Surrogate Models for Particle Accelerators

Andreas Adelmann

ICALEPCS - New York - 6. October 2019

- Polynomial Chaos Expansion (PCe)
- Artificial Neural Nets (ANNs)

References

- A. Adelmann, On Nonintrusive Uncertainty Quantification and Surrogate Model Construction in Particle Accelerator Modeling, SIAM/ASA Journal on Uncertainty Quantification, **7**(3), 2019
- N. Wiener, *The homogenous chaos*, Amer. J. Math. **30**, 897-936, (1938)
- A. Edelen, N. Neveu M. Frey Y, Huber, Ch. Mayes, A. Adelmann, Machine Learning to Enable Orders of Magnitude Speedup in Multi-Objective Optimizatin of Particle Accelerator Systems, submitted to PRAB, `https://arxiv.org/abs/1903.07759`
- N. Neveu, L. Spentzouris, A. Adelmann, Y, Ineichen, A. Kolano, C. Metzger-Kraus, C. Bekas, C, A. Curioni, P. Arbenz, Parallel general purpose multiobjective optimization framework with application to electron beam dynamics, Phys. Rev. Accel. Beams, **22**(5), 054602, 2019

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

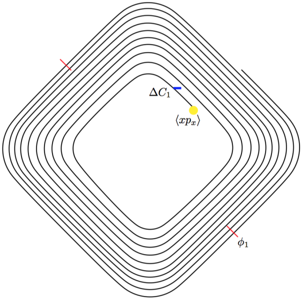
$$y(x) = \hat{y}(x) + \varepsilon$$

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

A Complicated Example (PCe)

[AA, On Nonintrusive UQ and SM Construction ... (2019)]

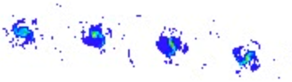
- **Goal**: model halo $h_x = \frac{\langle \boldsymbol{q}_x^4 \rangle}{\langle \boldsymbol{q}_x^2 \rangle^2} - C$ & $\tilde{x}$
- **Simplification**: 3 design parameters
  1. initial condition: $\langle x p_x \rangle$
  2. collimator setting: ΔC_1
  3. rf phase setting: ϕ_1.



A Complicated Example (PCe)

[AA, On Nonintrusive UQ and SM Construction ... (2019)]

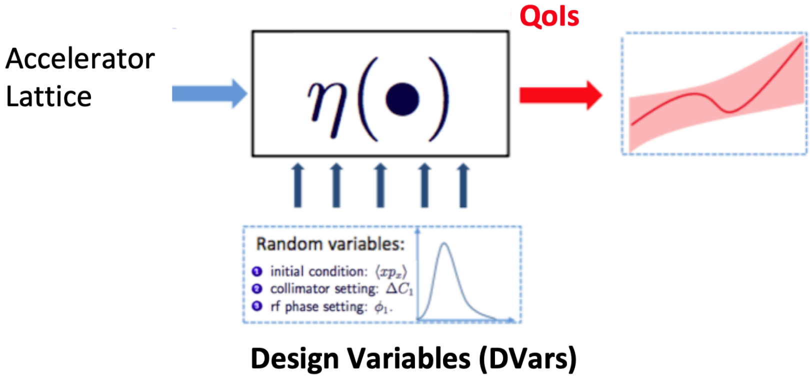
- **Goal**: model halo $h_x = \frac{\langle \boldsymbol{q}_x^4 \rangle}{\langle \boldsymbol{q}_x^2 \rangle^2} - C$ & $\tilde{x}$
- **Simplification**: 3 design parameters
  1. initial condition: $\langle x p_x \rangle$
  2. collimator setting: ΔC_1
  3. rf phase setting: ϕ_1.



This extensive search in the 3 dimensional parameter space requires PIC models with enough particles to estimate halo at a given location.

Illustration of the Basic Ideas (PCe)

Let η be the simulator



$$u^n = \eta(\xi^n)$$

Polynomial Chaos Expansions (PCe) I

All square integrable, second-order random processes with finite variance output, $y(\xi) \in L_2(\Omega, \mathcal{F}, \mathcal{P})$, can be written as [N. Wiener]

$$y = \sum_{k=0}^{\infty} \alpha_k \Psi_k(\xi).$$

- y: Random Variable (RV)
- α_k PC coefficients (deterministic)
- Ψ_k: Hermite polynomial, ξ: Gaussian RV

Expansion in terms of functions of random variables multiplied with deterministic PC coefficients.

Polynomial Chaos Expansions (PCe) I

[AA, On Nonintrusive UQ and SM Construction ... (2019)]

Algorithm: generate for each design variable, a PC surrogate model to order K

1. generate N samples (ξ^n) according to the sampling strategy of interest
2. create the **deterministic** training points with high fidelity simulations (non-intrusive)

$$u^n = \eta(\xi^n).$$

3. solve for α_k via
   - orthogonal Galerkin-projection
   - regression methods
   - Bayesian Compressive Sensing

Polynomial Chaos Expansions (PCe) II

[AA, On Nonintrusive UQ and SM Construction ... (2019)]

Given the computed α_k values one assembles $\hat{\eta}$

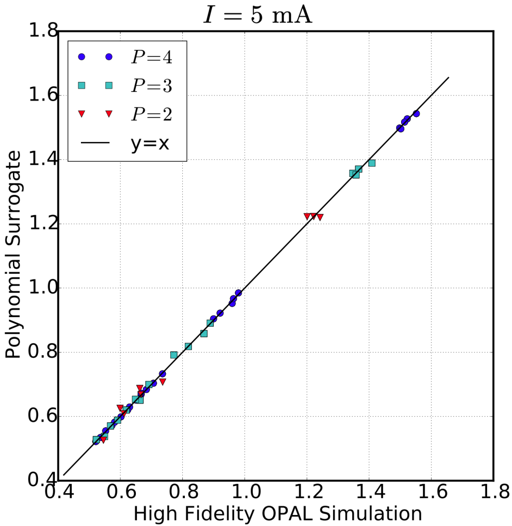
$$\boxed{\hat{\eta}(\xi) = \sum_{k=0}^{K-1} \alpha_k \Psi_k(\xi)}$$

$$S(\xi) = \frac{\sum_{k \in \mathcal{I}} \alpha_k^2}{\sum_{k=0}^{K-1} \alpha_k^2}$$

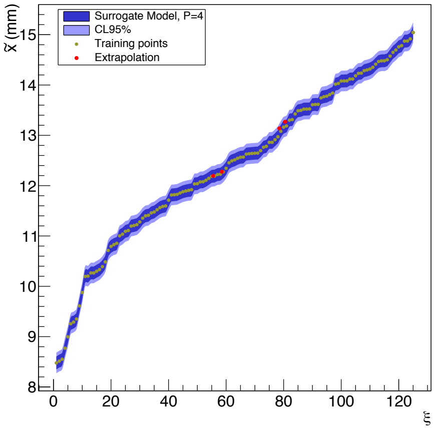
Surrogate Model $\hat{\eta}$

Global Sensitivity S

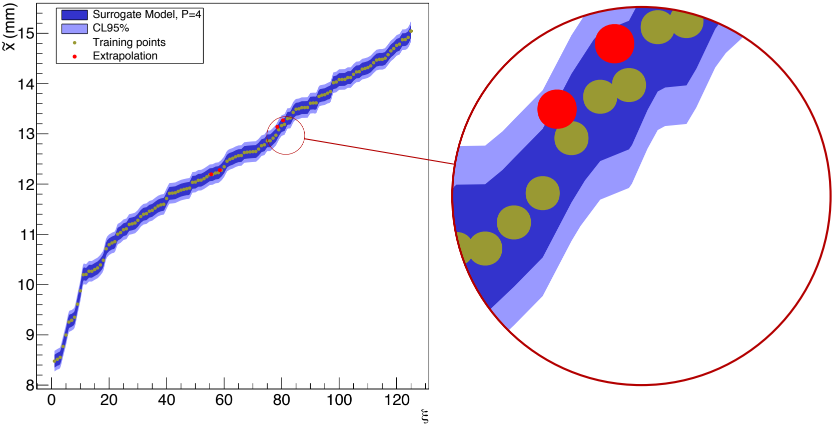
Predictions - h_x



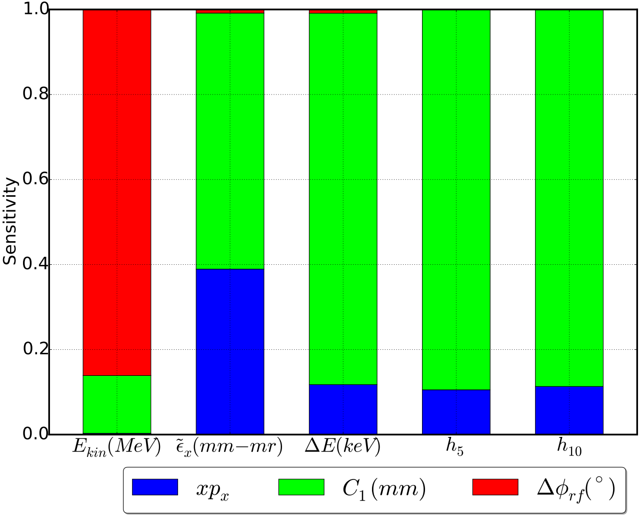
Predictions of $\tilde{x}$ with 95% CL



Predictions of $\tilde{x}$ with 95% CL

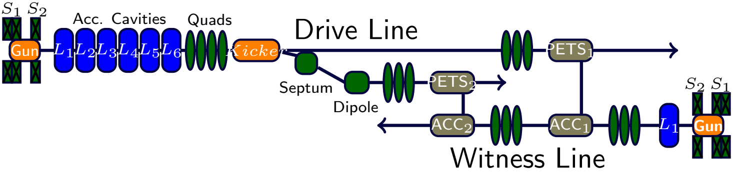


Sensitivities



MOGA for the Argonne Wakefield Accelerator

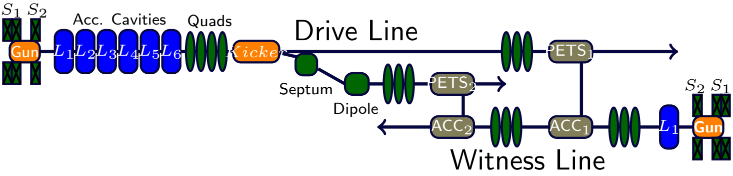
[N. Neveu, AA, et al. (2019)]



- 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

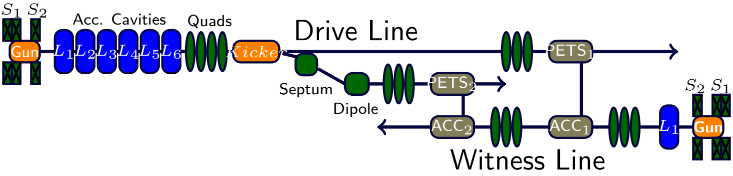
[N. Neveu, AA, et al. (2019)]



- 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

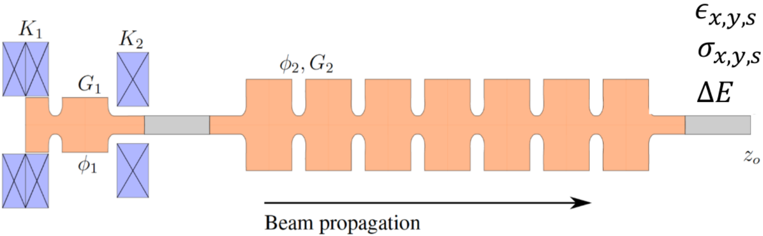
[N. Neveu, AA, et al. (2019)]



- OPAL MOGA: 24h on ≈ 5000 cores

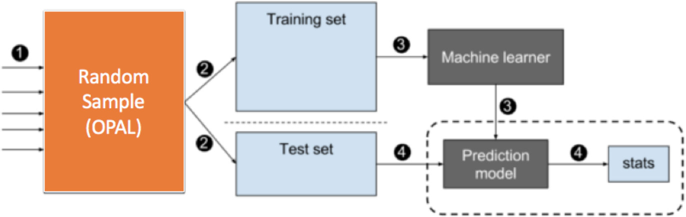
Machine Learning to Construct a cheap & accurate SM

[A. Edelen et al (2019)]



- **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

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

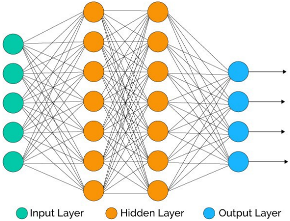
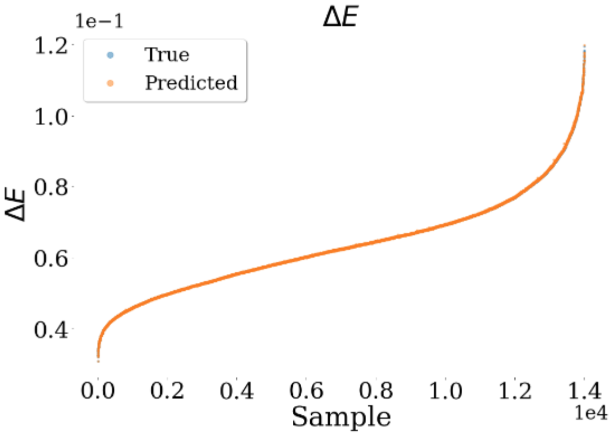
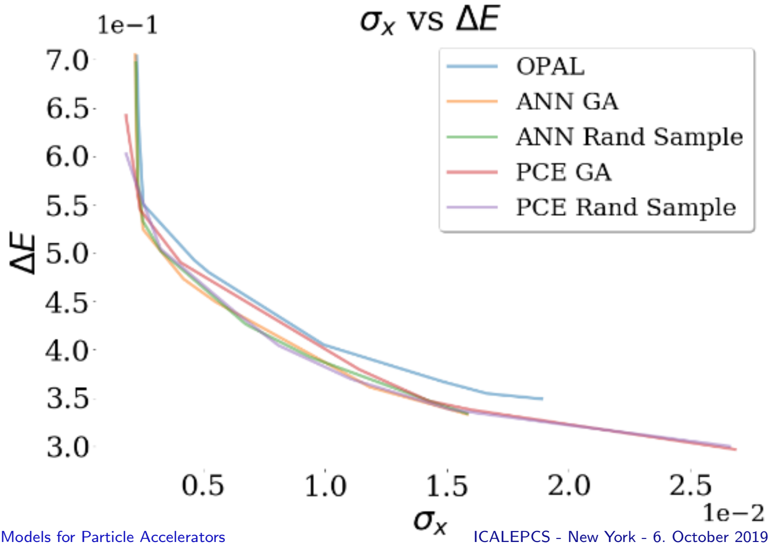


Figure: Neural Network scheme
https://towardsdatascience.com

Fidelity on the Test Data I



When all comes together ....



Take Home Points

OPAL MOGA: 24h on ≈ 5000 cores

Take Home Points

OPAL MOGA: 24h on ≈ 5000 cores

Train ANN once: $2-5$h on ≈ 128 cores

Take Home Points

OPAL MOGA: 24h on ≈ 5000 cores

Train ANN once: $2-5$h on ≈ 128 cores

ANN & MOGA : ≈ 30 minutes $\Rightarrow$

Take Home Points

OPAL MOGA: 24h on ≈ 5000 cores

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

ANN & MOGA : ≈ 30 minutes $\Rightarrow$

Take Home Points

OPAL MOGA: 24h on ≈ 5000 cores

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

ANN & MOGA : ≈ 30 minutes $\Rightarrow$

Speedup $>$ 1 000 000 & accurate

Take Home Points

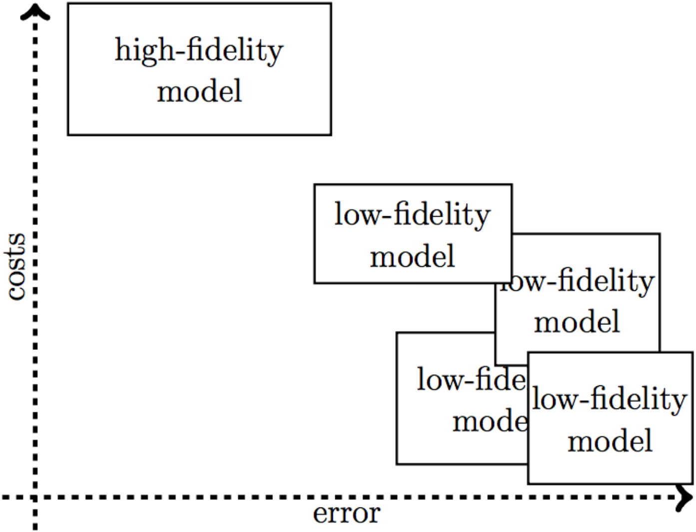
- Surrogate Models are the only way to achieve real-time performance & accuracy in complicated system!

- ANN & PCe are wonderful tools to achieve this

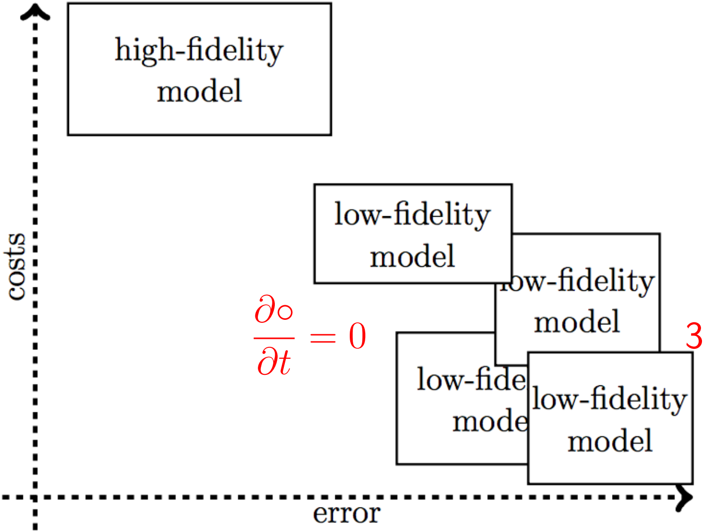
- Much to learn **robustness, training sizes, & accuracy**

Backup

Motivation


high-fidelity
model
low-fidelity
model
low-fidelity
model
low-fidelity
model
costs
error

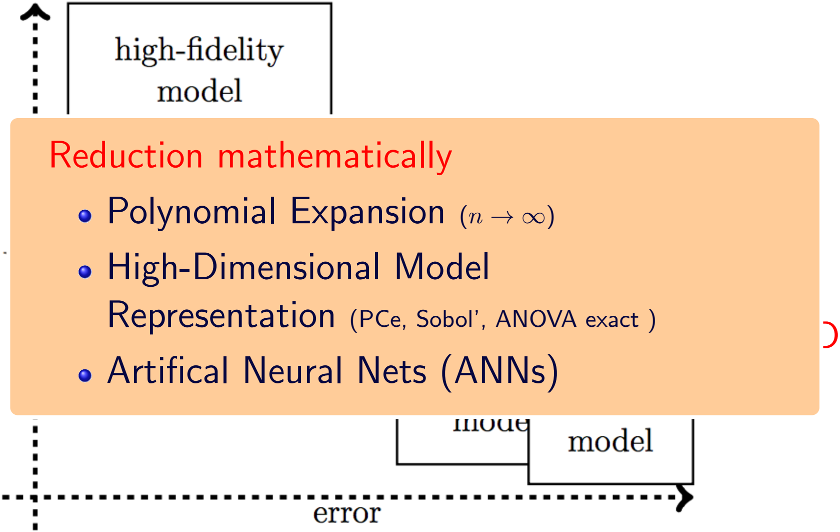
Motivation



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

3D $\rightarrow$ 2D

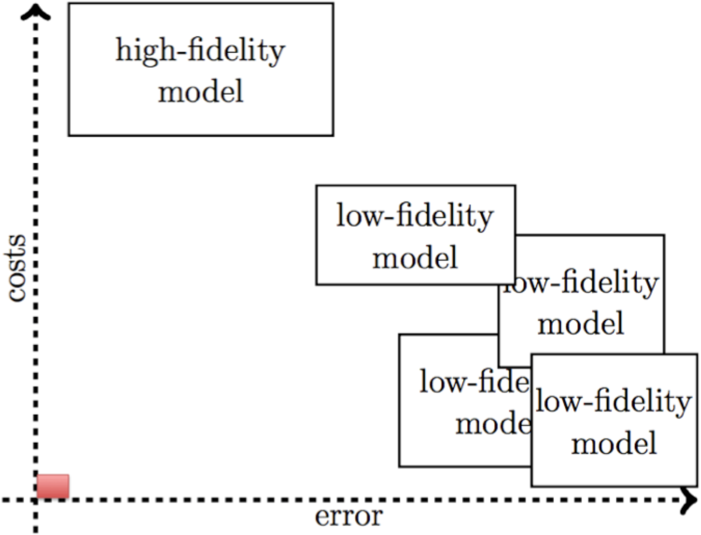
Motivation



Reduction mathematically

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

Motivation


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

Motivation

Weak vs. Strong Scaling

Motivation

Weak vs. Strong Scaling