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Optimization of muon EDM experimental setup using simulations

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MuEDM Experiment at PSI

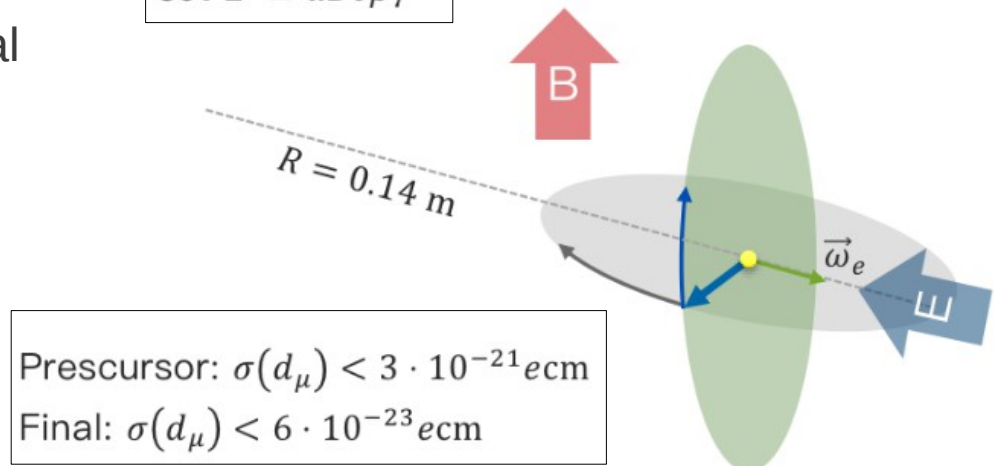
- PSI Muon EDM measurement using Frozen-Spin Technique
- Phase I demonstrates Frozen-Spin technique
- Injecting muons with right experimental design parameters essential for ensuring optimum storage
- Longitudinal asymmetry in positrons decaying from stored muons
→ signal for muon EDM

This talk → simulation studies to optimize initial parameters affecting injection efficiency

$$\vec{\Omega} = \frac{q}{m} \left[a\vec{B} - \left(a + \frac{1}{1-\gamma^2} \right) \frac{\vec{\beta} \times \vec{E}}{c} \right] + \frac{\eta q}{2m} \left[\vec{\beta} \times \vec{B} + \frac{\vec{E}}{c} \right]$$

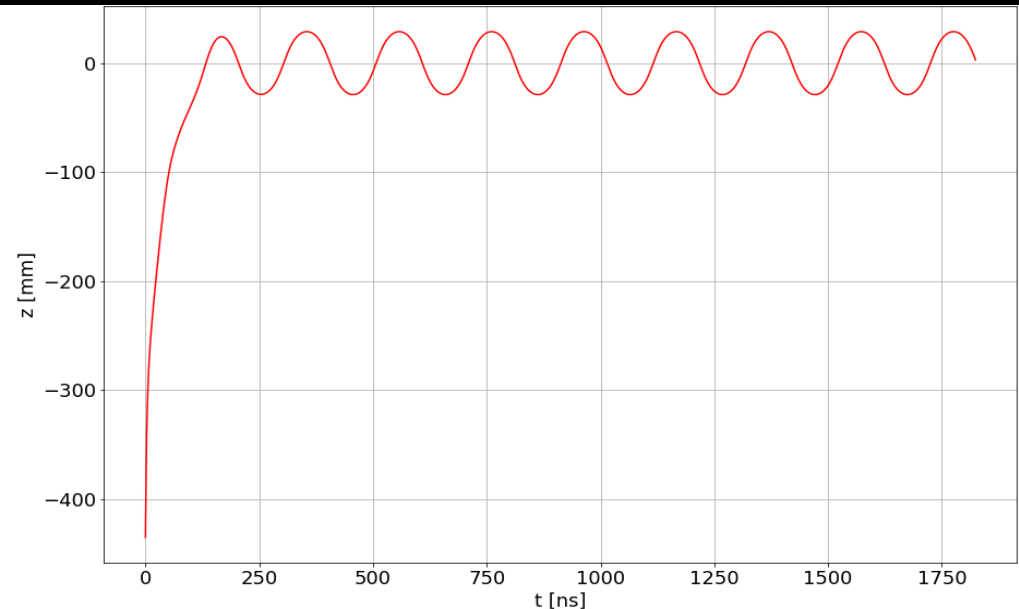
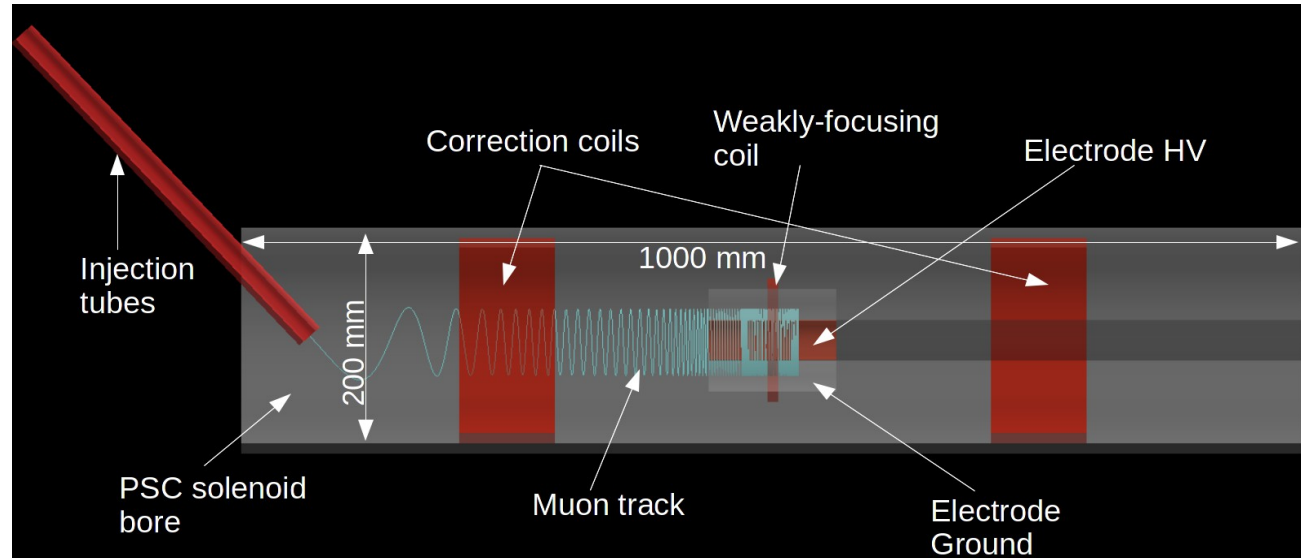
g-2 term
EDM term

$$\text{set } E \cong aBc\beta\gamma^2$$

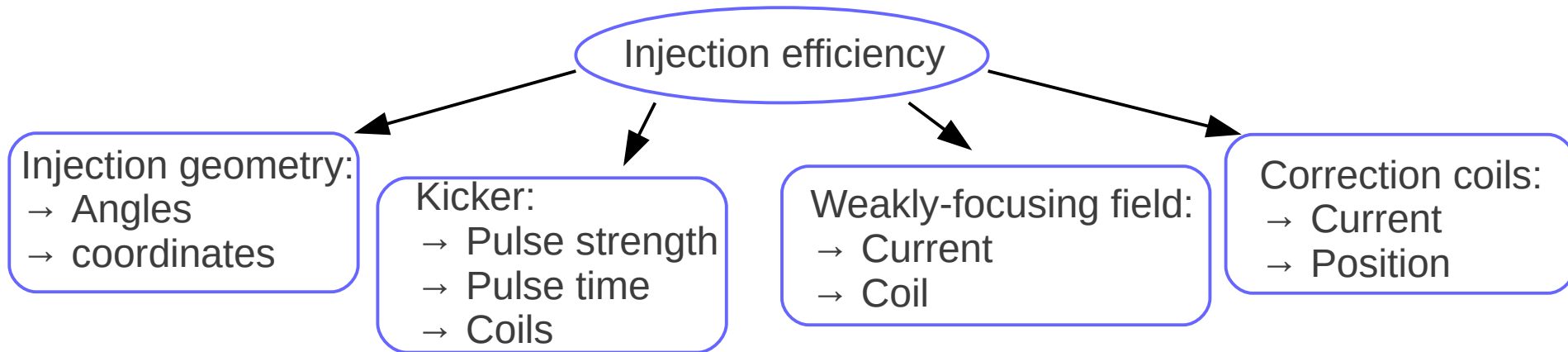


MuEDM Phase I in G4Beamline

- Muons are injected off-axis into 3 T solenoid
- Field gradient at injection corrected by correction coils
- Radial magnetic pulse generated by pair of anti-helmholtz coil
- Muons trapped in weakly-focusing magnetic field at the center generated by thin coils



Multivariate Optimization



- Multivariate optimization → computationally expensive
- G4Beamline simulation run for one configuration of input variables on HPC cluster takes ~6 hrs (for 1M muons)
- High fidelity simulations impossible to do given time constraint

PCE Based Surrogate Modelling

- Replace complex model with approximation → Surrogate Model
- Polynomial Chaos Expansion (PCE) :

$$Y = \sum_{i=0}^{\infty} \alpha_i \Psi_i (\vec{x})$$

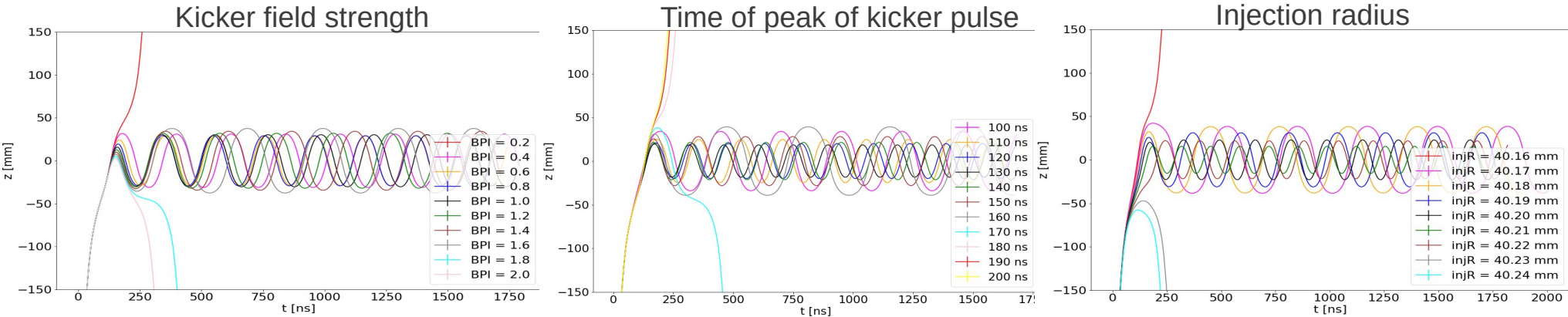
Y → Model response (injection efficiency), Ψ_i → Orthogonal polynomials
 x → input variables, α_i → expansion coefficients

- Polynomial basis based on input variable distribution
- Coefficients determined using regression based methods

$$\vec{\alpha} = \text{Argmin} \frac{1}{N} \sum_{j=1}^N \left\{ f(\vec{\xi}^j) - \sum_{i=0}^{P-1} \alpha_i \Psi_i (\vec{x}^j) \right\}^2$$

Initial Parameter Bounds

- Preliminary optimization with 8 parameters with range determined using rough scans in G4Beamline with the reference particle

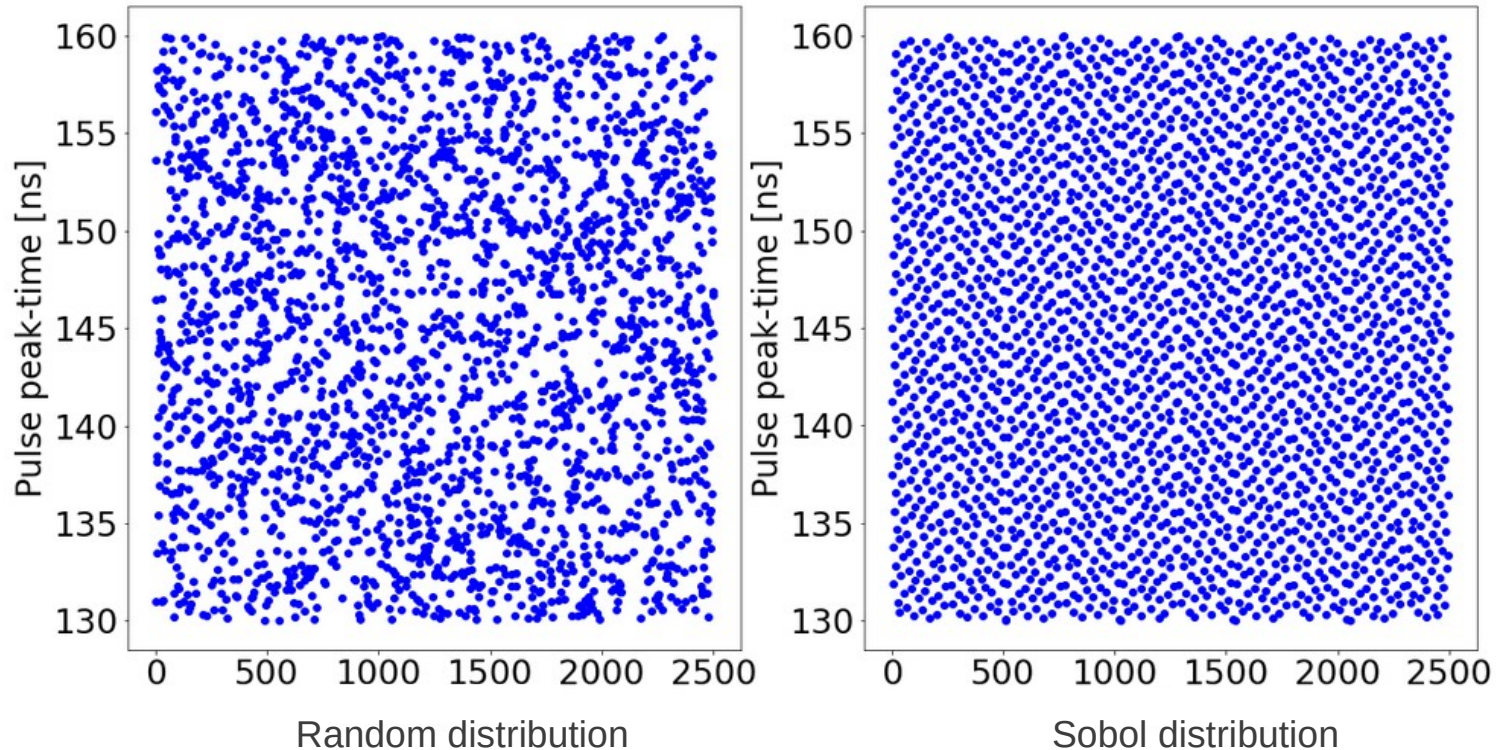


- Best guess input parameter range:

Parameter symbol	Physics Parameter	Lower bound	Upper bound
Theta	Injection angle (degrees)	47.38	47.45
Phi	Transverse angle (degrees)	5.4	5.9
InjR	Injection radius (mm)	40.0	40.4
Z	Longtudinal Injection coordinate (mm)	-437	-433
BPI	Kicker Field Strength (arb. unit)	-1.4	-0.2
KPT	Time of peak of Kicker Pulse (ns)	130	160
W	Width of the Kicker Pulse (ns)	15	55
WC	Weak Current*100 (A)	100	700

Initial Distribution: Sobol Points

- Monte Carlo techniques rely on random distribution of samples
- Prone to clusters and empty spaces, slow convergence, probabilistic error bounds



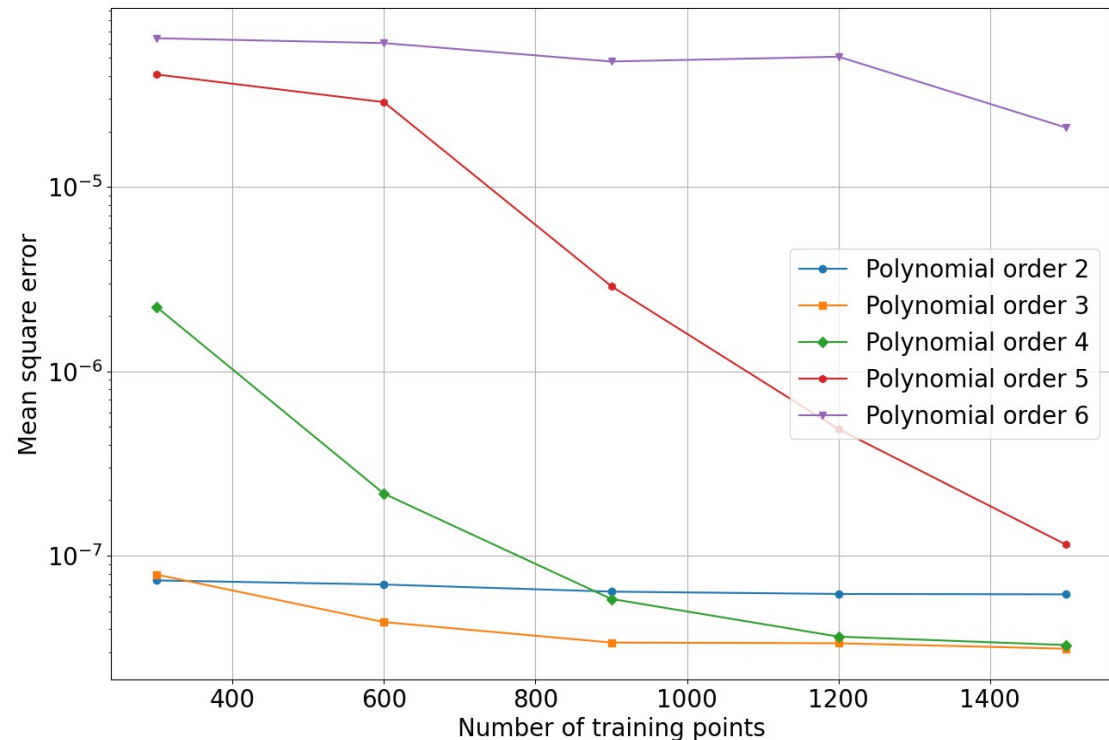
- Low discrepancy distributions like Sobol sequence preferred, deterministic error bounds, uniformly spans the given range

PCE Regression Analysis

- Run G4bl simulations with parameter sample space given by Sobol distribution
- For regression based estimation of coefficients, number of training samples is $N=(d-1)P$;
- $P \rightarrow$ terms in polynomial expansion: $P = \frac{(p+d)!}{p!d!}$, $d \rightarrow$ dimension, $p \rightarrow$ polynomial degree
- Storage criteria:

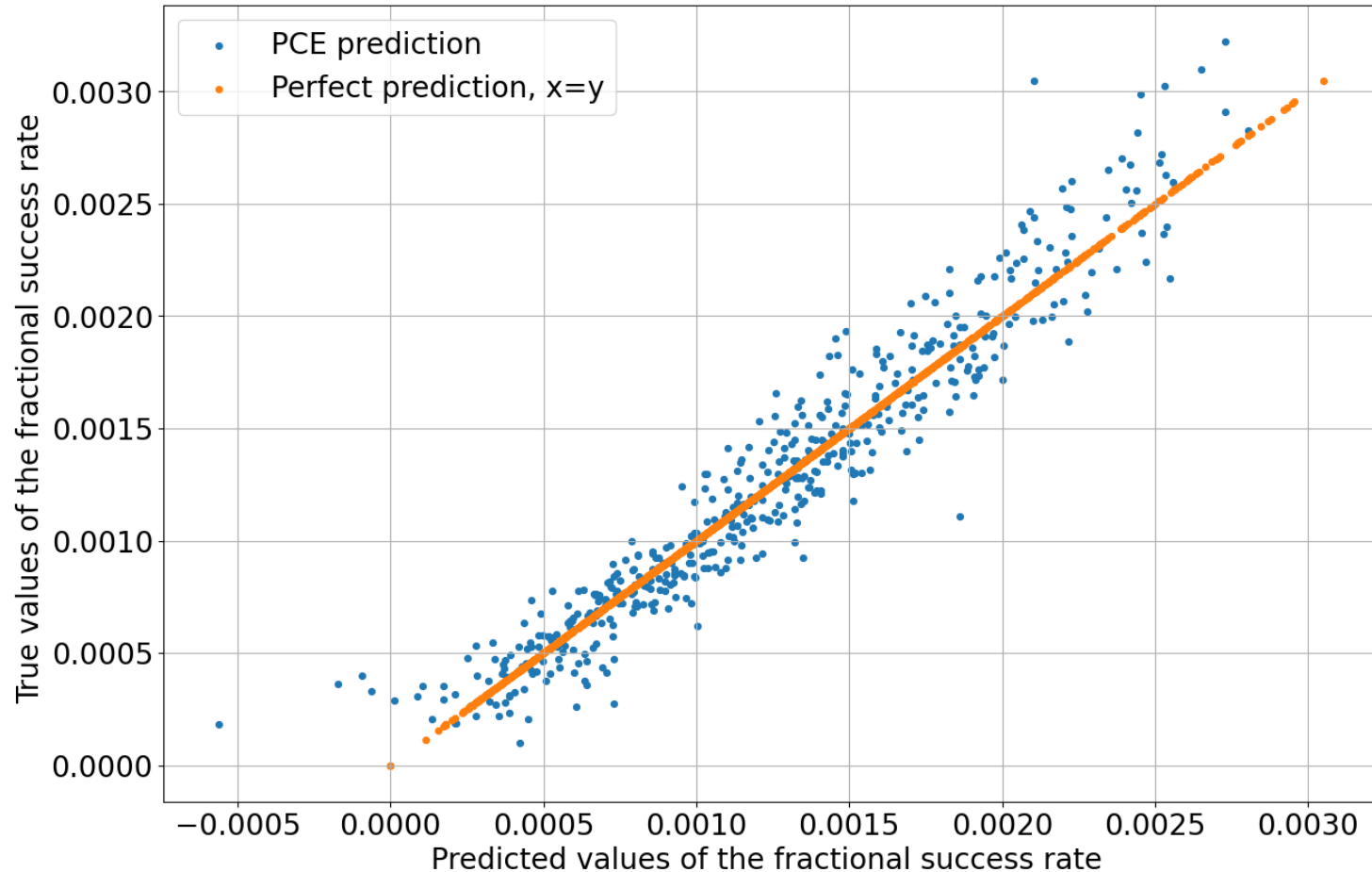
muon decaying/killed
with $-40\text{mm} < z < 40\text{mm}$
and $-0.5\text{MeV} < Pz < 0.5\text{MeV}$

- Python toolbox chaospy for generating expansion and regression fit
- Lowest MSE for poly order 3, poly order 4 converging fast
- ~1100 points needed for poly order 3,
~3500 points needed for poly order 4

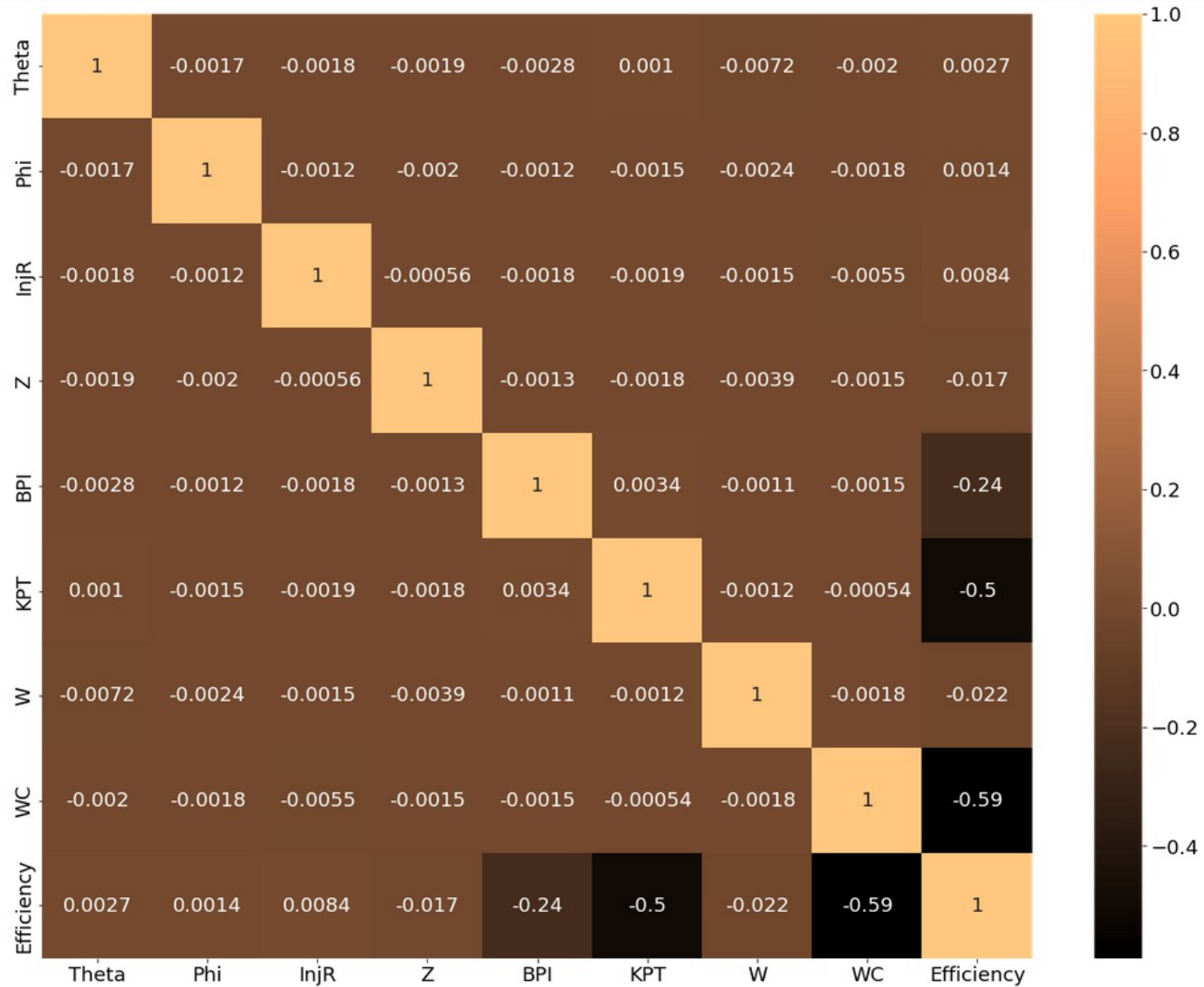


PCE Regression Analysis

- Comparison of true efficiency (orange) and model predicted efficiency (blue) for polynomial order 3

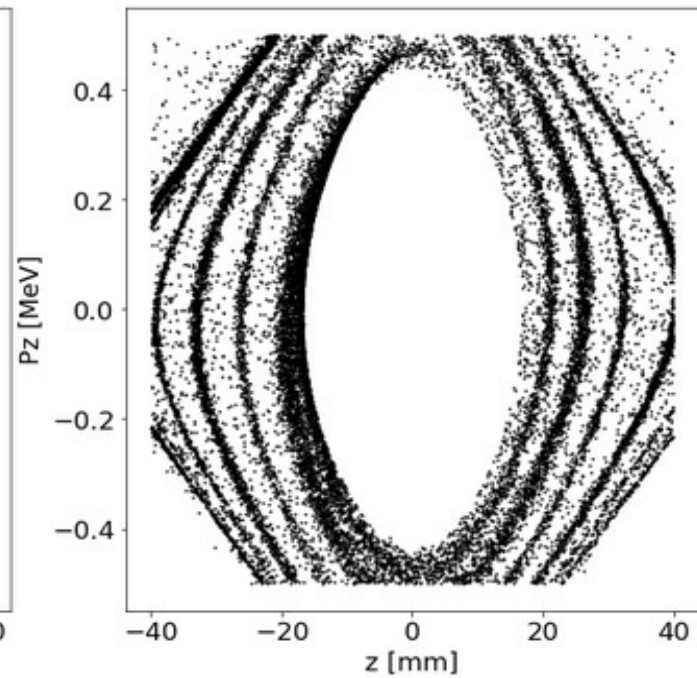
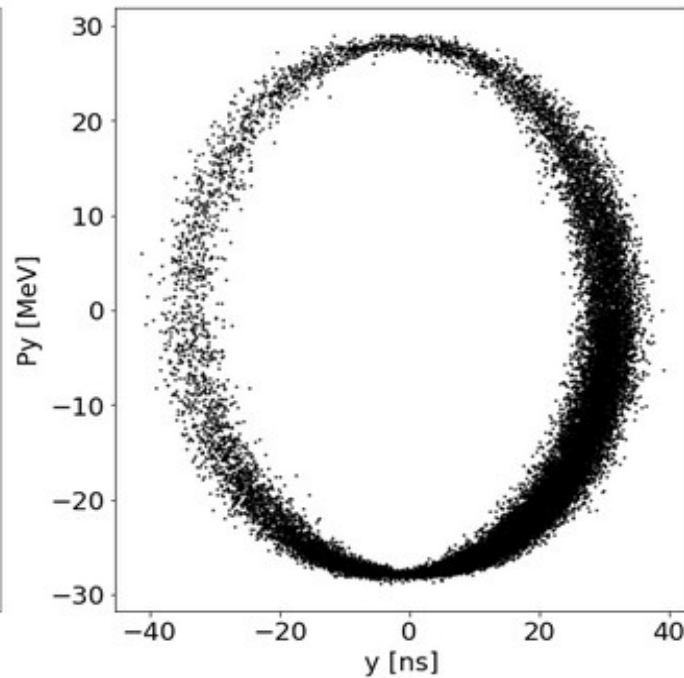
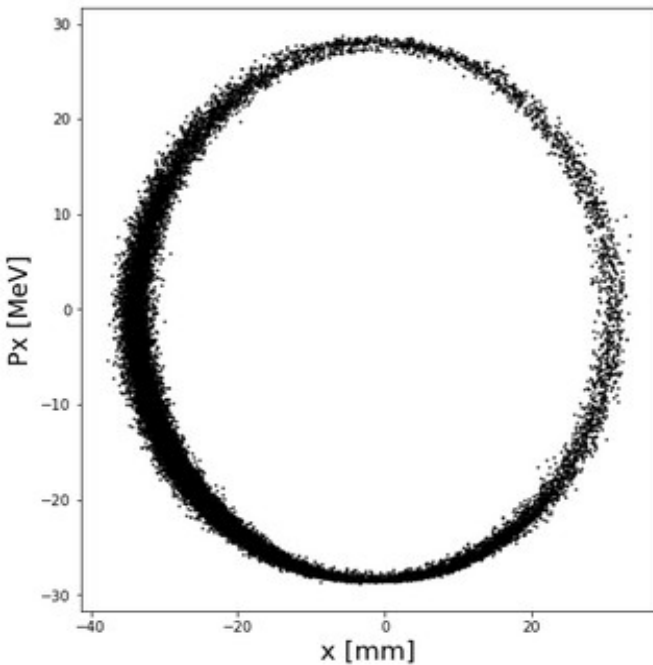


PCE Analysis Correlation Matrix



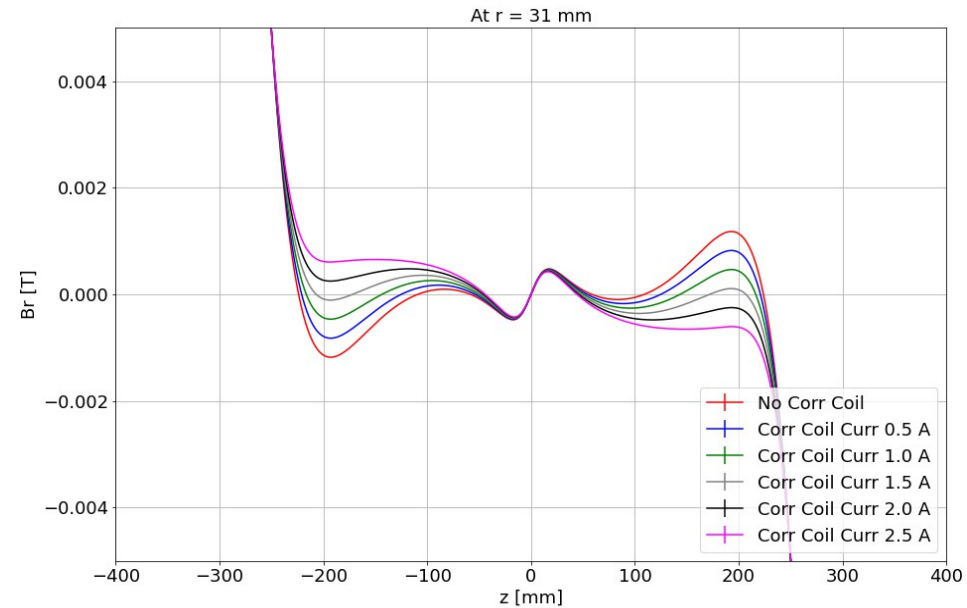
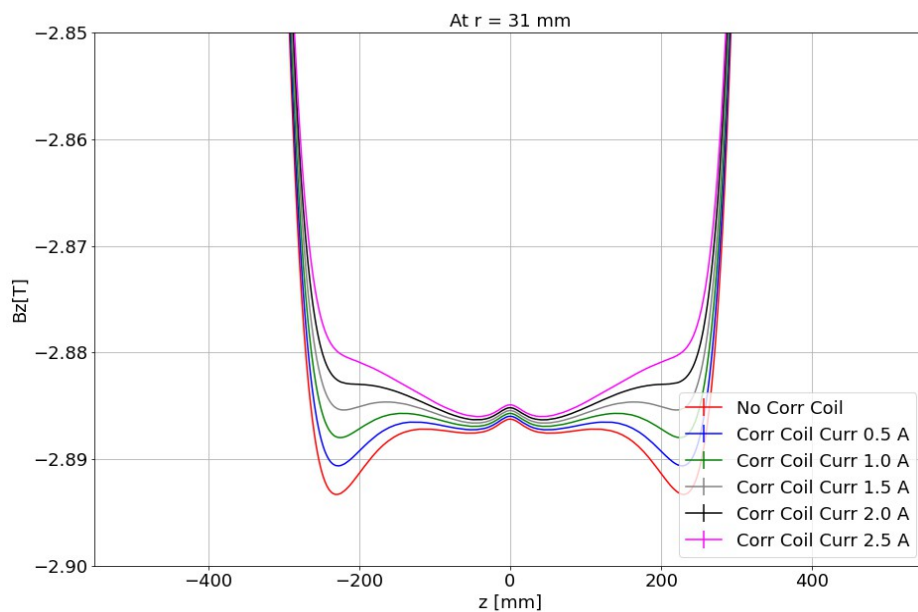
Current Status

- Need to generate muon distribution in storage region for detector design
- Currently trying to use the maximum efficiency parameters to generate distribution
- 3000 stored from 1M injected muons → Extrapolating to generate larger distributions



Current Status

- Currently running the next iteration of optimization → Excluded geometric parameters
- New parameter → distance between the pair of kicker coils, current in the correction coil
- Correction coils needed to reduce field gradient at injection



- Reduction in CC current desirable to control heat dissipation

Summary

- Injection efficiency depends on a range of design parameter
- Off-axis beam injection simulation in G4Beamline
- Maximize injection efficiency, determine acceptable input variable range
- Multivariate optimization problem → approximated by PCE based surrogate modeling
- Best modeled by polynomial degree 3, less sensitivity to geometric parameters
→ increase in training samples needed to reduce MSE
- Generate muon distribution in storage region based on the maximum efficiency parameters
- Optimize other input variables affecting injection efficiency

Thank You for Your Attention!

MuEDM Collaboration



Project funded by



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Confederaziun svizra

Swiss Confederation

Federal Department of Economic Affairs,
Education and Research EAER
**State Secretariat for Education,
Research and Innovation SERI**

Extra

Sensitivity indices: Example, when d=3

Response function representation:

$$Y = f(x_1, x_2, x_3) = f_0 + f_1(x_1) + f_2(x_2) + f_3(x_3) + f_{12}(x_1, x_2) + f_{13}(x_1, x_3) + f_{23}(x_2, x_3) + f_{123}(x_1, x_2, x_3)$$

Total variance:

$$D = \int_{\text{id}} f^2(x_1, x_2, x_3) dx_1 dx_2 dx_3 - f_0^2$$
$$= D_1 + D_2 + D_3 + D_{12} + D_{13} + D_{23} + D_{123}$$

with

$$D_1 = \int f_1^2(x_1) dx_1, D_2 = \int f_2^2(x_2) dx_2 \dots\dots$$

$$D_{12} = \int f_{12}^2(x_1, x_2) dx_1 dx_2, D_{23} = \int f_{23}^2(x_2, x_3) dx_2 dx_3, \dots\dots \text{and so on}$$

Sensitivity indices: $S_1 = D_1/D$, $S_{12} = D_{12}/D$, $S_{123} = D_{123}/D$, etc

and

$$S_1 + S_2 + S_3 + \dots + S_{123} = 1$$

Sensitivity Analysis in Surrogate Model

$$\text{PCE expansion: } Y = \sum_{i=0}^{\infty} \alpha_i \Psi_i(\vec{x}) \quad , \quad (\vec{x}) = (x_1, x_2, \dots, x_d) \quad , \quad d\text{-dimension}$$

For input variables

$$(x_1, x_2, \dots, x_d) \in I^d := [0, 1]^d$$

Model response Y can be represented by

$$Y = f(x_1, x_2, \dots, x_d) = f_0 + \sum_{i=1}^d f_i(x_i) + \sum_{1 \leq i < j \leq n} f_{ij}(x_i, x_j) + \dots + f_{12\dots d}(x_1, x_2, \dots, x_d),$$

if:

$$1. \quad f_0 = \int_{I^d} f(\vec{x}) d\vec{x}$$

$$2. \quad \int_0^1 f_{i_1, i_2, \dots, i_s}(x_{i_1}, x_{i_2}, \dots, x_{i_s}) dx_k = 0$$

where $k = i_i, \dots, i_d$ and $s = 1, 2, \dots, d$

The variance of the function is:

$$D = \int_{I^d} f^2(\vec{x}) d\vec{x} - f_0^2$$

$$\text{Alternatively } D = \sum_{i=1}^d D_i + \sum_{1 \leq i < j \leq n} D_{ij} + \dots + D_{12\dots d}$$

where

$$D_{i_1, i_2, \dots, i_s} = \int_{I^s} f_{i_1, i_2, \dots, i_s}^2(x_{i_1}, x_{i_2}, \dots, x_{i_s}) dx_{i_1} dx_{i_2} \dots dx_{i_s}$$

with $1 \leq i_1 < i_s \leq d$

Sobol sensitivity indices are defined as:

$$S_{i_1, i_2, \dots, i_s} = \frac{D_{i_1, i_2, \dots, i_s}}{D}$$

and satisfy the condition

$$\sum_{i=1}^d S_i + \sum_{1 \leq i < j \leq n} S_{ij} + \dots + S_{12\dots d} = 1$$

Sensitivity indices: Results

- Python Chaospy toolbox has built-in functions to calculate sensitivity indices
- First order, second order and total sensitivity indices can be calculated
- The input parameter distribution should be scaled to range [0,1]
- Main Sensitivity indices for poly order 3:

Parameter symbol	Physics Parameter	Main sensitivity index, Polynomial degree 3
Theta	Injection angle (degrees)	3.39230879e-08
Phi	Transverse angle (degrees)	3.86979007e-07
InjR	Injection radius (mm)	1.88544294e-06
Z	Longtudinal Injection coordinate (mm)	4.16966789e-08
BPI	Kicker Field Strength (arb. unit)	1.40754537e-04
KPT	Time of peak of Kicker Pulse (ns)	9.03986321e-04
W	Width of the Kicker Pulse (ns)	4.89511202e-02
WC	Weak Current*100 (A)	9.12374997e-01

Sum = 0.9624

- Relative sensitivities, dependent on initial range provided

Sensitivity indices: From PCE coefficients

$$\hat{S}_{i_1, i_2, \dots, i_s} = \frac{1}{\hat{D}} \sum_{\mathbf{i} \in I_{i_1, i_2, \dots, i_s}} \alpha_{\mathbf{i}}^2 \langle \Psi_{\mathbf{i}}^2 \rangle$$

where

$$I_{i_1, i_2, \dots, i_s} = \left\{ \mathbf{i} : \begin{array}{l} i_k > 0 \forall k = 1, \dots, s, k \in (i_1, \dots, i_s) \\ i_k = 0 \forall k = 1, \dots, n, k \notin (i_1, \dots, i_s) \end{array} \right\}$$

The variance, \hat{D} is given by

$$\hat{D} = \sum_{j=1}^{P-1} \alpha_{i_j}^2 \langle \Psi_{i_j}^2 \rangle.$$

From this, the main and total sensitivity is computed as

$$\hat{S}_j = \frac{1}{\hat{D}} \sum_{\mathbf{i} \in I_j} \alpha_{\mathbf{i}}^2 \langle \Psi_{\mathbf{i}}^2 \rangle$$

where $I_j = \{\mathbf{i} = (i_1, i_2, \dots, i_d) : i_k > 0 \forall k = j \wedge i_k = 0 \forall k \neq j\}$ and

$$\hat{S}_j^T = \frac{1}{\hat{D}} \sum_{\mathbf{i} \in I_j} \alpha_{\mathbf{i}}^2 \langle \Psi_{\mathbf{i}}^2 \rangle$$

where $I_j = \{\mathbf{i} = (i_1, i_2, \dots, i_d) : i_j > 0\}$, respectively.

Neural Network Regression

- No. of neurons: **512**

Hidden layers: **8**

Activation function:
Leaky ReLU

Scheduler:
ReduceLROnPlateau

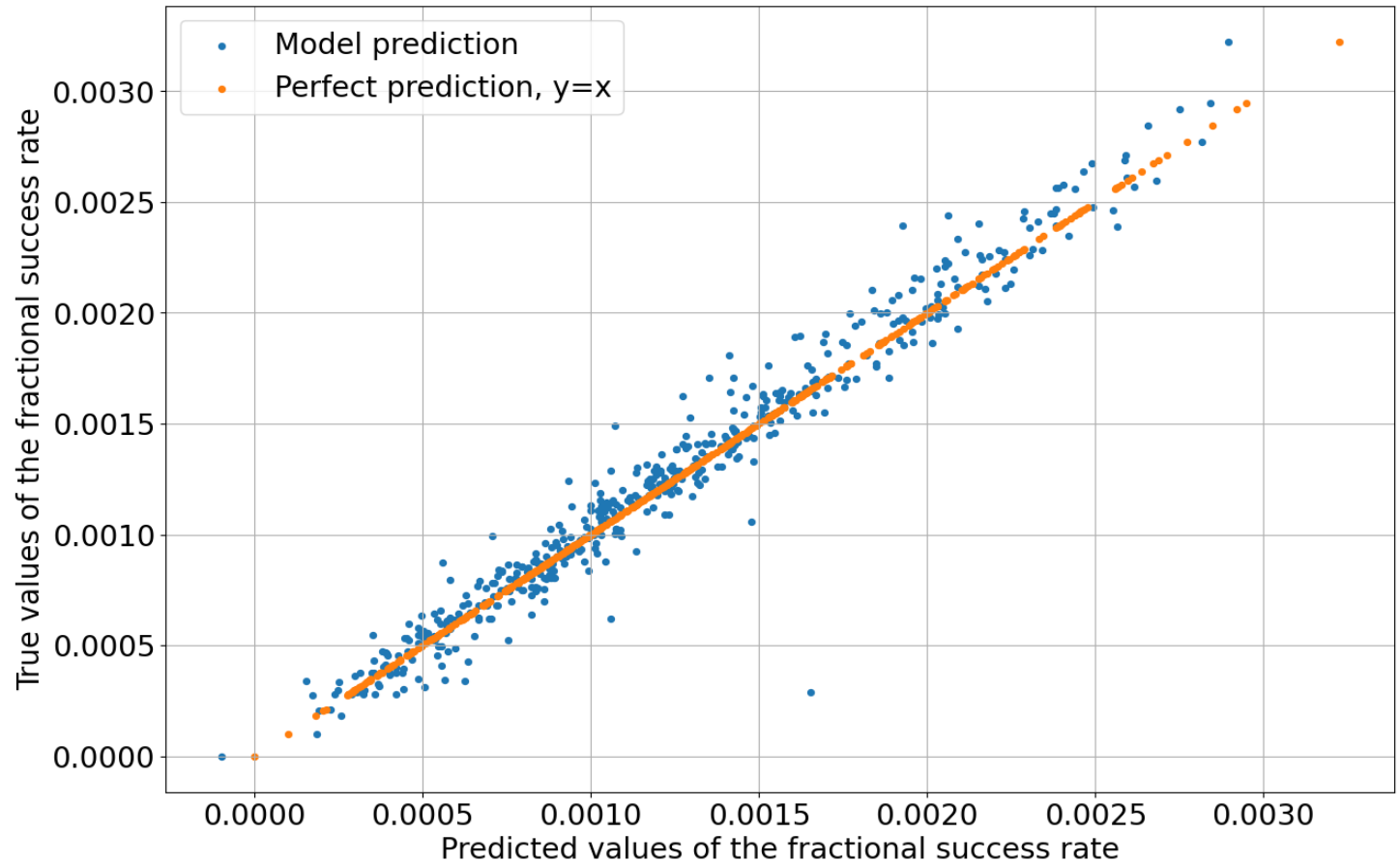
Batch size: **500**

Epoch: **400**

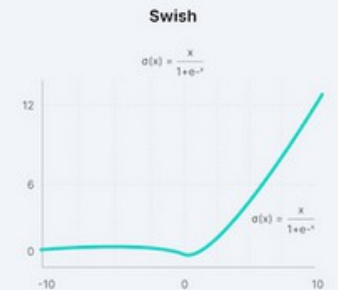
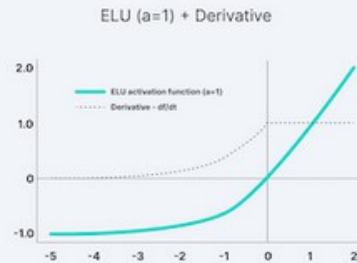
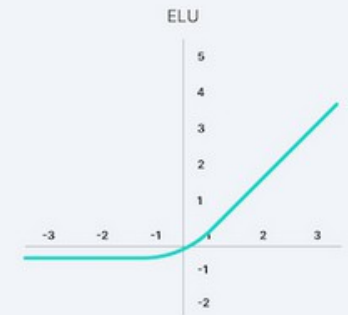
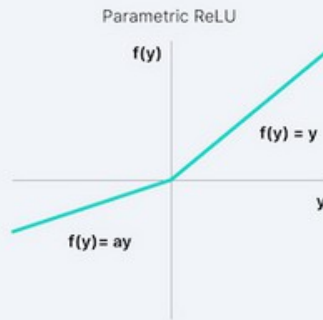
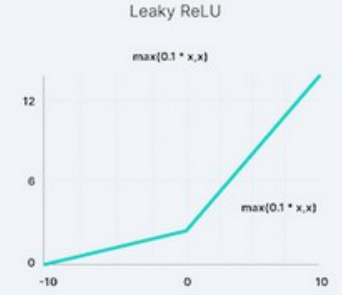
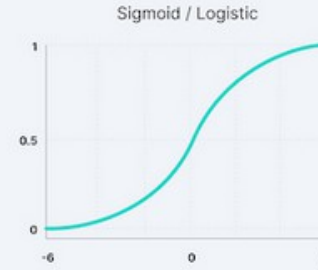
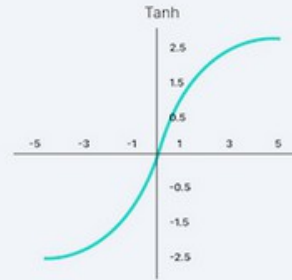
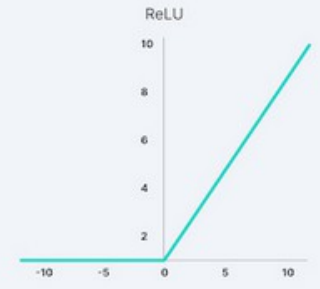
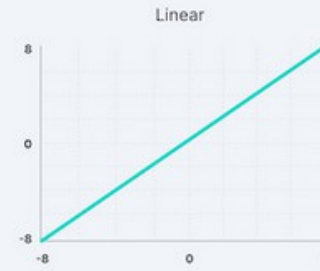
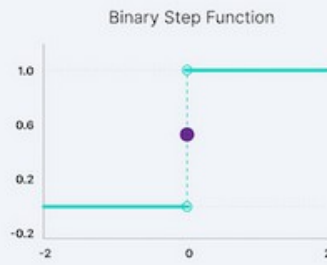
Optimizer: **Adam**

Dropout rate: **10%**

- Better agreement between true and predicted



Neural Network activation functions



Number of expansion coefficients, P and Integration points (sample size), N

d	p	P	N
6	3	84	420
6	4	210	1050
6	5	462	2310
7	3	120	720
7	4	330	1980
7	5	792	4752
8	3	165	1155
8	4	495	3465
8	5	1287	9009