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A PHYSICS-MOTIVATED SURROGATE FRAMEWORK FOR BEAM TRANSPORT OPTIMIZATION IN LINEAR ACCELERATORS

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Why Surrogate-Assisted Optimization?

Traditional Optimization Loop

Machine Parameters

⇩

High-Fidelity Simulation

⇩

Beam Properties
(σ, ε, Energy, Twiss, Transmission, ...)

⇩

Optimization Algorithm

Next Candidates

🔴 Every candidate → High-Fidelity Simulation

Computational Bottleneck

- One high-fidelity simulation per candidate
- Large number of repeated evaluations
- Runtime dominated by simulations

Surrogate-Assisted Optimization

Machine Parameters

⇩

Surrogate Model
Feasibility Screening
Fast Beam Prediction

⇩

High-Fidelity Simulation
(Verification)

⇩

Beam Properties
(σ, ε, Energy, Twiss, Transmission, ...)

⇩

Optimization Algorithm

Next Candidates

🟢 Only promising candidates → High-Fidelity Simulation

High-Fidelity Beam Dynamics Simulations

↓

Training Dataset

↓

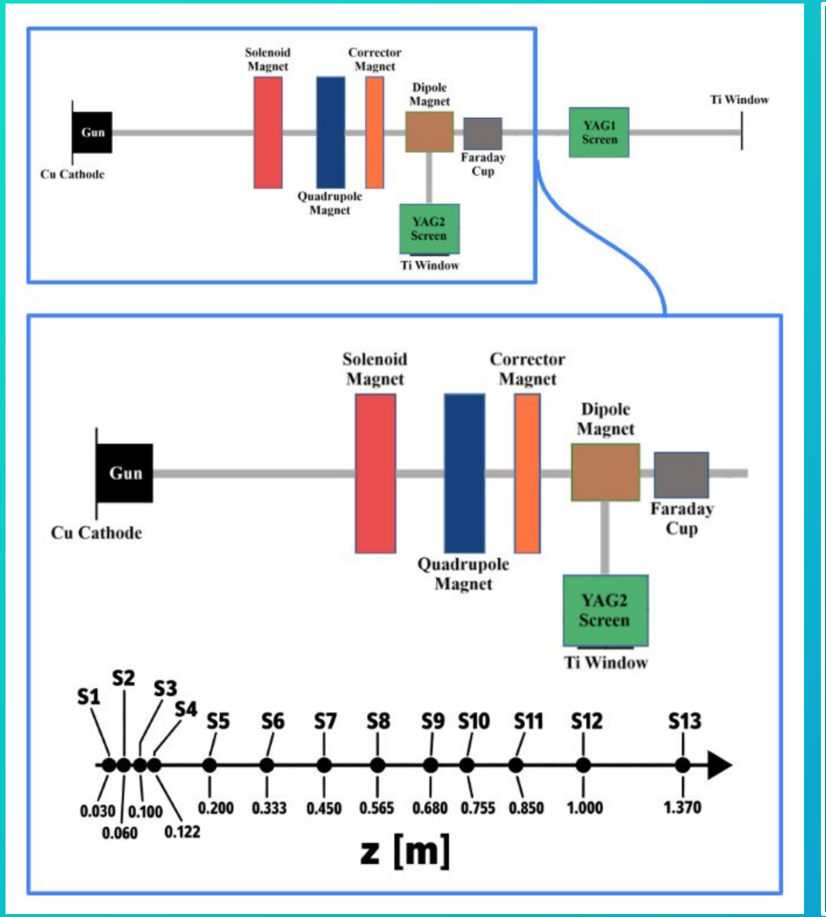
Surrogate Model

Surrogate Model

Classifier
Predicts whether a candidate machine setting is feasible

Regressor
Beam properties prediction for feasible candidates

AREAL Validation Case & Training Dataset



Predicted Beam Properties

Horizontal RMS Beam Size	σ_x
Vertical RMS Beam Size	σ_y
Longitudinal RMS Beam Size	σ_z
Horizontal Normalized Emittance	$\varepsilon_{n,x}$
Vertical Normalized Emittance	$\varepsilon_{n,y}$
Horizontal Twiss Alpha	α_x
Horizontal Twiss Beta	β_x
Vertical Twiss Alpha	α_y
Vertical Twiss Beta	β_y
Mean Energy	$\langle E \rangle$
Energy Spread	σ_E
Transmission	T

13 snapshots X 12 properties =
= 156 regression targets

Latin Hypercube Sampling
500,000 candidate machine settings

ASTRA Simulations
10,000 production attempts
8,000 macroparticles

Training Datasets
Classifier: 9,975 cases
Regression: 8,855 successful cases

Machine Parameters
Maximum on-axis RF field, RF Phase, Solenoid Field, Quadrupole Gradient

High-Fidelity Simulator:
ASTRA (A Space Charge **TR**acking **Al**gorithm**)**

Low-Energy Space-Charge-Sensitive Case
(150 pC, 1 - 3.6 MeV)

From Feasibility Screening to Direct Baseline

DANGEROUS MISS

=

Failed transport case classified as feasible

Sends candidate to regression where meaningful properties do not exist

Classifier Performance

839 → Correct PASS
47 → Conservative BLOCK
0 → Dangerous miss
112 → Correct BLOCK

100% Regressor Input Purity
94.7% Good Beam Retention

Direct Regression Experiment

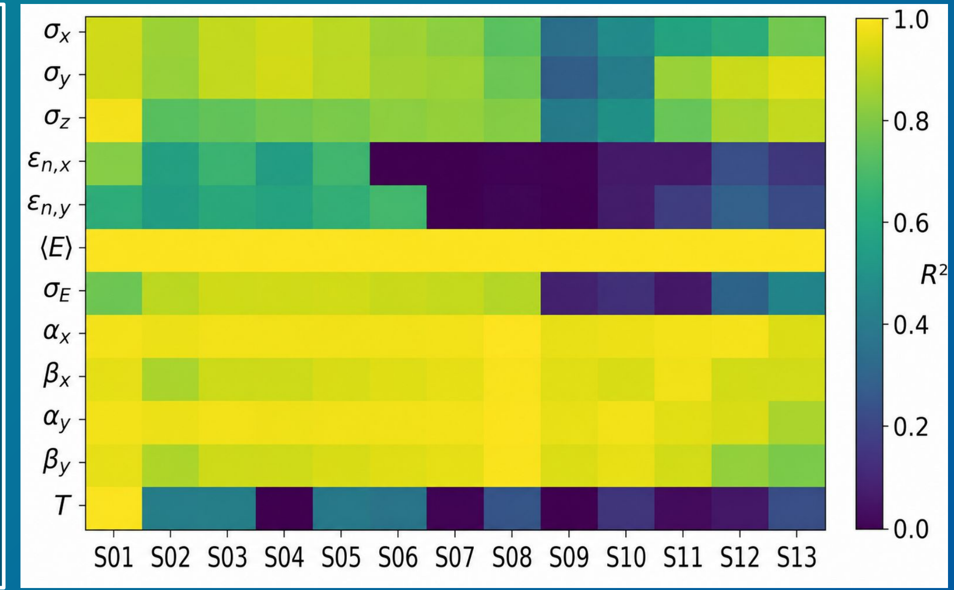
Machine Parameters
(E_0; ϕ; B_{sol}; Q_{grad})

↓

Regressor

↓

12 properties at snapshot S_k, where k = 1, 2, ..., 13



13 Regression Strategies Benchmarked

Dummy Regressor,
ExtraTrees Multi Output,
3 Different Size Shared MLPs,
3 Different Size Separate MLPs

Ridge ScaledX,
LightGBM Separate Per Target,
3 Different Size Multi Head MLPs,

Direct prediction is strongly property- and position-dependent, with the weakest performance observed for downstream emittance.

Beam-State Representation Matters

Direct Regression: $S_k = f(\text{machine parameters})$

Order 1 Full State: $S_k = f(\text{machine parameters}, S_{k-1})$

Order 2 Full State: $S_k = f(\text{machine parameters}, S_{k-1}, S_{k-2})$

Order 1 Delta: $S_k = f(\text{machine parameters}, \Delta S)$

Order 2 Full State + Delta: $S_k = f(\text{machine parameters}, S_{k-1}, \Delta S)$

(Where $\Delta S = S_{k-1} - S_{k-2}$)

- Same ExtraTrees regressor
- Same data split
- Only the input representation changes

Best: previous state + recent change

Property	Improvement (MAE Reduction)
σ_x	10.1x
σ_y	15.0x
σ_z	9.1x
$\varepsilon_{n,x}$	6.5x
$\varepsilon_{n,y}$	7.1x
α_x	19.2x
β_x	13.4x
α_y	17.6x
β_y	13.4x
σ_E	4.1x
T	2.6x

Thank you!

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