Surrogate Modelling for Laser Driven Ion Acceleration: A Transfer Learning Approach, Current Status

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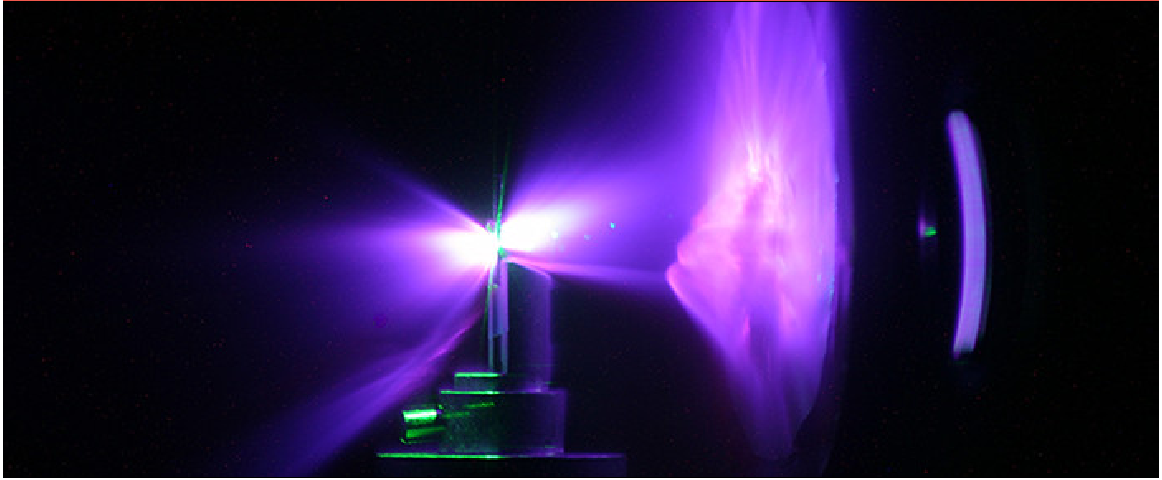

Nuclear Photonics

General Idea – Laser-driven Neutron sources
Pitcher-Catcher Setup

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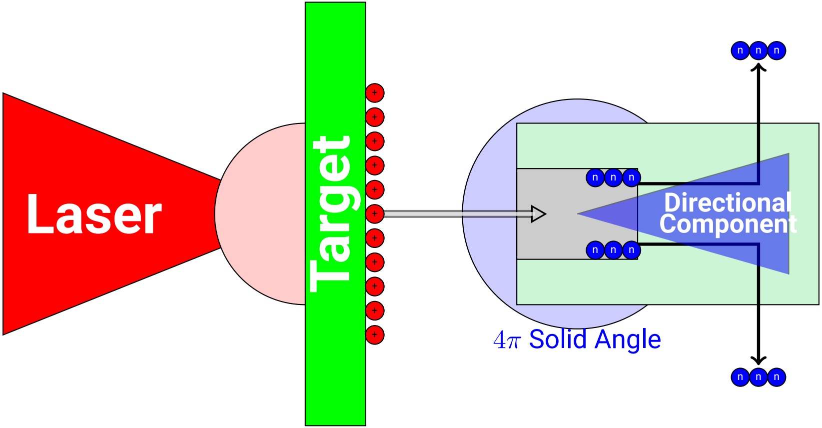

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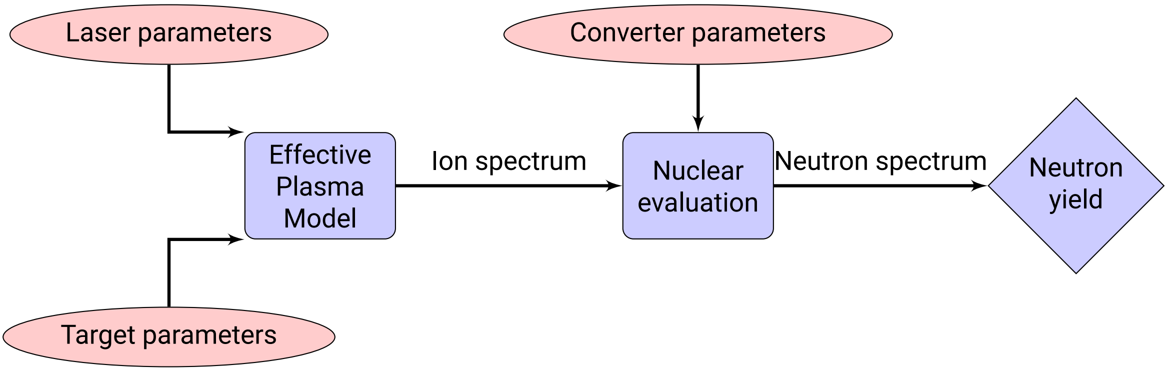
General Idea – Laser-driven Neutron sources
Effektiv Model



Part I: Laser Plasma Accelerators

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1. Basic Mechanisms
2. Issues / Uncertainties
3. Methodics

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Laser Component
Target Normal Sheath Acceleraion (TNSA)

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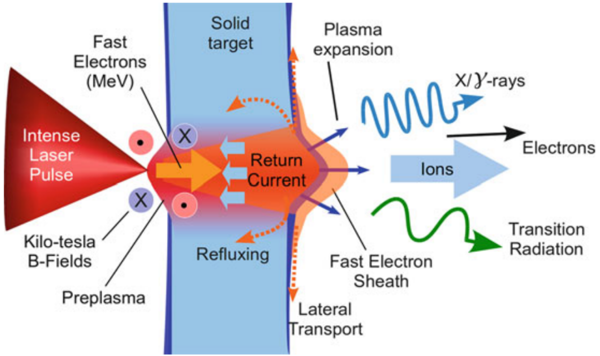
1. **Intense laser** hits target
2. **Ponderomotive force** accelerates electrons
3. **Electron Sheath** forms at the back
4. **Charge separation** accelerates Ions



Roth M., Schollmeier M. (2013) Ion Acceleration: TNSA.
In: Laser-Plasma Interactions and Applications. Springer, Heidelberg

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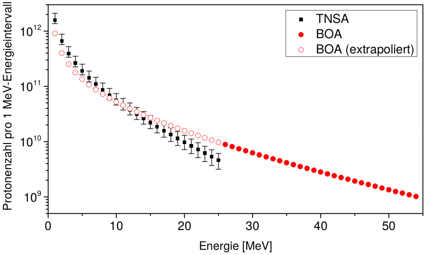
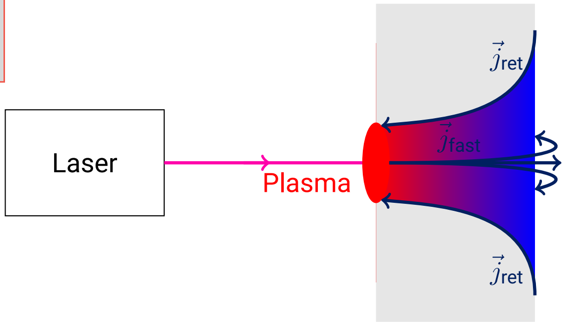
Laser Component Uncertainties

Ion spectrum deviates

- Reproducibility of laser pulse
- Instabilities in laser-plasma-interaction
- Nonlinear effects





Florian Wagner, PhD Thesis, 2014, TU Darmstadt

Plasma Physic Methods
Mathematical Formulation

- Vlasov-Maxwell EQS
- Many particles
- Sharp boundaries

⇒ Particle in cell simulations

⇒ Full 3D EM Solver

$$\frac{\partial f_\alpha}{\partial t} + \vec{v}_\alpha \cdot \nabla f_\alpha + q_\alpha \left(\vec{E} + \vec{\beta} \times \vec{B} \right) \cdot \frac{\partial f_\alpha}{\partial \vec{p}} = 0$$

$$\nabla \times \vec{B} = \frac{4\pi \vec{j}}{c} + \frac{1}{c} \frac{\partial \vec{E}}{\partial t}$$

$$\nabla \times \vec{E} = -\frac{1}{c} \frac{\partial \vec{B}}{\partial t}$$

$$\nabla \cdot \vec{E} = 4\pi \varrho$$

$$\nabla \cdot \vec{B} = 0$$

Plasma Physic Methods
Simulations and Surrogate Models

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- ⊗ Analytical Calculation? – Not possible.
- ~ (PIC) Simulations – Partly
  - 3D: Month on $\sim$ 100 Cores
  - 1.5D: Hours on $\sim$ 10 Cores
  - Approximation Errors
- ✓ Experiments
- ✓ Data driven surrogate models

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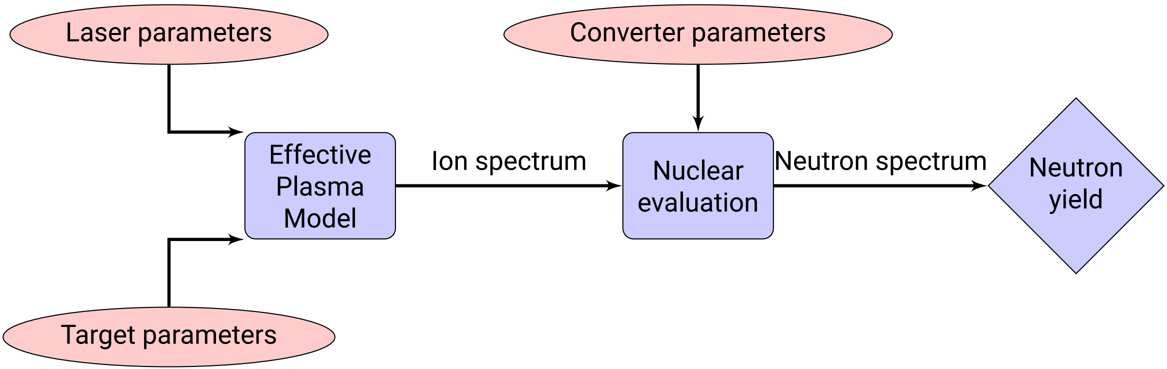
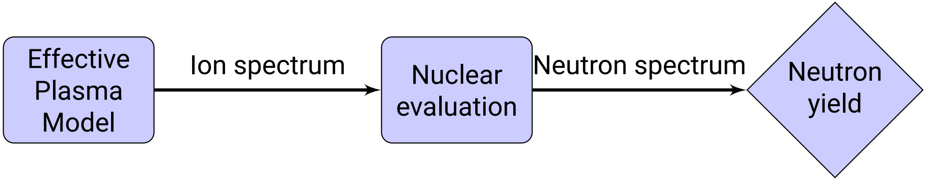
Laser-driven Neutron sources
Modelling and approaches



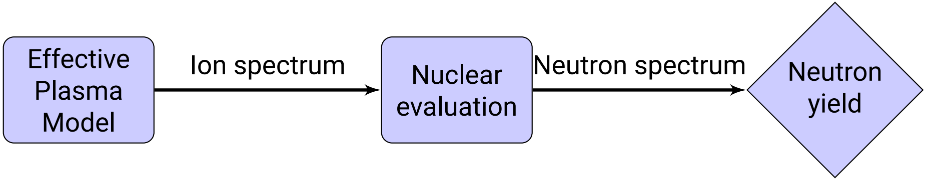
Laser-driven Neutron sources
Modelling and approaches



1. Experiments
2. Data driven Surrogate Model
3. PIC Simulations

1. Monte Carlo calculation
2. Experimental validation
3. Correction for nuclear MC

Laser-driven Neutron sources
Modelling and approaches



1. Experiments
2. **Data driven Surrogate Model**
3. PIC Simulations

1. Monte Carlo calculation
2. Experimental validation
3. Correction for nuclear MC

Surrogate Modeling

1. Definitions
2. Jupyter Tools
3. Dataset and Dataquality

Surrogate Modeling: Dataset Definitions

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$$\underbrace{Y}_{\text{Dependent V. Target Quantity}} = \underbrace{f}_{\text{Model Regression}} \underbrace{(x_0, ...x_i, ...x_n)}_{\text{Independent V. Features}}$$

- Each Y needs full set of x_i
- One model per target quantity
- Features:
  - Continuous distributed
  - Discrete distributed

Discrete Features:

- No interpolation useful
- Define disjunct **dataclasses**:
  - Cartesian Product
  - Datclasses will be compared to each other

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Surrogate Modeling: Dataset Tool 1

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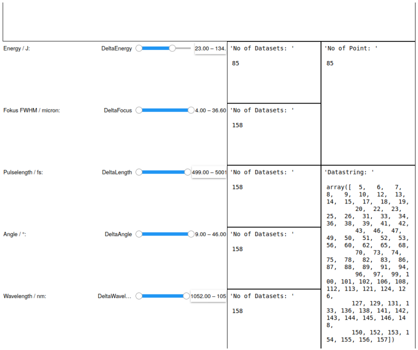
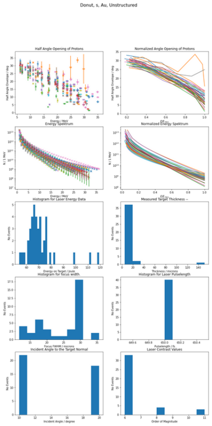
- Displays and investigates
  - features
  - data
- Allows to select data of interest





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Surrogate Modeling: Dataset Tool 2 – Resampling

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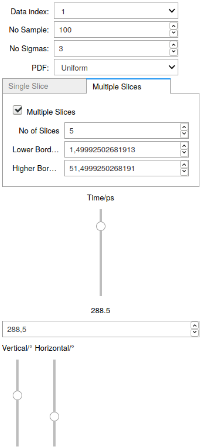
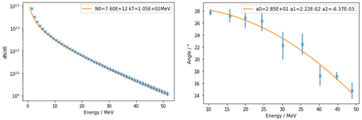
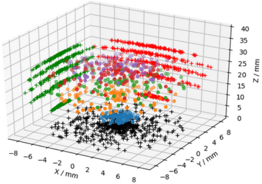
- Resampling of TNSA-ionbunches
  - Laminar expansion
  - Reproduces real data
  - Gaussian or uniform sampling
- Export to csv files







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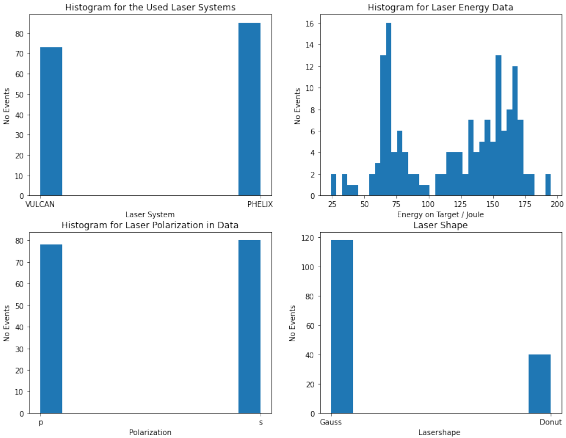
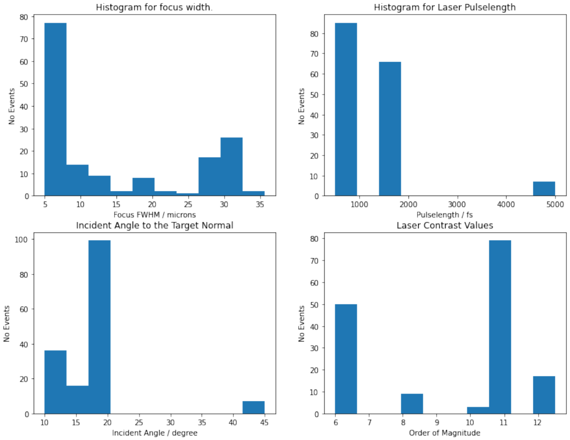
Surrogate Modeling: Dataset
Laser Features 1



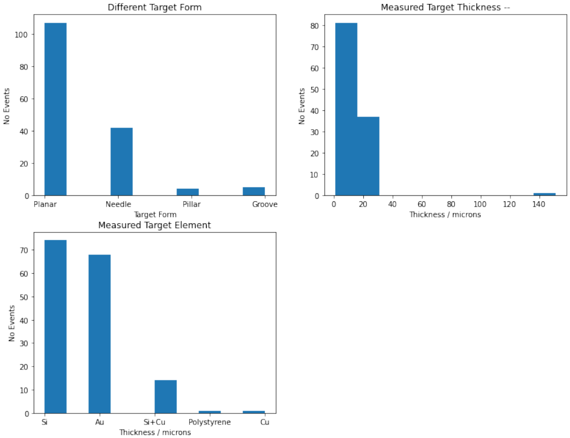
- Only 2 similar Lasersystems (Nd:Glass)
- On-target energy ...
- S and p polarized light $\approx 50 : 50$
- Mainly Gausslike spatial distribution

Surrogate Modeling: Dataset Laser Features 2



- Several different focus values
- Longpulses, other systems get down to 30 fs
- Mainly small incident angles
  - Gibbon et al.: 45° ideal?
- Contrast distributed between typical values
  - E-6 old value, not used anymore

Surrogate Modeling: Dataset
Target Features



- Different solid targets
  - mainly flat planar and needle targets
  - unstructured vs structured
- Mainly thin targets

Surrogate Modeling: Dataset Overview

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- State from: 18.08.2020:
  - 158 Datasets total (8 invalid, 1 Polysterene)
  - 149 usable Datasets
- 9 Dataclasses:

Gauss	s	Si+Cu	Structured	10
Gauss	s	Si+Cu	Unstructured	4
Gauss	s	Si	Unstructured	1
Gauss	s	Au	Unstructured	24
Gauss	s	Cu	Unstructured	1
Gauss	p	Si	Structured	34
Gauss	p	Si	Unstructured	31
Gauss	p	Au	Unstructured	4
Donut	s	Au	Unstructured	40

Metadata	Referenz	PHELIX	17640
Laser	Shape	Gauss	NaN
Laser	Energy/J	156.3	NaN
Laser	Polarization	s	NaN
Laser	Focus-FWHM/micron	5	NaN
Laser	Pulselength/fs	500	75
Laser	Incidentangle/deg	45	NaN
Laser	Contrast	E-12.5	NaN
Laser	Wavelength/nm	1054	0
Target	Form	Planar	NaN
Target	Thickness/micron	1	NaN
Target	Elements	Au	NaN
RCF	Composition	NaN	NaN
RCF	Distance/mm	50	NaN

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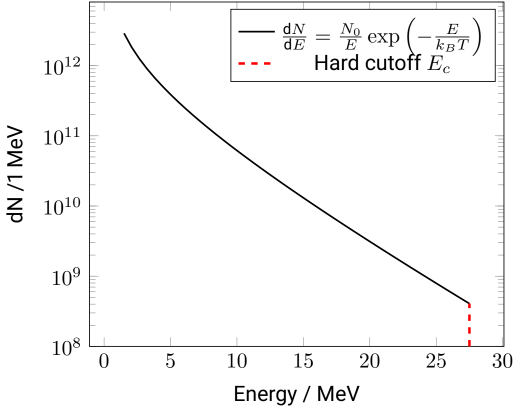
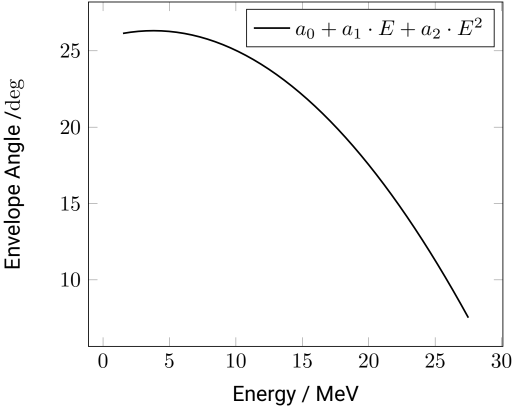
Surrogate Modeling: Dataset
RCF Results





Problem: Data not same length $\rightarrow$ Idea: Find model for fit parameters.

Surrogate Modeling: Dataset
RCF Results

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$$N_0 = f_1^i\left(E_L, W_L, \tau_L, \Theta_L, C_L, \lambda_L, d_T\right)$$
$$k_B T = f_2^i\left(E_L, W_L, \tau_L, \Theta_L, C_L, \lambda_L, d_T\right)$$
$$E_c = f_3^i\left(E_L, W_L, \tau_L, \Theta_L, C_L, \lambda_L, d_T\right)$$
$$a_0 = f_4^i\left(E_L, W_L, \tau_L, \Theta_L, C_L, \lambda_L, d_T\right)$$
$$a_1 = f_5^i\left(E_L, W_L, \tau_L, \Theta_L, C_L, \lambda_L, d_T\right)$$
$$a_2 = f_6^i\left(E_L, W_L, \tau_L, \Theta_L, C_L, \lambda_L, d_T\right)$$

$i \in \mathbb{N},$ index of dataclass

$\Rightarrow 6 \times \#$Classes functions needed!

To be taken into account:

- Noise of Parameters
- Region of Fit

Possible Methods:

- PCE: Polynomial Chaos Expansion
- GPR: Gaussian Progress Regression

Goals:

- Surrogate Model
- Sensitivity Analysis
- Correlation of the Observables
- Laser Uncertainties

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Surrogate Modeling: Dataset
Current Fazit

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Univariate Models

- Model depends on reference points.
- Variations are small.
- Sparse parameter space.
- Combined Dataclasses $\rightarrow$ bad prediction

Multivariate Models

- Variations are small.
- Sparse parameter space.
- Single Dataclasses $\rightarrow$ Overfitting!
- Difficult to use for sensitivity analysis.

Surrogate Modeling: What now?

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- Simpler models not sufficient
  ⇒ Acquire more data
- Transfer Learning
  ⇒ Add PIC simulations and neural network

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Surrogate Model with Sparse Data
Overview

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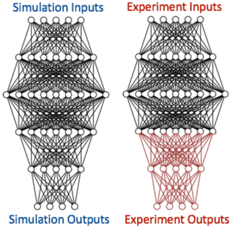
Idea

Find scalings in reduced simulations. → Fit to Experimental Data: several approaches

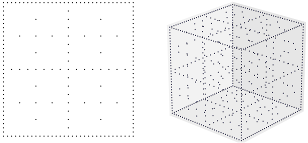
Neuronal Network



Train network
Fix most layers
Vary few layers

assumptions needed

Sparse Grids



Construct sparse grid
Interpolation on sparse grid
Fit to the experiment

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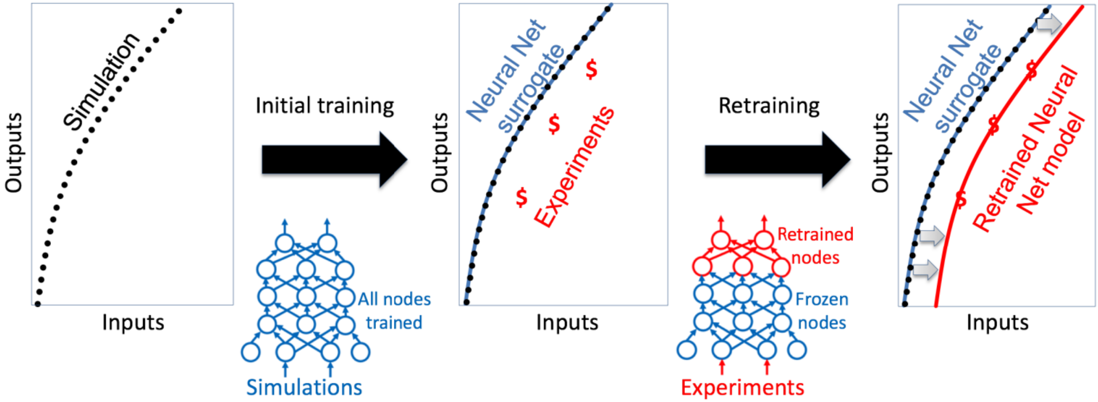
Surrogate Model with Sparse Data
Transfer Learning Concept



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Surrogate Model with Sparse Data
Problems and Solutions I

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- Large Parameter space
  - Real: 11D
  - 2D: 7D + 3Dk
  - 1.5D+boosted: 6D + 3Dk
  - 1.5D: 4D + 3Dk
- Random sampling

#	Element	Attribute	Range (real)	Range (1.5D)	Range (1.5D)	Range (2D)	Units
					Boosted		
1	Laser	Shape	{Gauss, Donut}	{Gauss}	{Gauss}	{Gauss}	
2	Laser	Energy	[1E-3, 2E+2]	[1E-3, 2E+2]	[1E-3, 2E+2]	[1E-3, 2E+2]	Joule
3	Laser	Focus-FWHM	[2, 20]	--	--	[2, 20]	micro meter
4	Laser	Pulselength	[15, 1000]	[15, 1000]	[15, 1000]	[15, 1000]	femto second
5	Laser	Polarization	{s, p}	--	{s, p}	{s, p}	
6	Laser	Incidentangle	{0, 85}	--	{0, 85}	{0, 85}	degree
7	Laser	Contrast	[1E-6, 5E-12]	--	--	--	
8	Laser	Wavelength	[550, 1100]	[550, 1100]	[550, 1100]	[550, 1100]	nano meter
9	Target	Form	{Planar, {Non-Planar}}	{Planar}	{Planar}	{Planar}	
10	Target	Thickness	[3E0, 2E3]	[3E0, 2E3]	[3E0, 2E3]	[3E0, 2E3]	nano meter
11	Target	Elements	{Si, Au, Cu, Si+Cu, Poly}	{Poly}	{Poly}	{Poly}	

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Surrogate Model with Sparse Data
Problems and Solutions II

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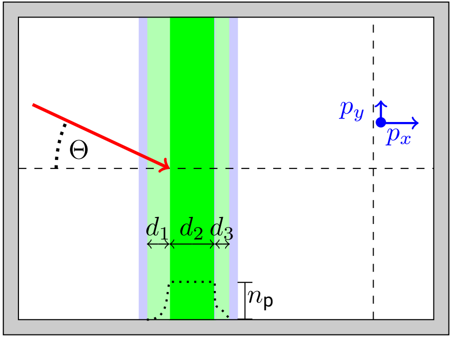
Reduce further: Introduce relevant analytical conditions

- TNSA Intensity:

$$\frac{E_L}{A_L \cdot \tau_L} = I \in \left[1 \times 10^{18}, 1 \times 10^{21}\right] \mathrm{W\,cm}^{-2}$$

- Lower boundary τ_L:
  $\Delta\tau \cdot \Delta\nu \geq K \quad K(\text{Shape})$
  $\Delta\nu$ dependent of lasermedium
- $\lambda \geq 550\,\mathrm{nm}$
- Incidentangle: ?
  - s-pol: Ideal close to 0°
  - p-pol: Ideal close to 45°



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Surrogate Model with Sparse Data
Problems and Solutions III

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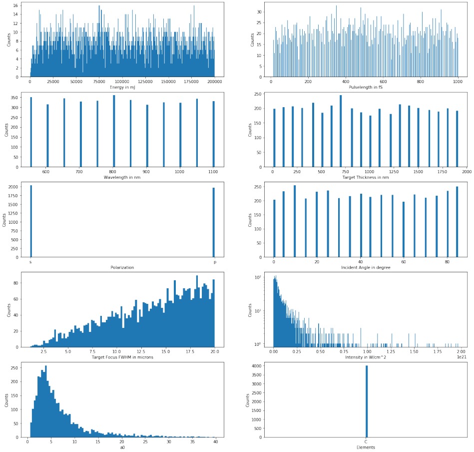
- Randomized parameter resampling
- Large number of Simulations

(+) Additional Parameterset

(+) Smoothness?



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Surrogate Model with Sparse Data
Problems and Solutions IV

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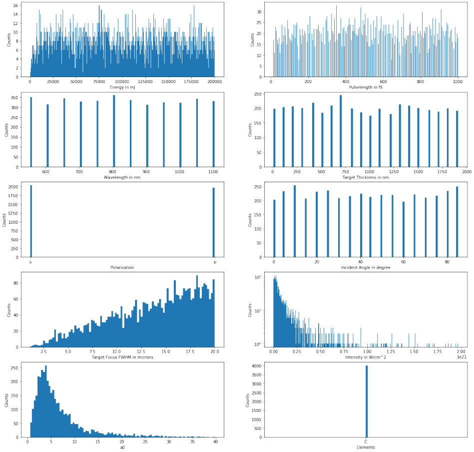
- Topology of NN
- Bayesian optimization for hyperparameters
- Physics informed NN?
- Incorporate contrast?



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Conclusion

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Status

- ✓ 149 Datapoints in 9 Dataclasses
- ✓ Model defined
  - 1.5D
  - 2D
- ✓ Start parameters found
- ✓ SMILEI tested

Outlook

- Additional Data (HHUD, Marvel Fusion, LIGHT)
- Model defined
  - 1.5D Lorentzboosted?
  - 3D azimuthal?
- SMILEI on Lichtenberg II and Virgo
- EPOCH tests from Marvel Fusion

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LOEWE
Exzellente Forschung für Hessens Zukunft

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