Machine Learning-based Data Analysis and Surrogate Modeling For COXINEL Experiment

A. Willmann[1], A. Ghaith[1], Y. Chang[1], A. Debus[1], M. LaBerge[1], M. Labat[4], P. Ufer[1,2], S. Schoebel[1,2], N. Hoffmann[1], M. Bussmann[1,3], M.-E. Couprie[4], U. Schramm[1,2], A. Irman[1]

[1] Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany
[2] Technische Universität Dresden, Dresden, Germany
[3] Center for Advanced Systems Understanding, Görlitz, Germany
[4] Synchrotron SOLEIL, Saint-Aubin, France

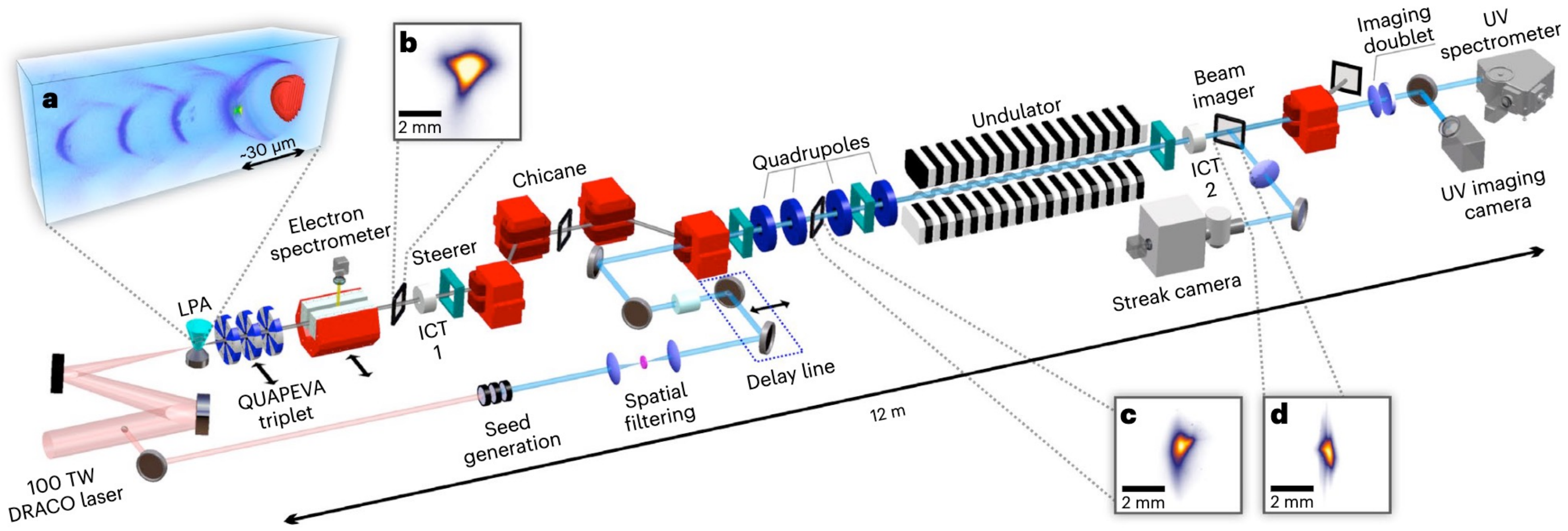
The 6th European Advanced Accelerator Concepts Workshop, 21.09.2023

Control and optimization of a laser-driven Free Electron Laser

COherent **X**-ray source **IN**ferred from **E**lectrons accelerated **L**aser

Challenges:

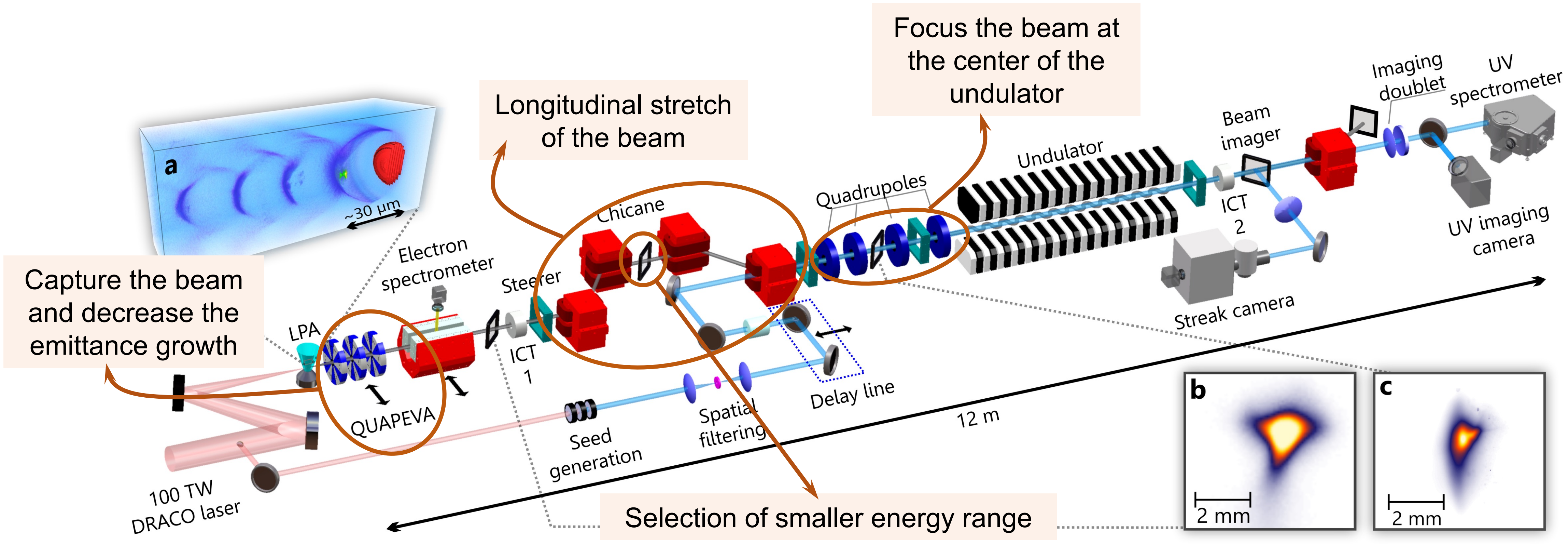
- Large parameter space
- Automatic exploration of design space
- Higher degree of control over radiation intensity



The experimental demonstration of a laser-plasma accelerator-driven free-electron laser in a seeded configuration at Helmholtz-Zentrum Dresden-Rossendorf.

Labat, Marie, et al. "Seeded free-electron laser driven by a compact laser plasma accelerator." *Nature Photonics* 17.2 (2023): 150-156.

COherent X-ray source INferred from Electrons accelerated Laser



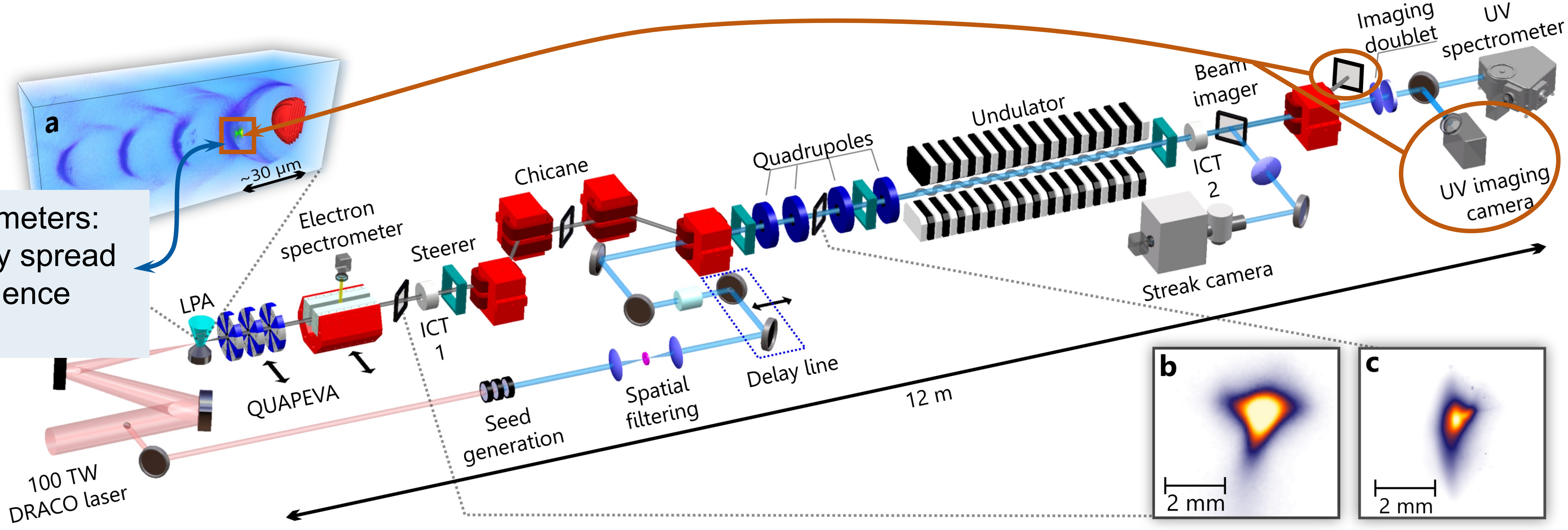
The experimental demonstration of a laser-plasma accelerator-driven free-electron laser in a seeded configuration at Helmholtz-Zentrum Dresden-Rossendorf.

Labat, Marie, et al. "Seeded free-electron laser driven by a compact laser plasma accelerator." *Nature Photonics* 17.2 (2023): 150-156.

Data Analysis Workflow for COXINEL Experiment

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

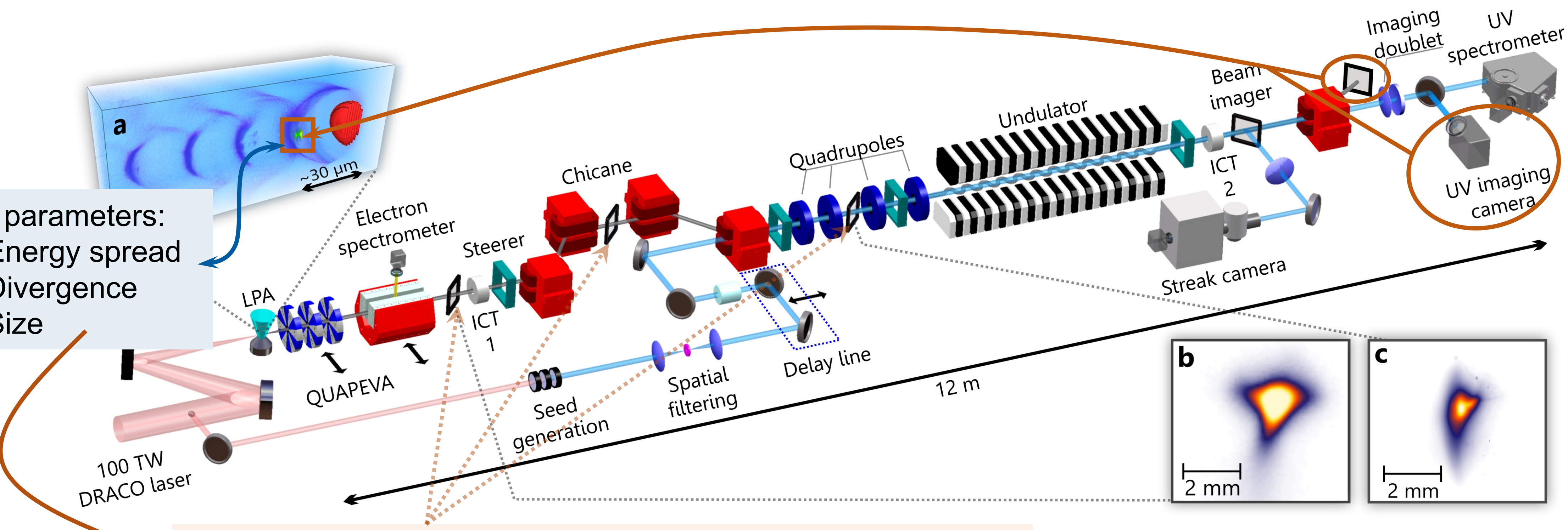
LPA parameters:
- Energy spread
- Divergence
- Size



Data Analysis Workflow for COXINEL Experiment

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

LPA parameters:
- Energy spread
- Divergence
- Size

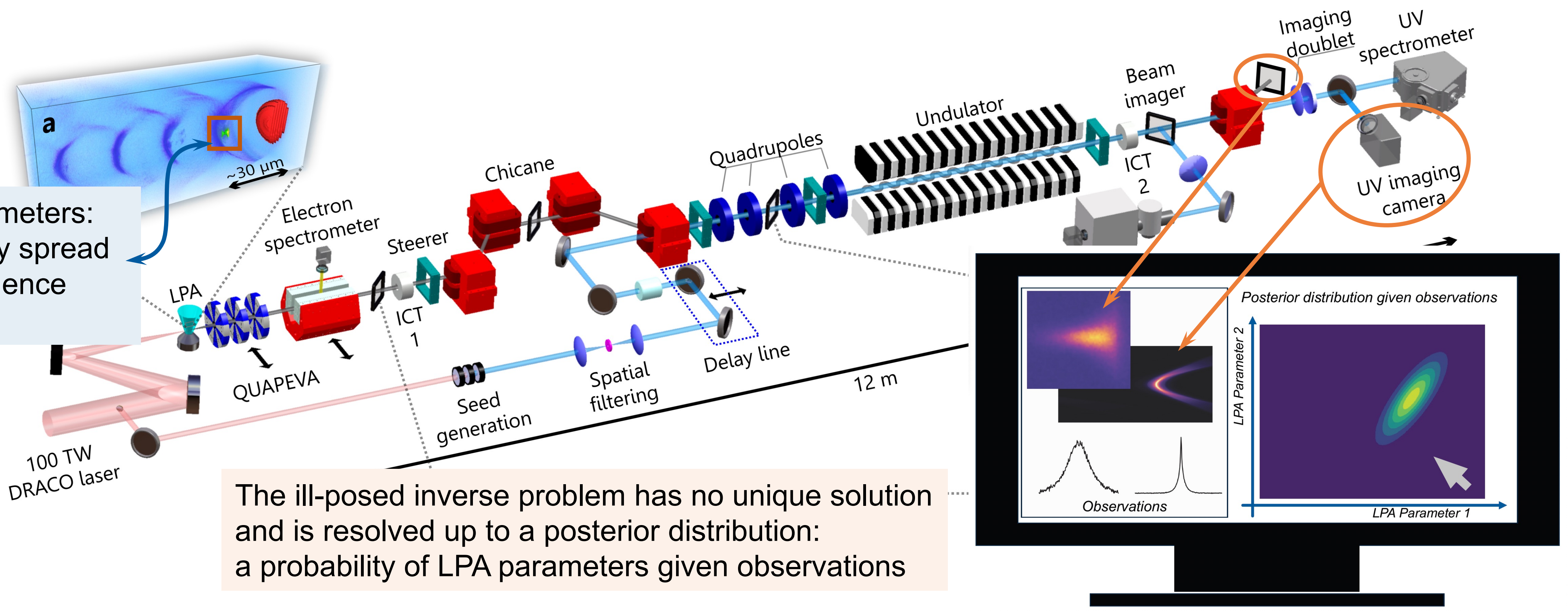


Virtual diagnostics provide data from all imagers in digital form with access to phase space of the beam in the beamline

Data Analysis Workflow for COXINEL Experiment

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

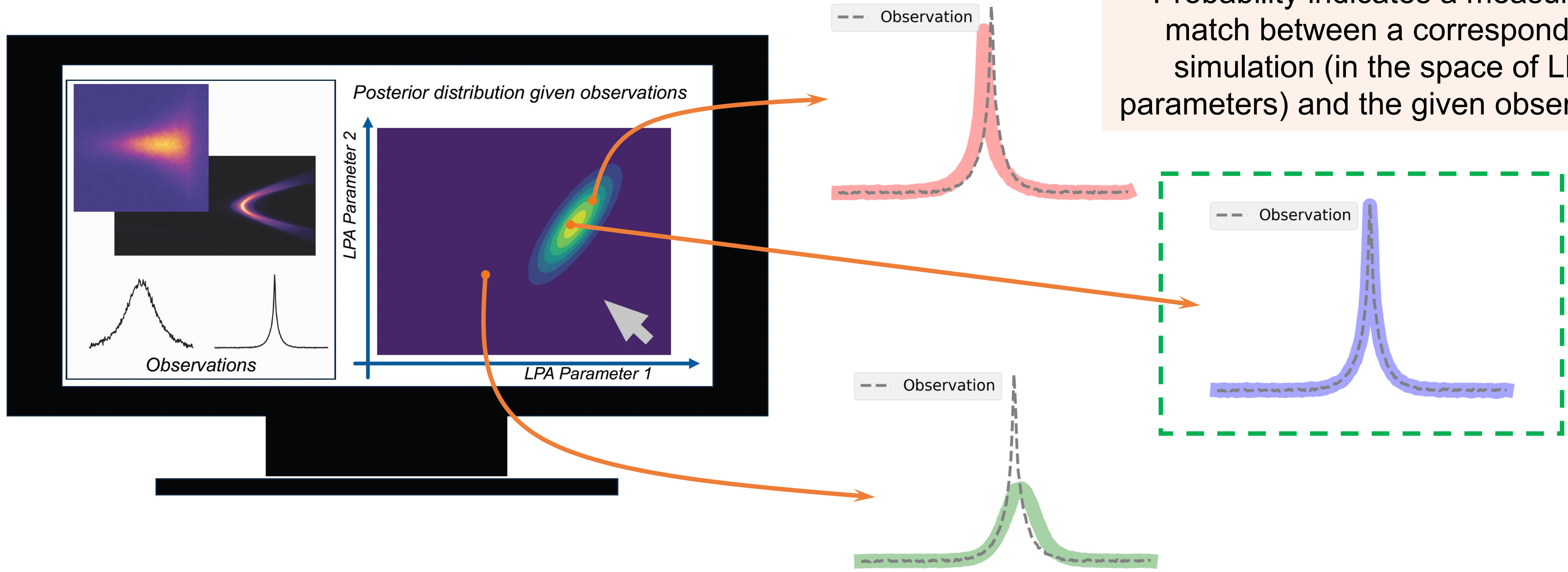
LPA parameters:
- Energy spread
- Divergence
- Size



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

Simulation-based Inference (SBI)

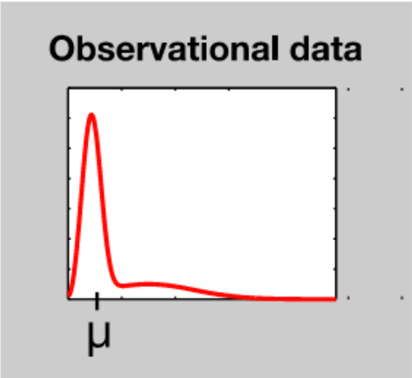
Infer the underlying model from experimental observations



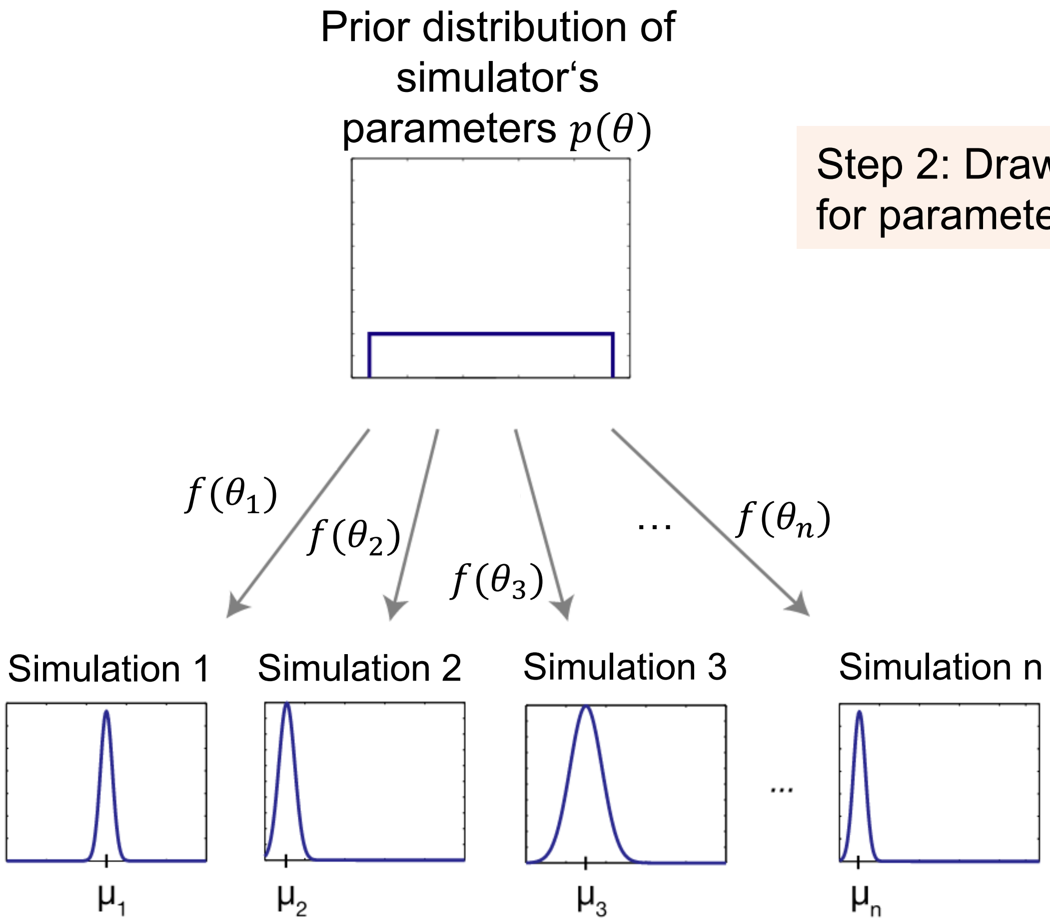
Probability indicates a measure of match between a corresponding simulation (in the space of LPA parameters) and the given observation

Bayesian Inference

Approximate Bayesian Computation (ABC) Rejection



Step 1: Compute a summary statistics μ for an observed sample



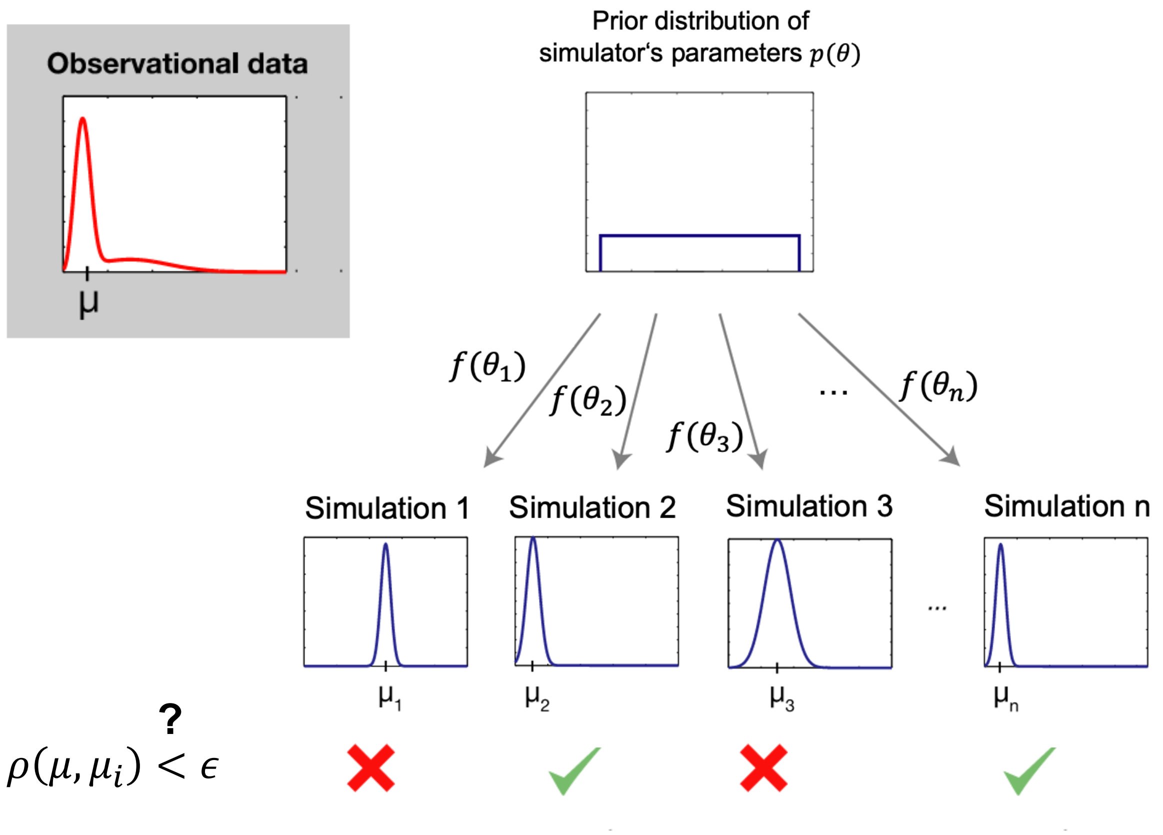
Step 2: Draw simulated samples for parameters $\theta_i \sim p(\theta)$

Step 3: Compute summary statistics μ_i for each sample

Image: https://astroautomata.com/blog/simulation-based-inference/

Bayesian Inference

Approximate Bayesian Computation (ABC) Rejection

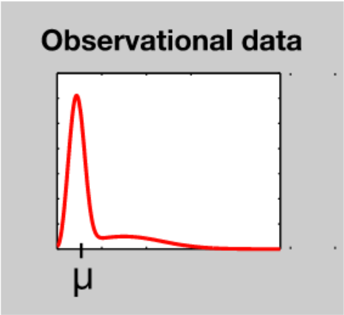


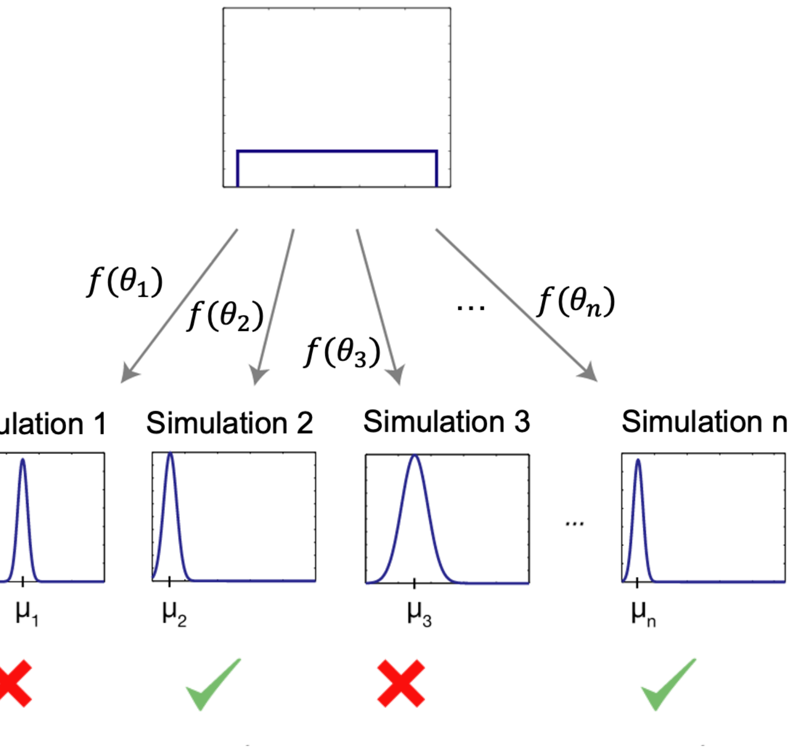
Step 4: Define rejection criteria $\rho(\mu, \mu_i) < \epsilon$ and reject all unsatisfactory samples

Image: https://astroautomata.com/blog/simulation-based-inference/

Bayesian Inference

Approximate Bayesian Computation (ABC) Rejection





Step 5: Based on accepted simulations, approximate posterior distribution of parameters θ given an observation x

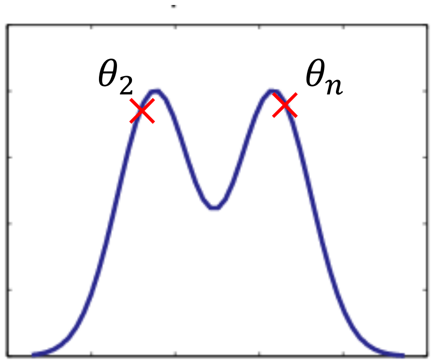


Image: https://astroautomata.com/blog/simulation-based-inference/

Bayesian Inference

Approximate Bayesian Computation (ABC)

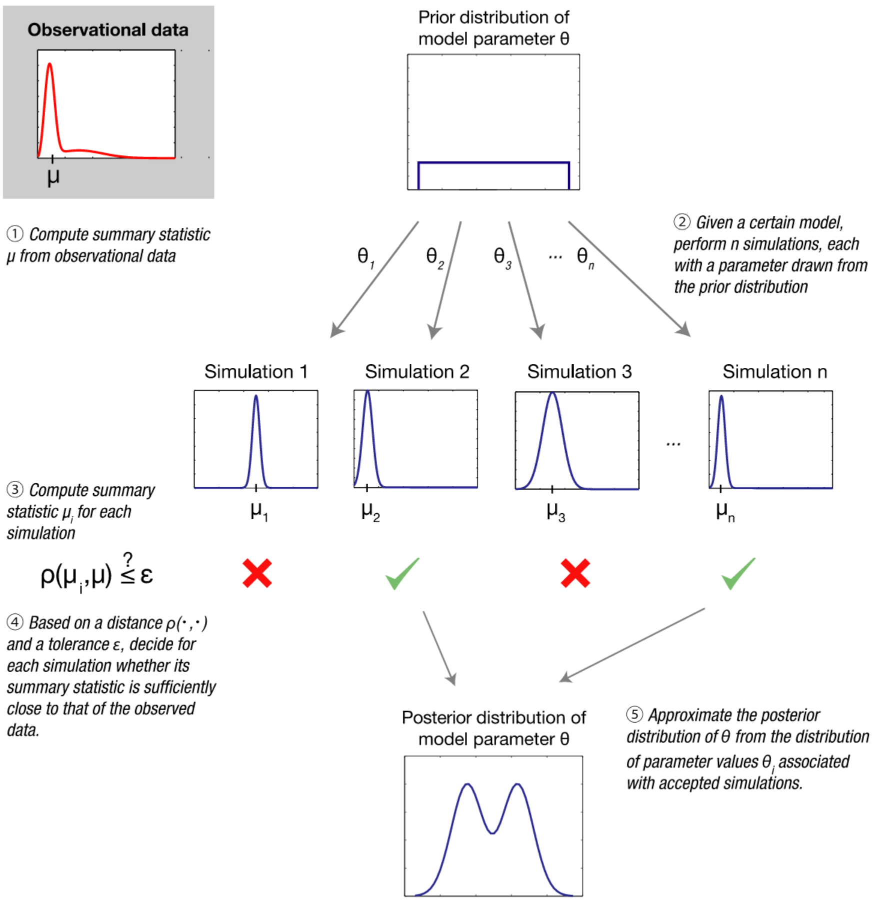


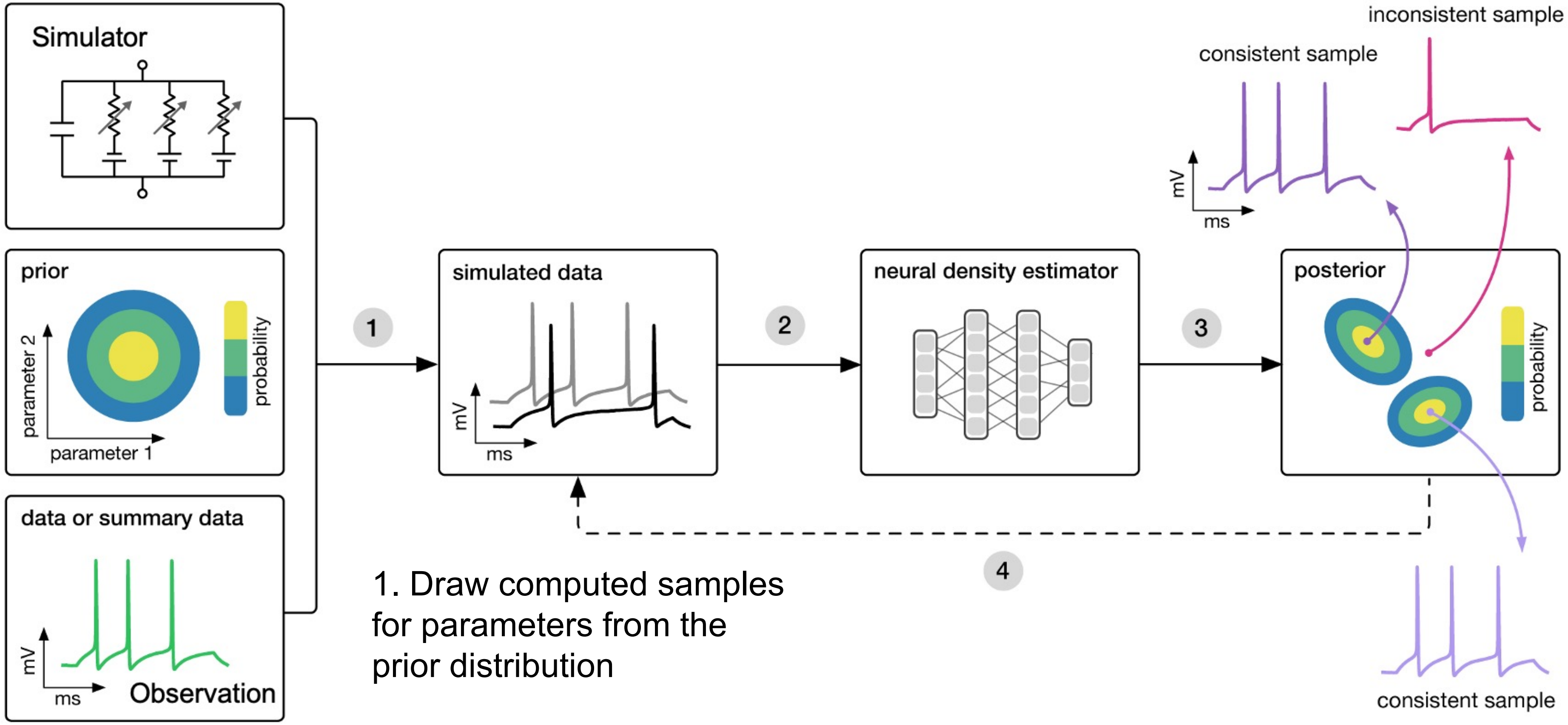
Image: https://astroautomata.com/blog/simulation-based-inference/

Problems:

- If the prior distribution $p(\theta)$ is too different from the posterior distribution $p(\theta|x)$, the acceptance rate might be very low, 5-15%
- In order to correctly approximate the posterior distribution $p(\theta|x)$ one has to run thousands of simulations
- The posterior distribution $p(\theta|x)$ is fixed to one observation, the procedure has to be repeated for each next collected observation

Simulation-based Inference

Sequential Neural Posterior Estimation (SNPE)

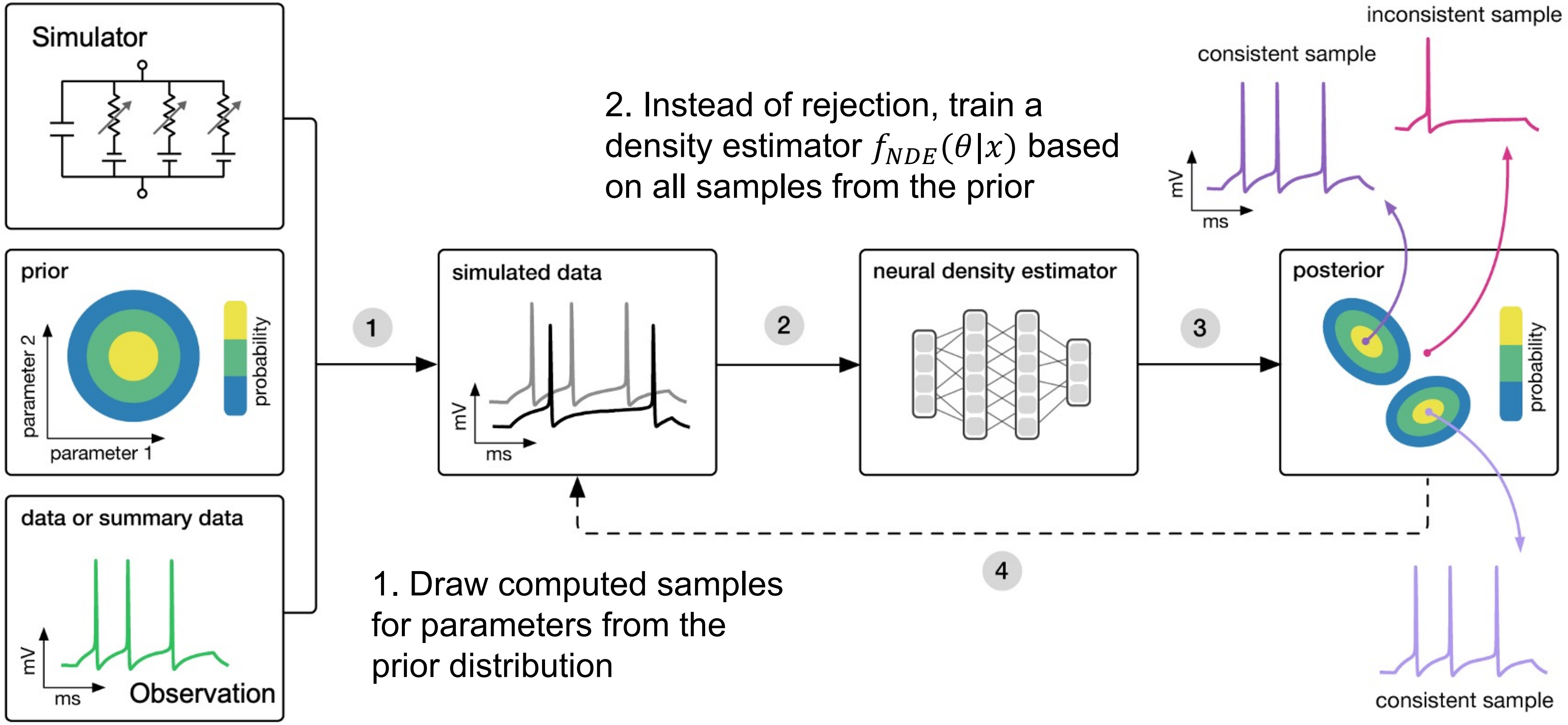


1. Draw computed samples for parameters from the prior distribution

Image: https://www.mackelab.org/sbi/

Simulation-based Inference

Sequential Neural Posterior Estimation (SNPE)



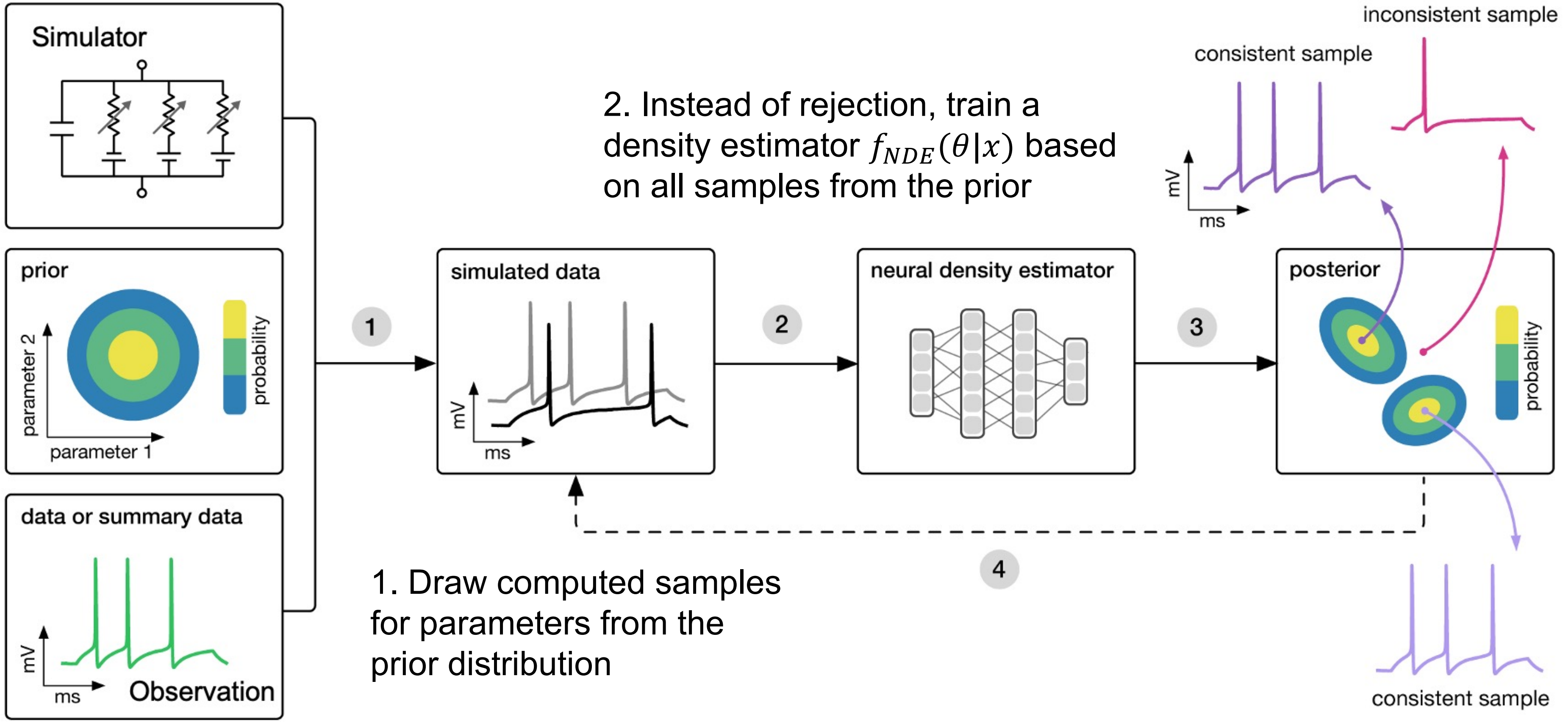
2. Instead of rejection, train a density estimator $f_{NDE}(\theta|x)$ based on all samples from the prior

1. Draw computed samples for parameters from the prior distribution

Image: https://www.mackelab.org/sbi/

Simulation-based Inference

Sequential Neural Posterior Estimation (SNPE)



2. Instead of rejection, train a density estimator $f_{NDE}(\theta|x)$ based on all samples from the prior

3. Neural Network $f_{NDE}(\theta|x)$ is a transformation between the posterior distribution and easy-to-sample distribution that allows easy sampling from $p(\theta|x)$

1. Draw computed samples for parameters from the prior distribution

Image: https://www.mackelab.org/sbi/

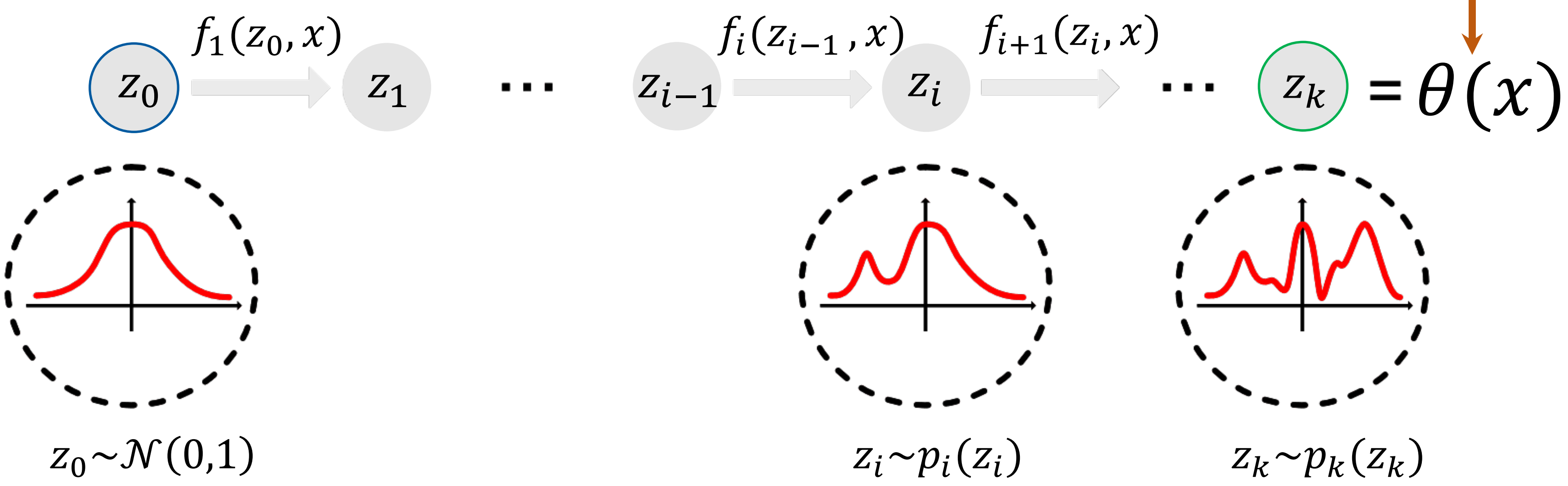
Simulation-based Inference

Neural Density Estimator: Normalizing Flows

Sequence of mappings f_i to transform a sample from the normal distribution into a sample θ (simulator parameters) from the custom distribution

For the posterior distribution estimation:
$\theta = f_K(f_{K-1}(\dots(f_1(z_0, x))))$, x is a given observation

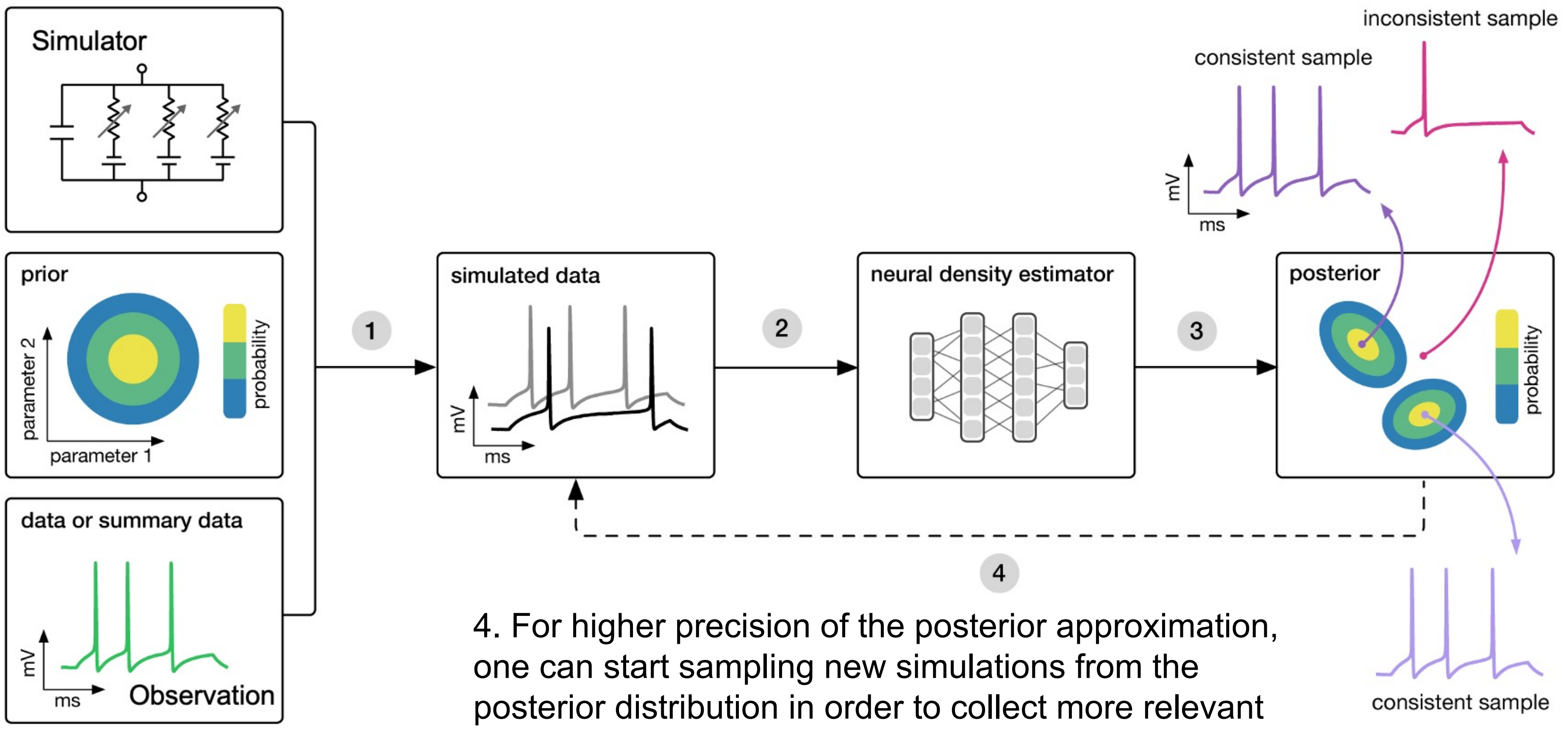
Simulator parameters for a corresponding observation x



https://lilianweng.github.io/posts/2018-10-13-flow-models/

Simulation-based Inference

Sequential Neural Posterior Estimation (SNPE)

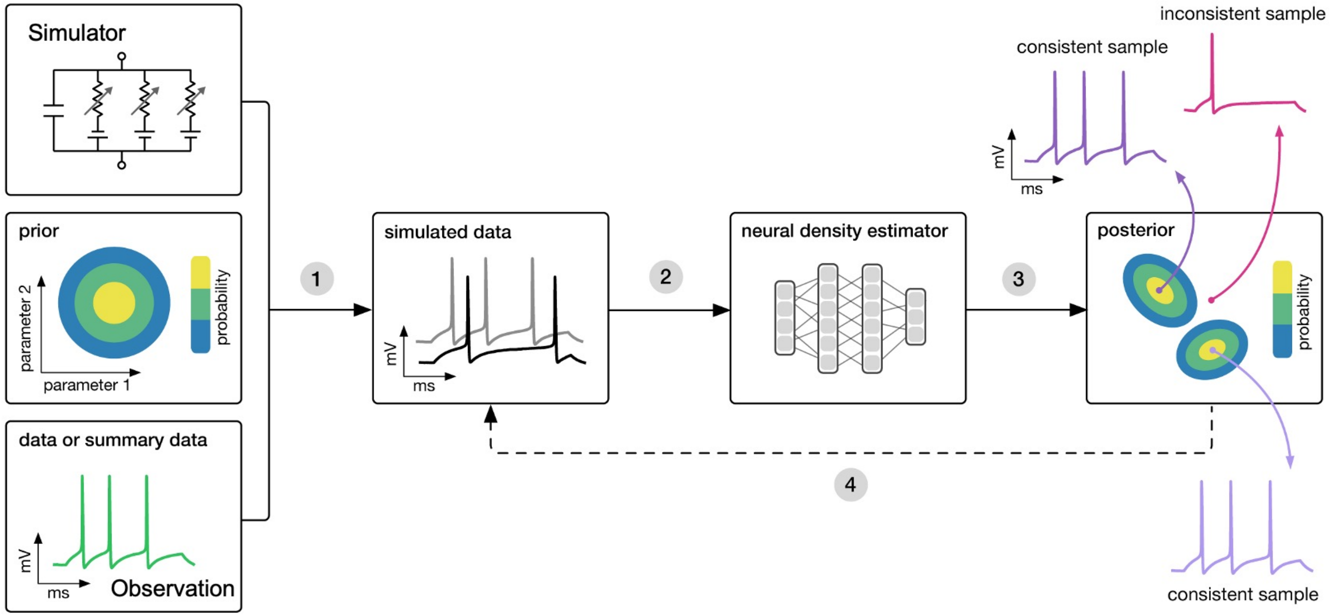


4. For higher precision of the posterior approximation, one can start sampling new simulations from the posterior distribution in order to collect more relevant to the given observation samples and adjust the NDE

Image: https://www.mackelab.org/sbi/

Simulation-based Inference

Sequential Neural Posterior Estimation (SNPE)



- Less simulations are required to approximate a posterior distribution
- Approximation of the posterior distribution can be used for any number of observations
- Available sampler from the posterior distribution helps to refine the posterior distribution w.r.t. a given observation

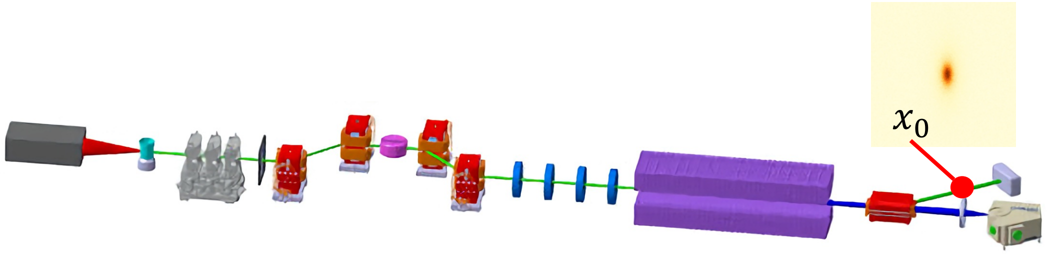
Image: https://www.mackelab.org/sbi/

Application of SBI to COXINEL experiment

Simulator:
`APS elegant code`* for simulation of beam transport

* Borland, Michael. Elegant: A flexible SDDS-compliant code for accelerator simulation. No. LS-287. Argonne National Lab., IL (US), 2000.

Observation:
A perturbed histogram of a simulated beam in the transverse plane (5% of noise) at the last imager

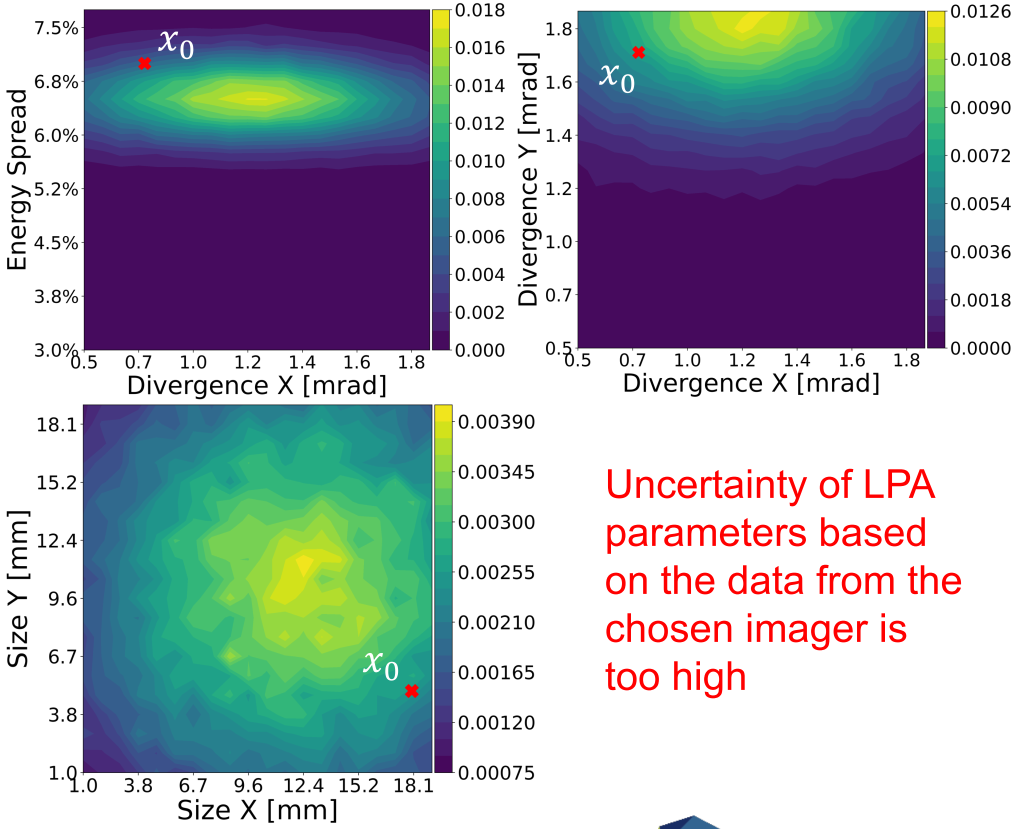


Used 10 000 simulations of beam transport sampled from a uniform prior defined by energy spread, divergence and beam size to train a neural density estimator

Figure:
Marie-Emmanuelle Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040

Inversion (LPA source parameters): $p(\theta|x_0)$

Computation time: 3.5h



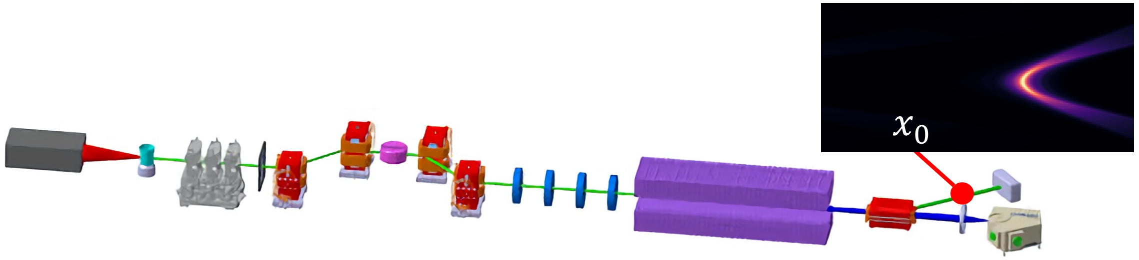
Uncertainty of LPA parameters based on the data from the chosen imager is too high

Application of SBI to COXINEL experiment

Simulator:
`SRW code`* for simulation of radiation intensity

* Chubar, O., and P. Elleaume. *Synchrotron Radiation Workshop (SRW)*. No. SRW; 002835MLTPL00. Brookhaven National Lab.(BNL), Upton, NY (United States), 2013.

Observation:
A perturbed spatio-spectral distribution of radiation intensity (5% of noise)

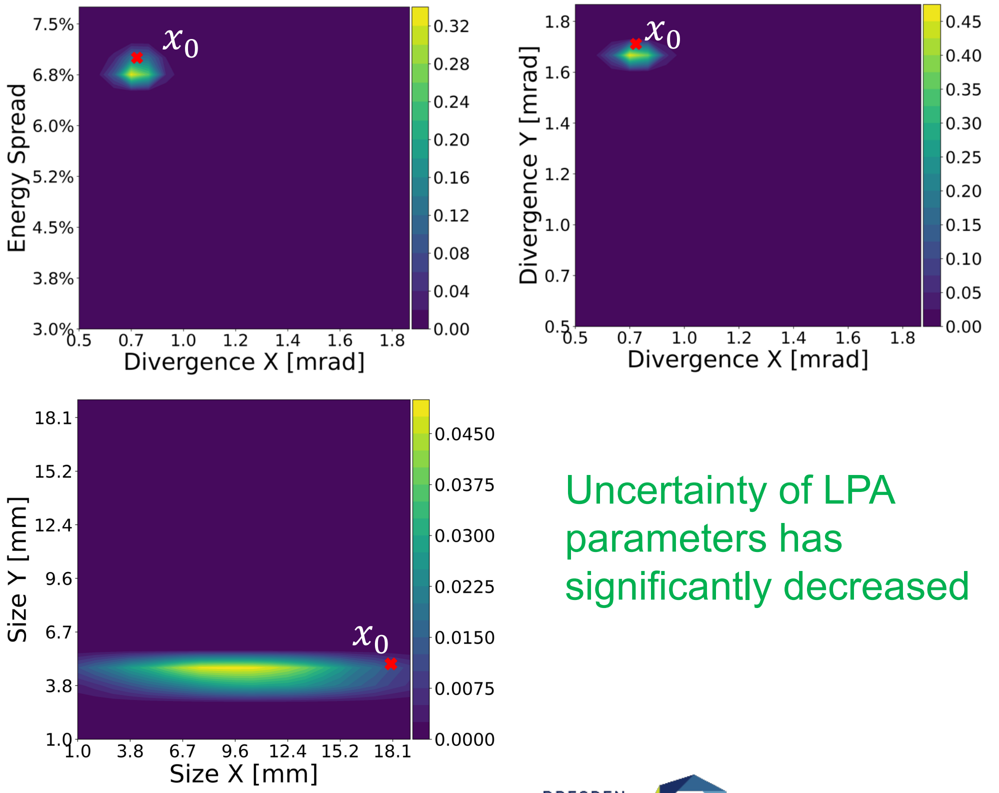


Used 10 000 simulations of beam transport sampled from a uniform prior defined by energy spread, divergence and beam size to train a neural density estimator

Figure:
Marie-Emmanuelle Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040

Inversion (LPA source parameters): $p(\theta|x_0)$

Computation time is estimated by 13 days, only inference on pre-computed simulations is possible



Uncertainty of LPA parameters has significantly decreased

Data-driven Surrogate Models for COXINEL

Simulation code is slowing down SBI analysis

In order to accelerate computations we can

- distribute simulations over many compute nodes
- replace simulations by surrogate models to reduce time and computational power consumption

Data-driven Surrogate Models for COXINEL

Simulation code is slowing down SBI analysis

In order to accelerate computations we can

- distribute simulations over many compute nodes
- replace simulations by surrogate models to reduce time and computational power consumption

Feasible to use in the experimental workflow due to fast response and low requirements to hardware

Data-driven Surrogate Models for COXINEL

Replace simulations by computationally cheap surrogate models

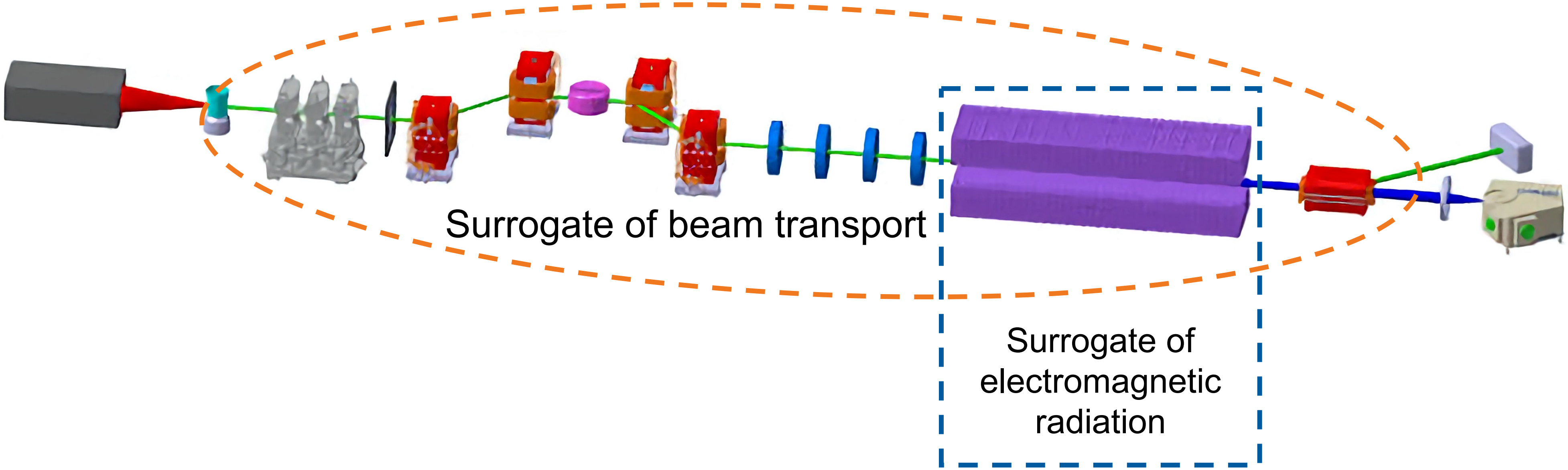
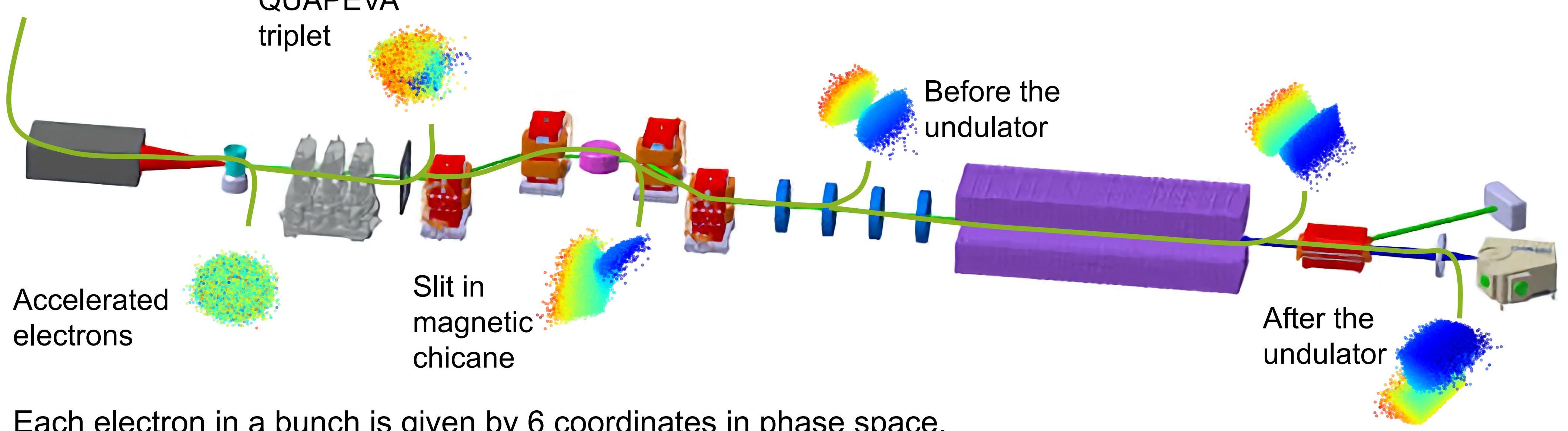


Figure:
Marie-Emmanuelle Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040

Surrogate Model of Electron Beam Transport

Reconstruct electron distributions at different positions in the beamline

Stated problem: reconstruct expected distributions of electrons at imagers in the beamline for the given LPA parameters

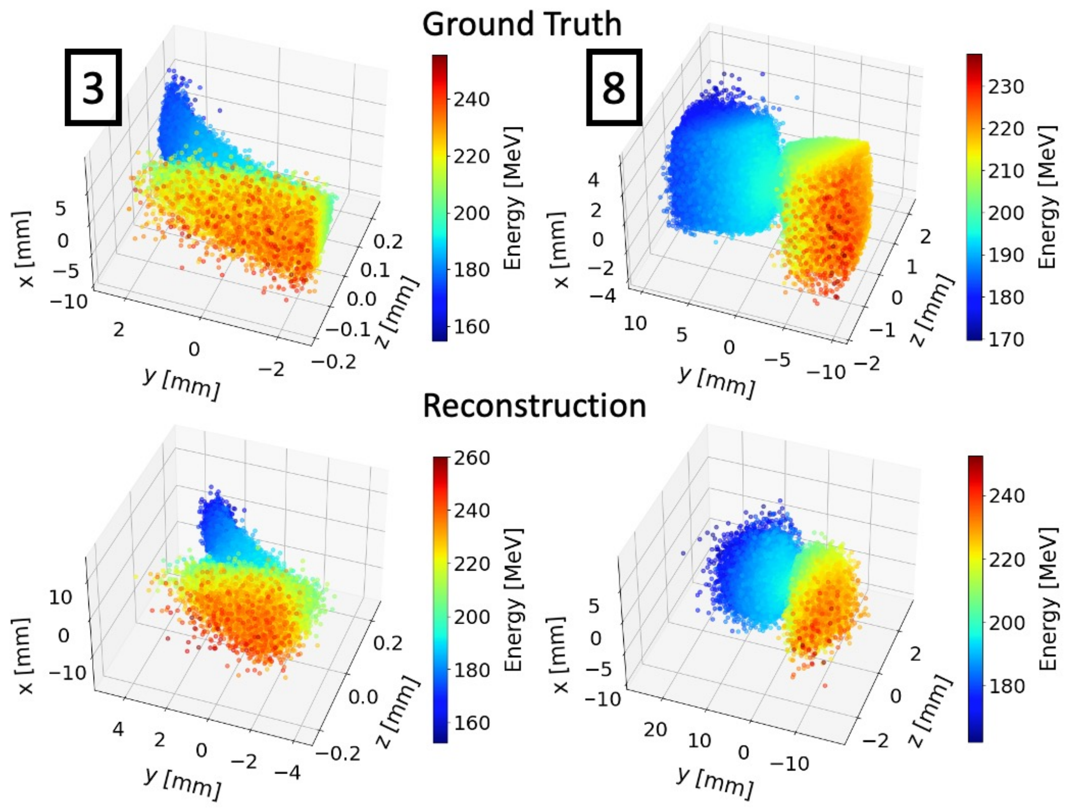


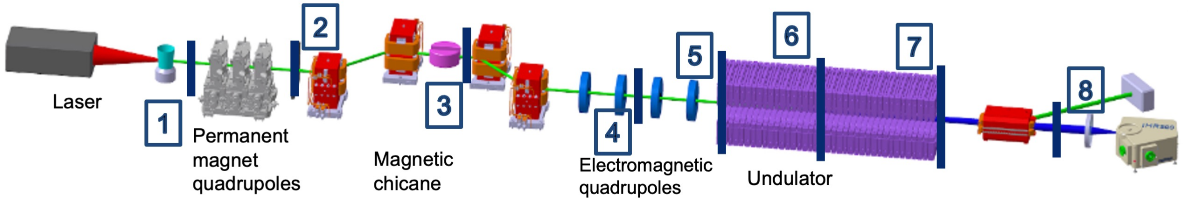
Each electron in a bunch is given by 6 coordinates in phase space.
Training/Validation data was simulated by `APS elegant`* for varying LPA parameters.

* Borland, Michael. Elegant: A flexible SDDS-compliant code for accelerator simulation. No. LS-287. Argonne National Lab., IL (US), 2000.

Surrogate Model of Electron Beam Transport

Reconstruction of phase space distribution at different locations along the beam transport line using normalizing flows[1] neural network architecture





- The model is limited to the given domain of parameters where training data is available
- Flexible inference w.r.t. number of electrons
- 10x faster inference than the numerical simulation (`APS elegant code`[2])

Figure:
Marie-Emmanuelle Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040

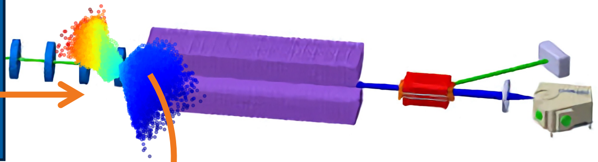
1 Papamakarios, G., Pavlakou, T., & Murray, I. (2017). Masked autoregressive flow for density estimation. *Advances in neural information processing systems*, *30*.

2 Borland, Michael. Elegant: A flexible SDDS-compliant code for accelerator simulation. No. LS-287. Argonne National Lab., IL (US), 2000.

Surrogate Model of Undulator Radiation

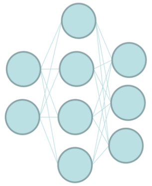
Undulator entrance

Surrogate model of Electron Beam Transport

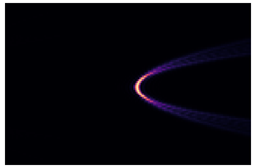


For each particle i

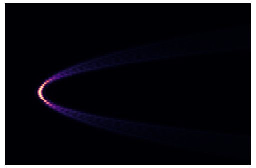
$$\begin{pmatrix} coordinate\ x_i, \\ coordinate\ y_i, \\ momentum\ xp_i, \\ momentum\ yp_i, \\ Energy_i \end{pmatrix}$$



Neural Network

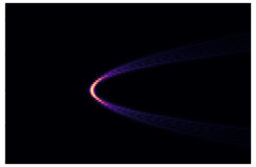


$i = 1$



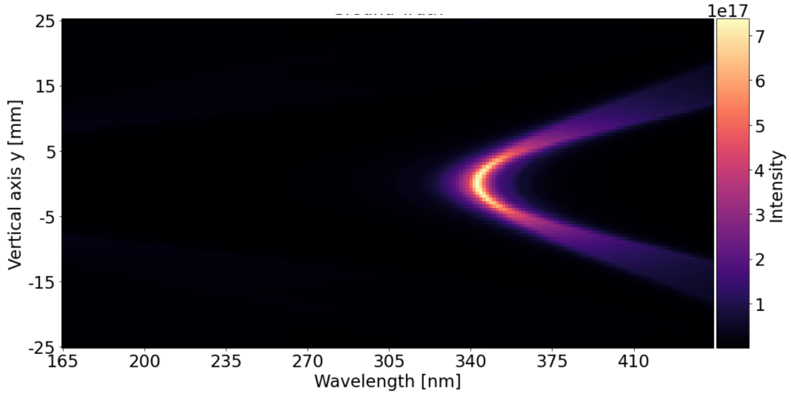
$i = 2$

...

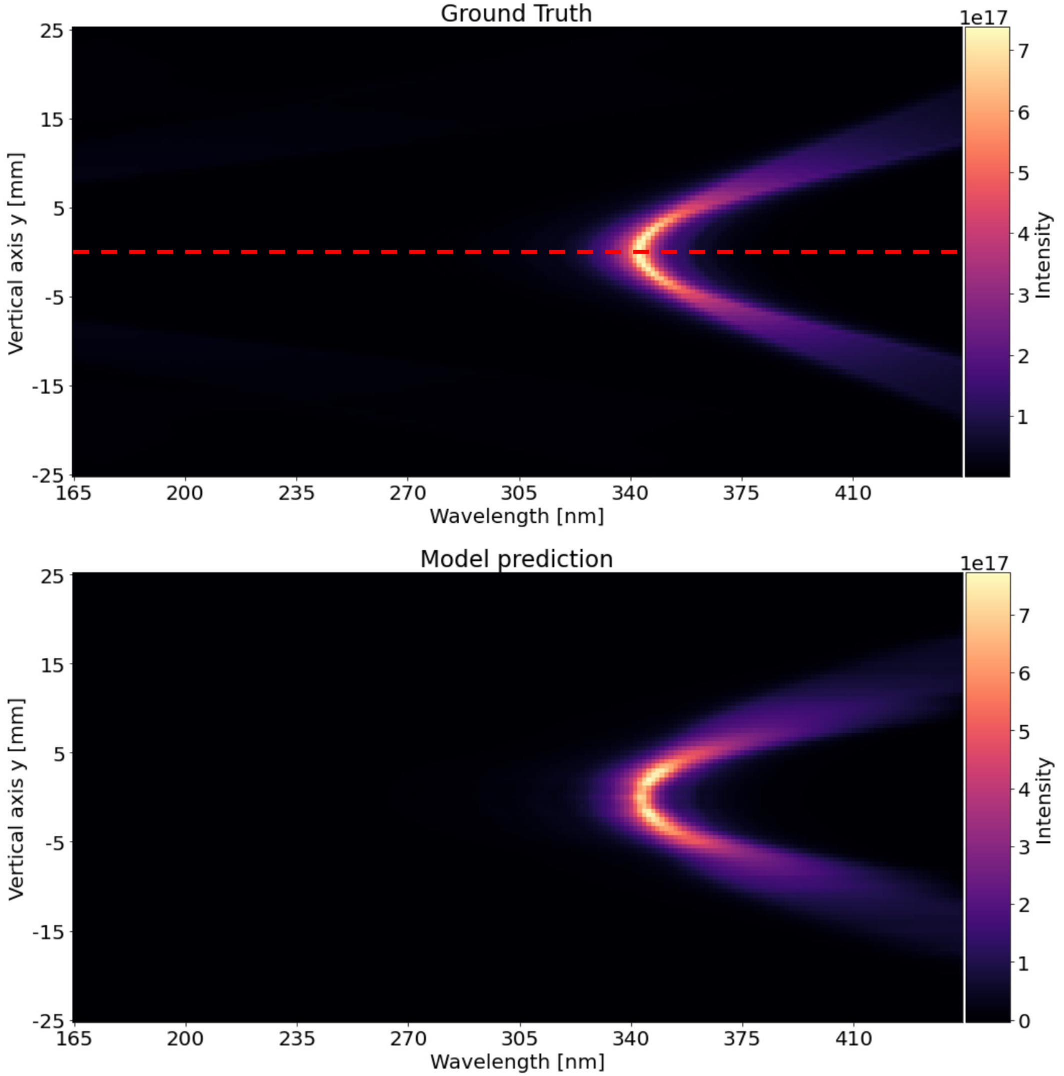


$i = n$

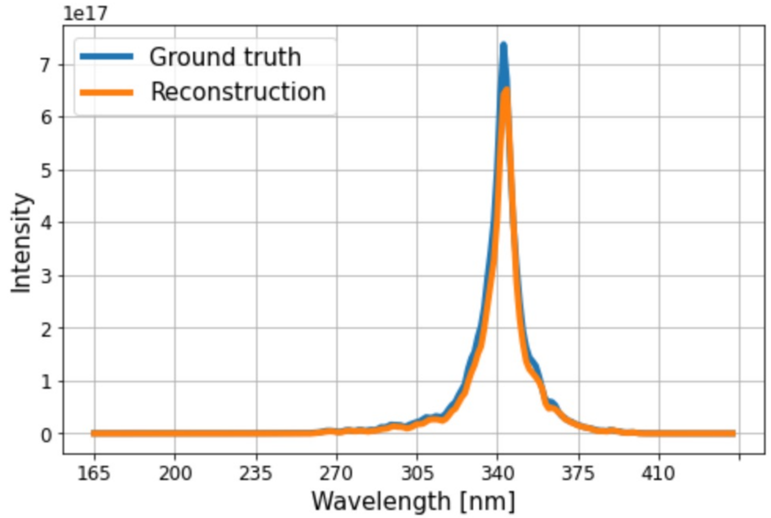
Sum of all particles‘ radiation



Surrogate Model of Undulator Radiation



Intensity at $y = 0$

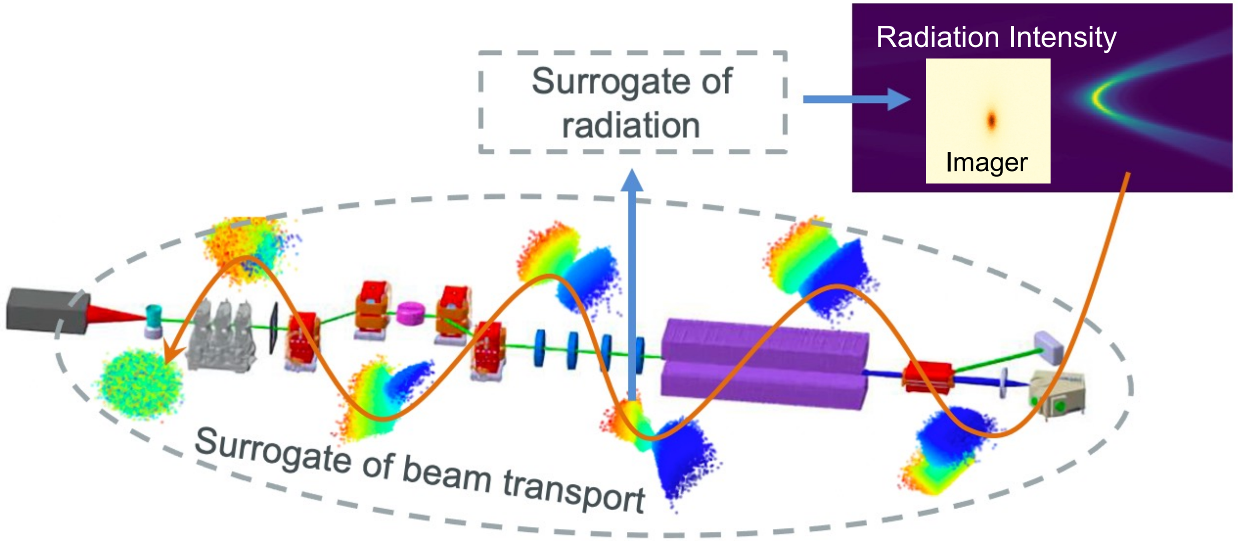


- The model is limited to the given domain of parameters where training data is available
- Surrogate model reconstructs the data structure correctly
- 390x faster than simulation code (`SRW`*)

* Chubar, O., and P. Elleaume. *Synchrotron Radiation Workshop (SRW)*. No. SRW; 002835MLTPL00. Brookhaven National Lab.(BNL), Upton, NY (United States), 2013.

Outlook and Summary

- Integration of the machine learning-based analysis workflow into the experimental results
- Virtual diagnostics in experiments can help to exploit correlations among all experimental data
- Identification of well-behaved operating states
- Feedback loop for experimental parameters to maintain the FEL performance
- Surrogate models are decreasing requirements to hardware and time consumption of data analysis



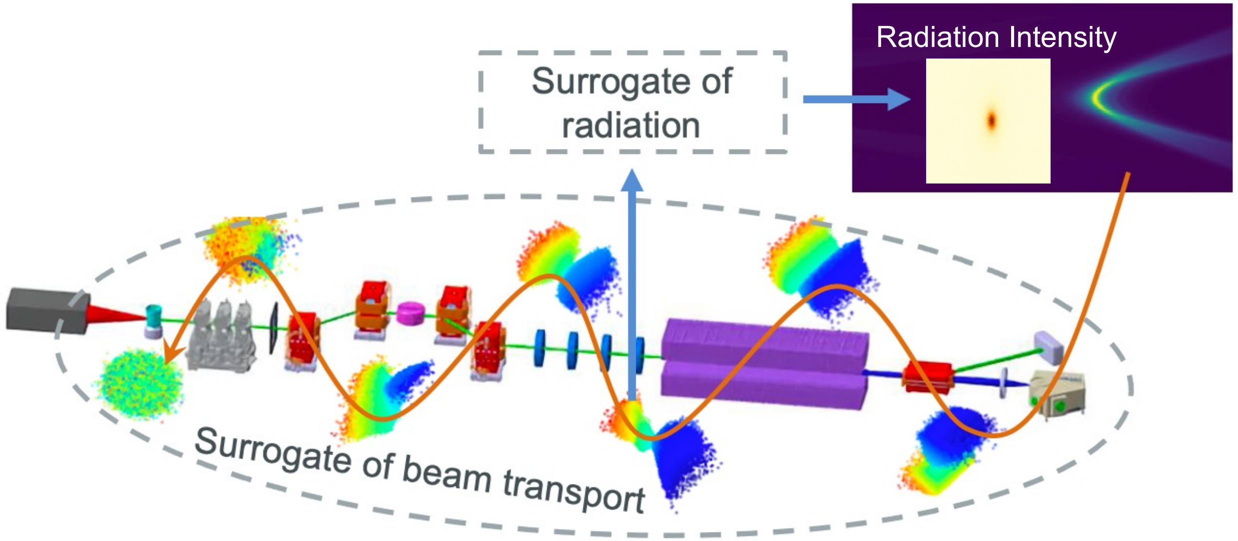
Outlook and Summary

- Integration of the machine learning-based analysis workflow into the experimental results
- Virtual diagnostics in experiments can help to exploit correlations among all experimental data
- Identification of well-behaved operating states
- Feedback loop for experimental parameters to maintain the FEL performance
- Surrogate models are decreasing requirements to hardware and time consumption of data analysis

Challenges:

Validation of inversion and surrogate models: how to define if result is accurate enough

Data-dependence of SBI method and surrogate models: the parameter ranges on input have to be chosen in advance bevor the experiment is running



Outlook and Summary

Thank you for your attention!

- Integration of the machine learning-based analysis workflow into the experimental results
- Virtual diagnostics in experiments can help to exploit correlations among all experimental data
- Identification of well-behaved operating states
- Feedback loop for experimental parameters to maintain the FEL performance
- Surrogate models are decreasing requirements to hardware and time consumption of data analysis

Challenges:

Validation of inversion and surrogate models: how to define if result is accurate enough

Data-dependence of SBI method and surrogate models: the parameter ranges on input have to be chosen in advance bevor the experiment is running