On Uncertainty Quantification in Particle Accelerator Modelling

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Cyclotrons 2016, September 12, Zürich

Motivation

- Uncertainties
  - physics model (position of a collimator ...)
  - numerical model (grid sizes, time steps ...)
  - new models **M. Frey, (THC02) Matched Distributions with Linear and Non-Linear Space Charge**
- Correlations
  - within the physics model (initial phase w.r.t. halo parameter)
  - within the physics & numerical model (grid sizes/ N_p w.r.t initial 6D phase space distribution)

With extensive sampling in the high dimensional parameter space, in principle, one can estimate uncertainties and correlations.

Caveats

- Models are usually **(very)** expensive to calculate

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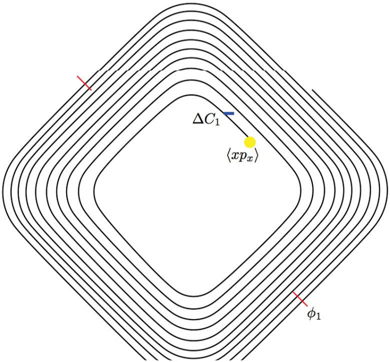
Motivation

- 3 model parameters
  1. initial condition: $\langle xp_x \rangle$
  2. collimator setting: ΔC_1
  3. rf phase setting: ϕ_1.
- **Goal**: minimise halo at the extraction



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

A. Kolano, (MOD03) A Precise 3D Beam Dynamics Model of the PSI Injector II

Illustration of the Basic Ideas

Let η be the simulator

- Sampling $u = \eta(\bullet)$ is expensive

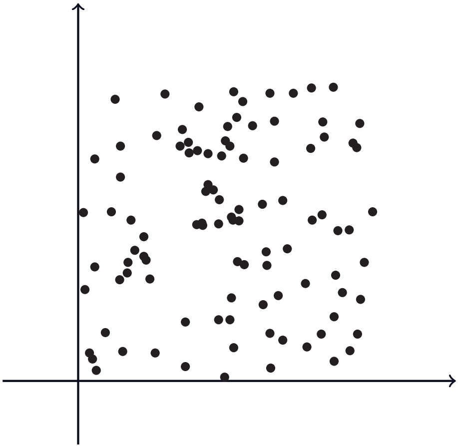
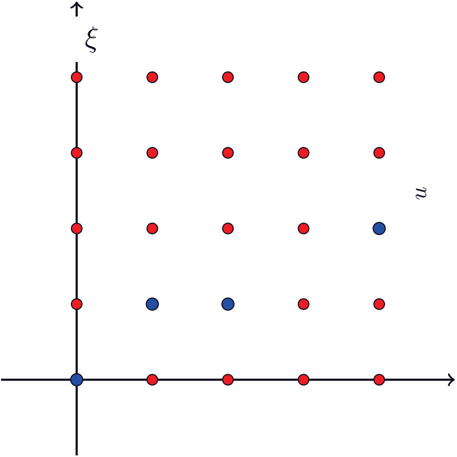


Illustration of the Basic Ideas

n training points $\bullet$ $\xi = \{x \in \mathbb{R}^d\}$ according to a statistics model
$\Longrightarrow$ the model output u is also a Random Variable (RV)



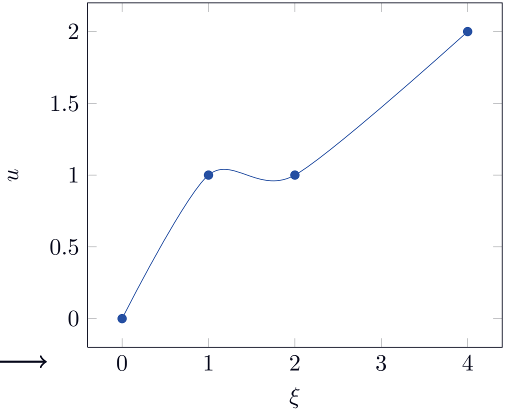


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Illustration of the Basic Ideas

Idea Spectral Approach represents u by a series expansion

You may very well think of

- Fourier decomposition
- approximation theory

The only difference is that we consider random variables.

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Polynomial Chaos Expansions (PCE)

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

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

- u: Random Variable (RV) represents 1D PCE
- α_k PC coefficients (deterministic)
- Ψ_k: 1D Hermite polynomial of order k, ξ: Gaussian RV

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

- set of deterministic PC coefficients fully describes RV
- separates randomness from deterministic dimensions

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Surrogate Model & Sensitivity Analysis I

[AA, UQ in Particle Accelerator Modelling (2015)]

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

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

$$u^n = \eta(\boldsymbol{\lambda}^n).$$

Surrogate Model & Sensitivity Analysis II

[AA, UQ in Particle Accelerator Modelling (2015)]

Given the computed α_k values for each k, one assembles the PCE (the surrogate model)

$$\hat{u} = \sum_{k=0}^{K-1} \alpha_k \Psi_k(\boldsymbol{\xi}).$$

3. calculate the expectation via orthogonal Galerkin-projection

$$\alpha_k = \frac{\langle u \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{1}{\langle \Psi_k^2 \rangle} \sum_{n=1}^{N} u^n \Psi_k(\boldsymbol{\xi}^n), \quad k = 0, \ldots, K-1.$$

d **Model Parameter** $\boldsymbol{\lambda}$

v-name	l-bound	u-bound
v_1	a_1	b_1
v_2	a_2	b_2
$\vdots$	$\vdots$	$\vdots$
v_d	a_d	b_d

N **Quadrature Points**

l **Design (controllable) Parameters** x

$$\boldsymbol{x} = \quad (x_1, \ldots, x_l)$$

lN **Model evaluations**
$\eta(\boldsymbol{\lambda}^n, \boldsymbol{x})$

Using N samples

$$u_i = \eta(\boldsymbol{\lambda}^n, \boldsymbol{x}) \approx \hat{u}_i = \mathcal{M}(\boldsymbol{\lambda}^n, \boldsymbol{x}) = \sum_{k=0}^{K-1} \alpha_{ki} \Psi_k(\boldsymbol{\xi}) \ .$$

$$S_i(x_i) = \frac{\sum\limits_{k \in \mathcal{I}} \alpha_{ki}^2}{\sum\limits_{k=0}^{K-1} \alpha_{ki}^2}$$

Surrogate Model $\mathcal{M}$

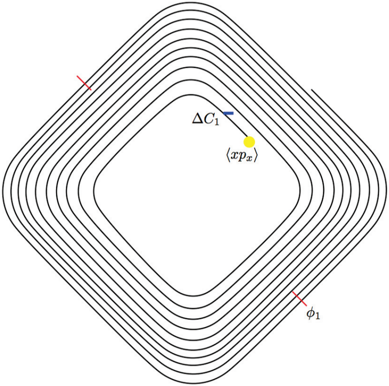
Global Sensitivity Analysis

Table: Summary of UQ related parameters for the presented results. The dimension for all the experiments is $d = 3$.

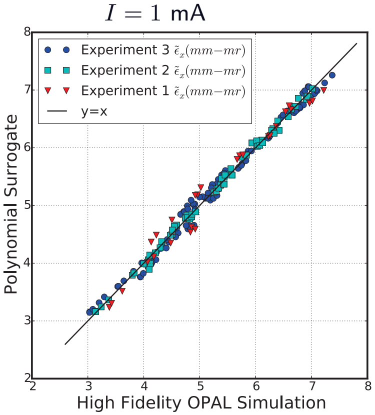
p	**order of surrogate construction**	2	3	4
	quadrature points per dimension $(p+1)$	3	4	5
N	quadrature points $N = (p+1)^d$	27	64	125
	number of high-fidelity runs	27	64	125
K	polynomial basis terms $K = (d+p)!/d!p!$	10	20	35

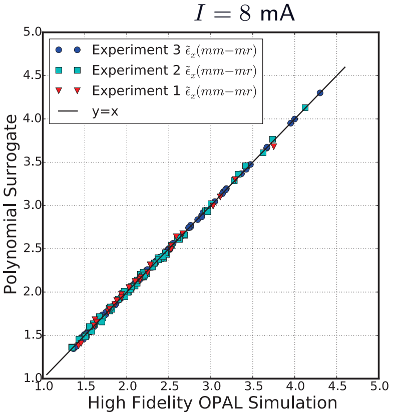
Realistic Model Problem

- PSI Injector 2 like central region
- OPAL as black box solver (η)
- I as controllable parameter
- 3 model parameters (d)
  1. initial condition: $\langle xp_x \rangle$
  2. collimator setting: ΔC_1
  3. rf phase setting: ϕ_1.
- Observables $\mathbf{u}$: **all** quantities η (OPAL) can compute
  - normalised emittance,
  - energy spread,
  - halo parameter
  - ...

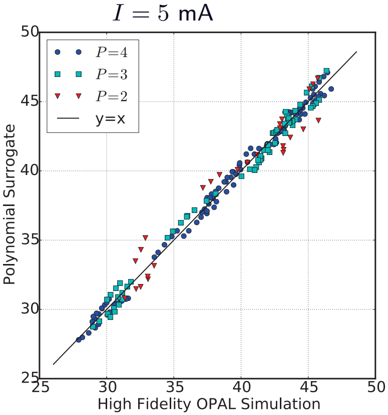


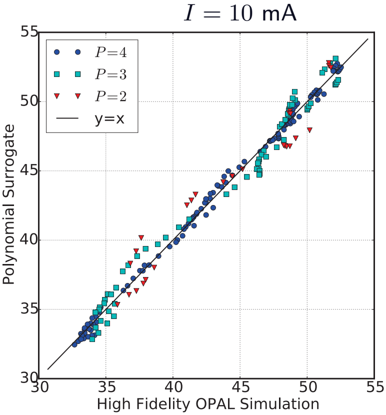
Results: Emittance (mm-mr normalized)



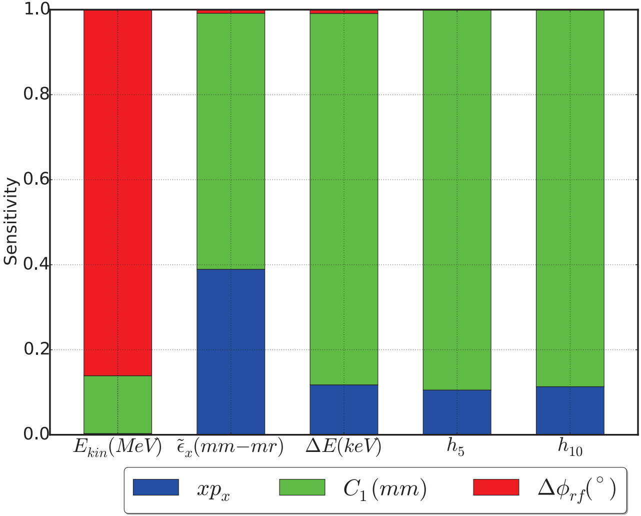


Results: Energy Spread (keV)





Results: Sensitivity (8 mA)



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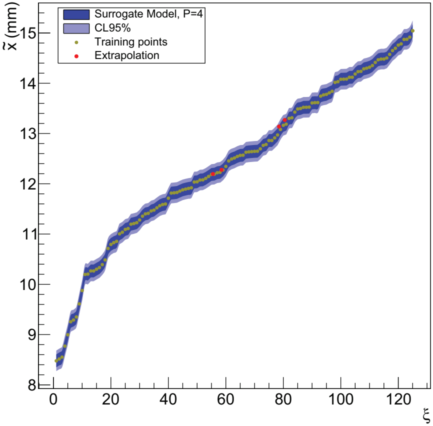
Predictions I

- appropriate number of training points $\rightarrow$ surrogate model
- N training points sample the input uncertainties of the design
- with the surrogate model we can evaluate any point, **not only** $\mathbf{N}$, within the bounds

v-name	l-bound	u-bound
v_1	a_1	b_1
v_2	a_2	b_2
$\vdots$	$\vdots$	$\vdots$
v_d	a_d	b_d

Predictions II

- the 95% CL is obtained by evaluating the Student-t test



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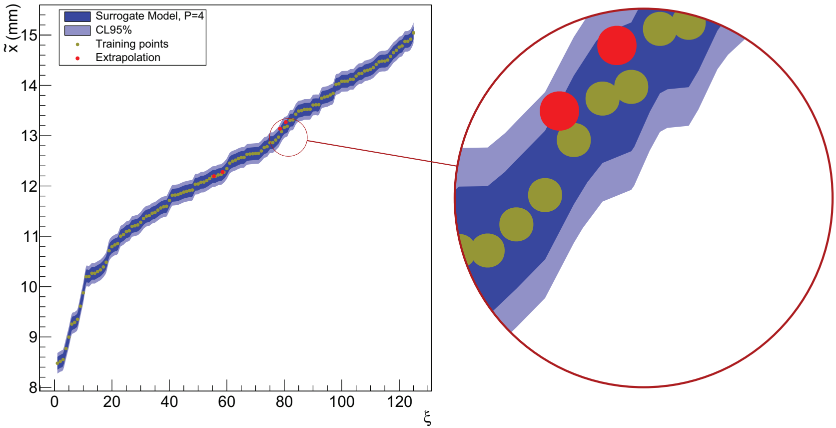

Take Home Points

- UQ with PCE is a well known technique in science
- This is the first application to beam dynamics, using [UQTk]
- You are getting:
  - a sound model for inherent uncertainties in the model
  - a cheap to evaluate surrogate model (speedup of many orders of magnitude)
  - without additional effort: a full sensitivity analysis
- UQ with PCE enables
  - multi objective optimization in a reasonable time
  - online modelling including non linear models

References

[AA, UQ in Particle Accelerator Modelling (2015)] A. Adelmann arXiv:1509.08130 & under review in JUQ

[N. Wiener] N. Wiener , *The homogenous chaos*, Amer. J. Math. **30**, 897-936, (1938)

[UQTk] UQ Toolkit (UQTk) `http://www.sandia.gov/UQToolkit/`