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RFQ BEAM DYNAMICS OPTIMIZATION USING MACHINE LEARNING

D. Koser*, J. M. Conrad, L. H. Waites, D. Winklehner, MIT, Cambridge, MA, USA
A. Adelmann, S. Mayani, PSI, Villigen, Switzerland
M. Frey, University of St. Andrews, St. Andrews, UK

Abstract

To efficiently inject a high-current H_2^+ beam into the 60 MeV driver cyclotron for the proposed IsoDAR project in neutrino physics, a novel direct-injection scheme is planned to be implemented using a compact radio-frequency quadrupole (RFQ) as a pre-buncher, being partially inserted into the cyclotron yoke. To optimize the RFQ beam dynamics design, machine learning approaches were investigated for creating a surrogate model of the RFQ. The required sample datasets are generated by standard beam dynamics simulation tools like PARMTEQM and RFQGen or more sophisticated PIC simulations. By reducing the computational complexity of multi-objective optimization problems, surrogate models allow to perform sensitivity studies and an optimization of the crucial RFQ beam output parameters like transmission and emittances. The time to solution might be reduced by up to several orders of magnitude. Here we discuss different methods of surrogate model creation (polynomial chaos expansion and neural networks) and identify present limitations of surrogate model accuracy.

INTRODUCTION

In modern ion accelerators radio-frequency quadrupoles (RFQs) typically are the first RF accelerator structure behind the low energy beam transport (LEBT) section and combine the following functions:

- The transversally defocusing effect of the space charge force has a $1/\gamma^2$-dependency and hence at low beam velocities efficient (and velocity-independent) transversal focusing is required. As shown in Fig. 1, the alternating electric quadrupole field leads to a focusing force along one of the transverse axes while defocusing occurs in the perpendicular direction, effectively constituting an alternating gradient focusing channel. The transversal focusing strength in an RFQ cell n is commonly characterized by the parameter B_n [1].

- By adding a sinusoidal modulation to the electrode shape, a longitudinal field component is generated which can be used to adiabatically bunch the DC input beam. This is a highly delicate procedure due to the high sensitivity of space-charge dominated beams to perturbations of the beam density. The consecutive modulation cells form a π-mode accelerator structure with a cell length of $\ell_c = \beta_c \lambda_{\mathrm{RF}}/2$. The extent of electrode modulation (corresponding to the magnitude of the longitudinal field component) of a cell n is parameterized by the modulation factor m_n.

- The synchronous phase $\phi_{s,n}$, which is adjusted by the cell lengths, determines the ratio of longitudinal bunching to acceleration and the overall phase space stability. By increasing $\phi_{s,n}$ along the RFQ, beam acceleration is gradually introduced.

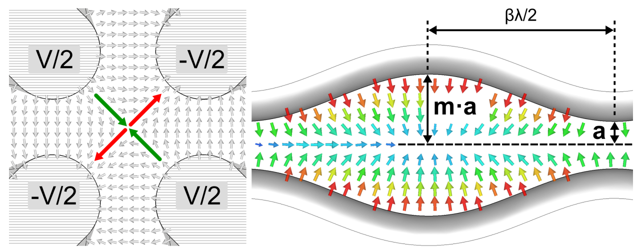

Figure 1: Transversal electric quadrupole field in an RFQ (*left*) with focusing/defocusing plane (green/red) and electrode cell modulation (*right*), resulting in a longitudinal field component.

Accordingly, the beam dynamics properties of an RFQ with a number of n cells are fully described by the parameter sets $\mathbf{B} = (B_1, \ldots, B_n)$, $\mathbf{m} = (m_1, \ldots, m_n)$ and $\boldsymbol{\phi}_s = (\phi_{s,1}, \ldots, \phi_{s,n})$.

Since finding an optimized beam dynamics design usually requires a very large number of simulation iterations, the design procedure of RFQs can be time consuming, especially when completely new solutions to meet the required beam output quality need to be explored. This is sometimes even the case for comparatively fast executing beam dynamics codes like PARMTEQM or RFQGen, but is definitely a problem when time consuming PIC simulations are used as the basis for optimization.

Most recently, uncertainty quantification (UQ) approaches have been developed to construct surrogate models that replicate the beam dynamics behavior in accelerators [2], using techniques based on polynomial chaos expansion (PCE) and neural networks (NN). By significantly reducing computational complexity compared to the corresponding physics simulation, surrogate models execute orders of magnitude faster. Optimizations based on surrogate models have already been demonstrated for different types of accelerator systems, such as ion injectors (linac), cyclotrons and electron accelerators [3, 4].

To optimize the beam dynamics design of the IsoDAR-RFQ, which is intended to be used for pre-bunching of a 5 mA H_2^+ beam for direct axial injection into a 60 MeV cyclotron [5], the developed machine learning techniques were applied to create a surrogate model of the RFQ and the applicability to different optimization problems was investigated (optimization of input beam twiss parameters, optimization of the entrance gap-field phase, full RFQ optimization).

* dkoser@mit.edu

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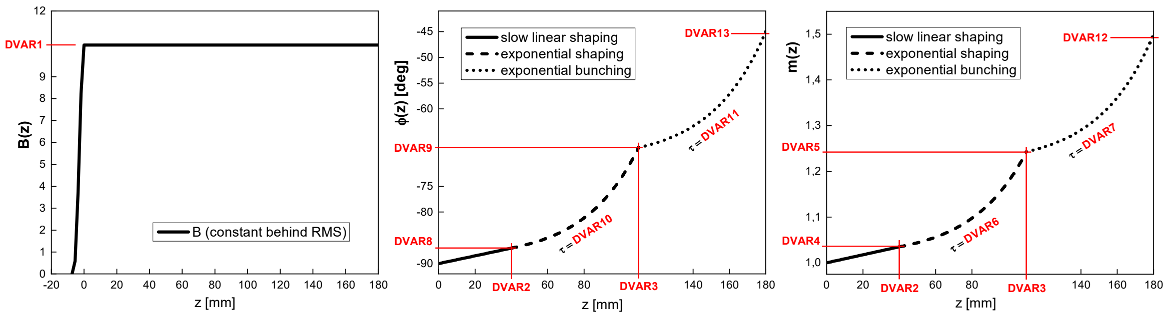

Figure 2: Parametrization functions $B(z)$, $\phi(z)$ and $m(z)$ of the RFQ cell properties.

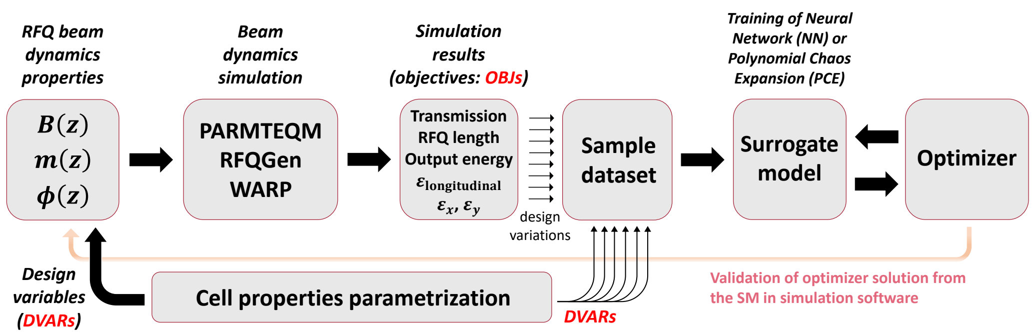

Figure 3: Machine learning optimization scheme for RFQ beam dynamics.

MACHINE LEARNING APPROACH TO RFQ BEAM DYNAMICS OPTIMIZATION

The optimization was based on beam dynamics simulations in PARMTEQM, which reads in the RFQ properties as an input table defining the functions $B(z)$, $\phi_s(z)$ and $m(z)$. For the case of the full RFQ optimization the RFQ was parameterized according to Fig. 2 by a total of 14 design variables (DVARs). The length of the RFQ is determined by **DVAR14**, being the cutoff energy after which PARMTEQM ends the electrode (always with a full RFQ cell).

As schematically depicted in Fig. 3, beam dynamics simulations were performed for a number of random RFQ design variations (randomized DVAR values), and the DVARs and corresponding simulated values of the objectives (transmission, RFQ length, output energy and emittances) for each run were stored in the sample dataset which was used to train either a neural network or use polynomial chaos expansion to create a surrogate model. Based on the surrogate model, an optimization was performed, the result of which (surrogate model output of the best found set of DVARs) was then compared to the result of the corresponding PARMTEQM simulation.

RESULTS – SURROGATE MODEL AND OPTIMIZATION ACCURACY

Different optimization problems have been studied:

- full RFQ optimization (14 DVARs)
- optimization of only the input beam twiss parameters (2 DVARs), the RFQ itself was not varied
- optimization of the entrance gap-field phase and the input beam twiss parameters (3 DVARs).

It was found that highly accurate (<1% mean average error, MAE) surrogate models can be obtained for the optimization of only the input beam twiss parameters (2 DVARs), as well as for a simplistic test case of a FODO lattice. For these simple cases, an optimization based on the surrogate model could be performed, with small deviation of the result to the beam dynamics simulation. In general, the use of neural networks leads to more accurate surrogate models compared to polynomial chaos expansion.

As shown in Fig. 4 and summarized in Fig. 5, the surrogate model for the full RFQ optimization suffers from much higher errors, especially regarding the emittances (>10%). This leads to unacceptable deviations of the SM optimization result compared to the PARMTEQM simulation of up to 40 %. In principle, this issue can be observed consistently in all optimizations where design variables are varied that directly affect the longitudinal phase space, such as the optimization of the phase of the longitudinal entrance gap-field which effectively pre-bunches the beam prior to entering the radial matching section of the RFQ. In none of the problematic cases did the error values improve significantly by switching off space charge (beam dynamics simulation with zero-current).

As depicted in Fig. 6, the surrogate model lends itself to performing sensitivity analyses investigating the impact of DVAR variation on the optimization objectives. Eventually, this allows evaluation of the cell properties parametrization model and to reduce the number of DVARs by omitting variable variations with little effect on the crucial optimization objectives.

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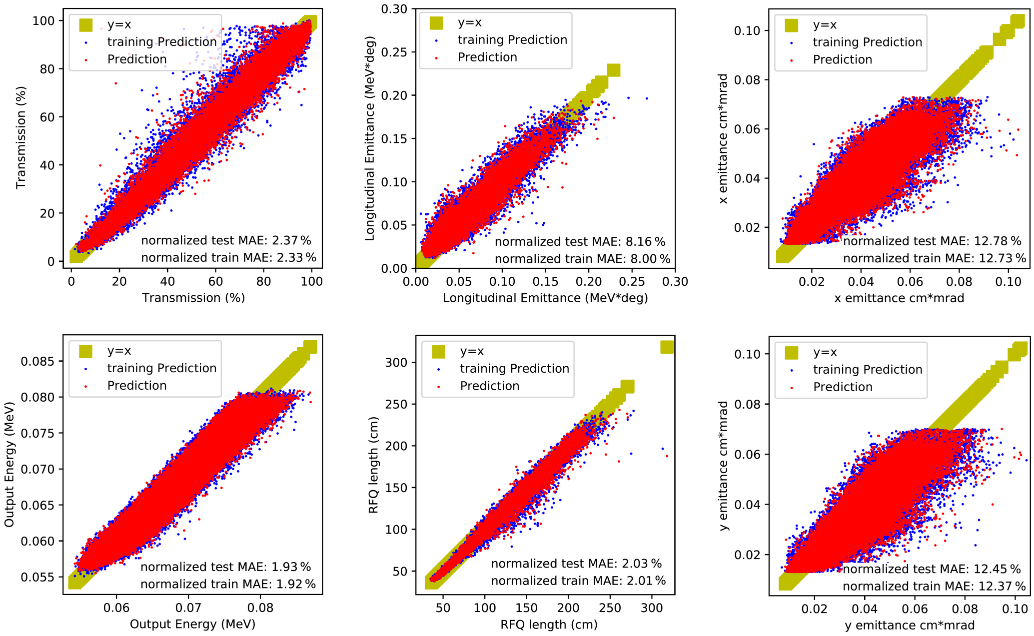

Figure 4: Surrogate model output (y-axis) vs. sample result value (x-axis) for the training and prediction datasets.

MAE's [%]	Input beam optimization (2 DVARs)		Full RFQ optimization (14 DVARs)	
	PCE	NN	PCE	NN
Transmission	0.17	0.15	3.45	2.37
$\varepsilon_{\text{longitudinal}}$	0.72	0.57	10.51	8.16
ε_x	1.85	0.55	13.19	12.78
ε_y	0.74	0.71	13.29	12.45
Output energy	*no variation*		1.82	1.93
RFQ length			1.16	2.03

Figure 5: Comparison between mean average errors (MAE's) for surrogate models based on polynomial chaos expansion (PCE) and neural networks (NN) for different optimization cases and objectives.

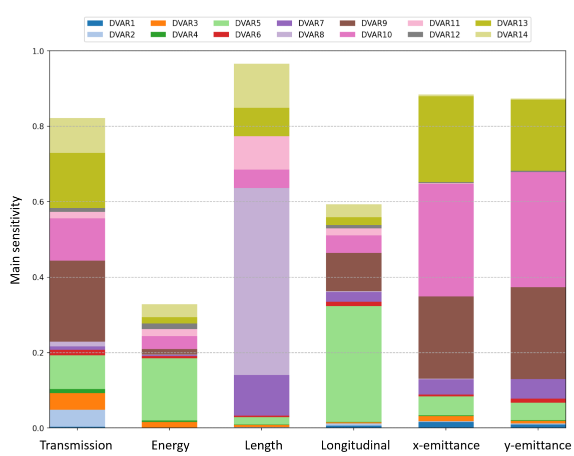

Figure 6: Sensitivity plot for the full RFQ optimization with 14 design variables (DVARs).

CONCLUSION & OUTLOOK

While some use cases (e.g. FODO lattice or RFQ input beam twiss parameters optimization) can already be modeled with high accuracy, the origin of the larger errrors regarding design parameter variations that affect the longitudinal phase space is currently being investigated. To allow an accurate surrogate model based optimization of the full RFQ, possible solutions such as a modification of the used neural network are being evaluated.

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