Surrogate Models for Particle Accelerators

Andreas Adelmann

RIKEN August 30, 2023

- Motivation
- Artificial Neural Nets (ANNs)

References I

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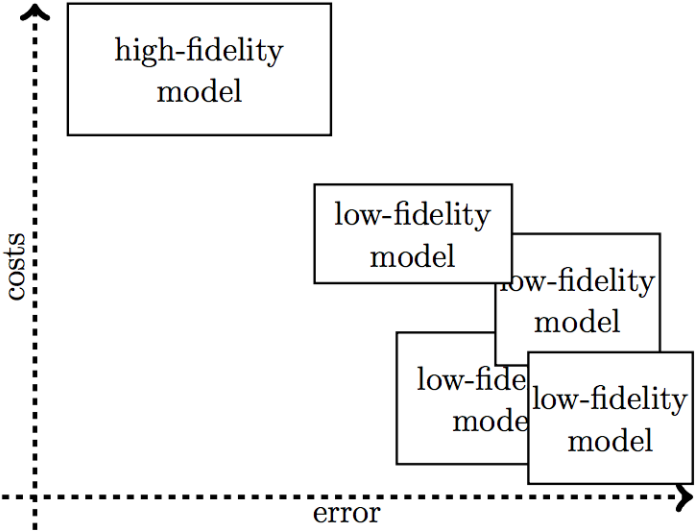
Motivation



high-fidelity model
low-fidelity model
low-fidelity model
low-fide mode
low-fidelity model
costs
error

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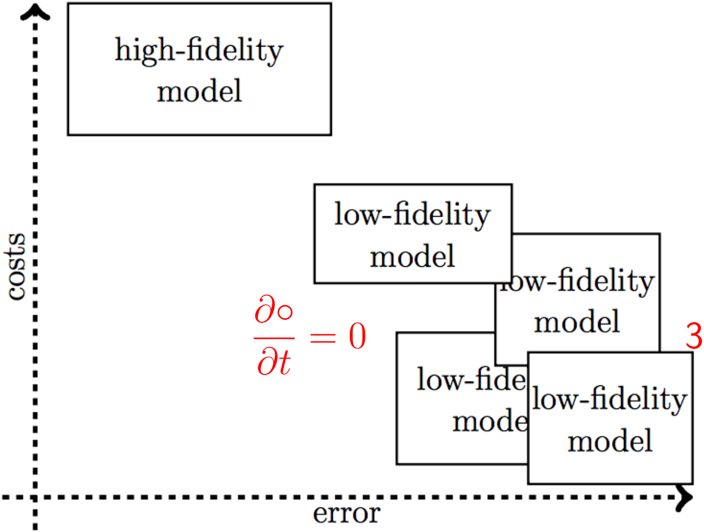
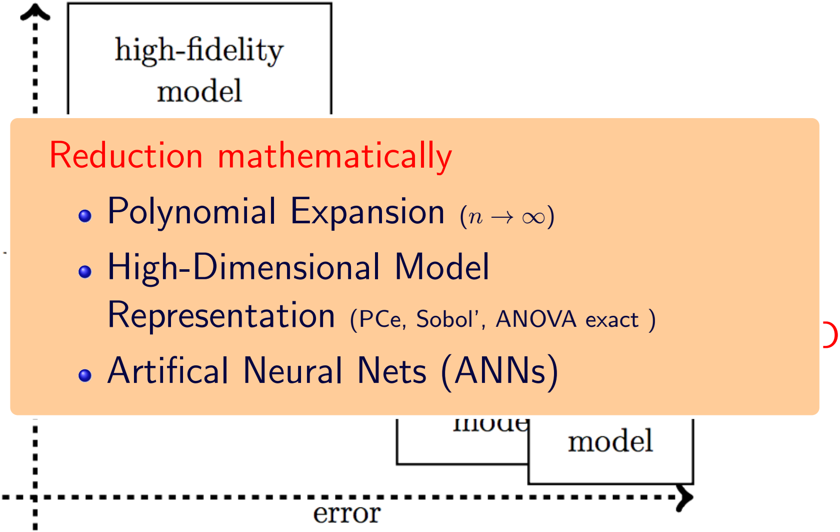
Motivation



$$\frac{\partial \circ}{\partial t} = 0$$

3D → 2D

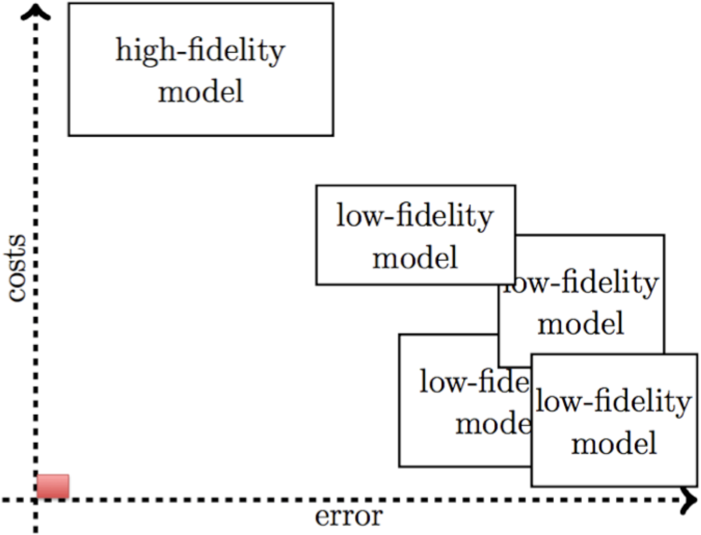
Motivation



Reduction mathematically

- Polynomial Expansion ($n \to \infty$)
- High-Dimensional Model Representation (PCe, Sobol', ANOVA exact)
- Artifical Neural Nets (ANNs)

Motivation



high-fidelity model
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Motivation

Weak vs. Strong Scaling

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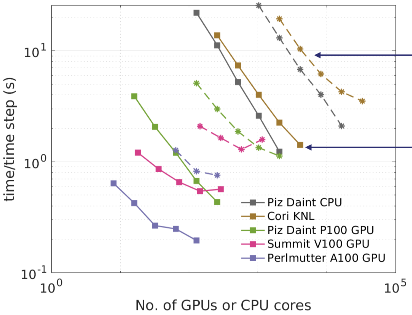
Motivation

Weak vs. Strong Scaling



Dashed:
1024^3 grid,
8B particles

Solid:
512^3 gri
1B partic

Surrogate Model a Simple Definition

Surrogate models (SMs) approximate a computationally expensive simulator η. Suppose

$$y(x) = \eta(x), \quad x \in \mathbb{R}^n, \quad y \in \mathbb{R}^m$$

then the SM is an approximation of the form

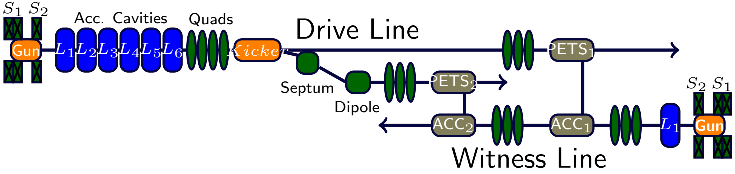
$$\hat{y}(x) = \hat{\eta}(x)$$

such that

$$y(x) = \hat{y}(x) + \varepsilon$$

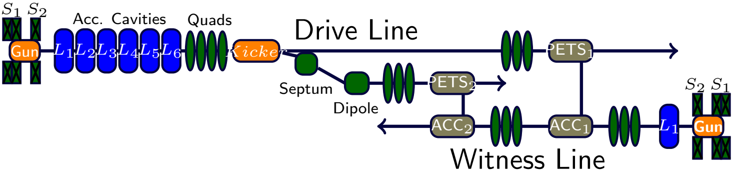
and $\hat{y}(x)$ **cheap** to evaluate.

MOGA for the Argonne Wakefield Accelerator [?]



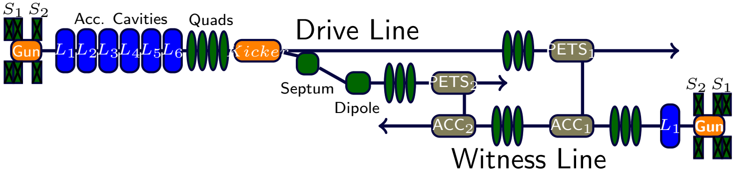
- Full 3D Start to End (S2E) needed
- OPAL Particle In Cell (PIC) model
- Very timeconsuming
- Parameter study / multi-objective optimisation expensive

MOGA for the Argonne Wakefield Accelerator [?]



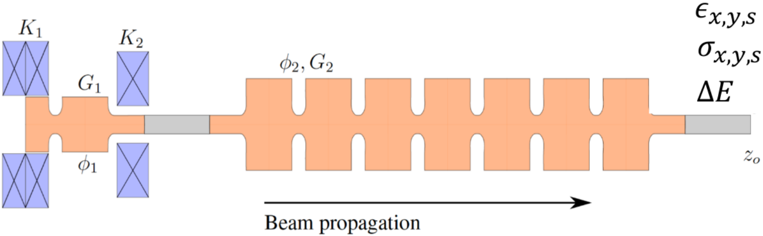
- One 3D medium fidelity S2E 3600 (s) on 32 cores
- $3 \ldots 7$ QoIs, $6 \ldots 15$ Dvars
- Genetic Algorithm setup: $G = 200, I = 100$

MOGA for the Argonne Wakefield Accelerator [?]



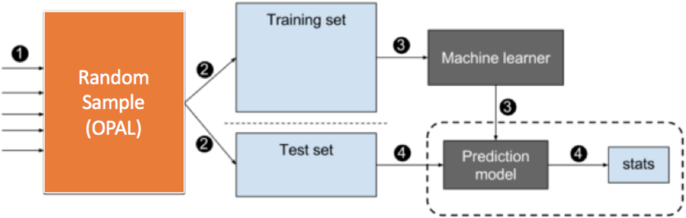
- OPAL MOGA: 24h on ≈ 5000 cores

Machine Learning to Construct a cheap & accurate SM [?]



- **optimise parameters at a given location**
- One 3D S2E 300 (s) on 8 cores
- 7 QoIs, 7 Dvars
- MOGA (in OPAL): $G = 200, I = 100 \Rightarrow$ ground truth

4 Step Process to Construct an ANN SM



1. generate random sample
2. split **labeled data** set (80%, 20%)
3. create ANN
4. understand quality

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Artificial Neural Network

- Fully connected and feed forward
- Hyperparameters
  - A lot of different architectures
  - Learning rate
- Best results using
  - 6-12-24-48-96-8
  - Adam optimizer with 0.0001 learn rate, trained for 30k epochs
  - Tanh as activation, no activation after output layer
  - Weights inverse proportional to the estimated density likelihood

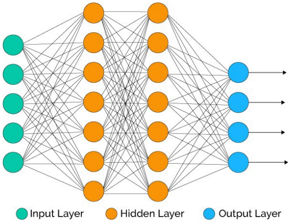
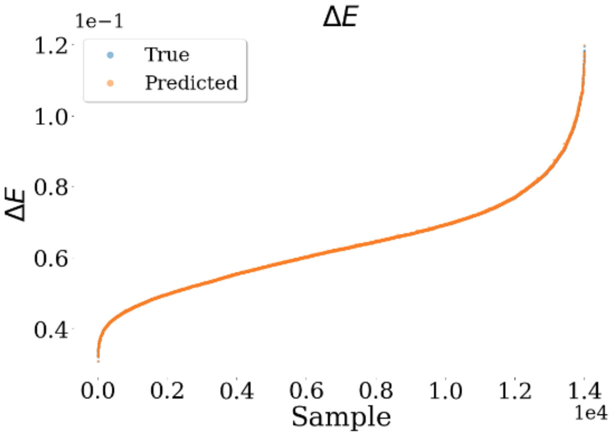


Figure: Neural Network scheme
https://towardsdatascience.com

Fidelity on the Test Data I



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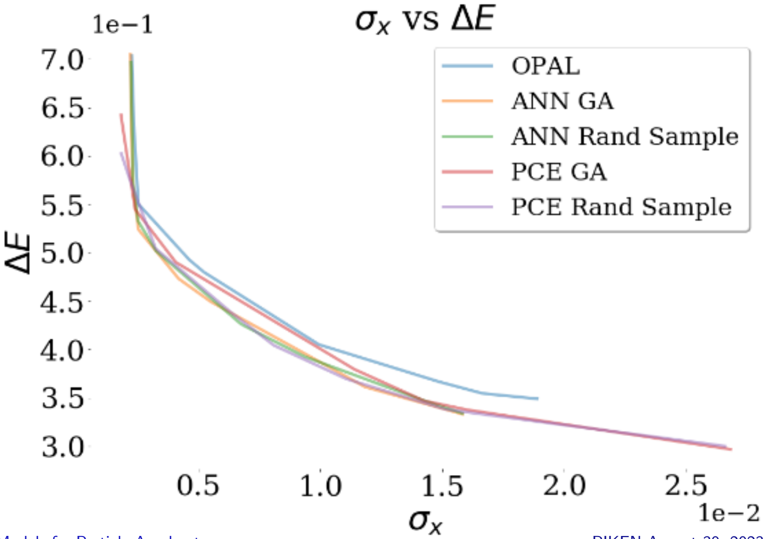
When all comes together ....



Take Home Points

OPAL MOGA: 24h on ≈ 5000 cores

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Train ANN once: $2 - 5$h on ≈ 128 cores

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ANN & MOGA : ≈ 30 minutes $\Rightarrow$

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Speedup $>$ 1 000 000 & accurate

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How Can OPAL Help?

`Sampler`, description see
https://gitlab.psi.ch/OPAL/Manual-2.1/wikis/sampler

Take Home Points

- Surrogate Models are the only way to achieve real-time performance & accuracy in complicated system!

- ANN & PCe are wonderful tools to achieve this

- Much to learn **robustness, training sizes, & accuracy**

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