UNIVERSITÀ DI PARMA

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OPTIMAL

Advanced process optimization using Artificial Intelligence (AI)

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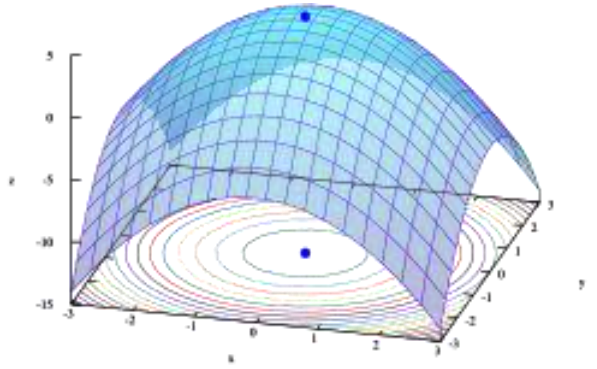
Process optimization

Optimization of **manufacturing processes** to make the best or most effective use of some specified set of parameters typically involves:

- Modelling or simulation of the process to predict outcomes.
- Experiments or testing to measure/determine outcomes.
- Modifying the process in an attempt to improve outcomes.



Process models can be:

- *Physics-based*, using physical relationships to describe a process. Physics-based models can be analytical (closed-form resolution of governing physical relationships) or numerical (discretization of domain and resolution of system of equations, e.g. Finite Element Method).
- *Data-driven* or statistical, using process data and/or observations from measurements.
- *Combined* physic-based and data-driven, combining both methods.

Characteristics of data-driven modelling:

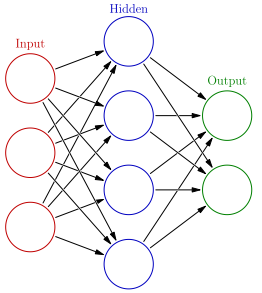
- Knowledge about underlying process is not necessarily required (although it usually helps).
- Can be used to discover previously unknown knowledge and relationships within data.
- Can be faster and simpler to implement that physics-based models.
- Can lack transparency (although there are methods to overcome this).

Artificial intelligence (AI) and machine learning (ML)

Artificial intelligence (AI): Intelligence exhibited by computer systems. The discipline of developing and studying methods and software that enable machines to perceive their environment and use learning and intelligence to take actions that maximize their chances of achieving defined goals, including:

- Reasoning and problem-solving
- Knowledge representation
- Planning and decision-making
- *Machine learning*
- Natural language processing
- …

Machine learning (ML): A field of study in AI concerned with the development and study of statistical algorithms that can learn from data and generalize to unseen data.



Given a 'training' dataset, a computer can use an ML algorithm to:

- Understand how data are distributed (unsupervised ML).
- Detect recurrent patterns in data (unsupervised ML).
- Map input data onto corresponding outputs (regression) or labels (classification) (supervised ML).

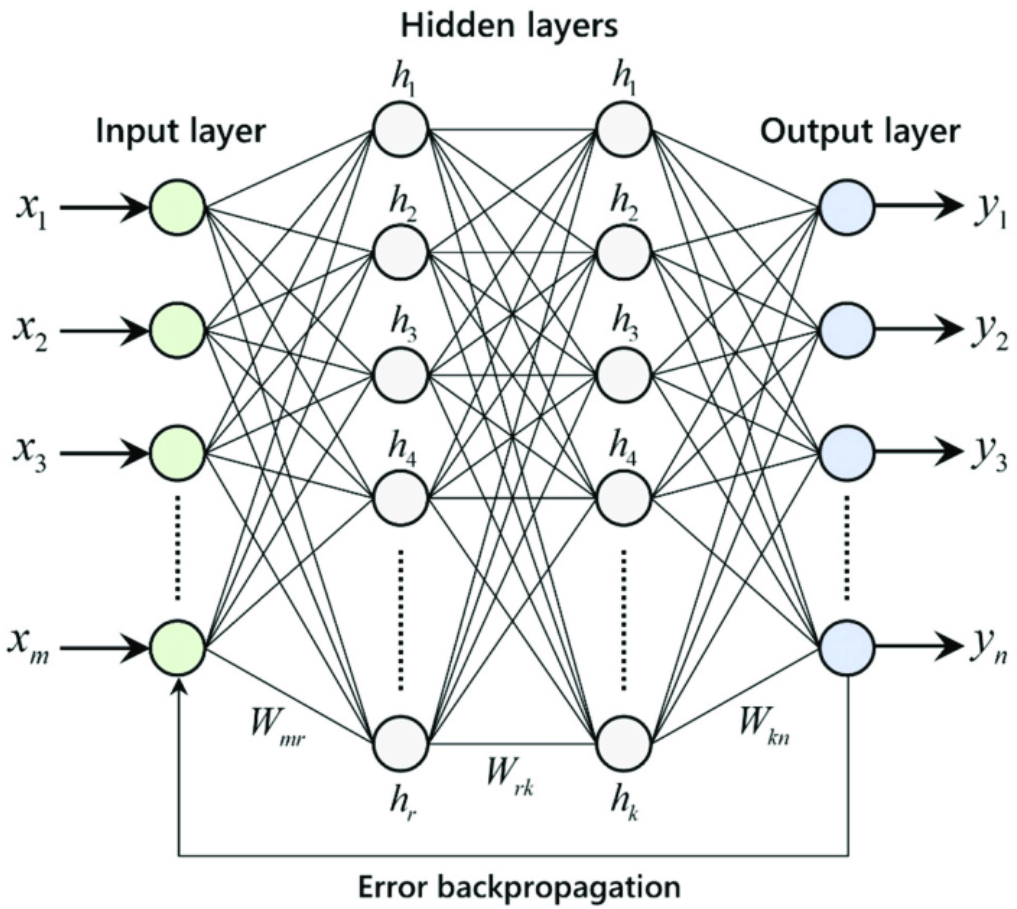
Artificial neural networks (ANN) for regression

ANNs are models inspired by the structure and function of biological neural networks, comprising a **series of connected nodes, or neurons,** that receive, process and emit signals to other connected neurons.

The structure and functionality of an ANN is governed by **hyperparameters**, including:

- Number of fully connected (hidden) layers
- Number of neurons per fully connected layer
- Types of activation functions
- Regularization type and strength
- …

In supervised learning, the ANN learns from labelled training data by iteratively updating its parameters to minimize a defined **loss function** (e.g. mean squared error), typically via gradient-based methods such as backpropagation.



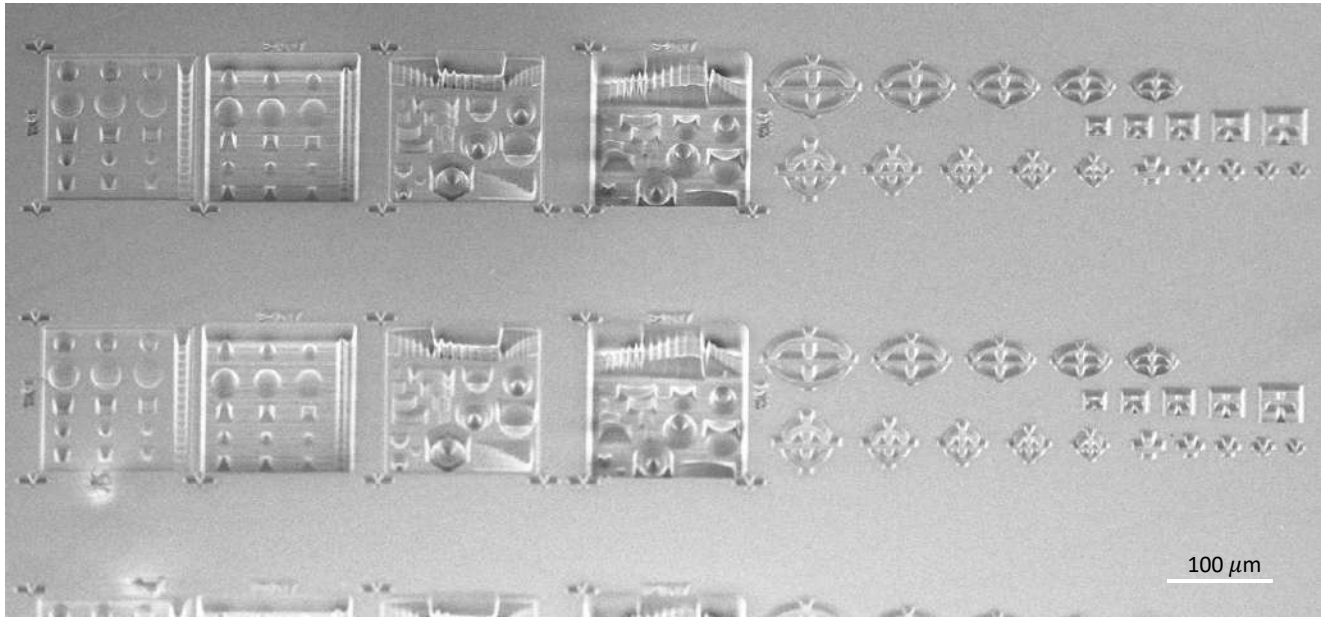
Fernández-Cabán, P.L. et al., Predicting roof pressures on a low-rise structure from freestream turbulence using artificial neural networks, Frontiers in Build Environment, 2018.

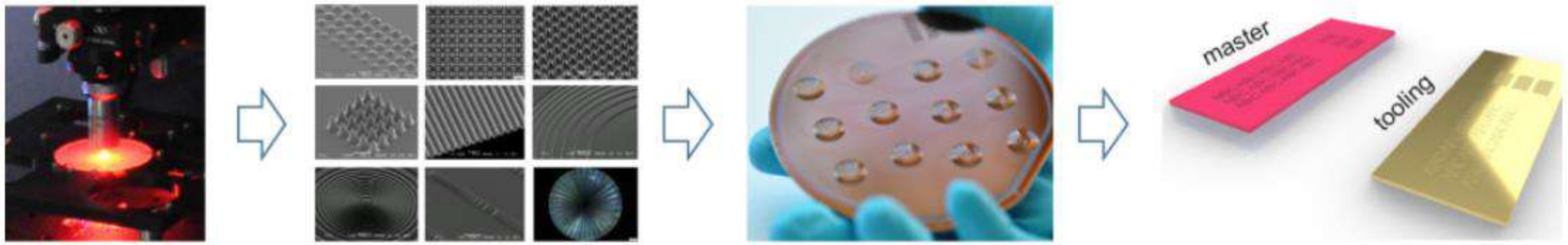
How can we apply ANNs to process optimization?

ANNs can be **applied as tools** for process optimization using standard libraries, toolboxes and functions:

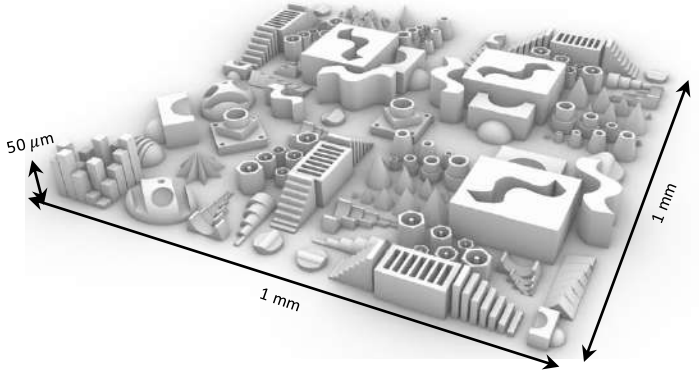
- **MATLAB**: *fitrnet, fitcnet, trainnet*
- **Python**: *TensorFlow*, *PyTorch*

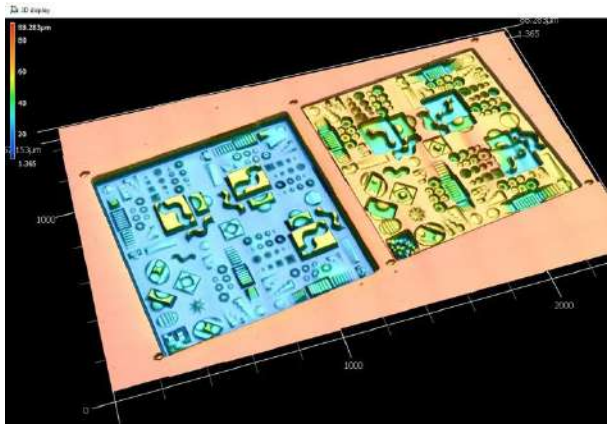
Case study: Optimization of process parameters in grayscale laser lithography to maximize build accuracy in OPTIMAL project.

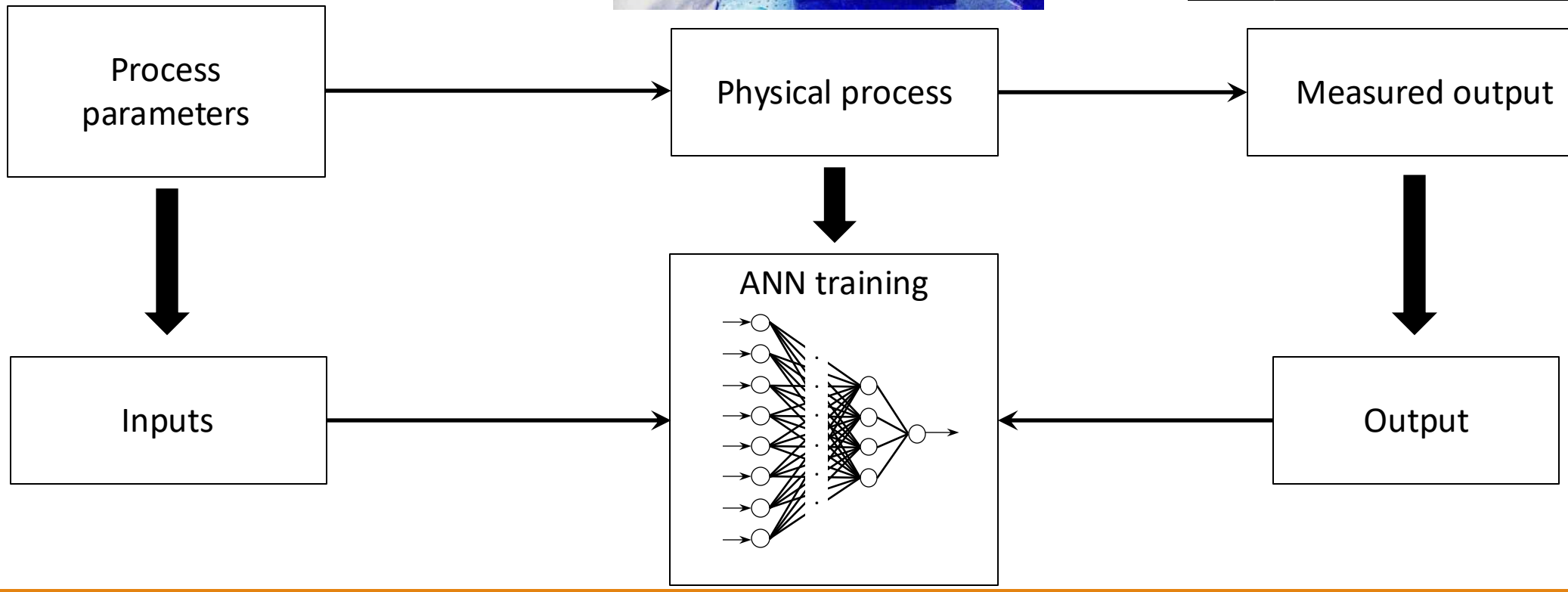




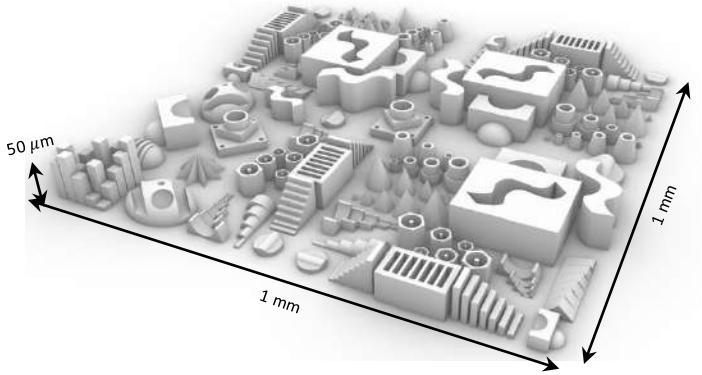
Training ANNs for process optimization





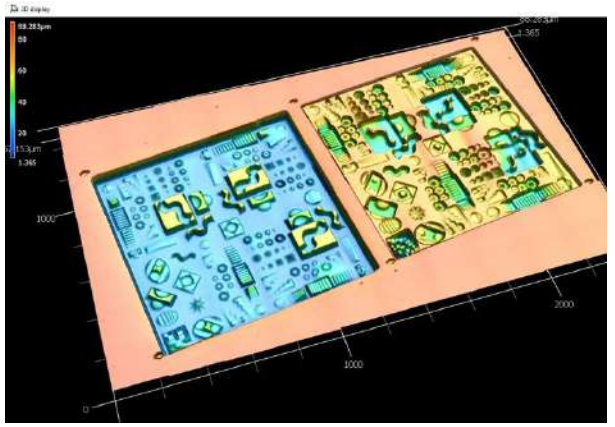


Training data



Process parameters = ANN inputs
Measured output = ANN output

Labelled training data must be **diverse, representative and of sufficient quantity**.



The quality of training data and its complete representation of the process is **critical**. *If you show a child 100 photos of cars then ask them to point out a motorbike, they'll point out a car.*

Training process parameters

Inputs

Measured output

Output

A high-quality dataset:

- Must contain all input parameters influencing outputs
- Parameter combinations must comprise the entire foreseeable range
- Must contain statistically representative data.

Hyperparameter optimization

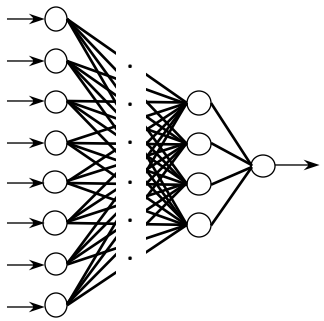
The structure and functionality of an ANN is governed by **hyperparameters**, including:

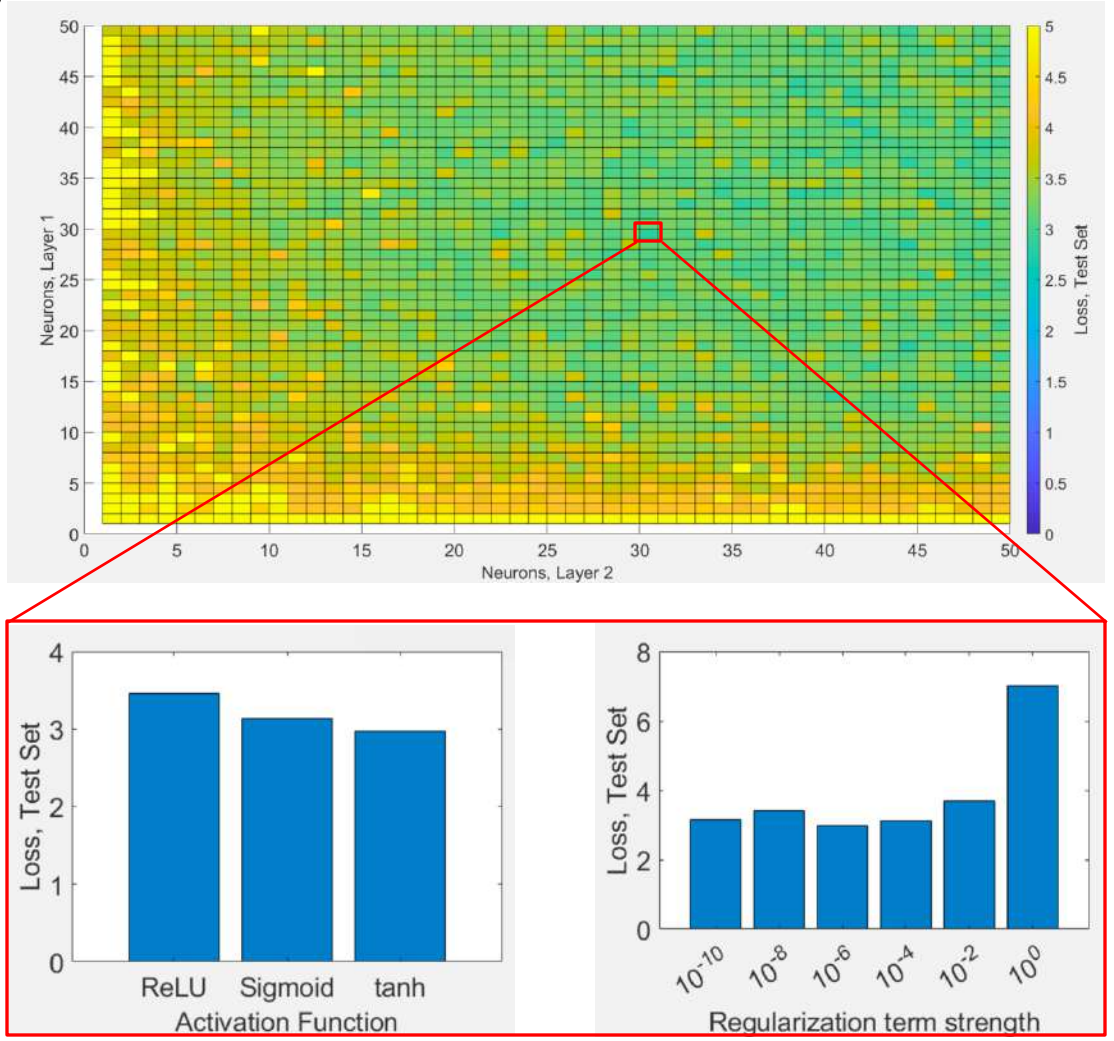
- Number of fully connected layers
- Number of neurons per layer
- Activation functions
- Regularization strength
- …

Hyperparameter optimization involves finding the configuration leading to best performance of the ANN.

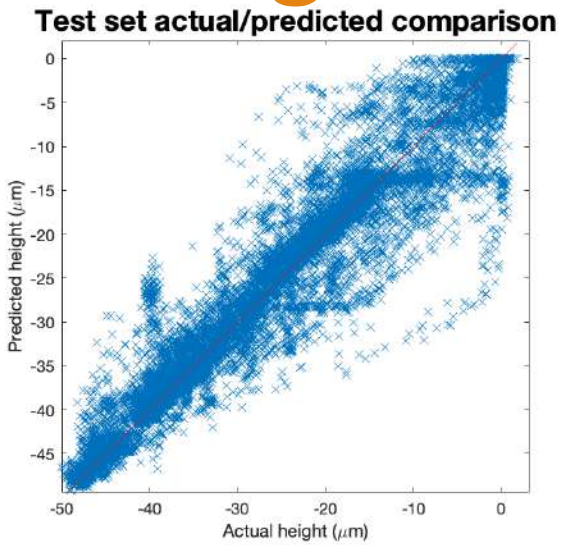
Typical hyperparameters optimization techniques:

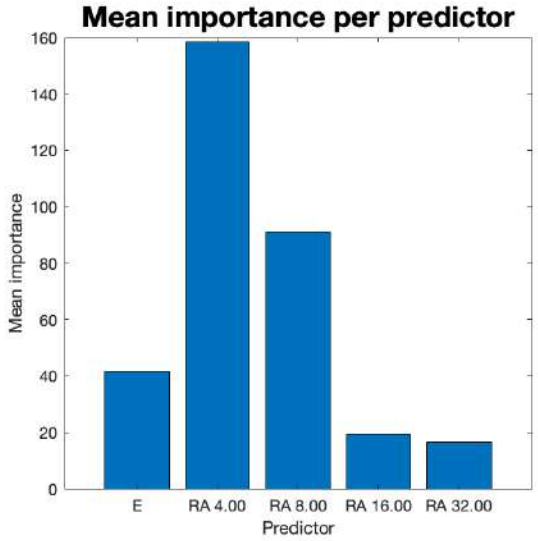
- Bayesian
- Grid
- Random

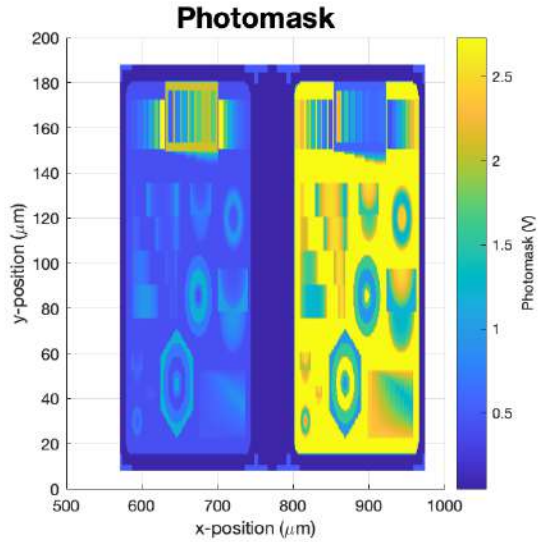


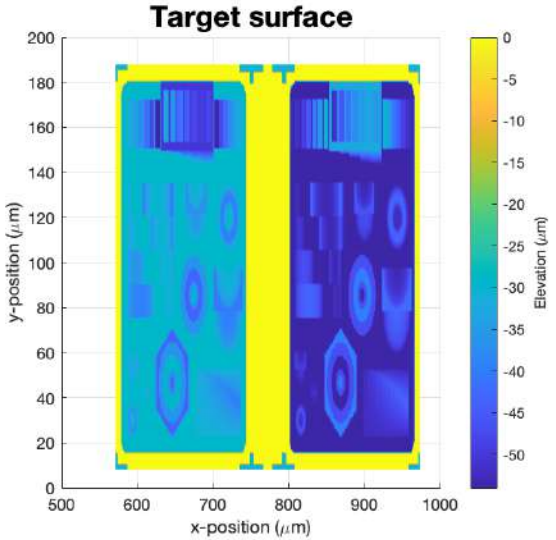


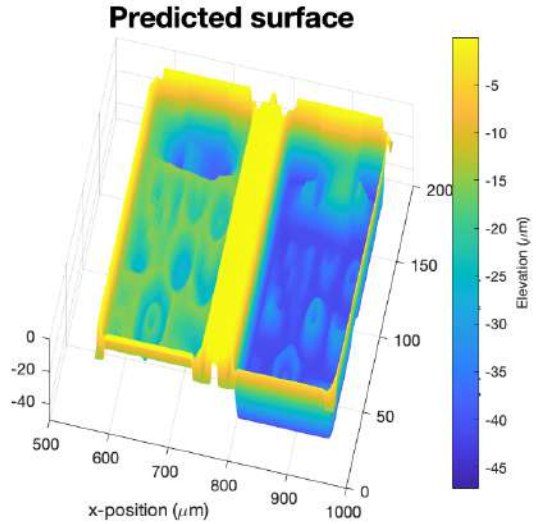
ANN training

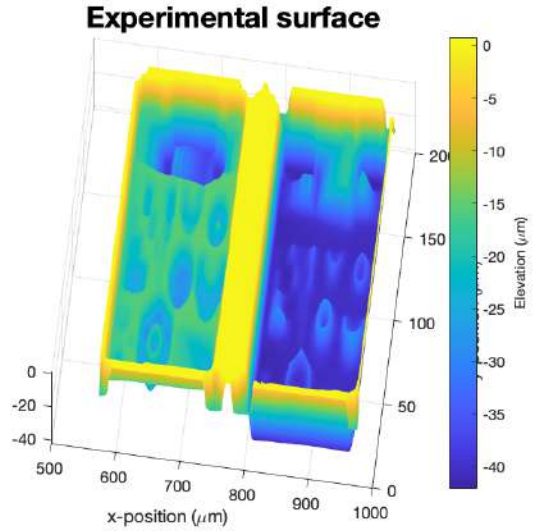








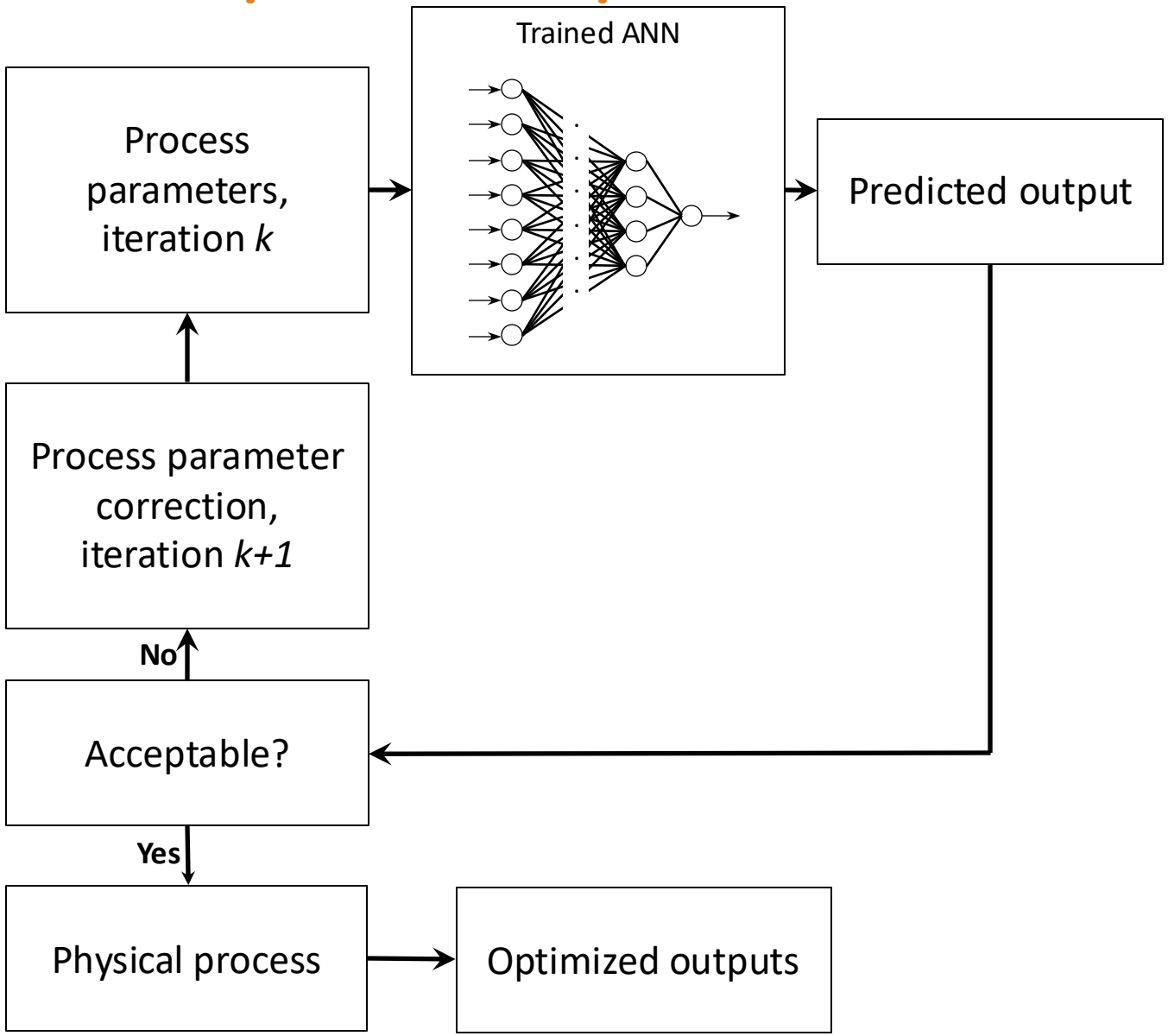




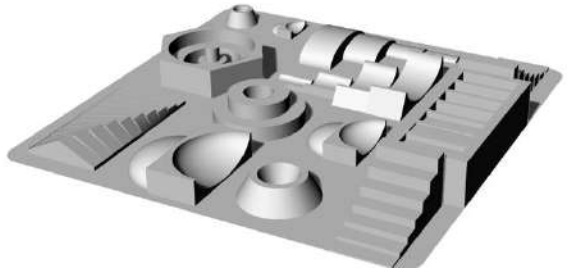
Implementation of ANNs for process optimization

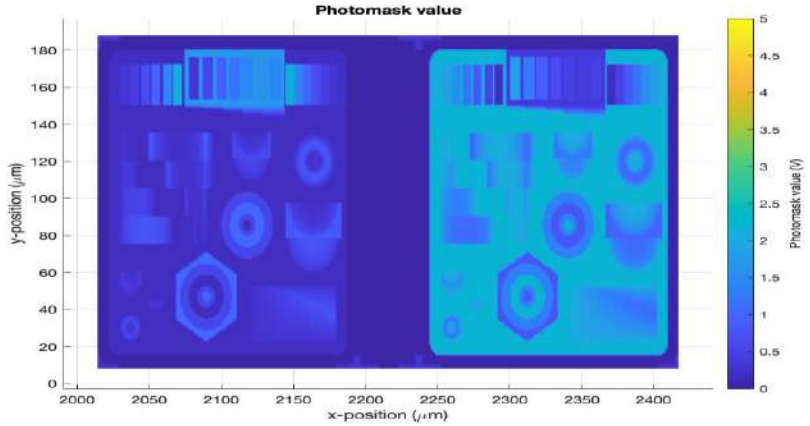
A trained ANN can replace experiments or physics-based models, providing fast prediction of an output for a given set of process parameters.

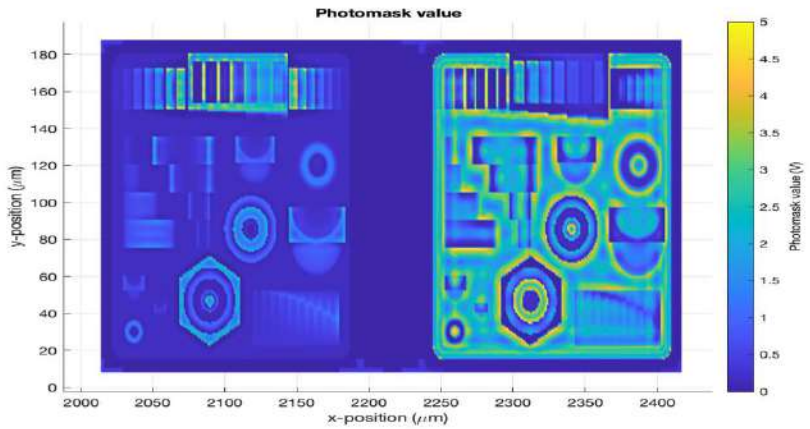
Successful process optimization **relies on knowledge of the process and how changing process parameters is likely to affect the predicted outcome**. *If the predicted surface elevation at some point is too high, should we increase or decrease laser power? By how much? What about surrounding points? Should any limits be placed on process parameters?*

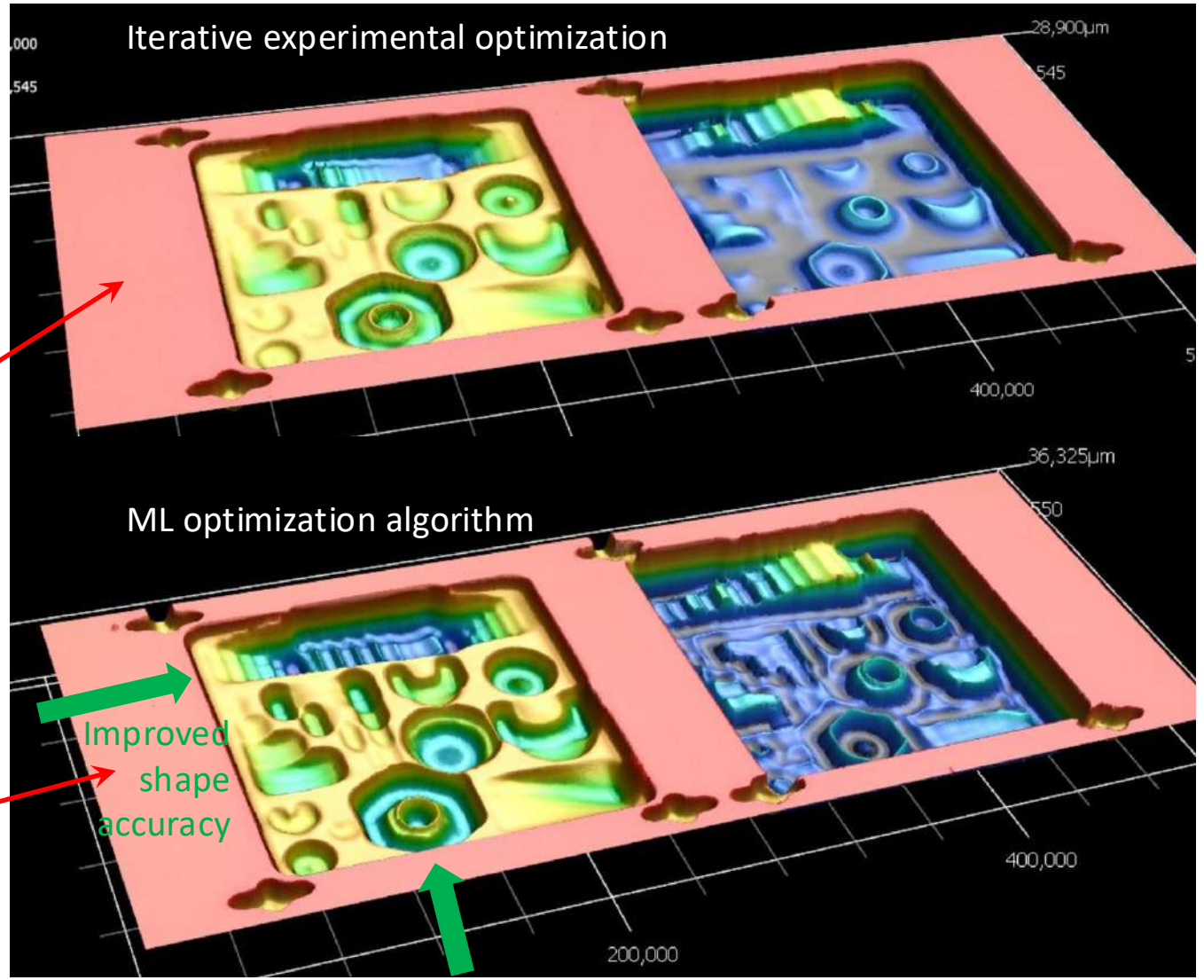


Implementation of ANNs for process optimization









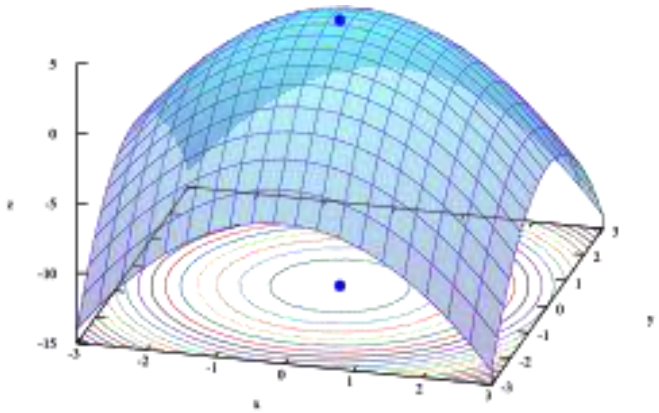
Conclusion

- **Data-driven process optimization** is a useful alternative to physics-based modelling and experiments where these are slow, complex, expensive or not sufficiently accurate.

- **AI** and **ML** can be applied relatively easily by engineers and scientists for process optimization using standard libraries, toolboxes and functions in Python and MATLAB.

- The accuracy of a data-driven model is strongly dependent on the **quality of data** employed for training (parameter selection, parameter ranges, statistical representation).

- Successful process optimization **relies on knowledge of the process** and how changing process parameters is likely to affect outcomes.



Thank you for your attention!

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