)



Learn posterior density from n simulated pairs

$$\mathcal{D} = \{< \theta_0, x_0 >, < \theta_1, x_1 >, \ldots, < \theta_{n-1}, x_{n-1} >\}.$$

Infer $\hat{\vartheta}$ given single new x_o!

Neural Posterior Estimation (NPE)

Inferred Parameter $\hat{\vartheta}$ ← **Density Estimator** $p(\vartheta|x) \propto p(x|\vartheta)p(\vartheta)$ ← Observed Data x

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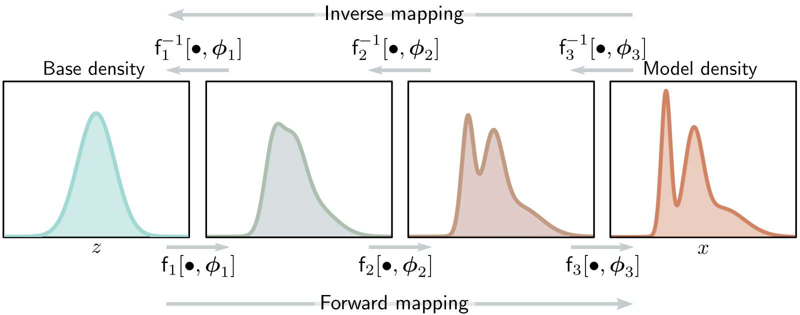
high n regime

- amortized inference regime
- reuse of density estimator
- use **Machine Learning** methods

ML for SBI: Normalizing Flows for density estimation



[Prince, 2023]

- flexible density learning with normalizing flows (conditional generation built-in) [Greenberg et al., 2019]
- strong guarantee to assess probabilities: $Pr(x|\phi) = \|\frac{\partial f[z,\phi]}{\partial z}\|^{-1} Pr(z)$
- if converged, represents full posterior estimate (log probs accessible)
- struggles with high-dimensional data (e.g. images)

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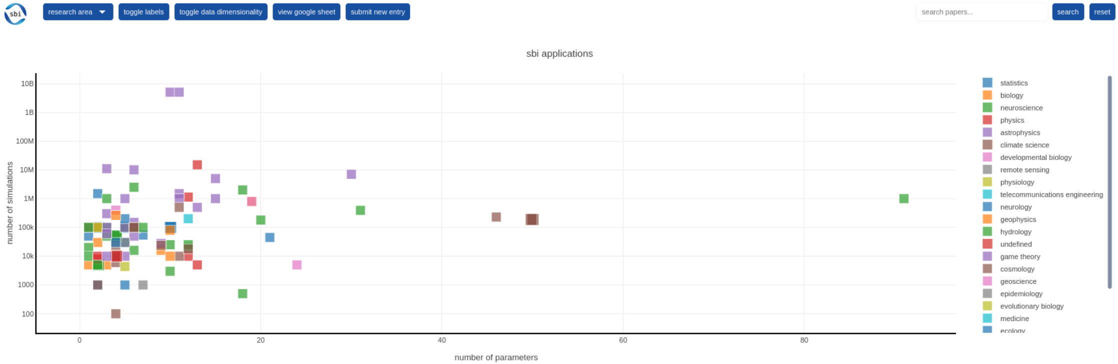
SBI Use Cases | Overview



Explore for yourself: sbi-applications-explorer.streamlit.app

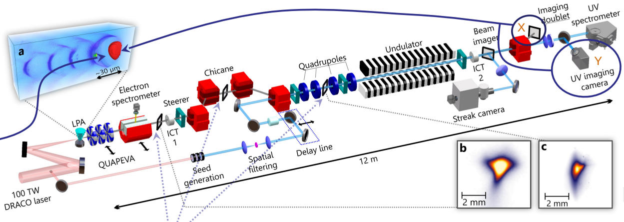
Control and Optimization of a laser-driven Free Electron Laser

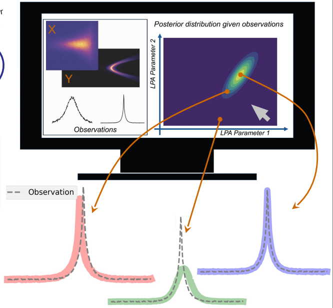
COXINEL[1]:
COherent **X**-ray source **IN**ferred from **E**lectrons accelerated **L**aser

Automatic inversion of experimental measurements from the last imager and UV imaging camera to beam parameters at the source

The ill-posed inverse problem has no unique solution and is resolved up to a posterior distribution (probability of LPA parameters given observations).

LPA parameters:
- Energy spread
- Divergence
- Size





Virtual diagnostics provide data from all imagers in a digital form with access to the phase space of the beam in the beamline

1. Labat, M. et al. (2023). Seeded free-electron laser driven by a compact laser plasma accelerator. Nat. Photon. 17, 150–156.

Laser Particle Acceleration | Concept

Method: Simulation-based Inference

Sample LPA parameters and pass them into the simulator

1

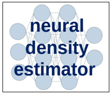
Prior distribution
of LPA parameters:
uniform if no assumptions are given

Simulator
Beam propagation:
`APS elegant`[3]
Undulator radiation: SRW[4]

2

Observation (X or Y)

Embedding Network

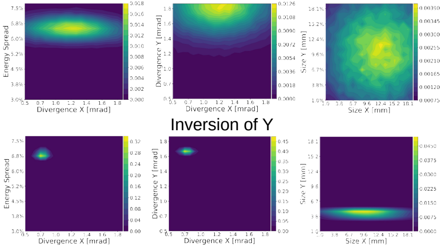


3

Compute simulations of a corresponding measurement (X or Y) for sampled parameters

Inversion of X

Inversion of Y



Estimation of the probability distribution of LPA parameters based on spectral observations from Imagers

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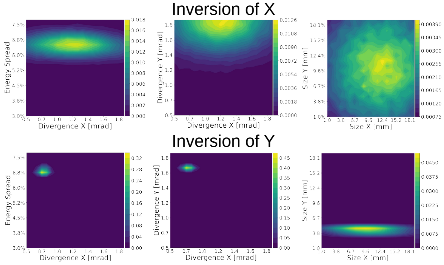


Estimation of the probability distribution of LPA parameters based on spectral observations from Imagers

dataset:

- $\vec{\vartheta} \in \mathbf{R}^{10}$
- $\vec{x} \in \mathbf{R}^{199\times 199}$

simulator:

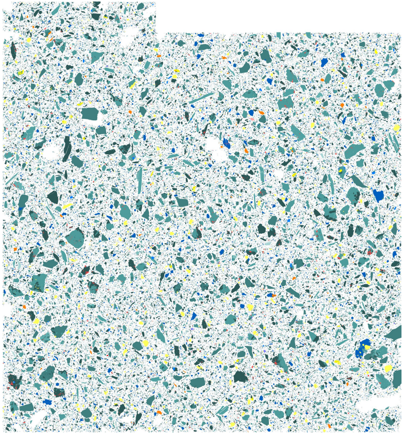
- 200k samples, each sample took 10s on 1c
- Elegant Software by [Borland, 2000]

sbi: simulator:

- amortized NPE on a single GPU
- automl search for good embedding net

HELMHOLTZAI DRESDEN concept HZDR

Physics of Stone | Idea & Motivation



Using a simulation, describe this stone powder!
(number of mineral types, size distribution, . . .)

Physics of Stone | First Failures

- simulations (in julia):
  $\vec{\vartheta} \in \mathbf{R}^{14}$
  $\vec{x} \in \mathbf{R}^{3500\times3500}$
- each sample: 1-2 minutes on single CPU
- simulation campaigns straight-forward to run

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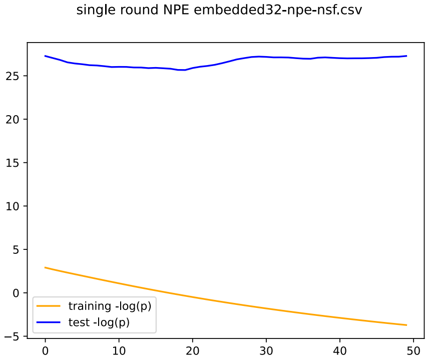
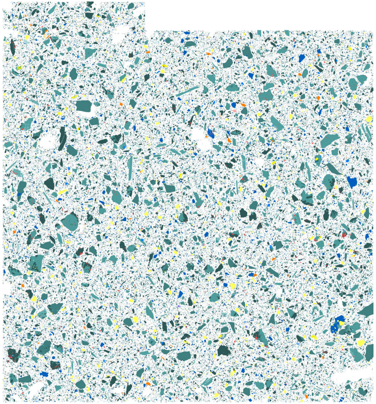
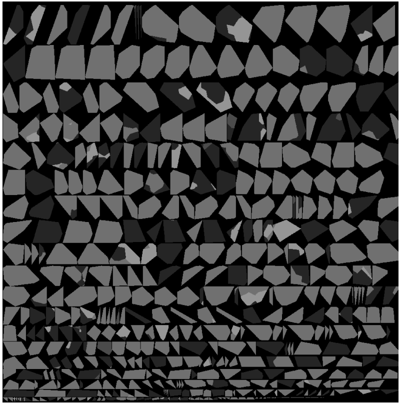


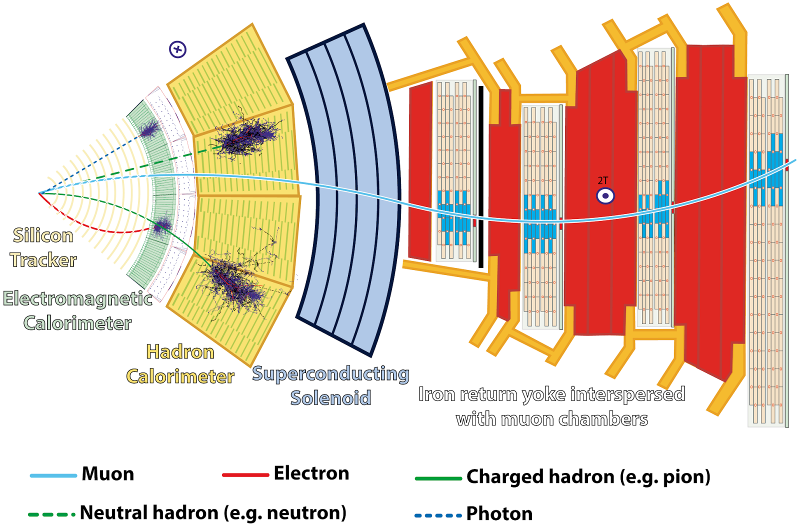
Physics of Stone | Observations and Simulations



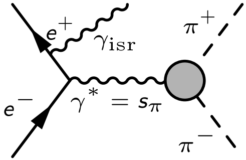


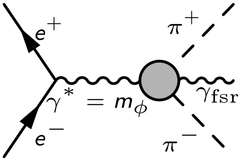
Currently exploring if statistics can bridge the Sim2Real gap.

Unfolding in Particle Physics | Motivation



Unfolding in Particle Physics | Evidence





- study cross-section measurement of $e^+e^- \to \pi^+\pi^-\gamma$
- smaller scale experiment (compared to LHC)
- unfolding: inferring simulated data from observations
- problem size: $\vec{\vartheta} = q^2_{MC} \in \mathbf{R}^1$, $\vec{x} = \{q^2, \dots\} \in \mathbf{R}^{10-15}$
- challenge: simulator inaccessible

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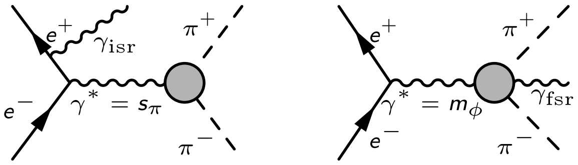

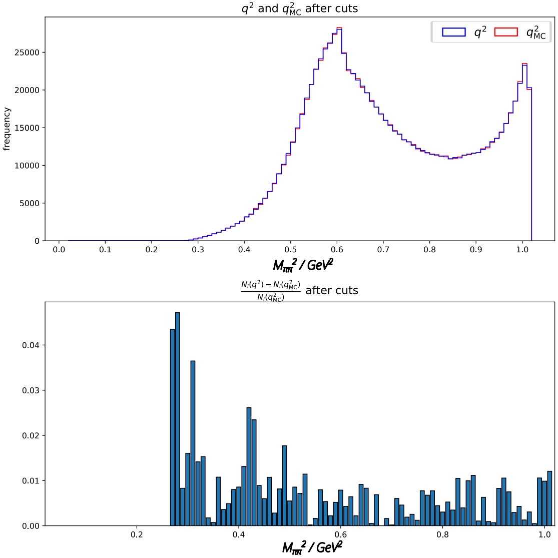

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Thank you for your attention!
Looking forward to questions, feedback and comments.

Want to get started?
[Deistler et al., 2025] sbi.readthedocs.io/en/latest/ Contact me!

Talk to us!

- helmholtz.ai/you-helmholtz-ai/ai-consulting/
- contact@helmholtz.ai for general questions
- consultant-helmholtz.ai@hzdr.de for questions regarding research field matter

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