# UKACM & GACM AUTUMN SCHOOL 2025

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UK Association for Computational Mechanics

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## Open-Source Codes for High-Performance Computing

## **Hands-on Session 4C & QUEENS**

30.09.2025 and 01.10.2025

4C
COMPREHENSIVE
COMPUTATIONAL
COMMUNITY
CODE

QUEENS

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# Update tutorial material

**Virtual machine:**

Pull the latest version from GitHub

1. Open a terminal in the virtual machine
2. Go to the folder with the tutorial material
3. Run:
   git pull --rebase origin

**Docker container:**

Pull the latest version from GitHub

1. Open a terminal on your machine
2. Go to the folder with the tutorial material
3. Run:
   git pull --rebase origin
4. (Re-)build the QUEENS Docker container.
   Follow the instructions here:
   https://github.com/mayrmt/UKACM_GACM_Tutorial_4C_QUEENS/blob/main/PREPARATION.md#queens-docker-container

See also the instructions on GitHub:
https://github.com/mayrmt/UKACM_GACM_Tutorial_4C_QUEENS/blob/main/PREPARATION.md

UKACM & GACM AUTUMN SCHOOL 2025
Open-Source Codes for High-Performance Computing
**Hands-on Session 4C & QUEENS**

# QUEENS

QUANTIFICATION OF UNCERTAIN EFFECTS IN ENGINEERING SYSTEMS

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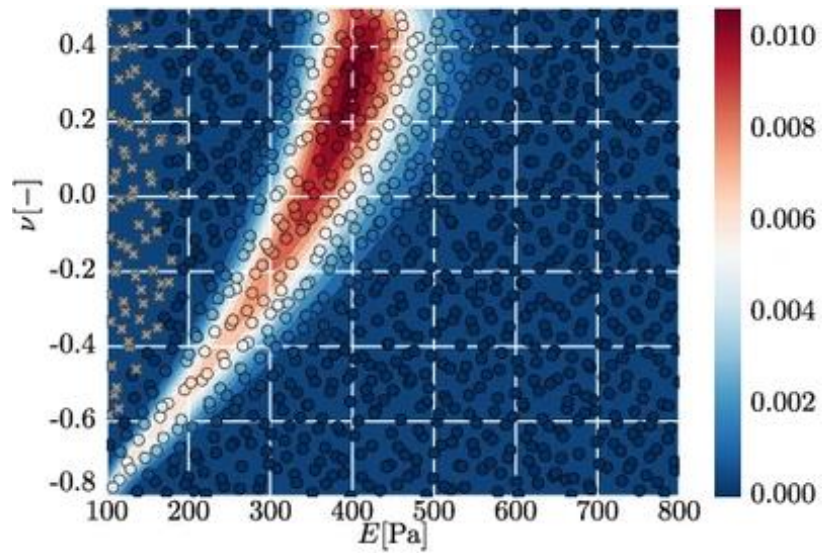
# QUEENS

is a Python framework for **solver-independent multi-query analyses** of large-scale **computational models**.



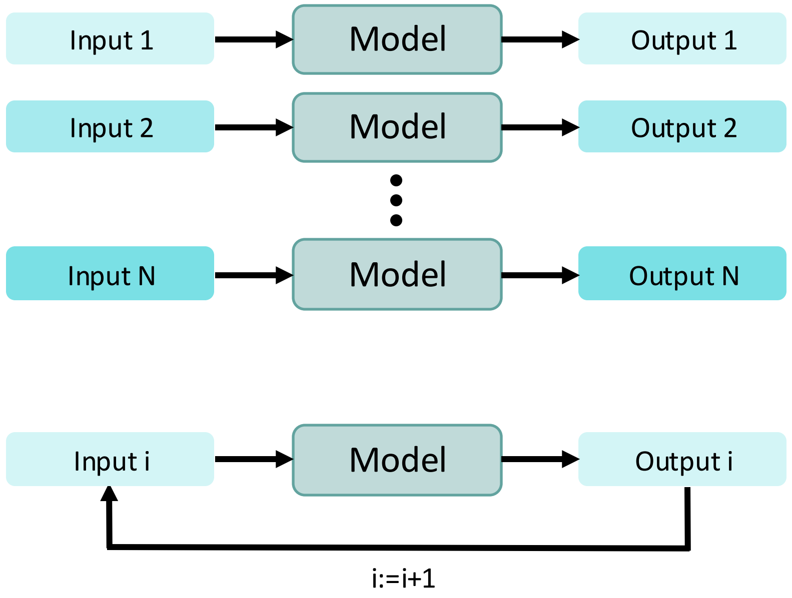

https://github.com/queens-py/queens

# Multi-Query Analysis

Examples of multi-query scenarios:

- **Open loop:** parameter studies, uncertainty quantification

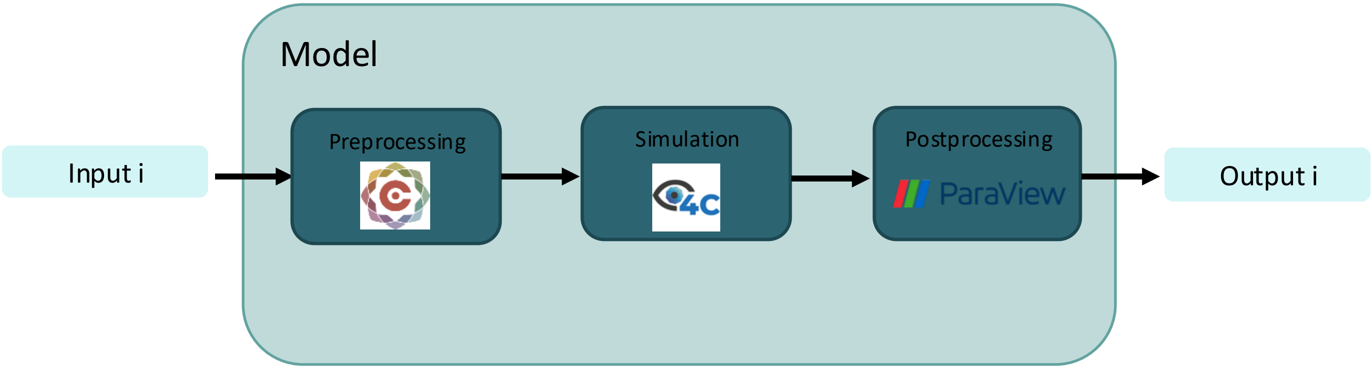
- **Closed loop:** optimization, (Bayesian) inverse problems




➢ Evaluation of the same model at **many input locations**

# Automation of model evaluations

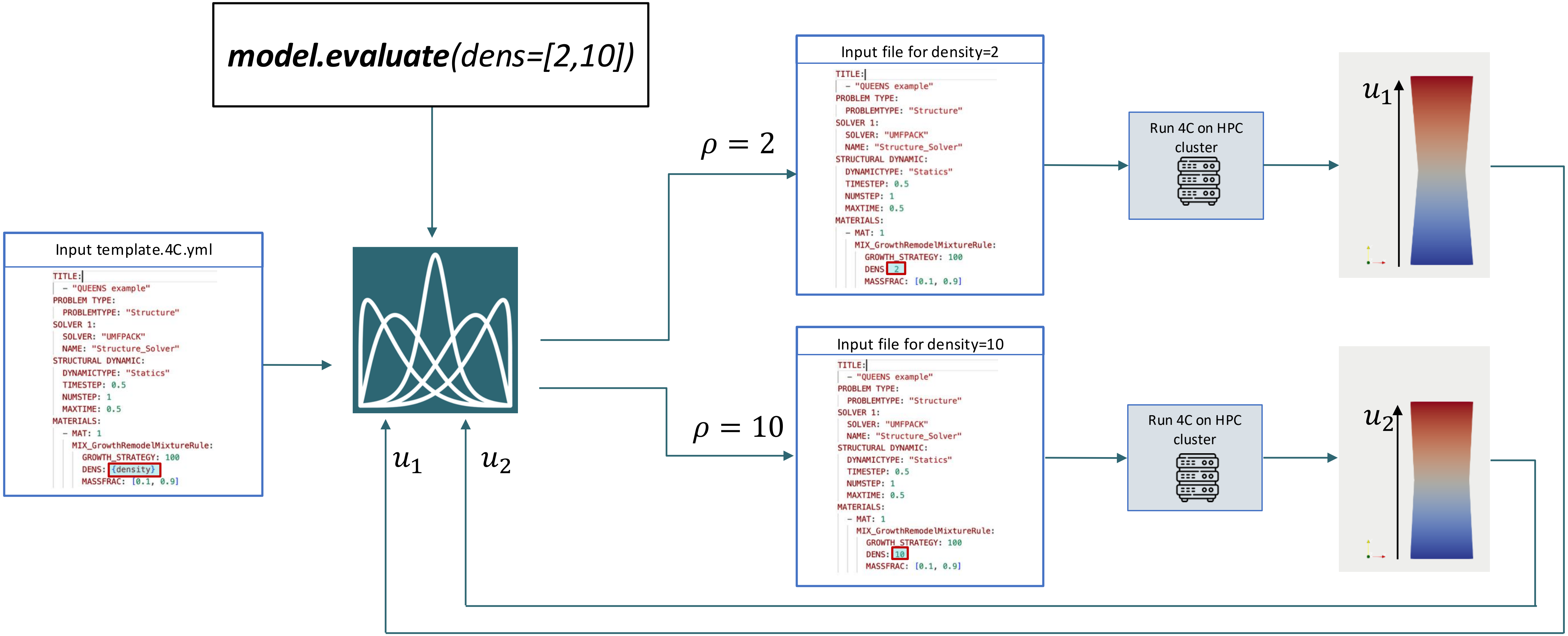
Each model evaluation involves numerous time-consuming manual sub-steps, e.g.,




➢QUEENS offers an abstract framework to **automate all of these sub-steps.**

# Run 4C with a single line of code

Essentially, everything you need is:



# Available analysis methods

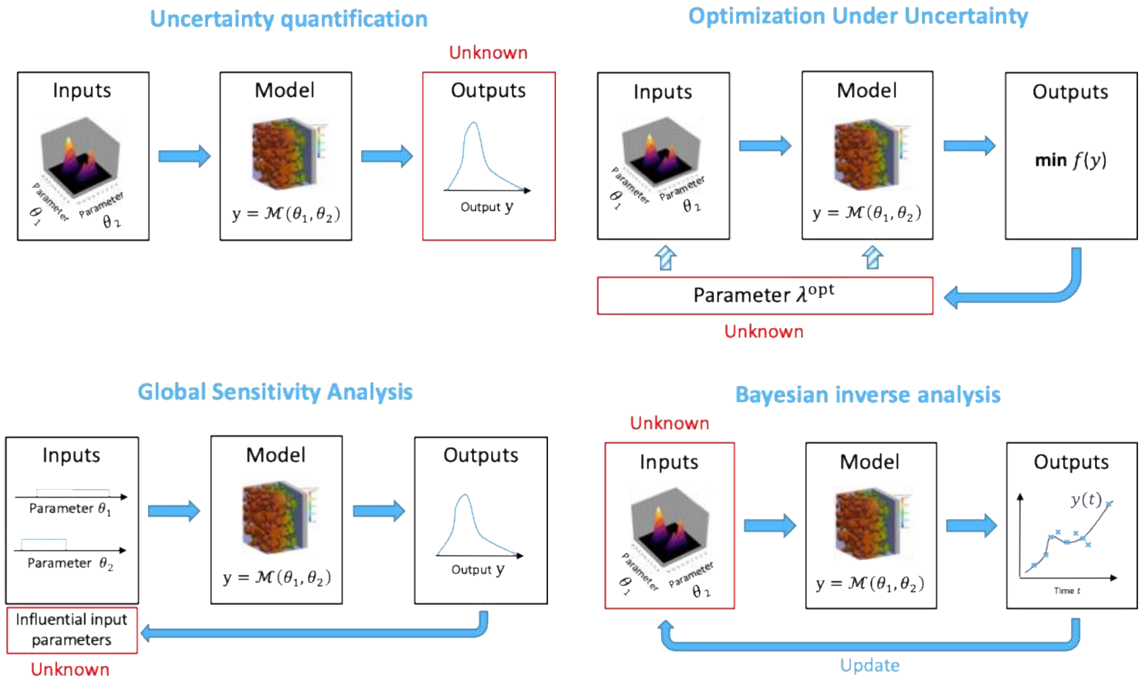
QUEENS offers a large collection of cutting-edge algorithms for deterministic and **probabilistic analyses**:

Methodological complexity

- parameter studies and identification
- sensitivity analysis
- surrogate modelling

⋮

- (multi-fidelity) uncertainty quantification
- Bayesian inverse analysis



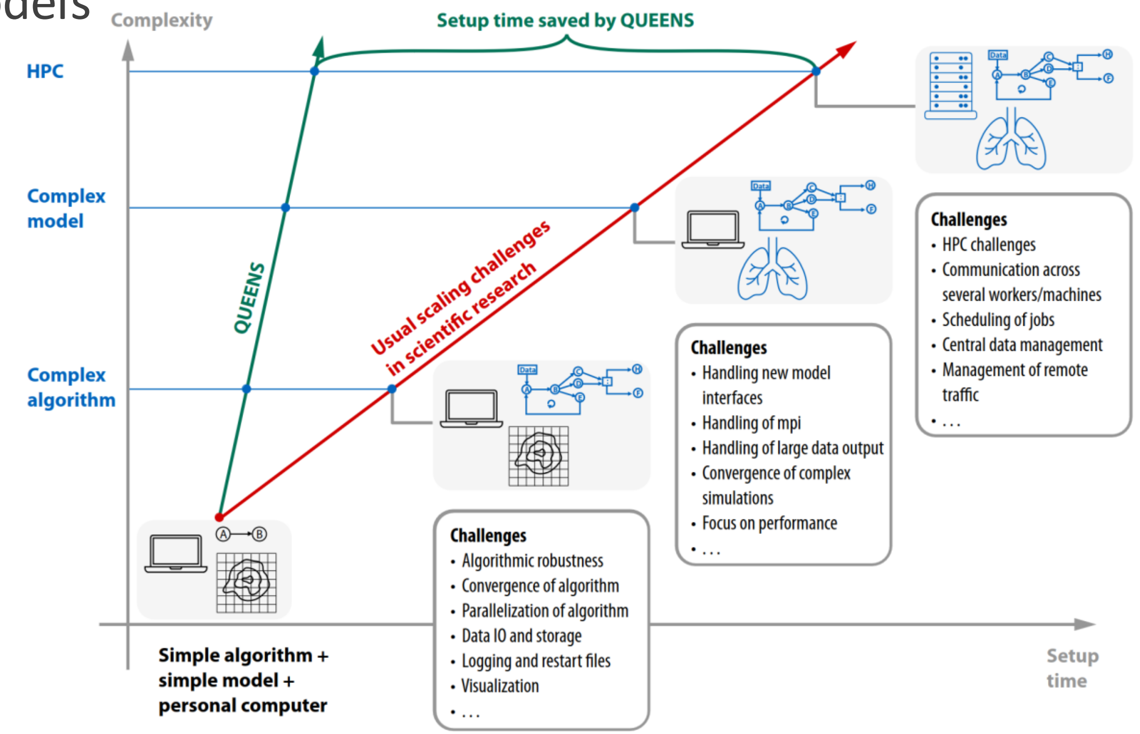

➢**A large variety of methods that are likely to be relevant to your research**

# Large-scale computational models

**QUEENS** is designed for the analysis of computational models in which a single evaluation requires **significant computational resources.**

It provides a modular architecture for:

- parallel queries of large-scale computational models
- robust data, resource, and error management
- easy switching between analysis types
- smooth scaling from laptop to HPC cluster



# Solver-independence

However, QUEENS is developed as a solver-independent platform.
It has also been interfaced with other solvers

- any Python package
- OpenFOAM
- Fenics
- deal.II-based codes
- and many others …

# Community

## Maintainer team

Sebastian Brandstäter

Maximilian Dinkel

Lea Häusel

Jonas Nitzler

Gil Robalo Rei

## Contributors

Daniel Wolff

Silvia Hervás Raluy

Regina Bühler

Bishr Maradni

Universität der Bundeswehr München

You are welcome to join!
Connect with us on GitHub.

[https://github.com/queens-py/queens](https://github.com/queens-py/queens)

# Workflow example

Experiment

Parameters

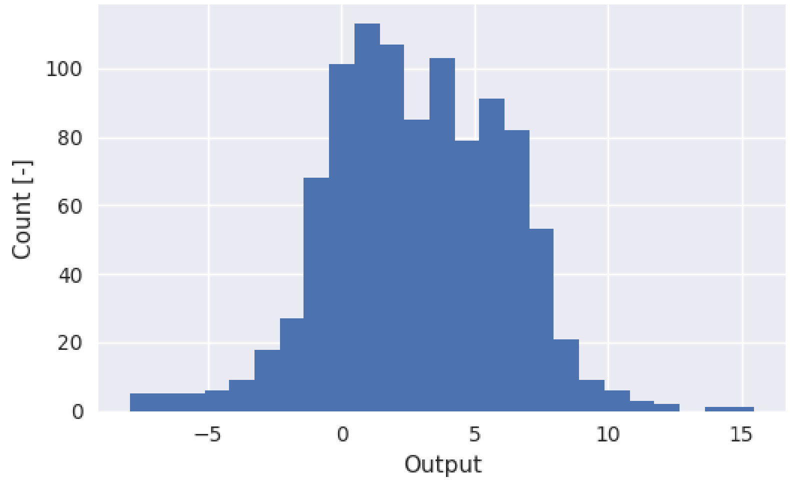
Model

Evaluation

Compute

Multi-query algortihm

```python
from queens.distributions import Beta, Normal, Uniform
from queens.drivers import Function
from queens.global_settings import GlobalSettings
from queens.iterators import MonteCarlo
from queens.main import run_iterator
from queens.models import Simulation
from queens.parameters import Parameters
from queens.schedulers import Local

if __name__ == "__main__":
    # Set up the global settings
    global_settings = GlobalSettings(experiment_name="monte_carlo_uq", output_dir=".")

    with global_settings:
        # Set up the uncertain parameters
        x1 = Uniform(lower_bound=-3.14, upper_bound=3.14)
        x2 = Normal(mean=0.0, covariance=1.0)
        x3 = Beta(lower_bound=-3.14, upper_bound=3.14, a=2.0, b=5.0)
        parameters = Parameters(x1=x1, x2=x2, x3=x3)

        # Set up the model
        driver = Function(parameters=parameters, function="ishigami90")
        scheduler = Local(
            experiment_name=global_settings.experiment_name, num_jobs=2, num_procs=4
        )
        model = Simulation(scheduler=scheduler, driver=driver)

        # Set up the algorithm
        iterator = MonteCarlo(
            model=model,
            parameters=parameters,
            global_settings=global_settings,
            seed=42,
            num_samples=1000,
            result_description={"write_results": True, "plot_results": True},
        )

        # Start QUEENS run
        run_iterator(iterator, global_settings=global_settings)
```



# Theory and background

Since some of you might not be familiar with probabilistic approaches…

We will first cover some theory and background to:

- Motivate the use of probabilistic approaches
- Explain the key concepts behind the hands-on examples

Don’t worry—we’ll keep the math to a minimum.

You’ll revisit these concepts during the tutorial, and most importantly, you’ll be able to follow the exercises even if some of the theory feels challenging.

# What are uncertainties?

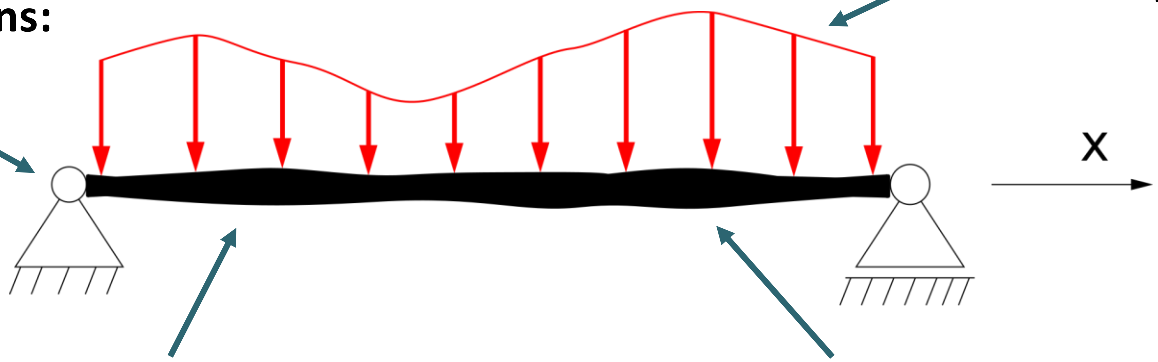
**Uncertainty is the lack of certainty about a quantity because it has more than one possible state**

- Can arise from **inherently random effects**

- Can arise from **lack of information/knowledge**

**External forces:**
loads q(x)?

**Boundary conditions:**
support type?




**Material parameters:**
Young's modulus E(x)?

**Geometry:**
cross section A(x)?

# Why should I care about uncertainties?

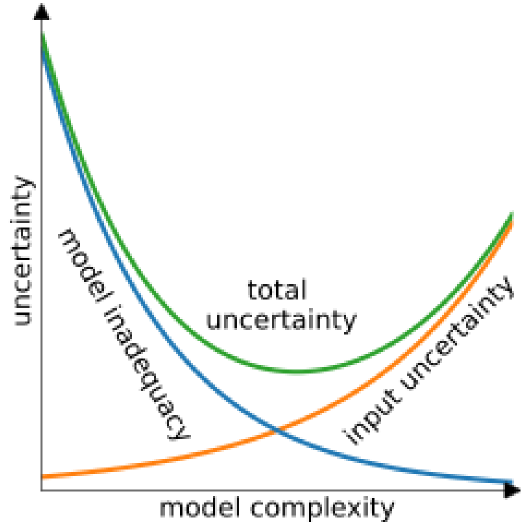
To make **meaningful predictions**, uncertainty needs to be incorporated:

Every model is only an **approximation of reality**

- Uncertainty through **model**

Even if a model is perfect, numerically **precise results can be meaningless** if model parameters are not known precisely

- Uncertainty through **parameters**




**With uncertainties, we can tell what we know, but also what we do not know.**

# How to handle uncertainties?

**How engineers used to handle uncertainties:**

- Redo analysis or measurements,
  analyse mean and standard deviation
- Propagation of significant figures
- Propagation of tolerances
- Post process data (filters, interpolation, ...)
- Use of safety factors
- Playing around with input parameters

**Probabilistic approach:**

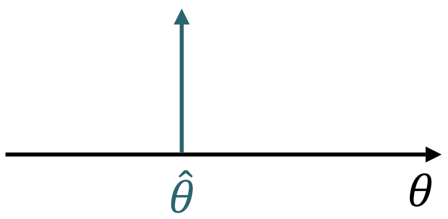
- Use **probability theory** to describe uncertainty
- Use **random variables** to model uncertain parameters

Systematic approach

# What are random variables?

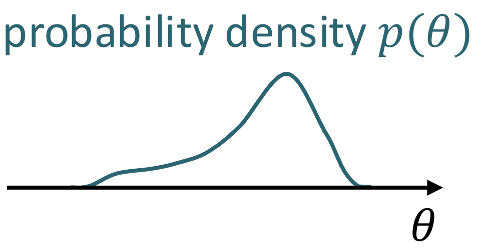
For example, $\theta$ is a model parameter:

**Deterministic:**




- $\theta$ assumes a **single value.**

**Random variables:**




- $\theta$ can assume **many values**, but with varying probability.

# What are random fields?

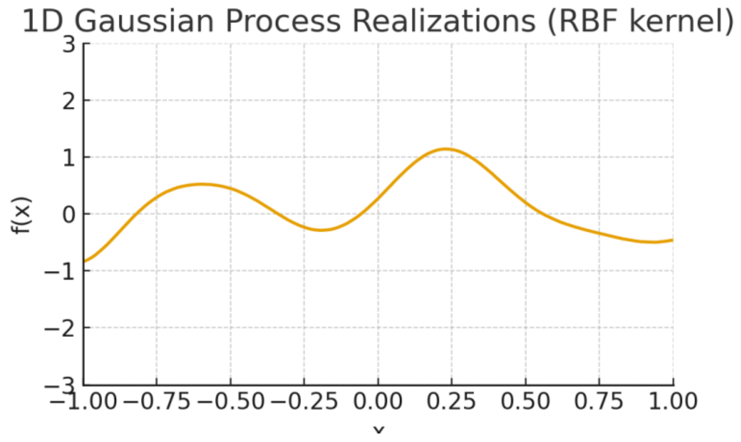
## Random variables:

- A random variable is a single random number.
  $\theta$ can assume **many values**,
  but with varying probability.

$$\theta = -0.694$$

## Random field:

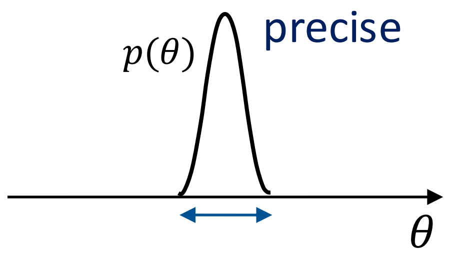
- A random field is the extension to functions: instead of a random number,
  you get a whole random function.
  Each realization of a random field is just one specific function.

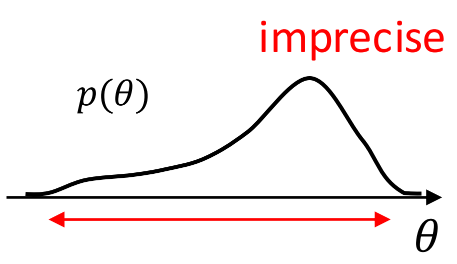


# Advantages of probabilistic approaches

## Information Quality

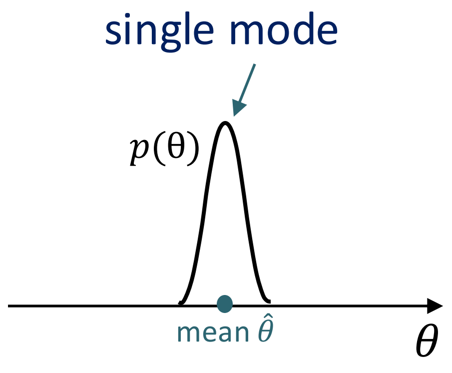
*How precise can we measure?*

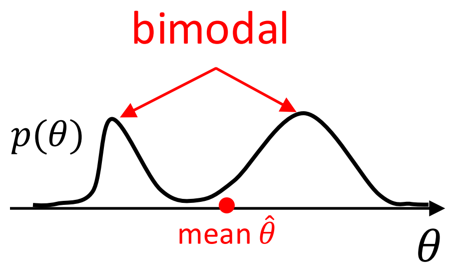



## System Preferences

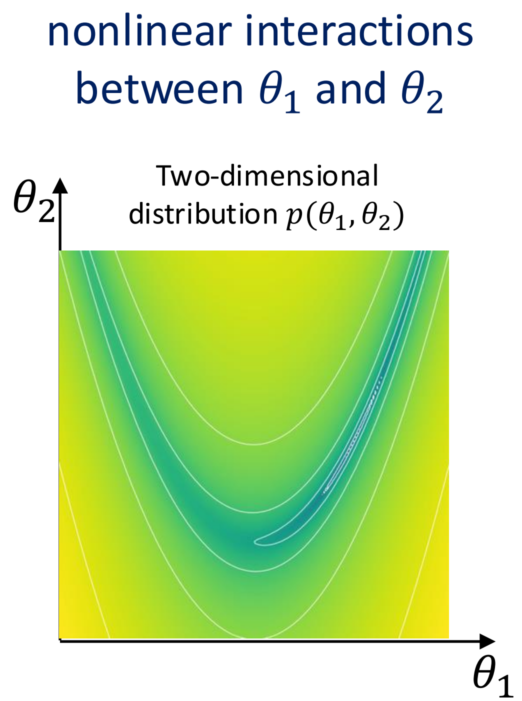
*Are there multiple preferred configurations?*




## Interactions

*Is there a correlation of parameters?*

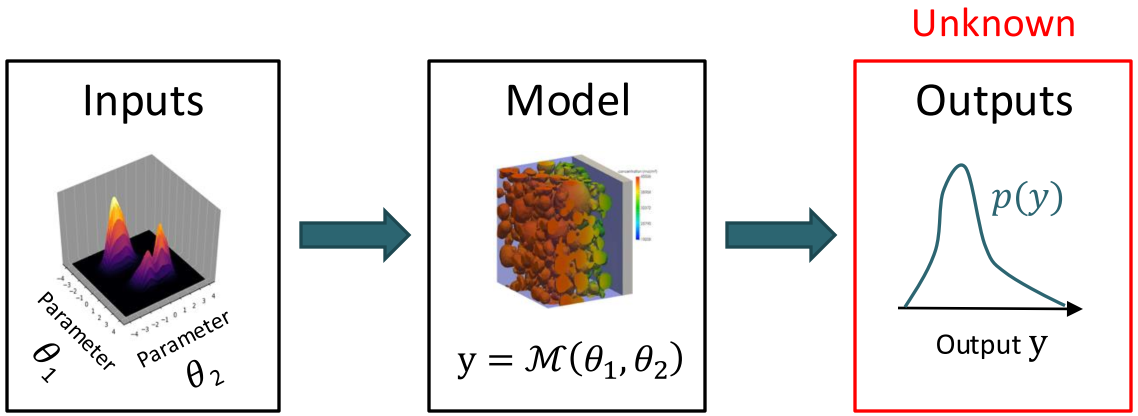



And many more…

# How to quantify uncertainties?

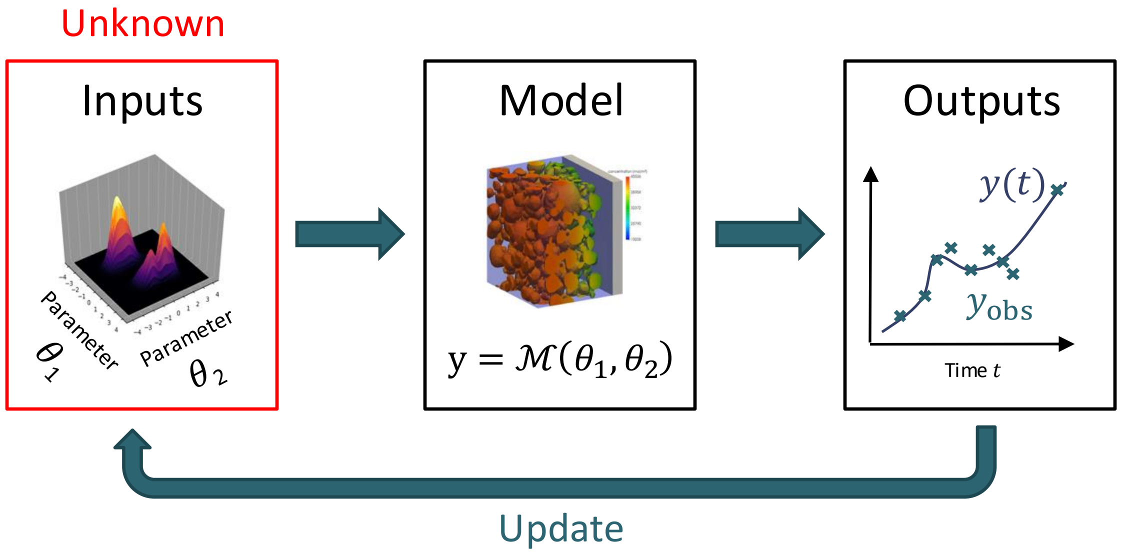
**Uncertainty Propagation**
**Forward Uncertainty Quantification (UQ)**
Quantification of uncertainties in the output

**Forward UQ**




**Inverse Analysis (IA)**
**Backward Uncertainty Quantification (UQ)**
Quantification of uncertainties in the input

**Backward UQ**



# Forward Uncertainty Quantification

**Goal:**
Propagate uncertainties from input quantities $\theta$ to output quantities $y$ using a computational model $\mathcal{M}$

$$p(y) = \mathbb{E}_{p(\theta)}[\delta(\mathcal{M}(\boldsymbol{\theta}) - y)]$$

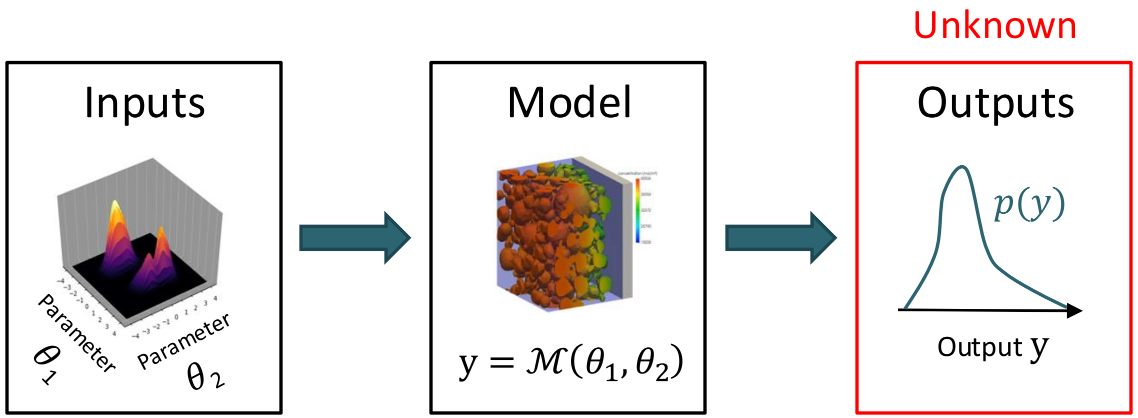
$\delta(.)$ is the Dirac mass delta.

Known:

- Probability density function $p(\boldsymbol{\theta})$ of uncertain model inputs $\boldsymbol{\theta}$
- Model $\mathrm{y} = \mathcal{M}(\boldsymbol{\theta})$

Unknown:

- Probability density function $p(y)$ of uncertain output $y$



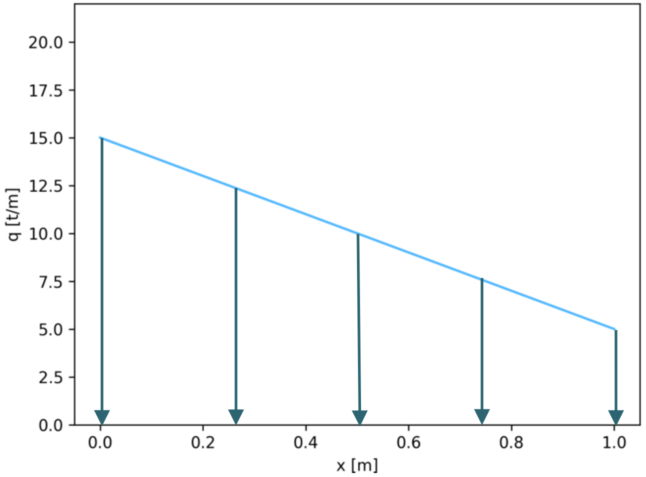
# Beam example - deterministic

**Inputs**

$$\boldsymbol{\theta} = [\theta_1, \theta_2]^{\mathrm{T}}$$

$$\theta_1 = \quad 15.0\ t/m$$
$$\theta_2 = -10.0\ t/m^2$$

load $q(x, \boldsymbol{\theta}) = \theta_1 + \theta_2 x$

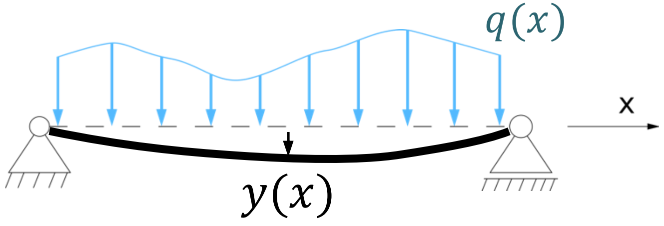



**Model**

$$y(x) = \mathcal{M}(x, \boldsymbol{\theta})$$

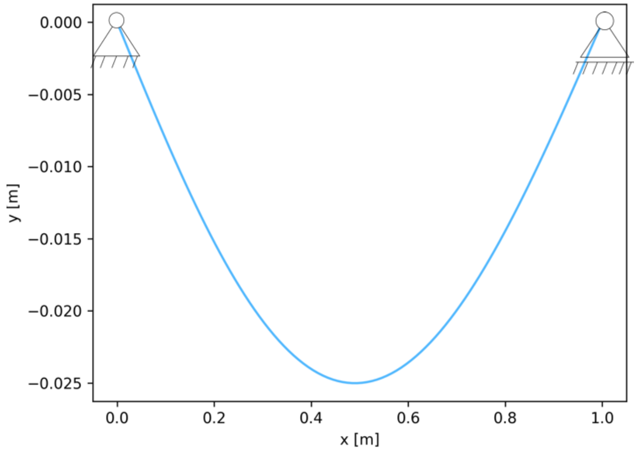
Where $\mathcal{M}(x, \boldsymbol{\theta})$ models a static Euler-Bernoulli beam:

$$EI \frac{\partial^4 y}{\partial x^4}(x) = q(x, \boldsymbol{\theta})$$




**Outputs**

bending line y$(x)$



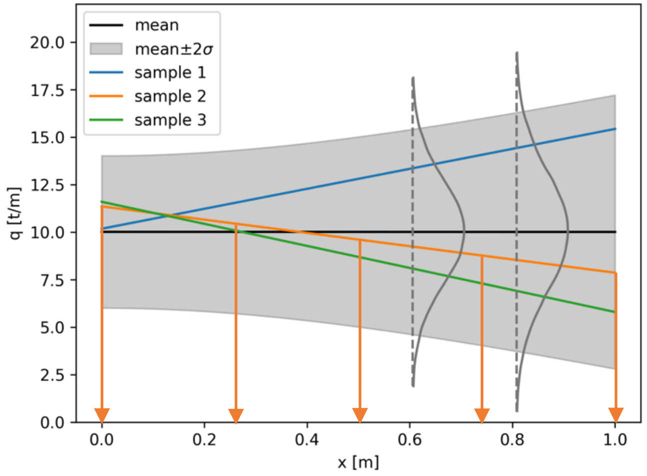
# Forward UQ – Beam example

**Inputs**

$$\boldsymbol{\theta} = [\theta_1, \theta_2]^{\mathrm{T}}$$

$$\theta_1 \sim \mathcal{N}(\mu = 10.0,\ \sigma^2 = 4.0)$$
$$\theta_2 \sim \mathcal{N}(\mu = 0.0,\ \sigma^2 = 9.0)$$

load $q(x, \boldsymbol{\theta}) = \theta_1 + \theta_2 x$

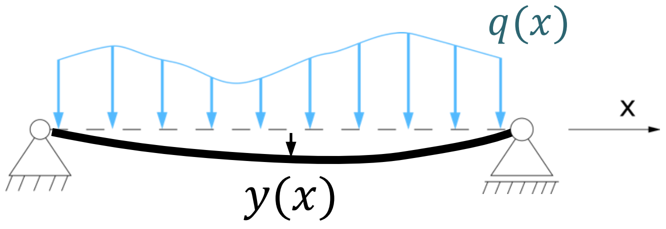



**Model**

$$y(x) = \mathcal{M}(x, \boldsymbol{\theta})$$

Where $\mathcal{M}(x, \boldsymbol{\theta})$ models a static Euler-Bernoulli beam:

$$EI \frac{\partial^4 y}{\partial x^4}(x) = q(x, \boldsymbol{\theta})$$

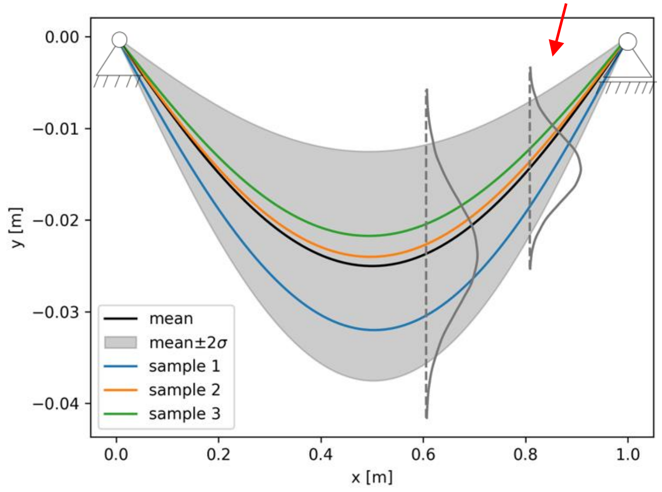



Unknown

**Outputs**

bending line $y(x)$

Variance smaller towards support



# Bayesian inverse analysis / Backward UQ

**Goal:**
Given experimental data $y_{\mathrm{obs}}$ and a model $\mathcal{M}$, estimate the unknown input quantities $\theta$ and the uncertainty in this estimate

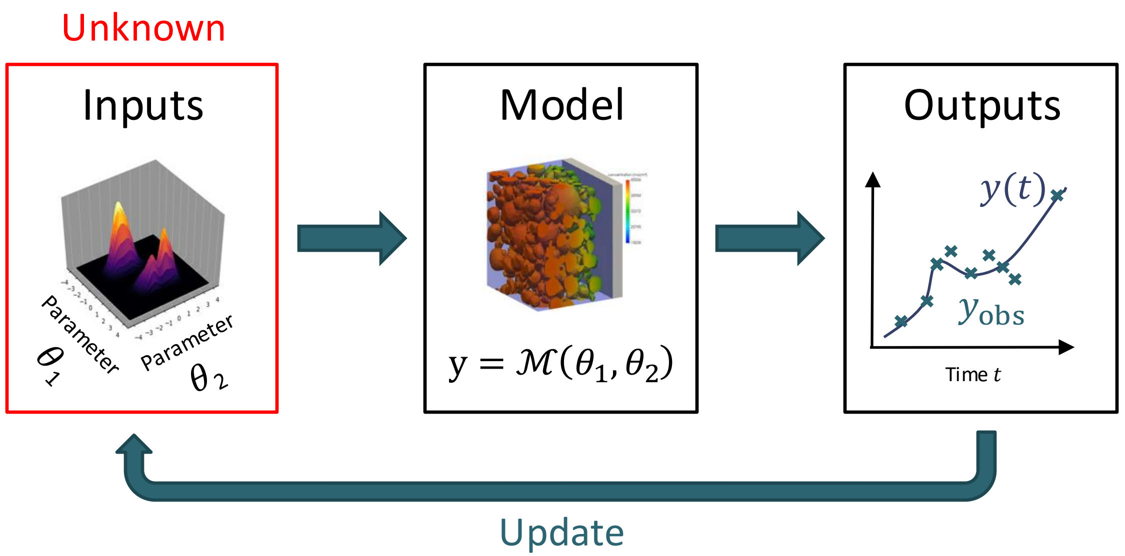
Bayes' rule: $p(\theta|y_{obs}) = \frac{p(y_{obs}|\theta)p(\theta)}{p(y_{obs})}$

Known:

- Observations $\boldsymbol{y}_{\mathrm{obs}}$
  e.g. from experiments
- Prior $p(\boldsymbol{\theta})$
  over uncertain model inputs $\boldsymbol{\theta}$
- Model $\mathrm{y} = \mathcal{M}(\boldsymbol{\theta})$
- *Optional but desirable:*
  Model derivative $\frac{\partial \mathcal{M}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$

Unknown:

- Posterior $p(\boldsymbol{\theta}|\boldsymbol{y}_{\mathrm{obs}})$
  over uncertain model inputs $\boldsymbol{\theta}$



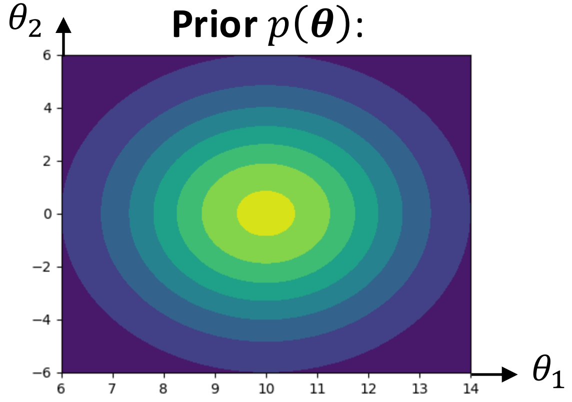
# Bayesian inverse analysis – Beam example

**Inputs**

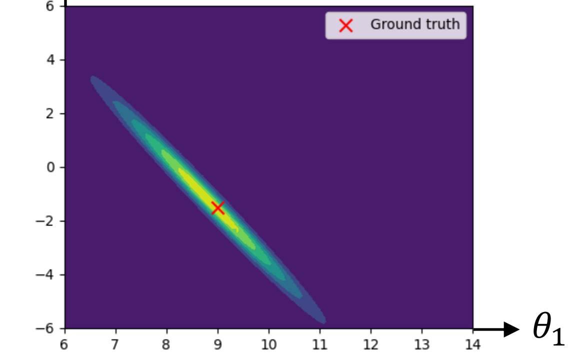
$\boldsymbol{\theta} = [\theta_1, \theta_2]^{\mathrm{T}}$

load $q(x, \boldsymbol{\theta}) = \theta_1 + \theta_2 x$

**Prior** $p(\boldsymbol{\theta})$:




**Posterior** $p(\boldsymbol{\theta}|y_{\mathrm{obs}})$:



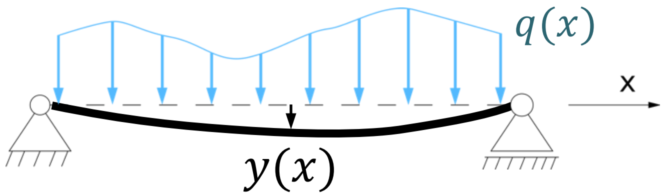

Unknown

**Model**

$$y(x) = \mathcal{M}(x, \boldsymbol{\theta})$$

Where $\mathcal{M}(x, \boldsymbol{\theta})$ solves:

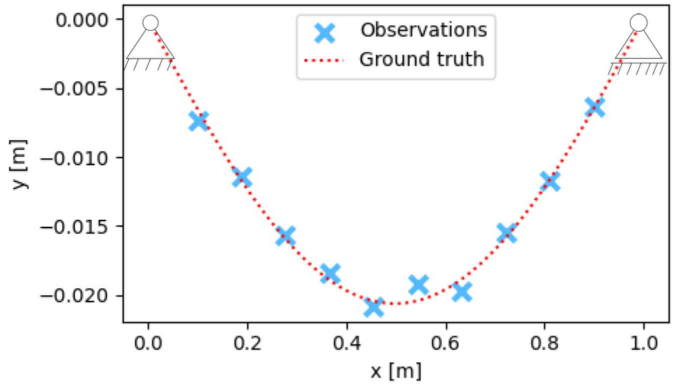
$$EI \cdot \frac{\partial^4 y}{\partial x^4}(x) = q(x, \boldsymbol{\theta})$$




**Outputs**

bending line $y(x)$

Observations $\mathrm{y}_{\mathrm{obs}}$:



# Hands-on Sessions on ZOOM

09:30 - 11:00 QUEENS 1: From Grid studies to deterministic optimisation

11:00 - 11:15 Break

11:15 - 12:15 QUEENS 2: Uncertainty propagation and quantification

12:15 - 13:15 Lunch break

13:15 - 14:45 4C & QUEENS 1: Simulation analytics - Orchestrating 4C simulations with QUEENS

14:45 - 15:00 Break

15:00 - 16:30 4C & QUEENS 2: Quantifying uncertainty due to heterogeneous material fields

16:30 - 17:00 State-of-the-art research with QUEENS

Link: https://unibw.zoom-x.de/j/64722868182?pwd=V4bEWtP43aJy9NOx2TfkdPbwMuebqY.1
Meeting-ID: 647 2286 8182
Passcode: 409537