Inverse Uncertainty Quantification in nuclear engineering

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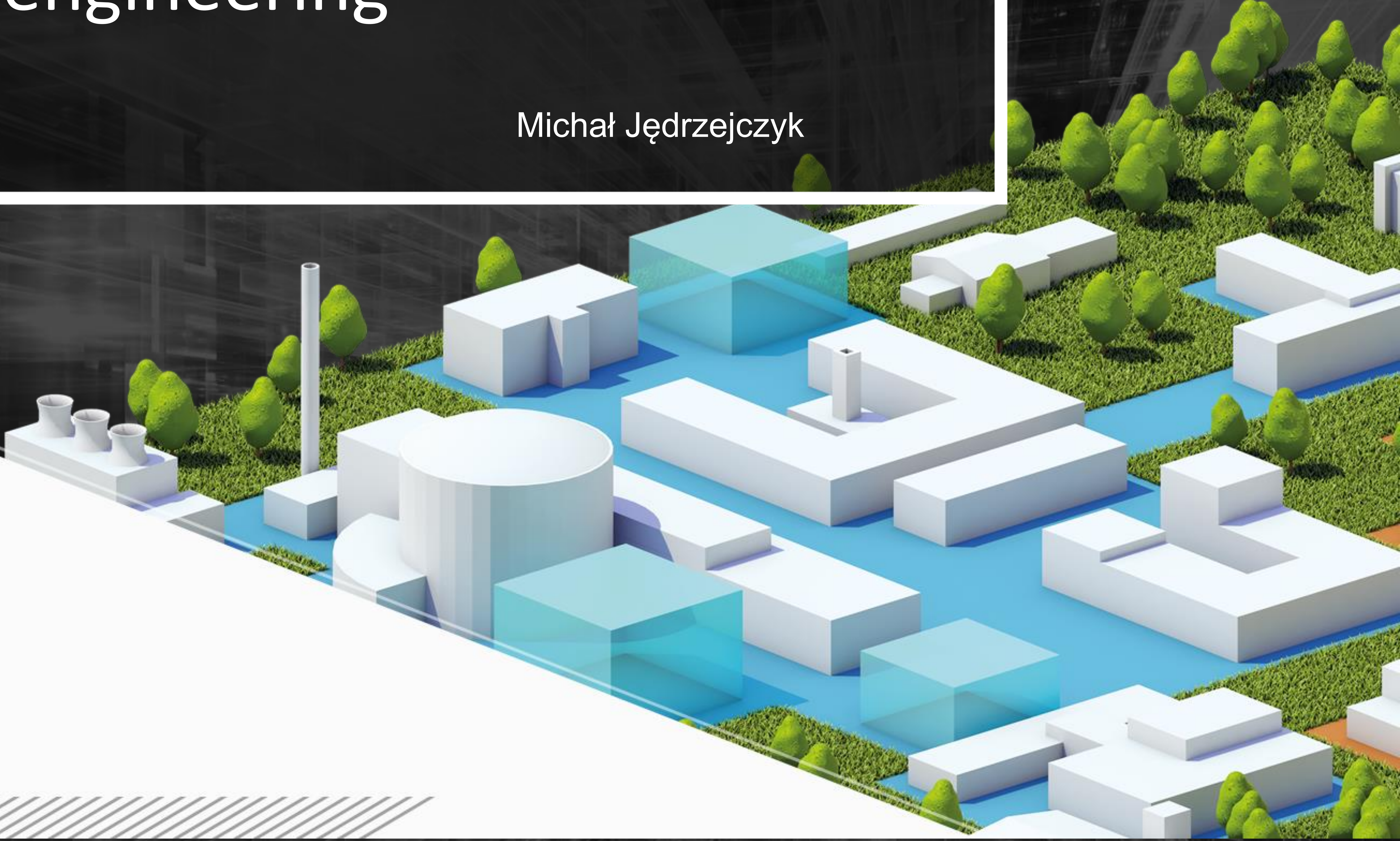

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Presentation plan

- What is Inverse Uncertainty Quantification (IUQ)?
- Nuclear reactor licensing criteria
- What is uncertainty quantification (UQ)?
- IUQ types
- Introduction to Approximate Bayesian Computation (ABC)
- Advanced ABC and coffee cup cooling example
- Limitations of IUQ

Problem definition

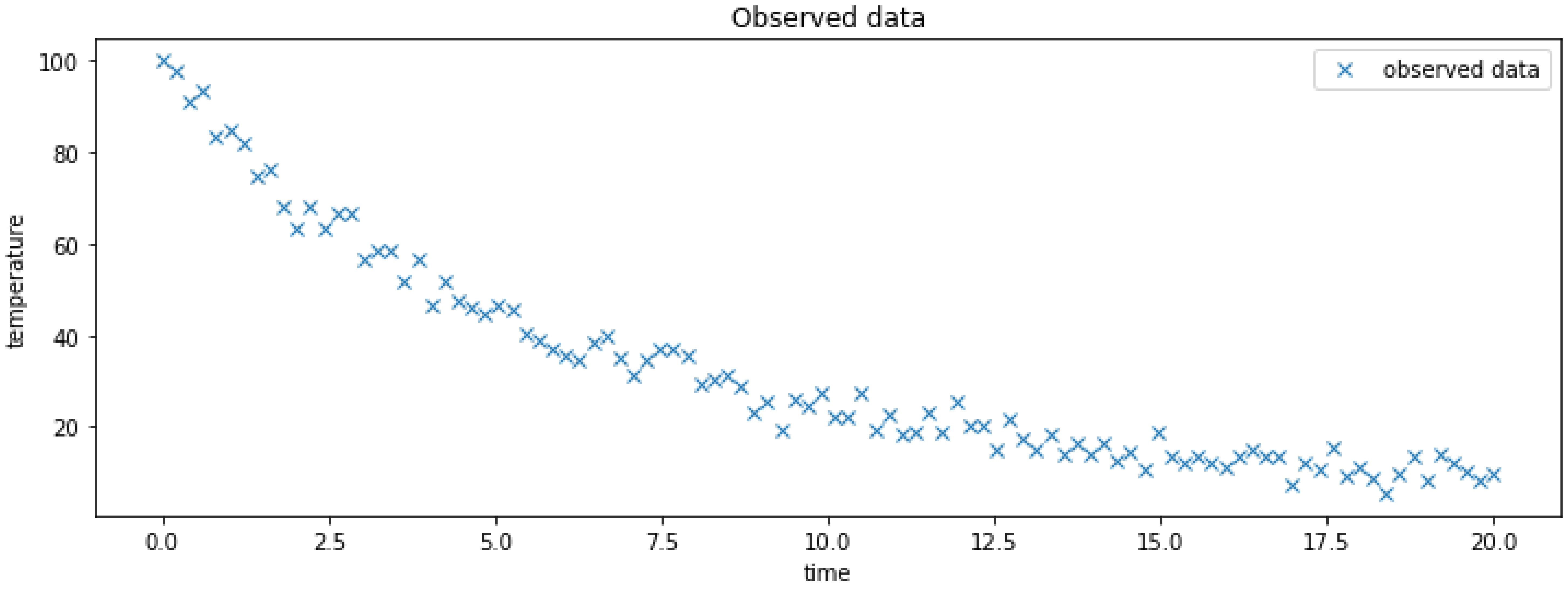
Consider a general computer model $y^M = y^M(x, \theta)$, where y^M is the model output.

x denotes design variables – like physical dimensions of an experiment, its material properties.

θ denotes calibration parameters – these may or may not have physical meaning but influence the model output. They have unknown true values invariant of the experiments

A coffee cup example:

$$\frac{dT}{dt} = -k\left(T_{cup} - T_{env}\right) - f * \left(T_{cup}^4 - T_{env}^4\right).$$



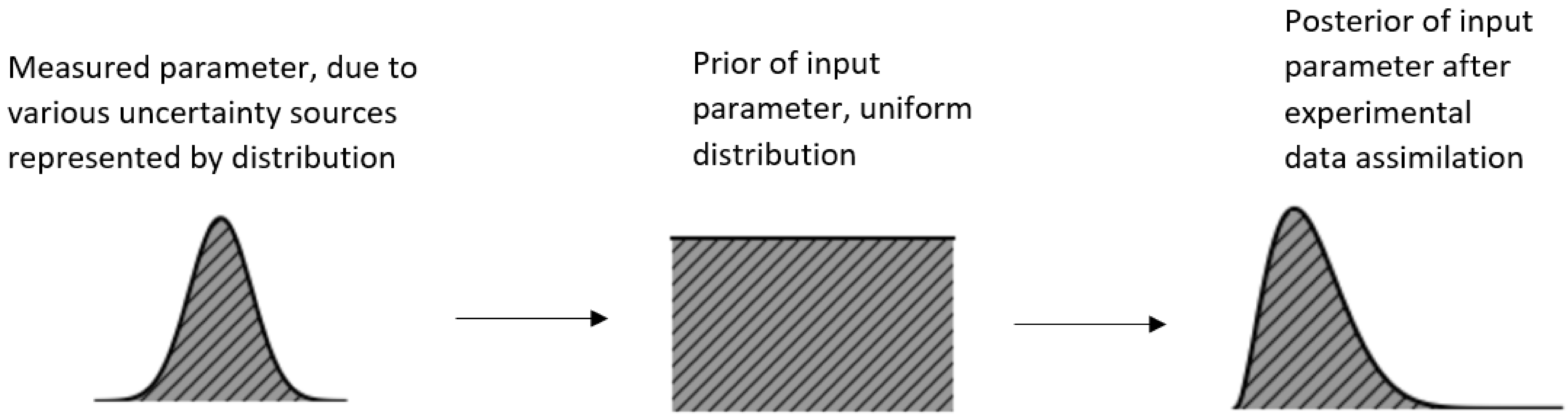
Task: find distributions of k and f based on experiment.

What is Inverse Uncertainty Quantification (IUQ)?

Determination of input parameter uncertainty based on simulations of experimental data and Bayesian statistics

Two possible cases:

1. We only have a point estimate of input parameter or a rough idea in what range its value should be
2. There is some known uncertainty in input parameters and we want to decrease it – then it is called Bayesian calibration



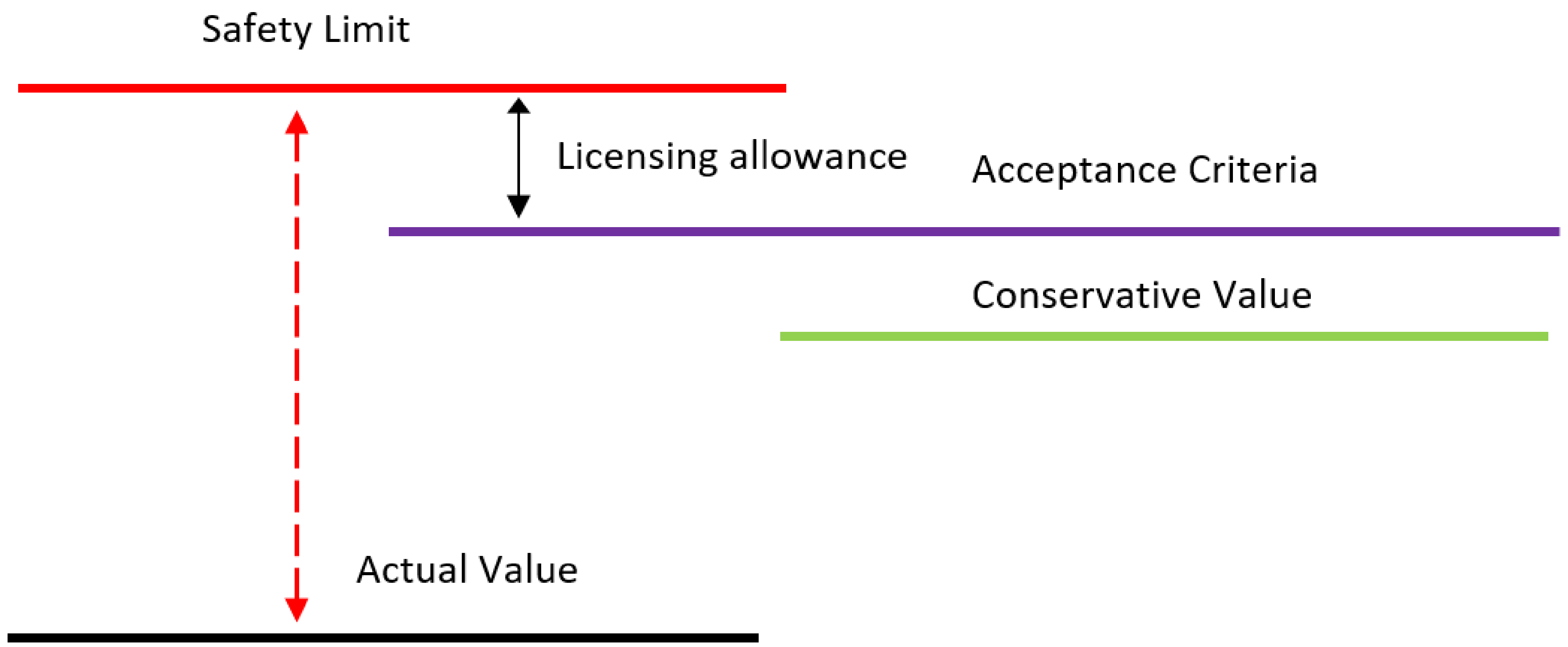
Unknown uncertainties in nuclear engineering problems

Thermohydraulic simulation for a Boling Water Reactor, maximum temperature example:

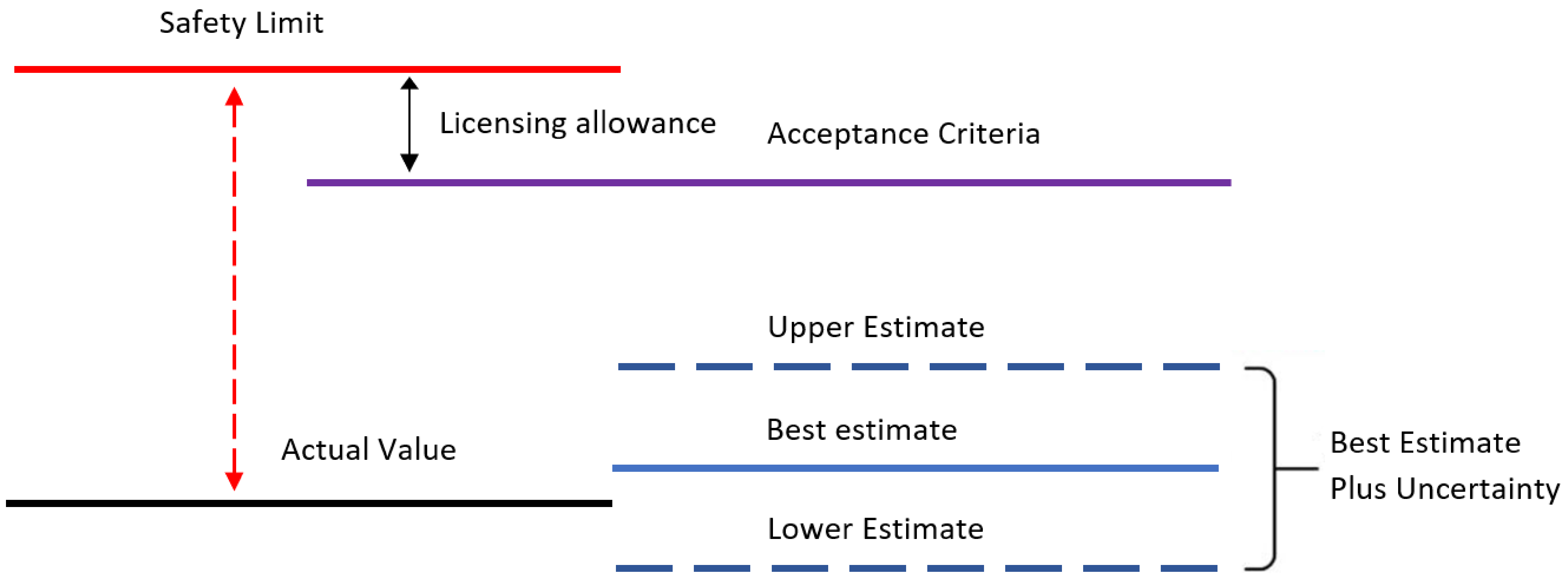
x – dimensions of a reactor, material properties, boundary conditions

θ – heat transfer coefficient of single phase liquid to wall, subcooled boiling heat transfer coefficient, wall drag coefficient, interfacial drag between water bubbles and fuel rods

Old licensing norms



Modern licensing norms



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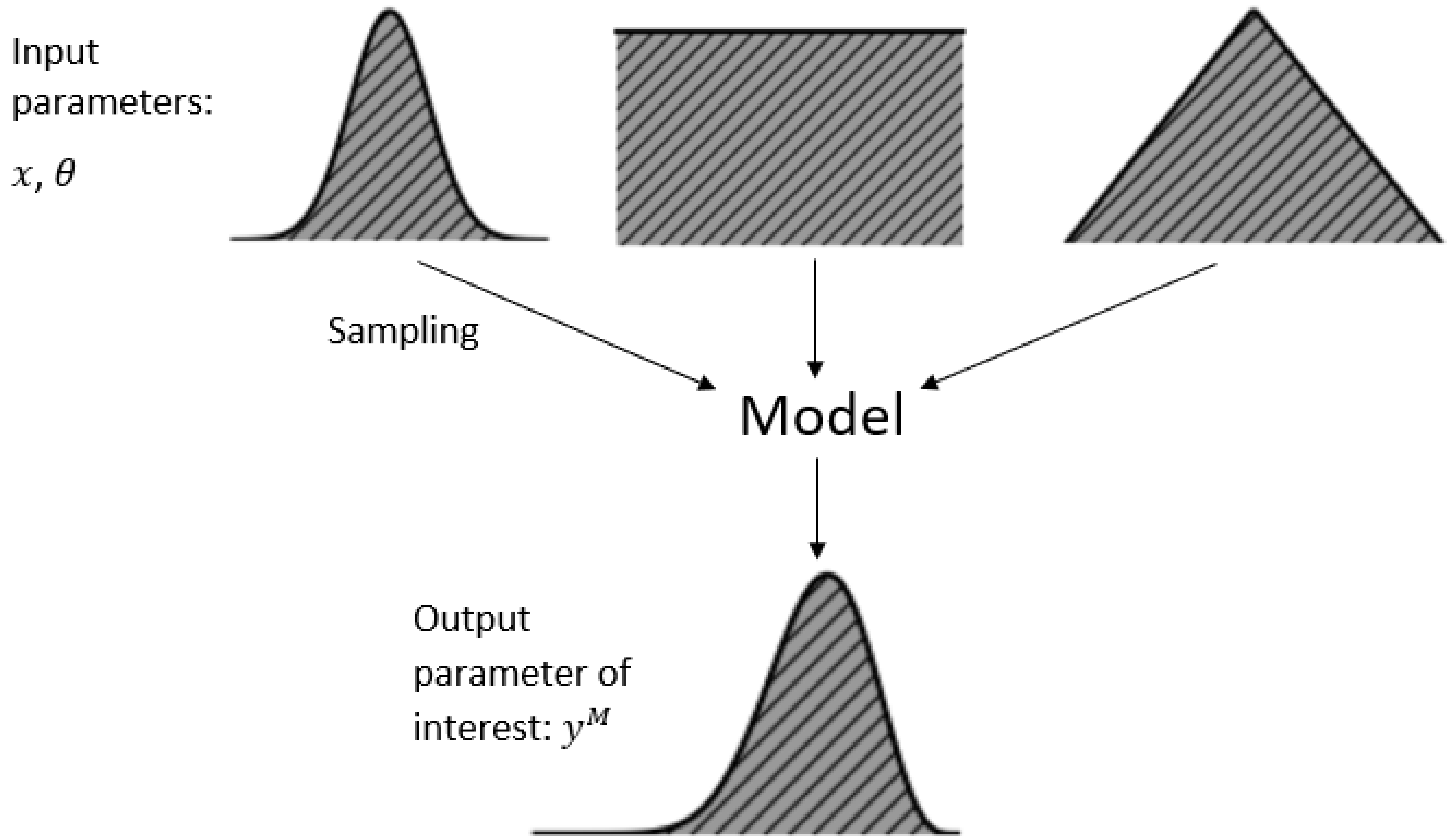
Determining uncertainty in model outcome - Uncertainty Quantification (UQ)

Error propagation from input parameters to calculated parameters of interest

Example: uncertainty in uranium cross-sections to multiplication factor in a nuclear reactor



IUQ types

IUQ type	Deterministic	Bayesian	Empirical
Method	Optimization	Bayesian updating	Trial-and-error
Prior distribution of input parameter	Uniform	Uniform	Uniform
Posterior	Assumed in advance – normal / lognormal	Any distribution, including multimodal	Uniform
Sampling	Based on optimization scheme	MCMC or its derivative	Monte Carlo sampled from uniform

Bayesian is the most rigorous and the most computationally expensive.

Bayesian statistics

$$\text{Bayes}'\text{theorem: } P(\theta|y_0) \propto P(y_0|\theta)P(\theta)$$

$P(\theta)$ - prior (initial belief about probability or distribution of θ)

$P(\theta|y_0)$ - posterior (probability or distribution of θ given data y_0)

$P(y_0|\theta)$ - likelihood (probability of the data y_0 as a function of θ)

Approximate Bayesian Computation (ABC) – a class of computational algorithms used to update prior beliefs on a distribution by assimilating experimental data. ABC allows for solving problems, where it is hard or impossible to calculate likelihood analytically.

Likelihood is approximated with a summary statistic: $\delta(y^M(\theta), y_0|\epsilon)$

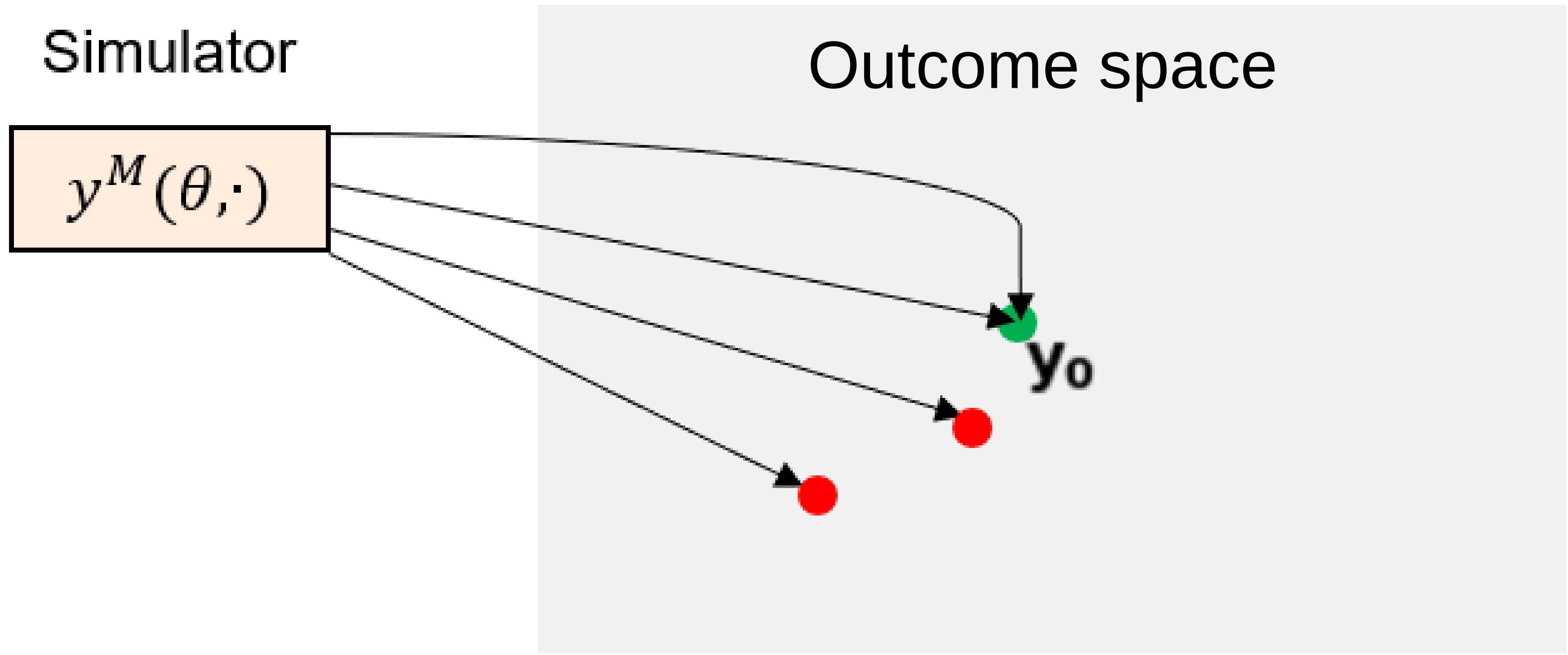
We get: $\mathrm{p}(\theta|y_0) = \delta(y^M(\theta), y_0|\epsilon)p(\theta)$

For $\epsilon = 0$, we get $\delta(y^M(\theta), y_0|\epsilon) = p(y_0|\theta)$

Basic ABC algorithm

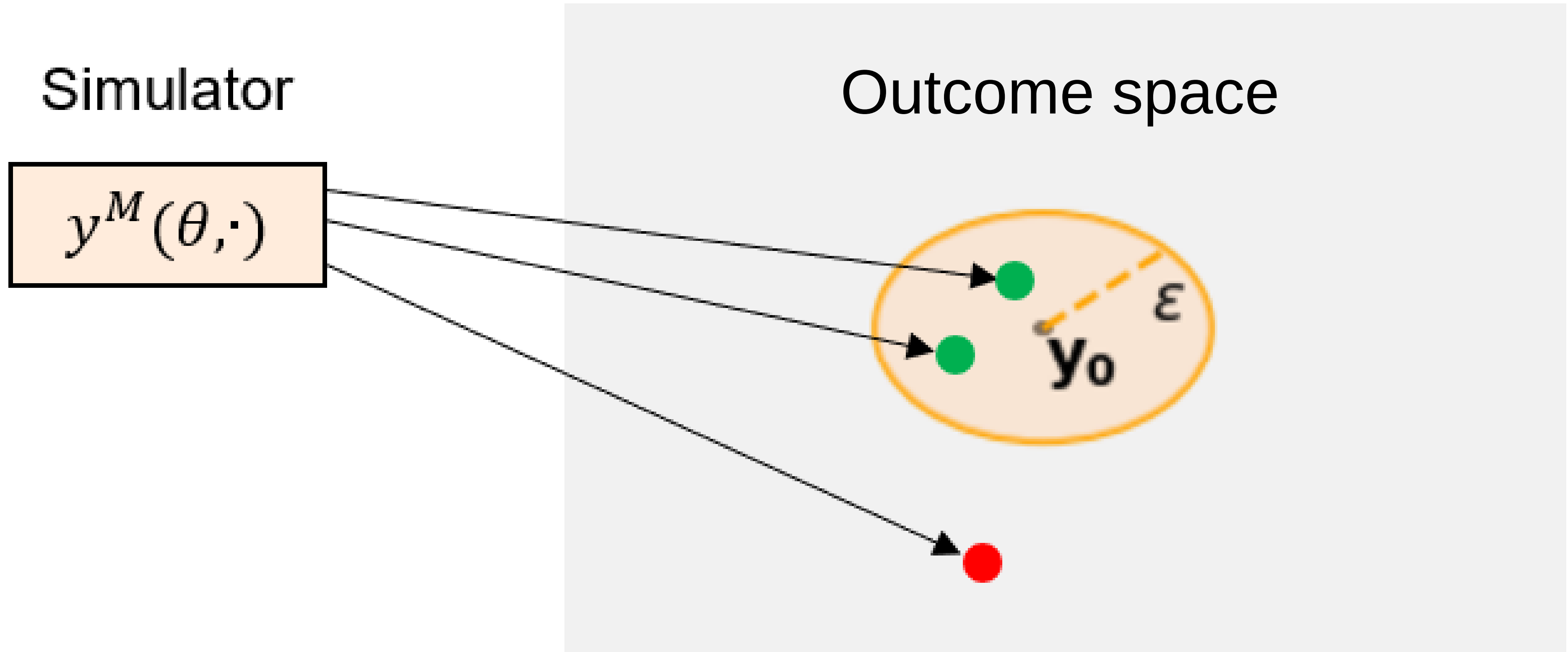
Basic rejection algorithm:

for $i = 1$ *to* N *do*
  reapeat
    Generate θ *from the prior* $p(\cdot)$
    Generate $y^M(\theta,\cdot)$ *from the simulator*
  until $y^M(\theta,\cdot) = y_0$
  $\theta^i \leftarrow \theta$
end for



An ABC rejection algorithm:

for $i = 1$ *to* N *do*
  reapeat
    Generate θ *from the prior* $p(\cdot)$
    Generate $y^M(\theta,\cdot)$ *from the simulator*
  until $\delta(y^M(\theta,\cdot), y_0) \leq \epsilon$
  $\theta^i \leftarrow \theta$
end for



Example of a stochastic inverse problem

Imagine a scenario where we flipped a coin 200 times and got tail 133 times. Can we determine for sure whether the coin is biased?

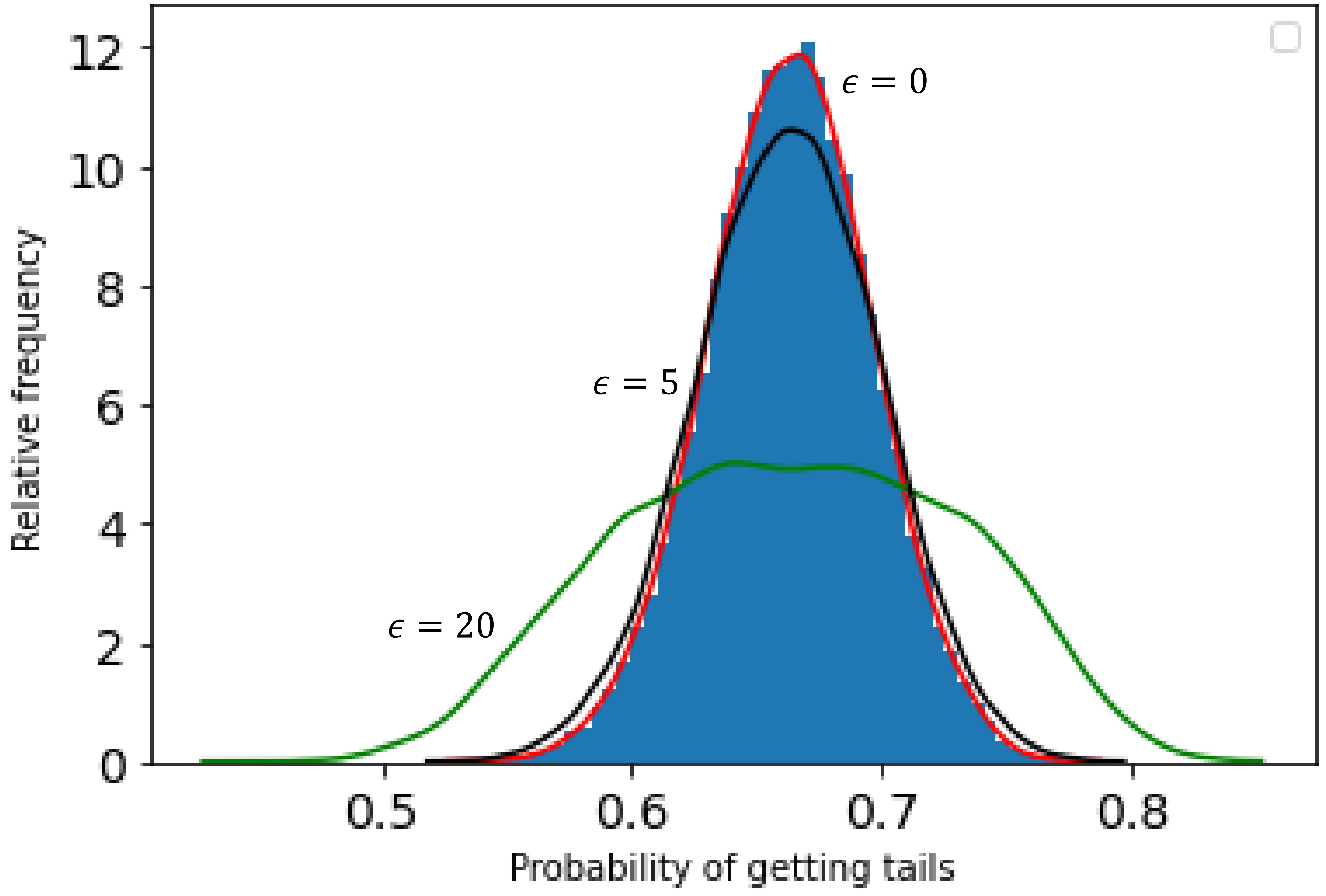
First, we establish a prior: probability of getting tails (θ) is sampled from a uniform prior with bounds (0,1).

Secondly, we construct a mathematical model: a binomial distribution $y^M = y^M(\theta,\cdot)$, where we get either 0 or 1 with probability sampled from prior. Randoming number 1 represents getting tails. The model generates 200 numbers, corresponding to 200 coin tosses.

We choose a summary statistic: a sum.

Lastly, we choose the threshold value and the number of samples that we want to construct posterior from.

The case with $\epsilon = 5$ requires 10x less sampling than the pure rejection algorithm.



True probability of getting tails: 0.7

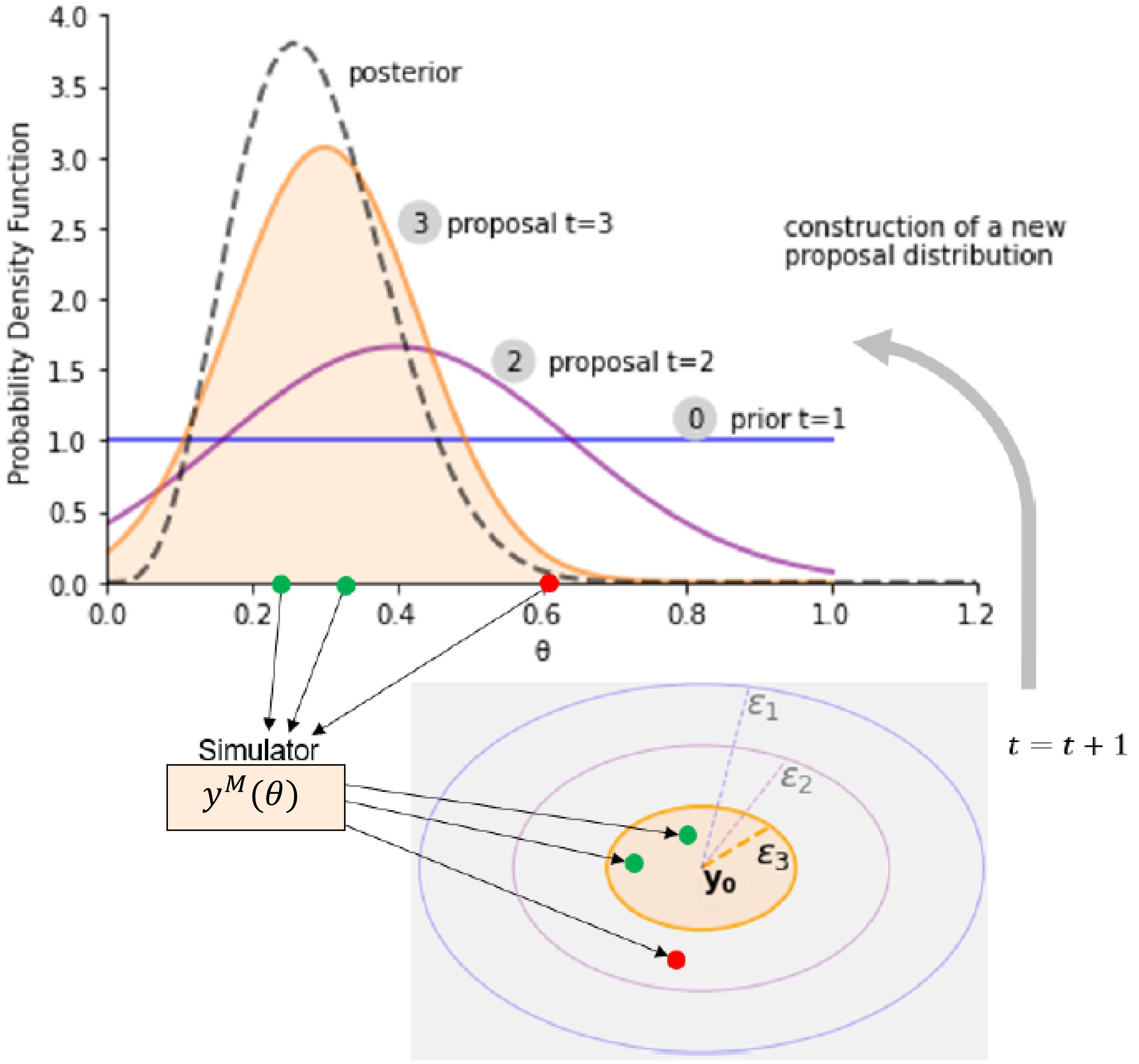
Advanced ABC algorithm for non-stochastic problems

Sequential Monte Carlo – Approximate Bayesian Computation:

Require: specify a decreasing sequence of thresholds $\epsilon_1 > \epsilon_2 > \cdots > \epsilon_T$

for $i = 1$ *to* N *do*
  reapeat
    Generate θ *from the prior* $p(\cdot)$
    Generate $y^M(\theta)$ *from the simulator*
  until $\delta(y^M(\theta), y_0) \leq \epsilon_1$
  $\theta^i \leftarrow \theta$
  $\omega_1^i \leftarrow N$
end for
$\Sigma_1 \leftarrow 2Cov(\theta_1)$

for $t = 2$ *to* T *do*
  for $i = 1$ *to* N *do*
    repeat
      Draw θ^* *from among* θ_{t-1} *with probabilities* ω_{t-1}
      Generate θ *from* $Normal(\theta^*, \Sigma_{t-1})$
      Generate $y^M(\theta)$ *from the simulator*
    until $\delta(y^M(\theta), y_0) \leq \epsilon_t$
    $\theta_t^i \leftarrow \theta$
    $\omega_t^i \leftarrow p(\theta)/(\Sigma_{k=1}^N \omega_{t-1}^k Normal(\theta|\theta_{t-1}^k, \Sigma_{t-1}))$
  end for
  $\Sigma_t \leftarrow 2Cov(\theta_t)$
end for

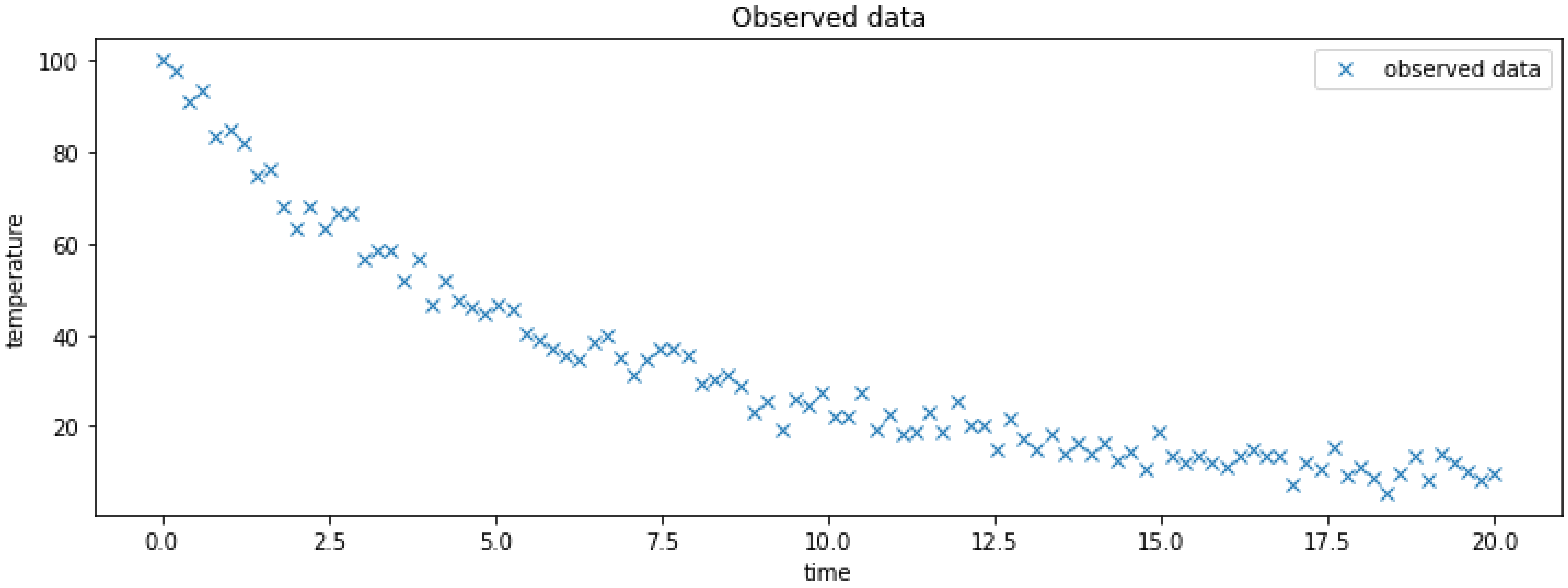


Coffee-cooling problem

Consider a problem of finding the constants describing the cooling of a coffee cup:

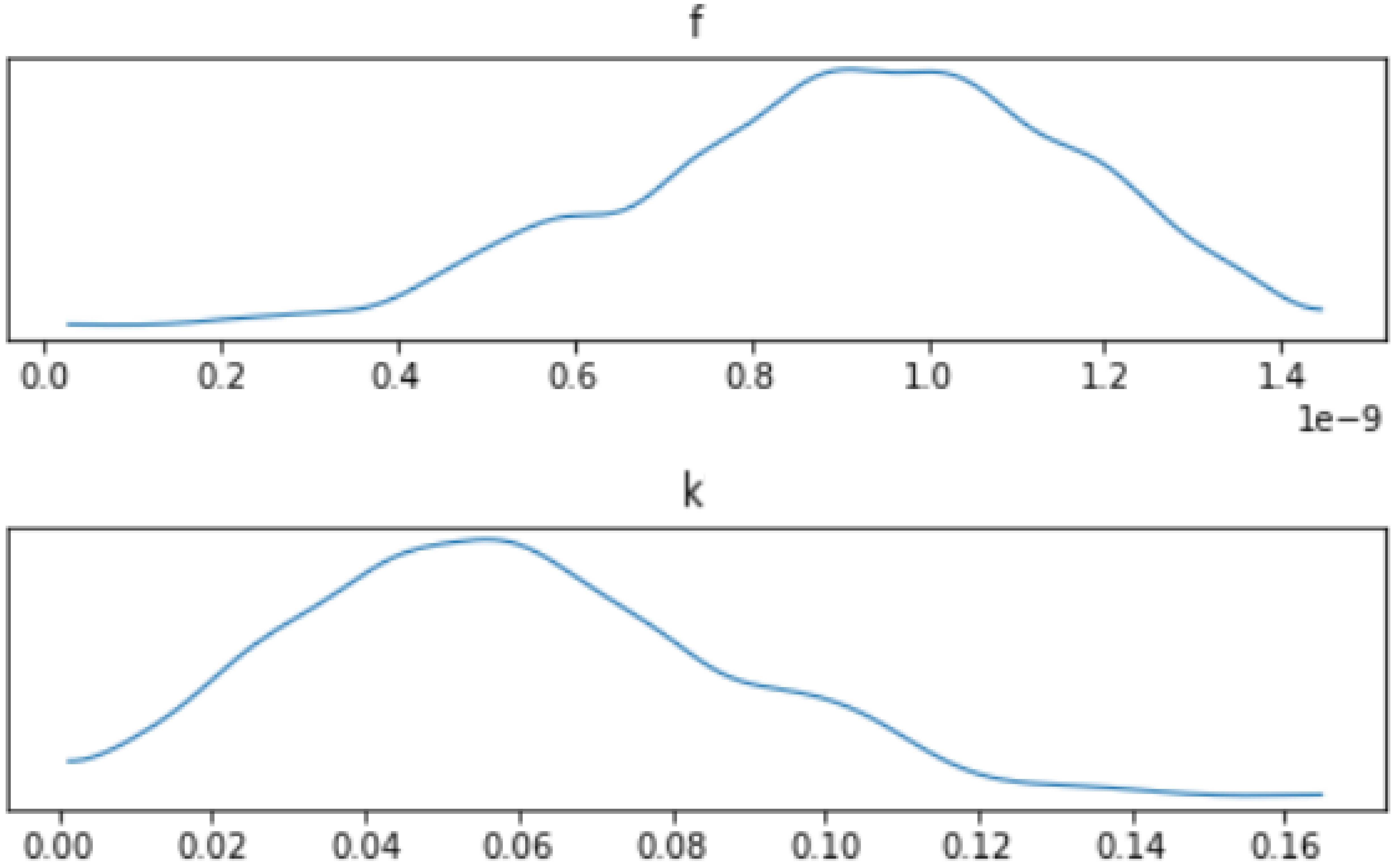
$$\frac{dT}{dt} = -k\left(T_{cup} - T_{env}\right) - f * \left(T_{cup}^4 - T_{env}^4\right).$$

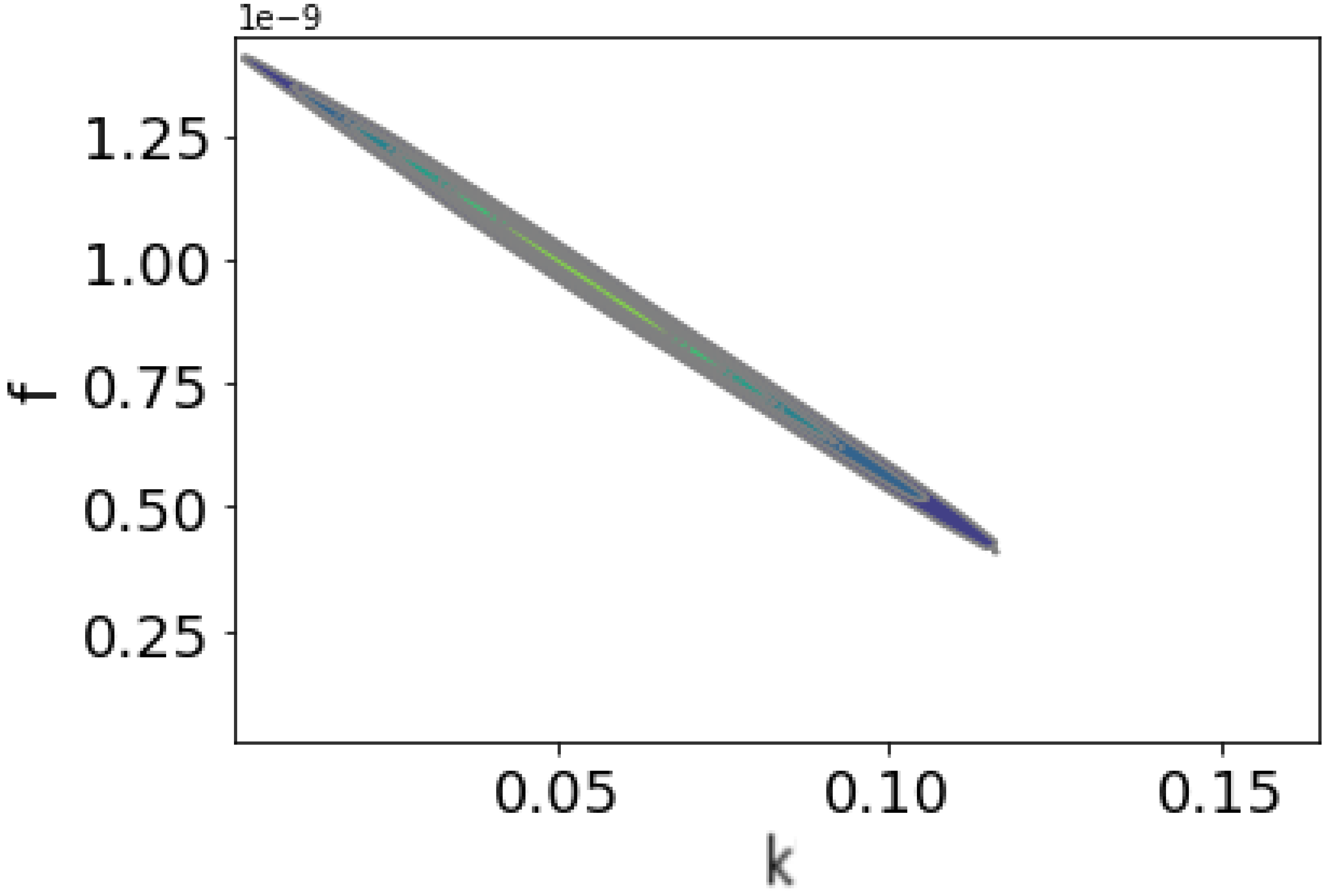
We want to be able to conduct UQ afterwards.



Assuming priors:
$0 < k < 5$
$0 < f < 10^{-7}$,
Defining ϵ as thermocouple error

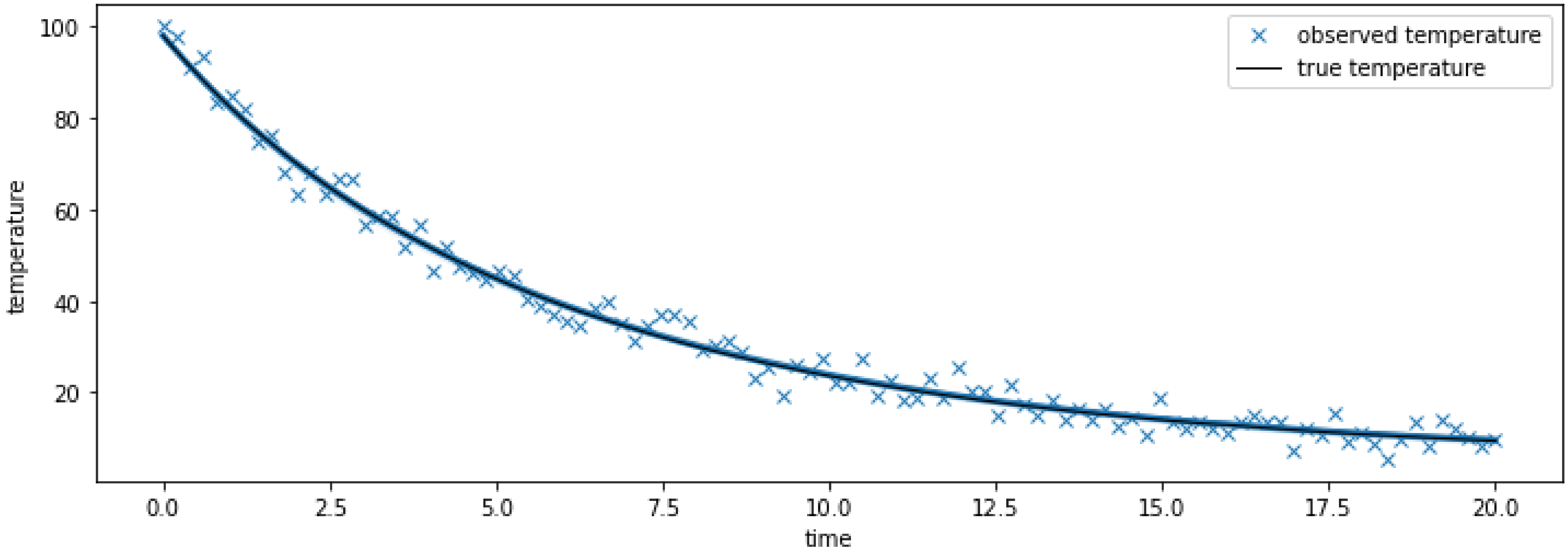
Posterior distributions





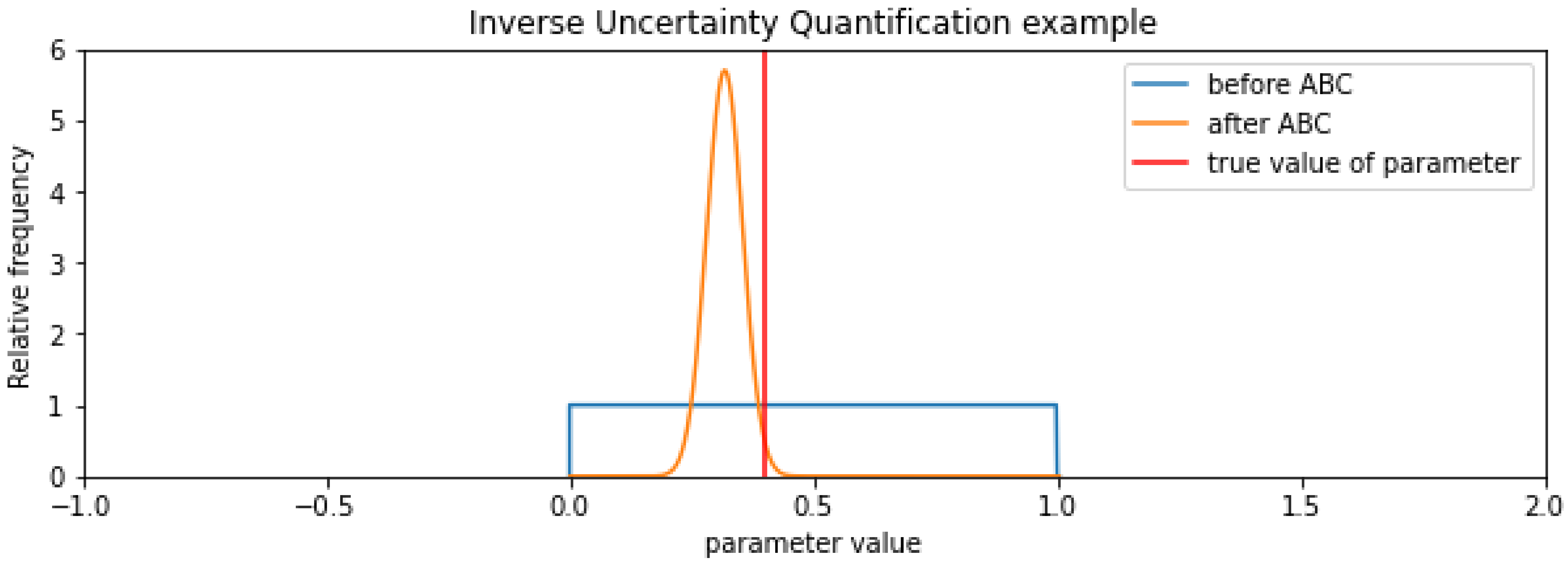
True values of the parameters: $k = 0.0667$, $f = 8.5 * 10^{-9}$.

Error propagation



How do we know if we can find input values with available measurements?

Identifiability problem answers the question on whether available measurement data is enough to find the true value of uncertain input parameters.



Identifiability assessment

When is identifiability weak?

- In cases where output parameters are not sensitive to some input parameters or one input parameter is dominant sensitivity-wise
- When measurements are not diverse enough
- When there are too few measurements

Validation techniques

Two techniques are available to determine whether IUQ was successful

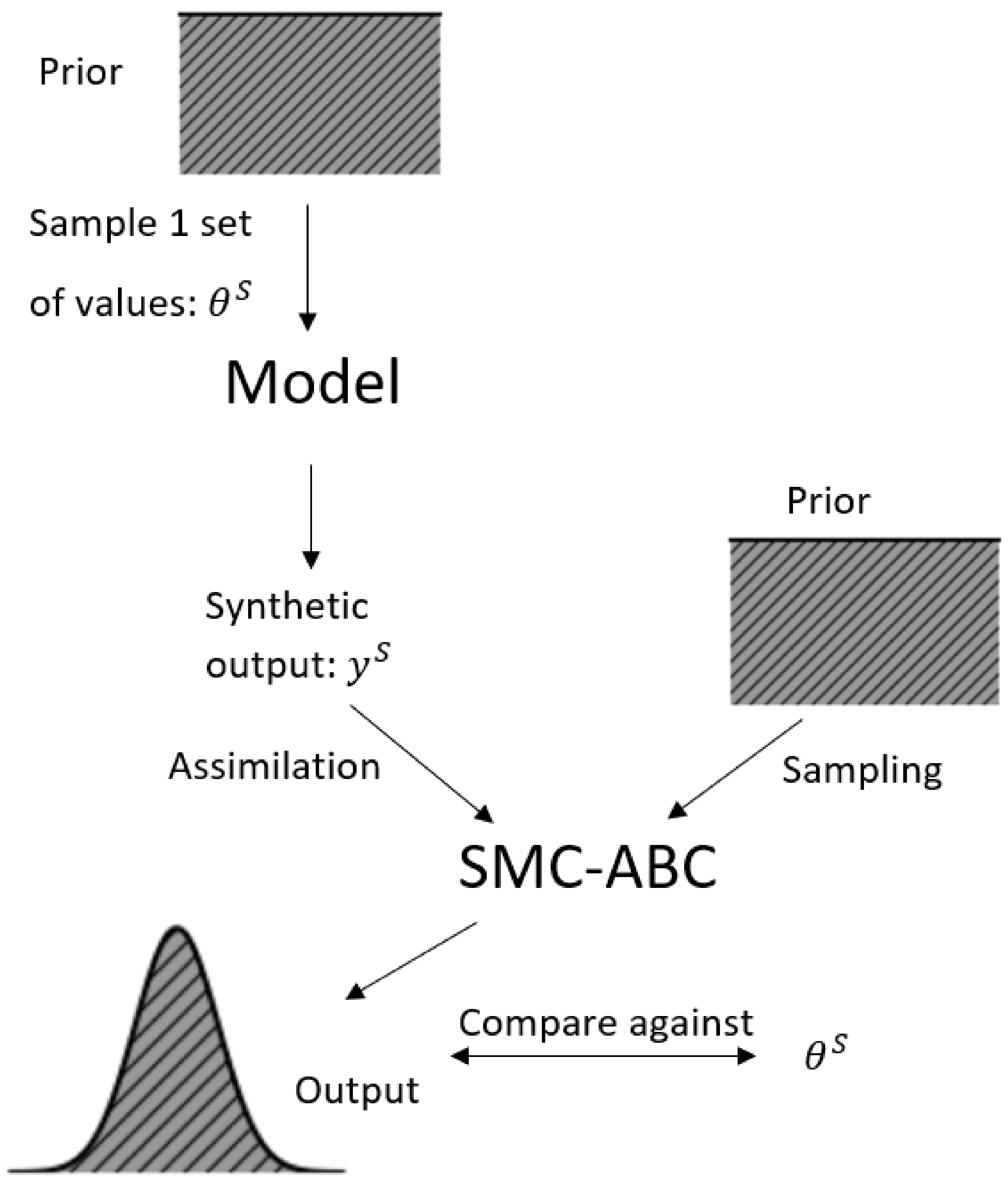
- Validation using unassimilated experiments – checking if experimental data is within bounds determined by UQ
- The use of so-called synthetic experiments

Validation with synthetic experiments

Synthetic exsperiments are simulation outputs generated computationally, based on inputs sampled from the prior. We assimilate the outputs and check how close posteriori values are to the sample from the prior.

Procedure:

1. Sample input values θ^S from prior distribution. Document the values.
2. Compute outputs $Y_S(\theta^S,\cdot)$
3. Treat $y_S(\theta^S,\cdot)$ as observed data, assimilate with an ABC algorithm
4. Assume the same threshold (uncertainties) as for the validated case
5. Set the same SMC-ABC parameters as for the validated case
6. Compare posterior of θ with θ^S



Limitations of ABC

- Computational requirements rise exponentially with the number of calibrated parameters: „curse of dimensionality”
- Computing model discrepancy may be very difficult for some models
- Only viable for computer models which do not take too much time to compute (< 5 mins)

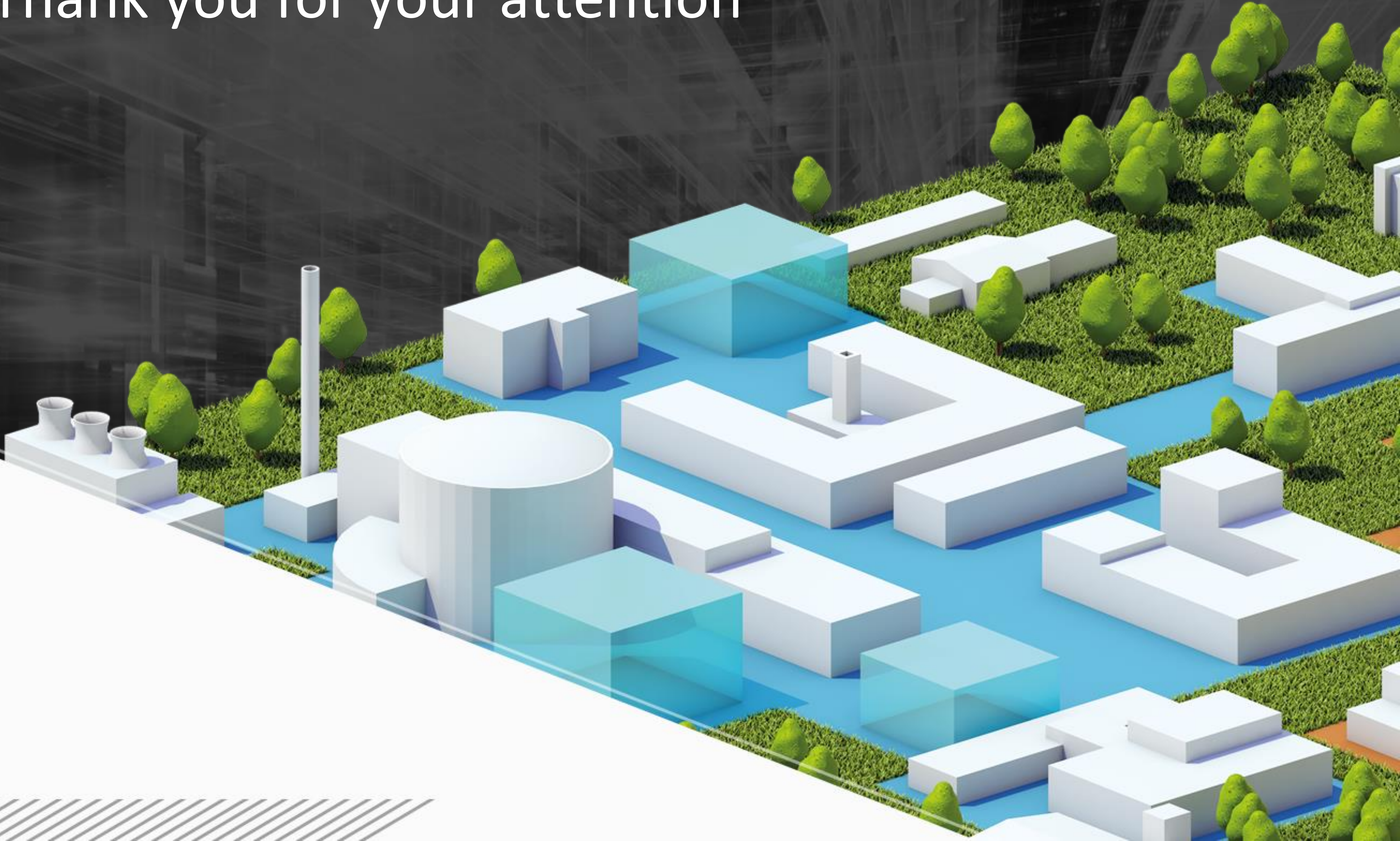
Some examples of publications with IUQ or SMC-ABC

Wu, X., Kozlowski, T., Meidani, H., & Shirvan, K. (2018). Inverse uncertainty quantification using the modular Bayesian approach based on Gaussian Process, Part 2: Application to TRACE. *Nuclear Engineering and Design*, *335*, 417-431. https://doi.org/10.1016/j.nucengdes.2018.06.003

Xie, Z., Jiang, W., Wang, C., & Wu, X. (2022). Bayesian inverse uncertainty quantification of a MOOSE-based melt pool model for additive manufacturing using experimental data. *Annals of Nuclear Energy*, *165*, 108782. https://doi.org/10.1016/j.anucene.2021.108782

My publication using SMC-ABC to reduce uncertainties in cross-section values is under review in Nuclear Engineering and Design.
23 MV normal input variables, 24 experiments, 3 minutes to simulate experiment: 3 months with 4000 cores on NCBJ cluster.

Thank you for your attention



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