7th European Advanced Accelerator Conference

Sep 21 – 27, 2025Hotel Hermitage, La Biodola Bay, Isola d'Elba, Italy

Unlocking High-Dimensional Parameter Spaces: Bayesian Optimization in Beam-Driven Plasma Accelerators

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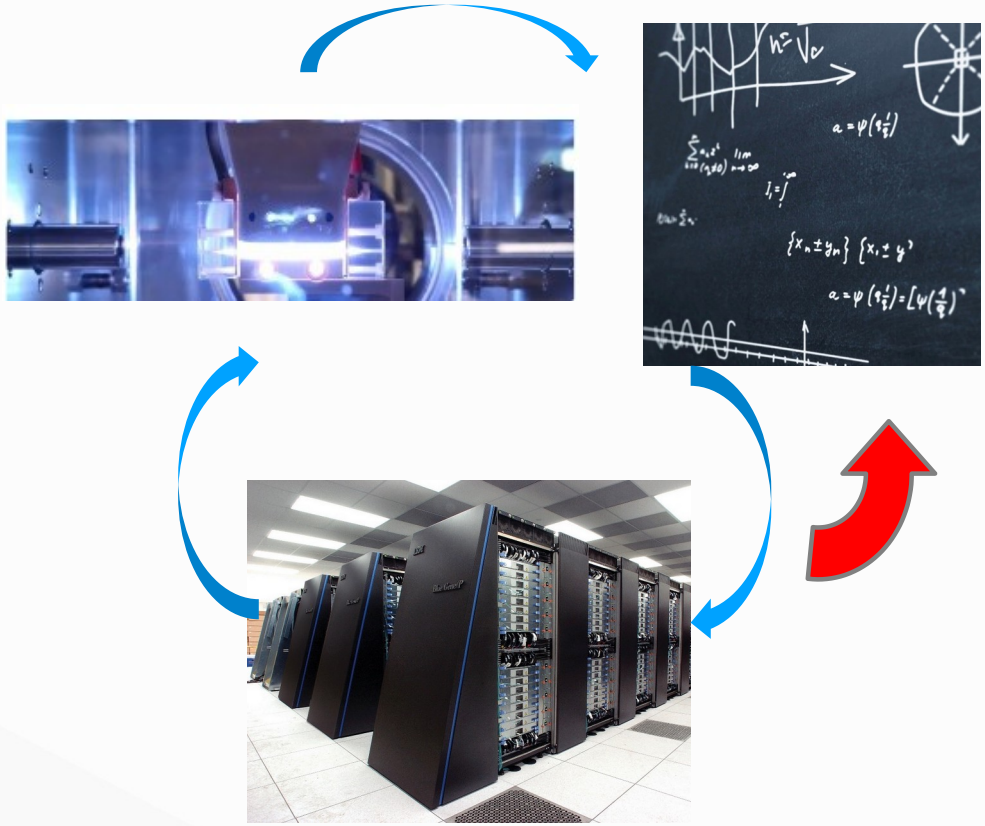
Challenges in plasma based particle accelerators

- **Strong coupling between parameters:** plasma density, laser/beam energy, shape and dynamics
- **Phenomenology:** try to capture the essential features by reducing the degrees of freedom of the theory
- **Computers simulations:** provide numerical experiments

Challenges in plasma based particle accelerators

- **Can we use “ab-initio” numerical solutions to unlock phenomenology?**
- **This has been done in many other fields:** nuclear and sub-nuclear physics, biophysics, mathematical physics (non linear and ODE problems solution), ect …



Bayesian optimization

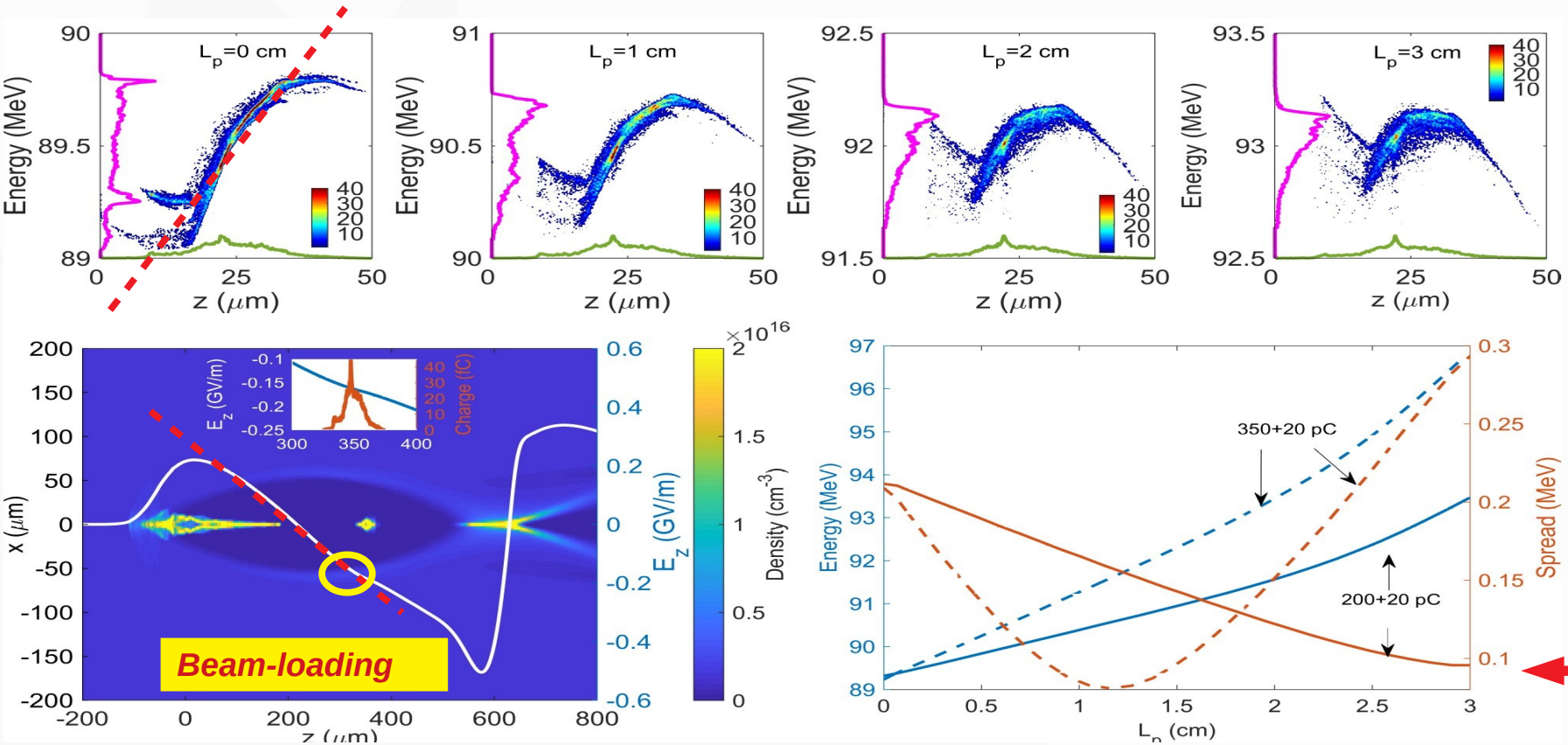
Bayesian probability theory offers a powerful framework for optimizing plasma wakefield acceleration systems while simultaneously uncovering underlying physics.

- BO uses **probabilistic surrogate models** (e.g., Gaussian processes) able to capture parameters uncertainty.
- Iteratively updates models with sparse data to guide efficient parameter exploration in high dimensional space.
- Supports multi-objective and multi-fidelity optimization, balancing competing goals and simulation costs.
- **This approach facilitates data-driven discovery and validation of scaling laws governing plasma wakefiled acceleration physics.**

Pompili, Riccardo, et al. "Energy spread minimization in a beam-driven plasma wakefield accelerator." Nature Physics 17.4 (2021): 499-503.

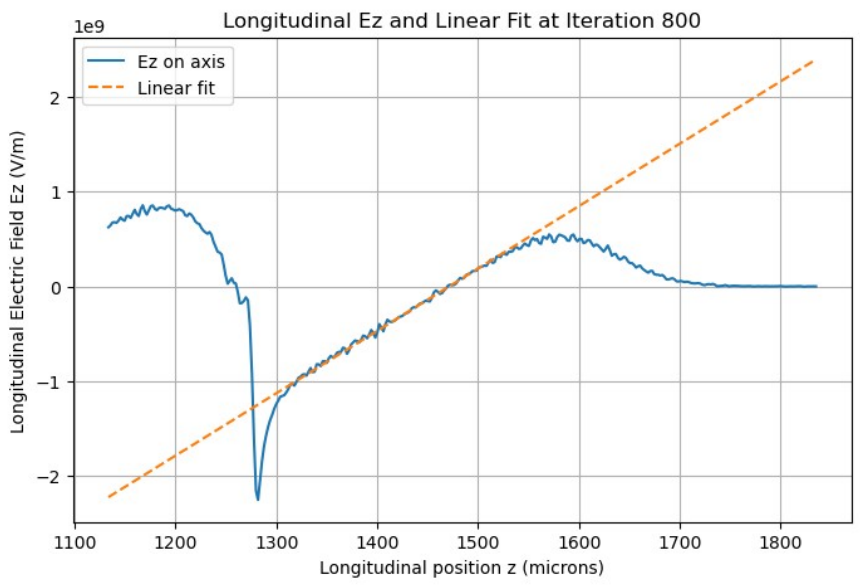
Simulated plasma acceleration

Pre-chirp to compensate wakefield slope



Longitudinal electric field retrieving

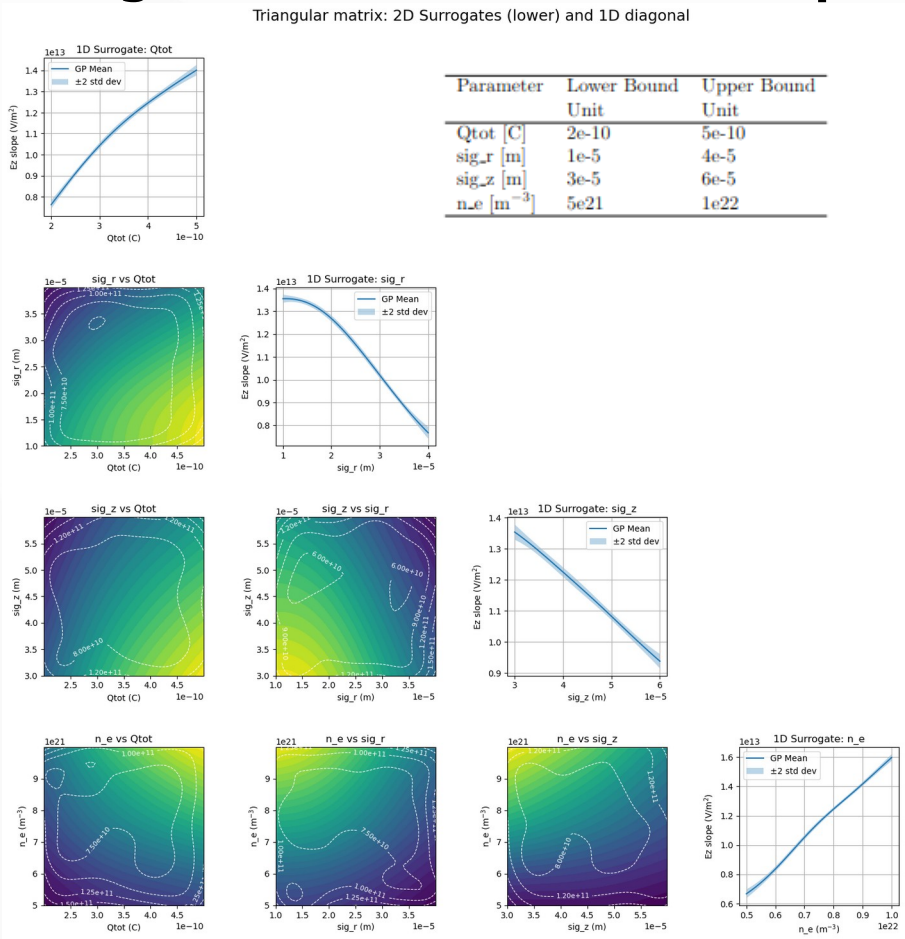
- The idea is to retrieve the longitudinal electric field generated by a driver electron bunch interacting with a plasma.



Software setup and integration:

- **PIC or fluid codes**
  for simulating beam-plasma interaction
- **OpenPMD**
  for post-processing
- **Botorch for Bayesian framework**
  (library built on PyTorch, featuring scalable **Gaussian Process models** via GPyTorch, Monte Carlo acquisition functions, GPU acceleration, and a modular design for easy customization).

4D surrogate model of the field slope



Parameter	Lower Bound Unit	Upper Bound Unit
Qtot [C]	2e-10	5e-10
sig_r [m]	1e-5	4e-5
sig_z [m]	3e-5	6e-5
n_e [m^{-3}]	5e21	1e22

- Gaussian processes model the objective function f(**x**) as a random function whose value at any finite set of points ($\mathbf{x}_1,\ldots,\mathbf{x}_n$) follow a multivariate gaussian distribution

$$\mathbf{f} = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n)) \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{K})$$

μ is a mean vector and **K** a covariance matrix modeled by a kernel function.

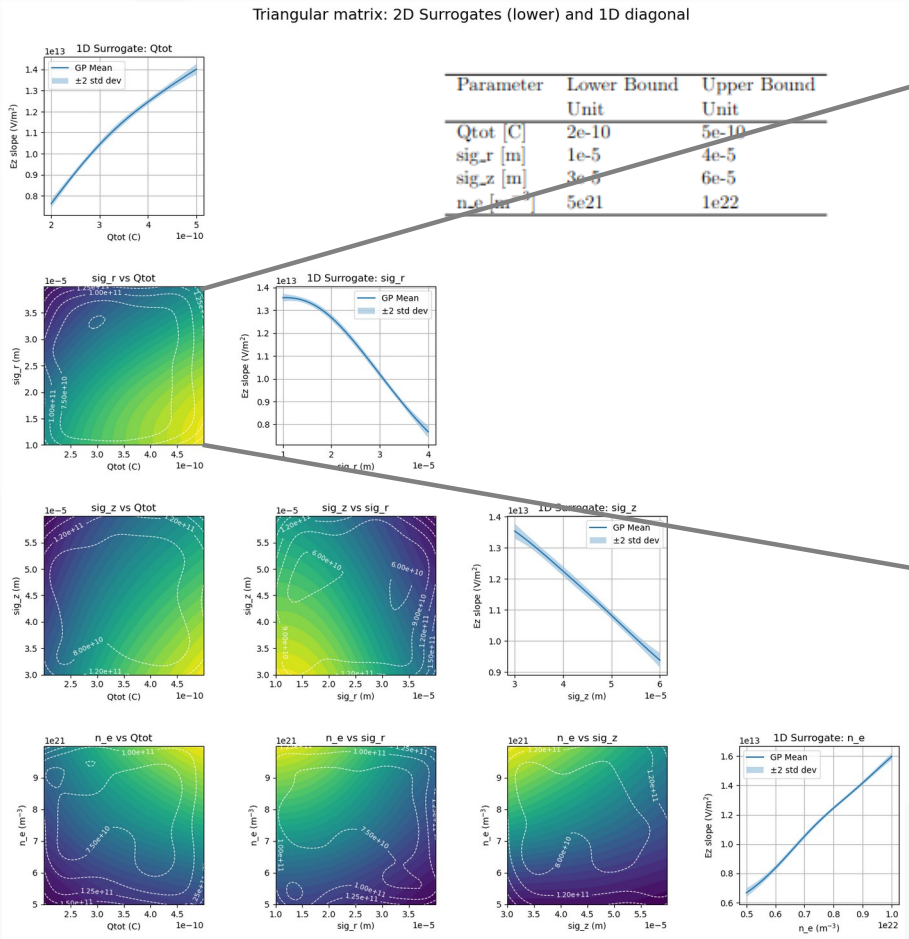
- Given observations it is possible to calculate the posterior predictive distribution for any new point in the space $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$

$$\mu(\mathbf{x}_*) = \mathbf{k}_*^T (\mathbf{K} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{y}$$

$$\sigma^2(\mathbf{x}_*) = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^T (\mathbf{K} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{k}_*$$

- In order to optimize f some **acquisition function** for selecting the next point in the space must be adopted.

Information extraction from 4D to 2D representation



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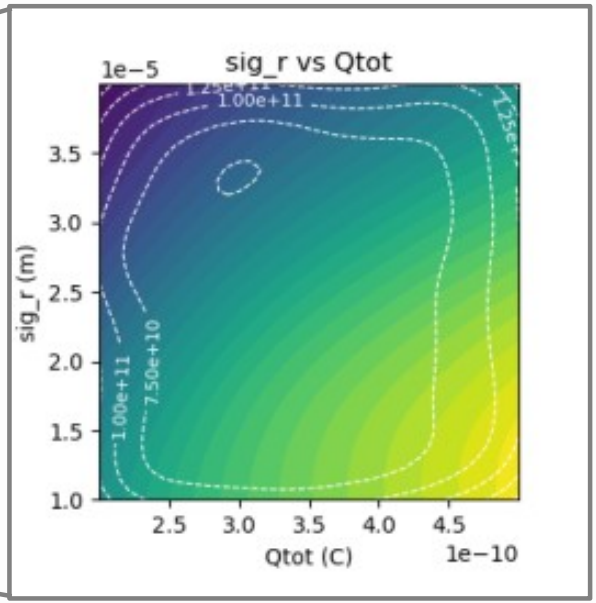
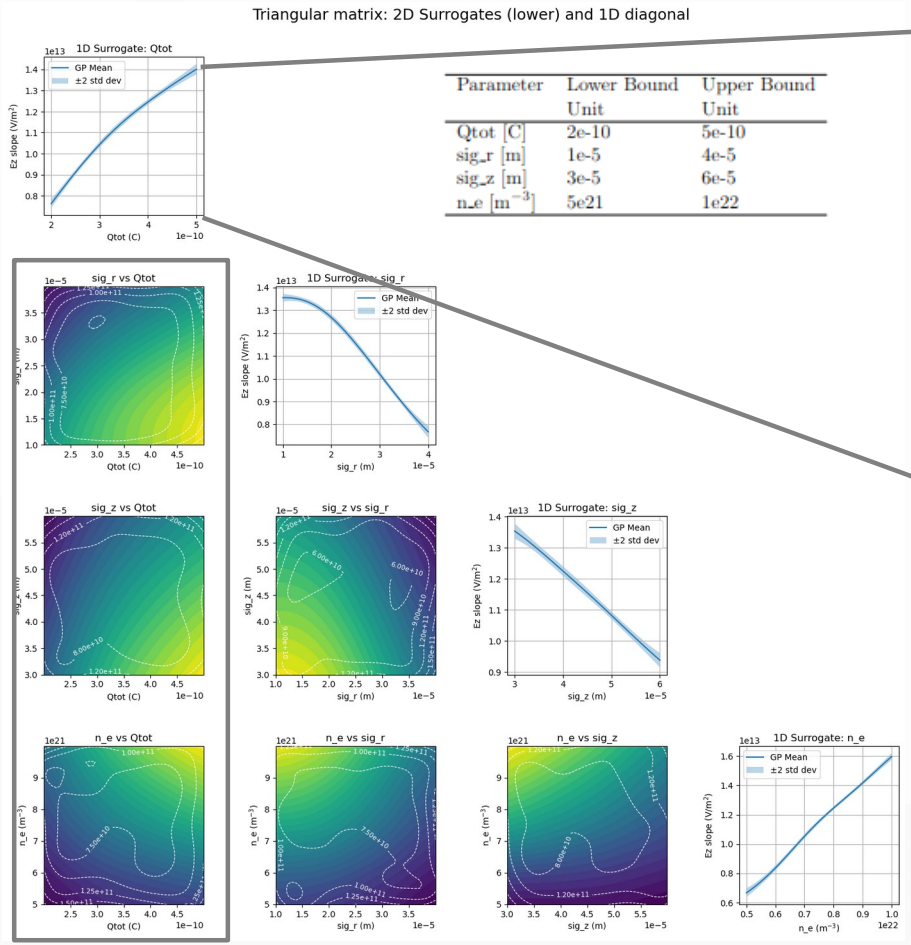


- **Fixing two of the four variable of the function f, we can slice the 4D space**
- **n_e and sig_z fixed** at the center of the intervals

Information extraction from 4D space to 1D



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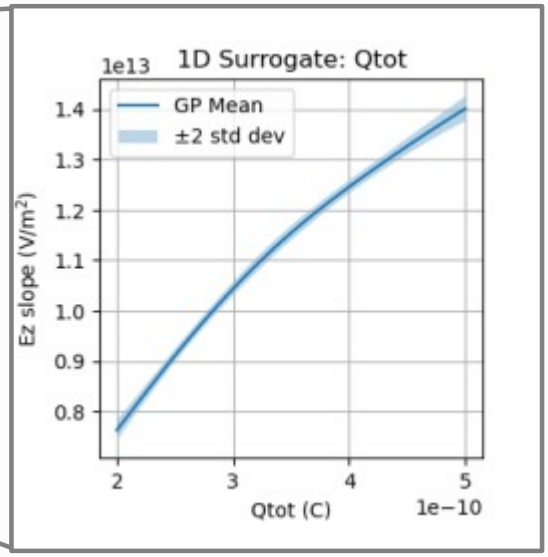
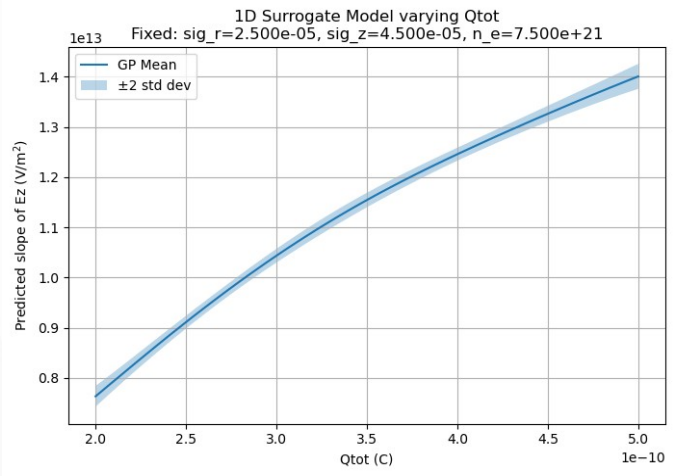
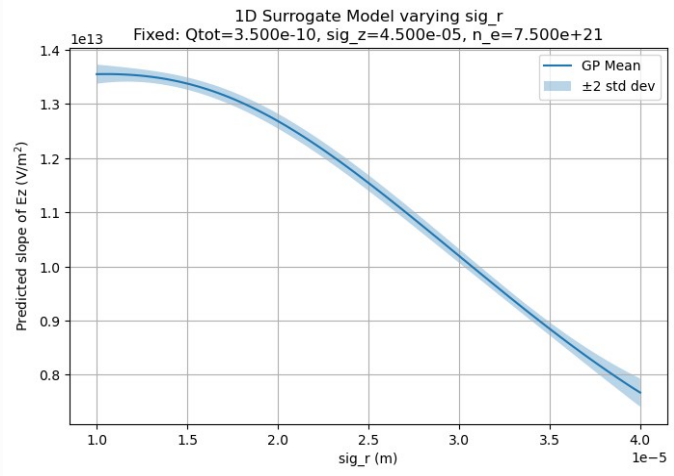


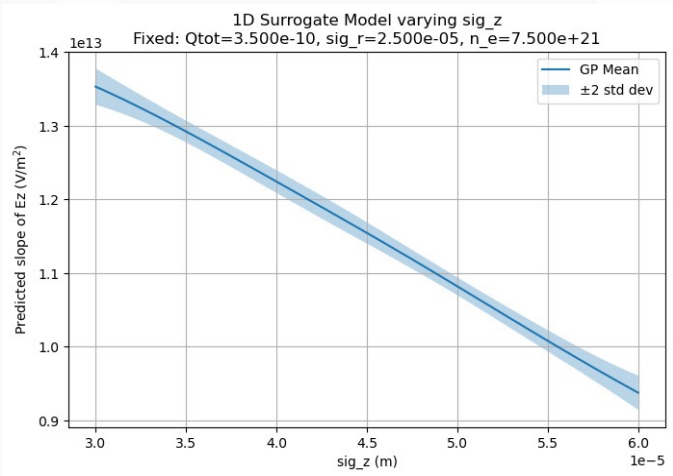
Fixing three of the four variable of the function f, we can go to 1D scaling laws

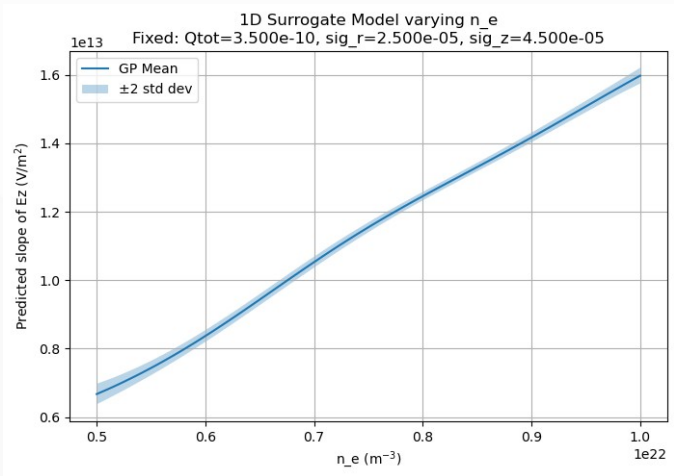
n_e ,sig_z, sig_r fixed at the center of the intervals

1D scaling with parameters



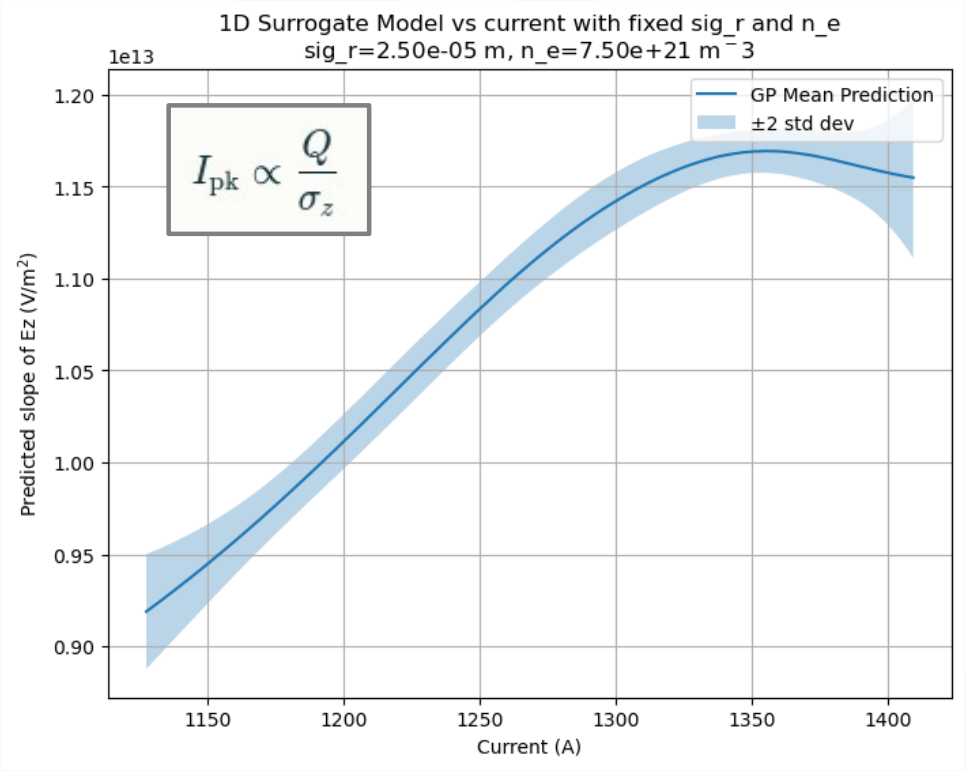


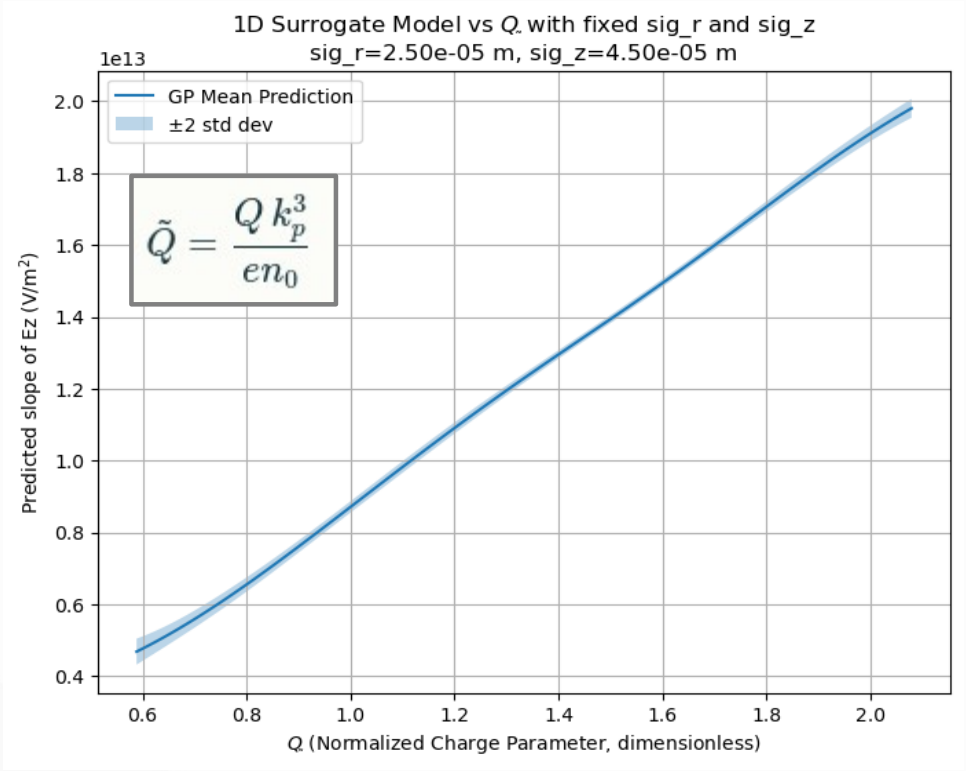




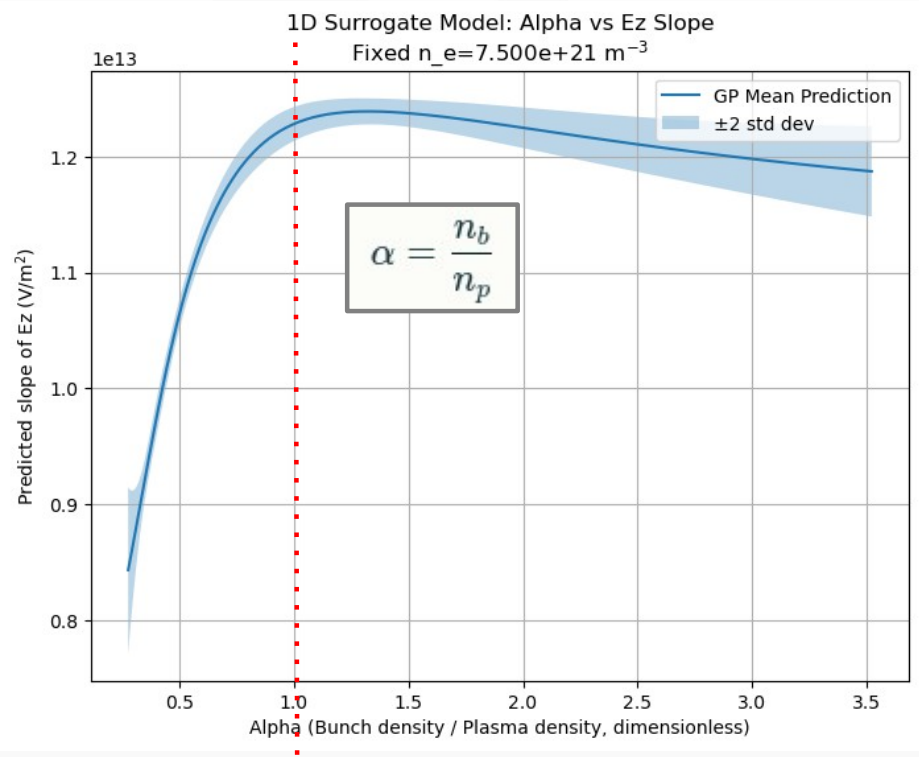
- Field slope increase almost linearly with the plasma density
- The dependence on the driver charge has a **square root-like behavior**
- There is also a clear dependence on the longitudinal, **but also transverse** size of the driver bunch

More 1D interesting quantities





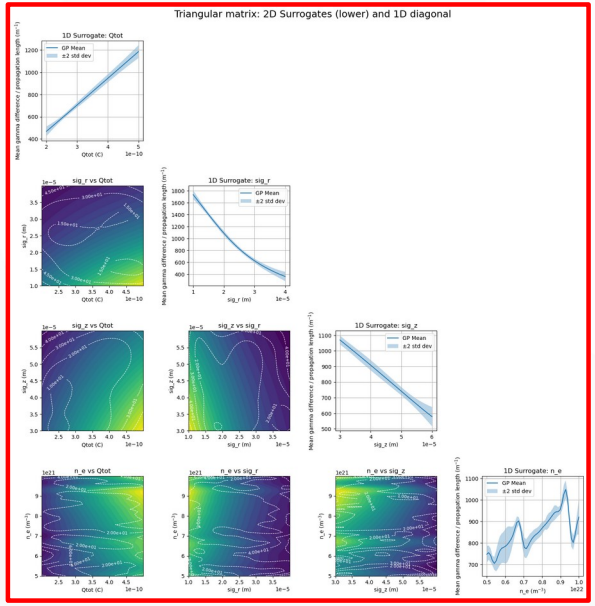
What about bunch charge density?

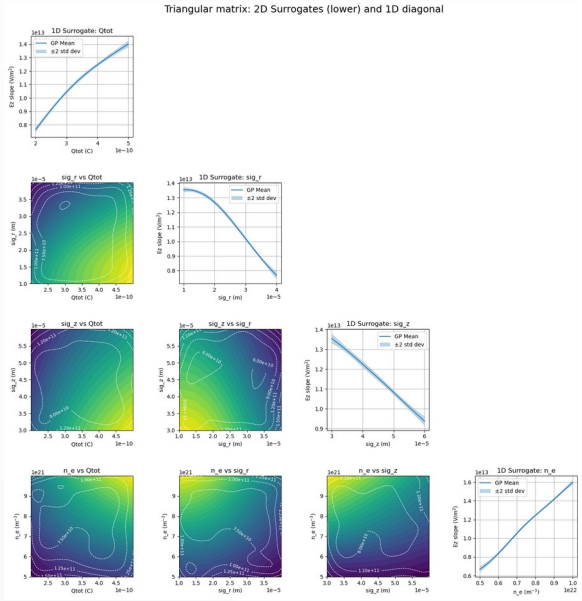


- **Plasma density is fixed**, therefore we are looking at the field slope as a function of the bunch charge density
- The field increases (almost linearly) up to alpha = 1
- For alpha > 1 the field slope is almost constant

What can we measure (ongoing activity)?

- Can we measure the field slope in the lab? **No!**
- **We can only measure quantities related with the driver bunch, i.e. the energy loss**





Thank for your attention