

TTK31 - Design of Experiments (DoE), metamodelling and  
Quality by Design (QbD)  
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Big Data Cybernetics Gang



## Metamodelling - introduction

- A multivariate metamodel maps the output behavior of a mechanistic model from different input conditions
- The metamodel describes the mechanistic model's behavior
- The mechanistic model might be a first-principle based model or a simulation model
- Typically, thousands of simulation evaluations are required and one single evaluation may take a couple of minutes to hours of computing time
- Time-consuming simulations may be tolerated in the design phase, but is not acceptable in the daily operational optimisation
- Once the metamodel has been established, the input-output relationship makes it possible to circumvent the mechanistic model input-output relationship is established by use of multivariate regression or any other suitable method

# What are the objectives with metamodelling?

- Different ways to apply metamodels
  - ① Understand and verify underlying relationships in the mechanistic model
  - ② Speed up mechanistic and simulation models to enable online use
  - ③ Invert model to estimate internal states
  - ④ Combine metamodel outputs with empirical measurements for a hybrid modelling approach that combines “the best of both worlds”
  - ⑤ Investigate if interaction and square terms might influence the output of the mechanistic model
- Numerical optimization with constraints serve as a basis for verification runs

# Design of Experiments as a tool in metamodeling

- One of the essential tools in meta- and hybrid- modelling is Design of Experiments (DoE)
- Proper use of DoE ensures that the parameter space in the mechanistic and simulation-based models is described with a minimum number of combinations of the parameters of interest
- Procedure
  - 1 Construct an experimental plan of the different simulation input parameter settings that are to be tested using DoE
  - 2 Simulate the system with the given input parameter values
  - 3 Train the multivariate method using the simulated input-output samples
- The designs to use are typically:
  - Multifactor, multilevel designs
  - Optimal designs with constraints

## Illustration of the metamodeling procedure

