Machine-learning strategies in laser-plasma physics



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- ² Max Planck Institute for Quantum Optics (MPQ)
- ³ Faculty of Physics, Oxford University

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Data-driven Optimization of Laser Physics and Interactions



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Collaborators in Oxford

Peter Norreys

Robin Wang



Machine learning in laser-plasma physics



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- Held 1st online workshop on control systems and machine learning in January 2022 (150+ registered participants)
- Special issue in High-Power Laser Science and Engineering.
- Pre-print of review paper (30+ pages) recently published on arXiv

1. A. Döpp et al. Data-driven Science and Machine Learning Methods in Laser-Plasma Physics, arXiv:2212.00026 (2022)

Data-driven Science and Machine Learning Methods in Laser-Plasma Physics

Andreas Döpp,^{1,*} Christoph Eberle,¹ Sunny Howard,^{1,2} Faran Irshad,¹ Jinpu Lin,¹ and Matthew Streeter³

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Leger plasma physics has developed rapidly even the past few decades as legers have become be

Laser-plasma physics has developed rapidly over the past few decades as lasers have become both more powerful and more widely available. Early experimental and numerical research in this field was dominated by single-shot experiments with limited parameter exploration. However, recent technological improvements make it possible to gather data for hundreds or thousands of different settings in both experiments and simulations. This has sparked interest in using advanced techniques from mathematics, statistics and computer science to deal with, and benefit from, big data. At the same time, sophisticated modeling techniques also provide new ways for researchers to deal effectively with situation where still only sparse data are available. This paper aims to present an overview of relevant machine learning methods with focus on applicability to laser-plasma physics and its important sub-fields of laser-plasma acceleration and inertial confinement fusion.

CONTENTS C. Downhill simplex method and gradient-based algorithms D. Genetic algorithms I. Introduction E. Bayesian optimization A. Laser-Plasma Physics F. Reinforcement learning B. Why data-driven techniques? V. Unsupervised Learning II. Modeling & prediction A. Clustering A. Predictive models 1. Centroid-based clustering 1. Spline Interpolation 2. Distribution-based clustering 2. Regression B. Correlation analysis 3. Probabilistic models C. Dimensionality reduction 4. Gaussian process regression 1. Principal component analysis 5. Decision trees and forests 2. Autoencoders 6. Neural networks 7. Physics-informed machine learning VI. Image analysis models A. Classification B. Time series forecasting 1. Support vector machines 1. Classical models 2. Convolutional neural networks 2. State-Space Models B. Object detection 3. Forecasting networks C. Segmentation C. Prediction and Feedback VII. Conclusions III. Inverse problems Acknowledgements A. Least squares solution B. Statistical inference References C. Regularization D. Compressed sensing

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E. End-to-end deep learning methods

F. Deep unrolling

A. General concepts

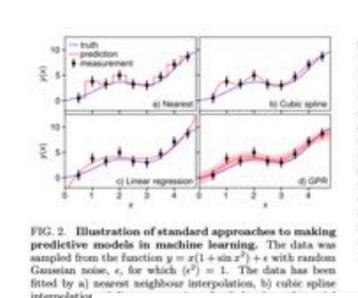
Objective functions
 Pareto optimization
 Grid search and random search

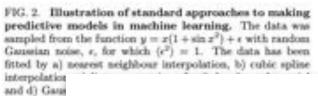
IV. Optimization

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Machine learning in laser-plasma physics

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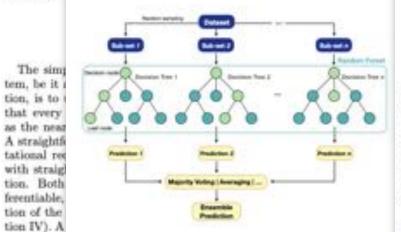


FIG. 4. Sketch of a random forest, an architecture for regression or classification consisting of multiple decision trees, whose individual predictions are combined using into an ensemble prediction e.g. via majority voting or averaging.

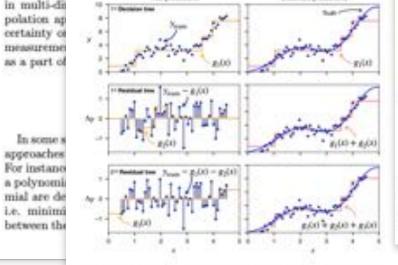


FIG. 5. Example of gradient boosting with decision trees. First, a decision tree g_i is fitted to the data. In the next step, the residual difference between training data and decision tree g_2 . This process is repeated n times, with each new tree q. learning to correct only the remaining difference to the training data. Data in this example sampled from same function as in Fig. 2 and each tree has a maximum depth of two decision layers.

in regression settings or entropy and information gain in a classification setting. At each decision point the data set is split and subsequently the metric is re-evaluated for the resulting groups, generating the next layer of decision nodes. This process is repeated until the leaves are reached. The more layers decision layers are used, called the depth of the tree, the more complex relationships can

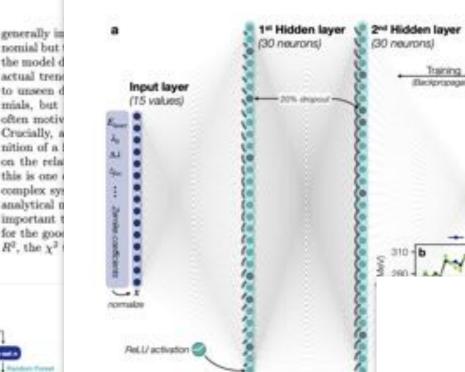


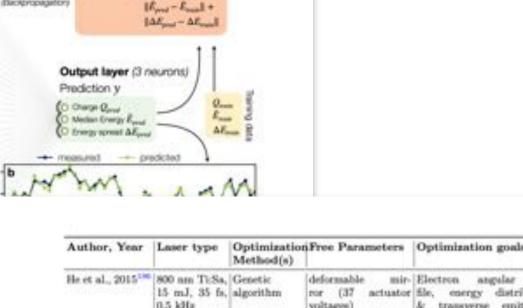
FIG. 7. Real-world example of a multilayer perceptr consists of 15 input neurons, two hidden layers with 30 neuron The input is derived from parasitic laser diagnostics (laser p $\Delta\lambda$, longitudinal focus position z_{fec} and Zernike coefficients 20% of neurons drop out for regularization during training. evaluate the accuracy of the model, in this case using the m the loss function is then propagated back through the netwo median energy (E) and (c) measured and predicted energy: b-c adapted from Kirchen et al.29

model incorporating a trained neural network was used to provide an additional computation package to the Geant4 particle physics platform. Neural networks are also trained to assist hohlraum design for ICF experiments by predicting the time evolution of the radiation temperature, in the recent work by McClarren et al.117. In the work by Simpson et al. 113, a fully-connected neural network with three hidden layers is constructed to assist the analysis of a x-ray spectrometer, which measures the x-rays driven by MeV electrons produced from high-power laser-solid interaction.

7. Physics-informed machine learning models

The ultimate application of machine learning for modeling physics systems would arguably be to create an "artificial intelligence physicist", as coined by Wu and Tegmark¹¹⁴. One prominent idea at the backbone of how

ing decision tree as an initializer are Deep Jointly-Informed Neural Networks (DJINN) developed by Humbird et al. 20, which have been widely applied in the high power laser community, especially The algorithm first constructs a tree or a random forest with tree depth set as a tunable hyperparameter. It then maps the tree to a neural network, or maps the forest to an ensemble of networks. The structure of the network (number of neurons and hidden layer, initial weights, etc.) reflects the structure of the tree. The neural network is then trained using back-propagation. The use of decision trees for initialization largely reduces the computational cost while maintaining comparable performance to optimized neural network architectures. The DJINN algorithm has been applied to several classification and regression tasks



450 mJ, 40 fs, Nelder-Mead or

800 nm Ti:Sa, Bayesian

800 nm Ti:Sa, Bayesian

2.6 J, 39 fs. 1 optimization

TABLE I. Summary of a few representative papers on machine-learning-aided optimization in the context of laser-plasma acceleration and high-power laser experiments.

ispersive filter

0.245 J, 45 optimization & length, laser dis-Electron charge within ac-

(H₂ front and back,

 N_1); focus position

and laser energy

∂(d), focus position ray counts

Gas cell flow rate Total electron beam energy

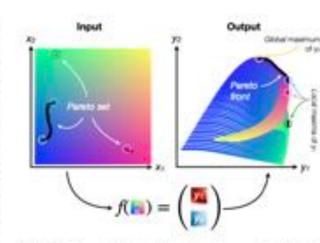
persion $(\partial_{\omega}^2 \phi, \ \partial_{\omega}^3 \phi, \ \text{ceptance angle, Betatron X-}$

Gas cell flow rates Spectral charge density

distributions, in this case the electron energy distribution. While simple at the first glance, these objectives need to be properly defined and there are often different ways to do so²⁰¹. In the example above, energy and bandwidth are examples for the central tendency and the statistical dispersion of the energy distribution, respectively. These can be measured using different metrics such as weighted arithmetic or truncated mean, the median, mode, percentiles and so forth for the former; and full width at half maximum, median absolute deviation, standard deviation, maximum deviation, etc. for the latter. Each of these seemingly similar measures emphasises different features of the distribution they are calculated from, which can affect the outcome of optimization tasks. Sometimes one might also want to include higher order momenta as objectives, such as the skewness, or use integrals, e.g. the total beam charge.

2. Pareto optimization

multiple sometimes competing objectives g_i. As the objective function should only yield a single scalar value, one has to condense these objectives in a process known as scularization. Scalarization can for instance take the form of a weighted product $g = \prod g_i^{\alpha_i}$ or sum $g = \sum \alpha_i g_i$ of the individual objectives g, with the hyperparameters o, describing its weight. Another common scalarization technique is ϵ -constraint scalarization, where one seeks to reformulate the problem of optimizing multiple objectives into a problem of single-objective optimization conditioned on constraints. In this method the goal is to optimize one of the g, given some bounds on the other objectives. All of these techniques introduce some explicit bias in the optimization which may not necessarily repre-



function f(x) = y acts on a two-dimensional input space $x = (x_1, x_2)$ and transforms it to the objective space y = (y_1, y_2) on the right. The entirety of possible input positions is uniquely color-coded on the left and the resulting position in the objective space is shown in the same color on the right d solutions form the Pareto front, indicate on the right, whereas the corresponding set of coordinates in the input space is called the Pareto set. Note that both Pareto front and Pareto set may be continuously defined locally, but can also contain discontinuities when local maxima get involved. Adapted from Irshad et al. 2021.

FIG. 12. Pareto front. Illustration how a multi-objective

sent the desired outcome. Because of this, the hyperparameters of the scalarization may have to be optimized themselves by running optimizations several times.

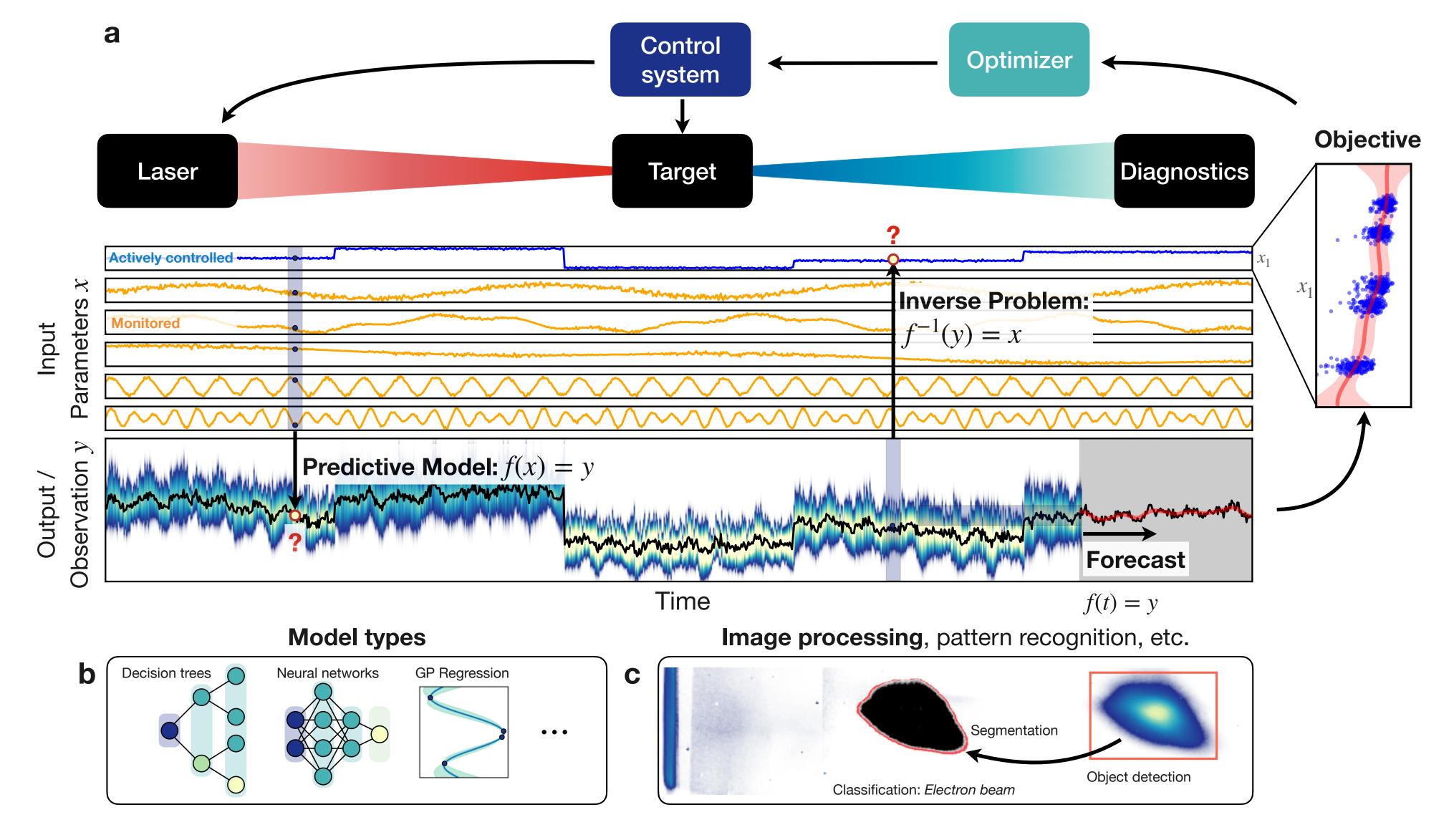
A more general approach is Pareto optimization, where the entire vector of individual objectives $g = (g_1, \dots, g_N)$ is optimized. To do so, instead of optimizing individual objectives, it is based on the concept of dominance. A

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Machine learning strategies

General use cases

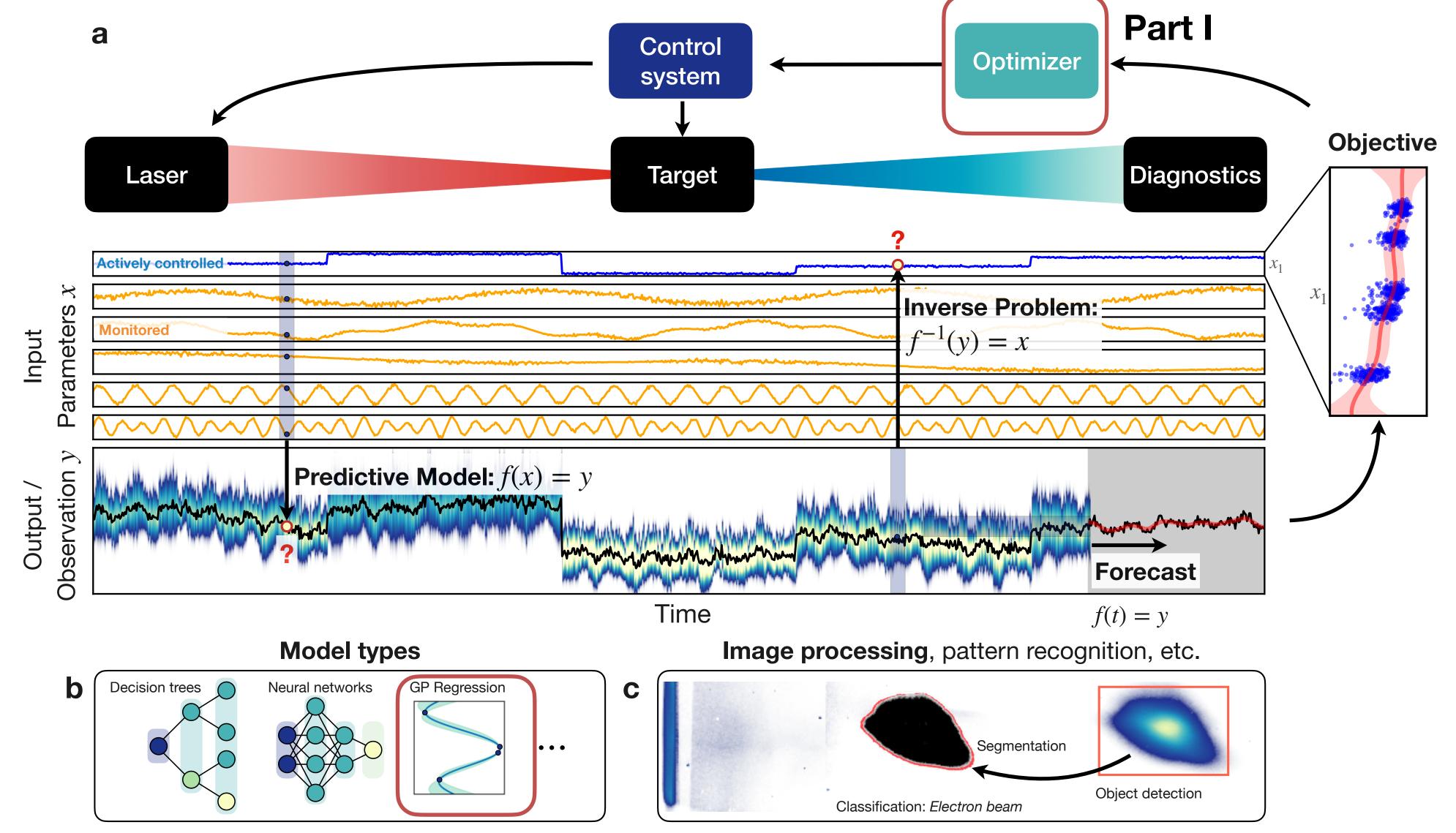




Machine learning strategies

General use cases

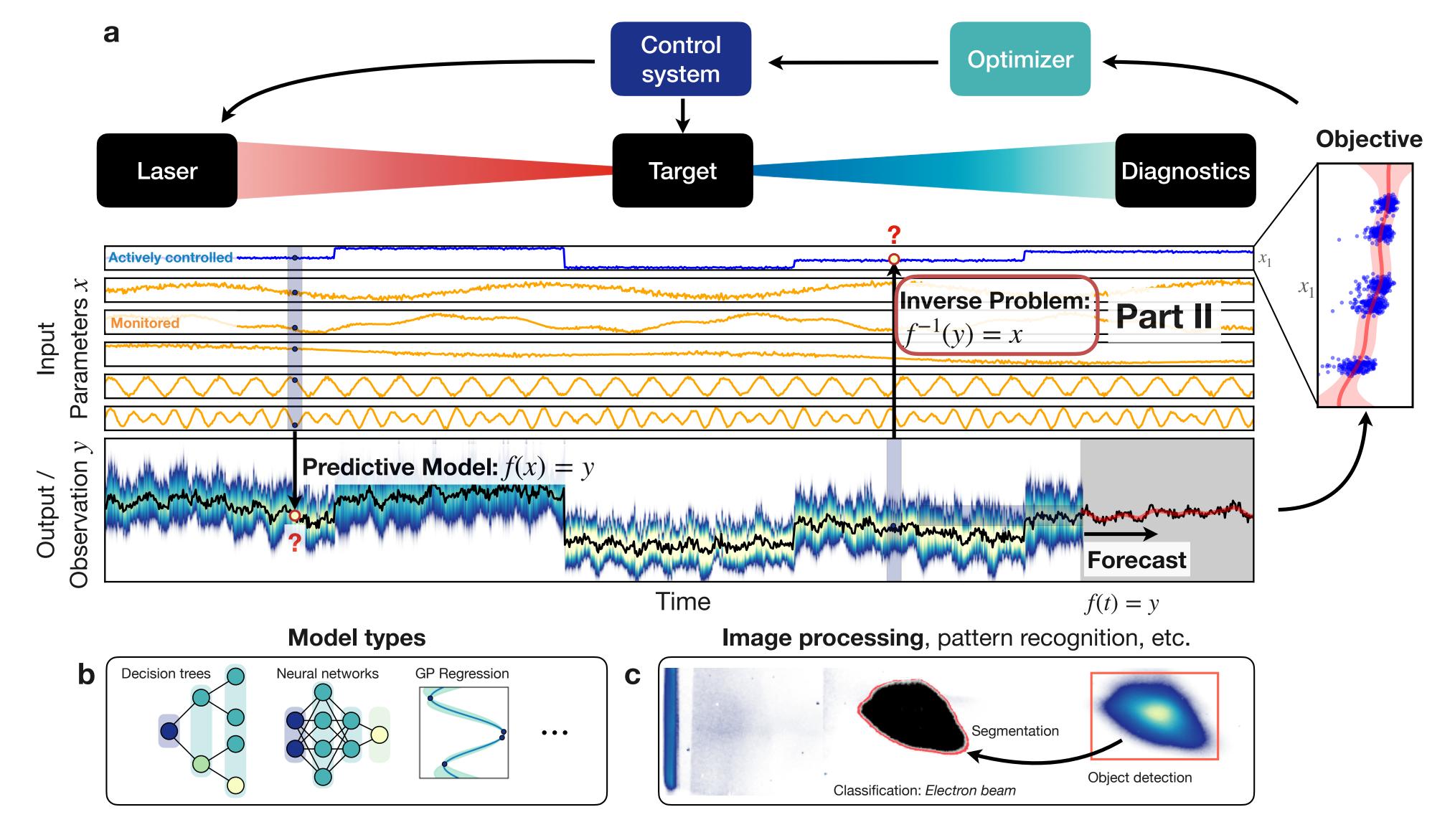




Machine learning strategies

General use cases







Part 1

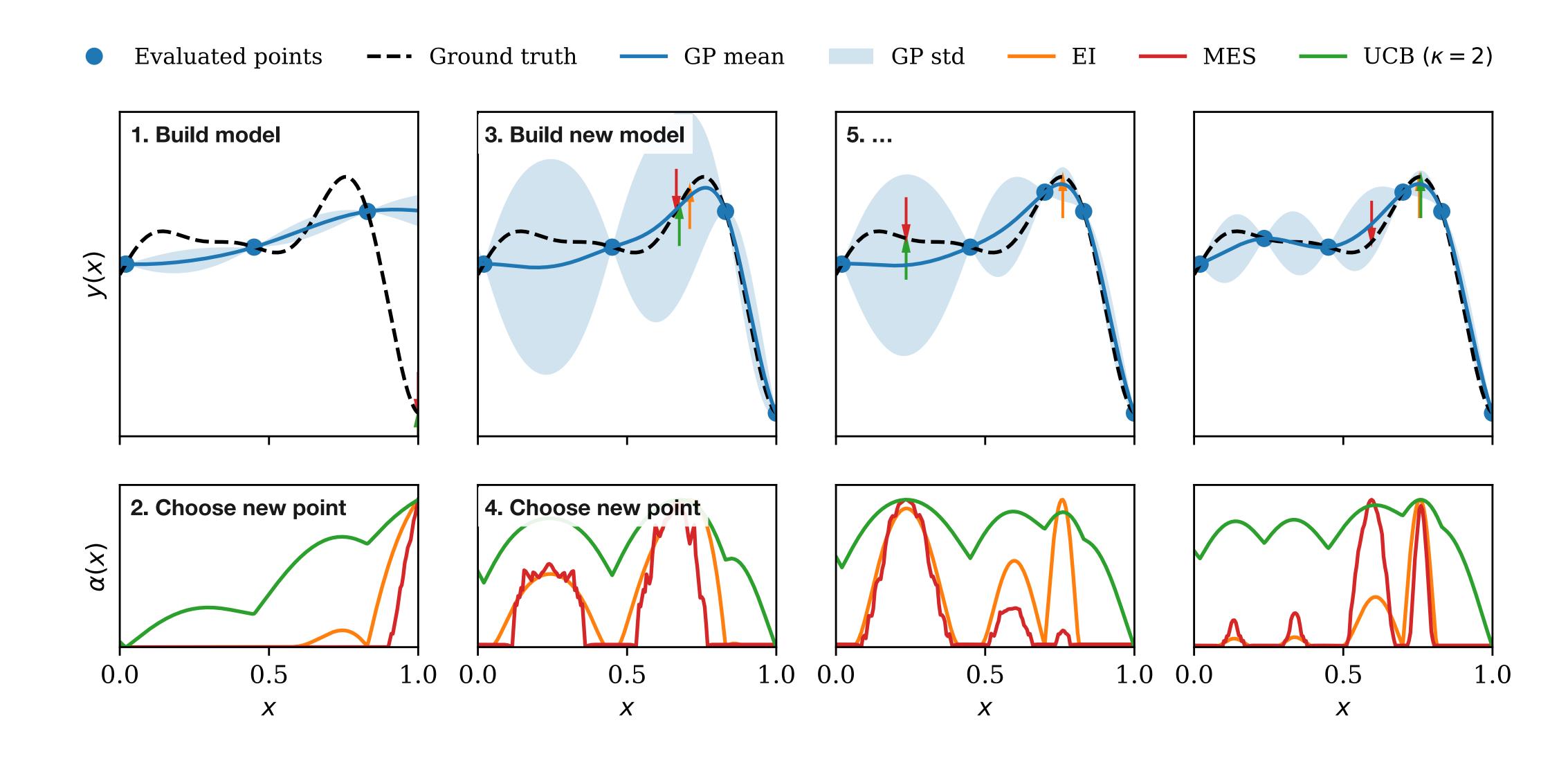
Multi-objective, multi-fidelity

Bayesian optimization

Bayesian optimization

Sequential surrogate-based optimization

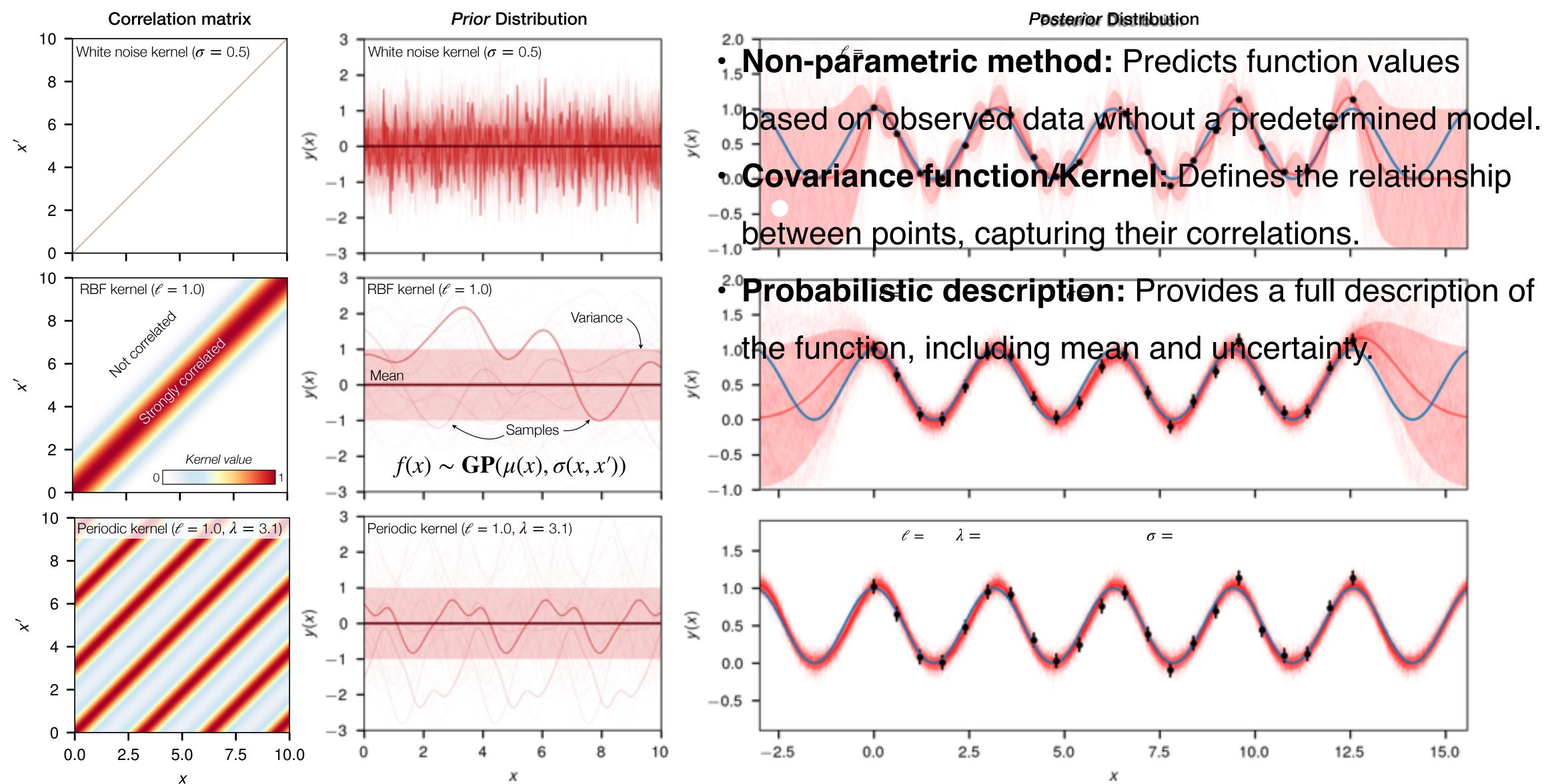




Gaussian process regression

Modeling functions via correlations

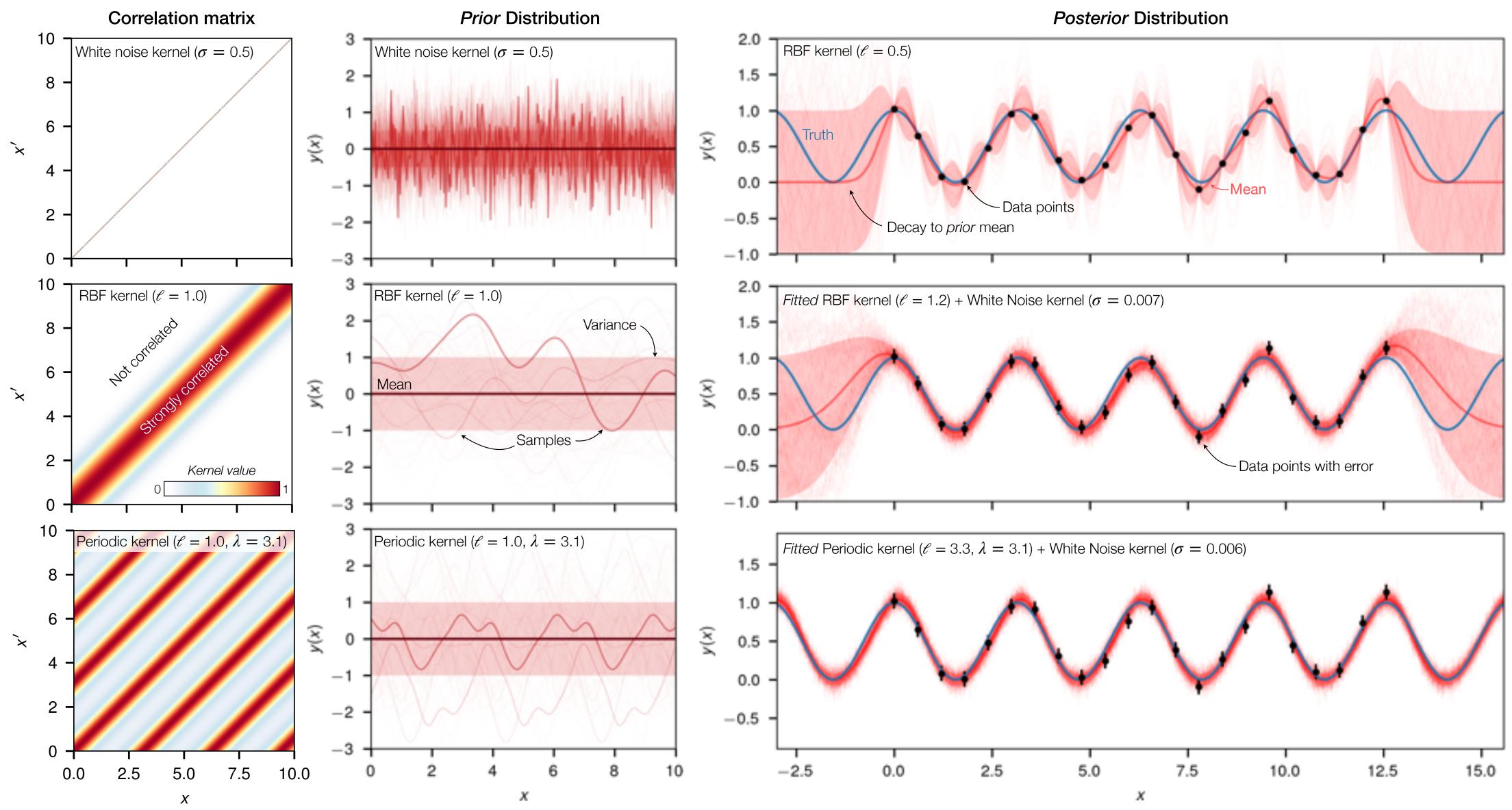




Gaussian process regression

Modeling functions via correlations

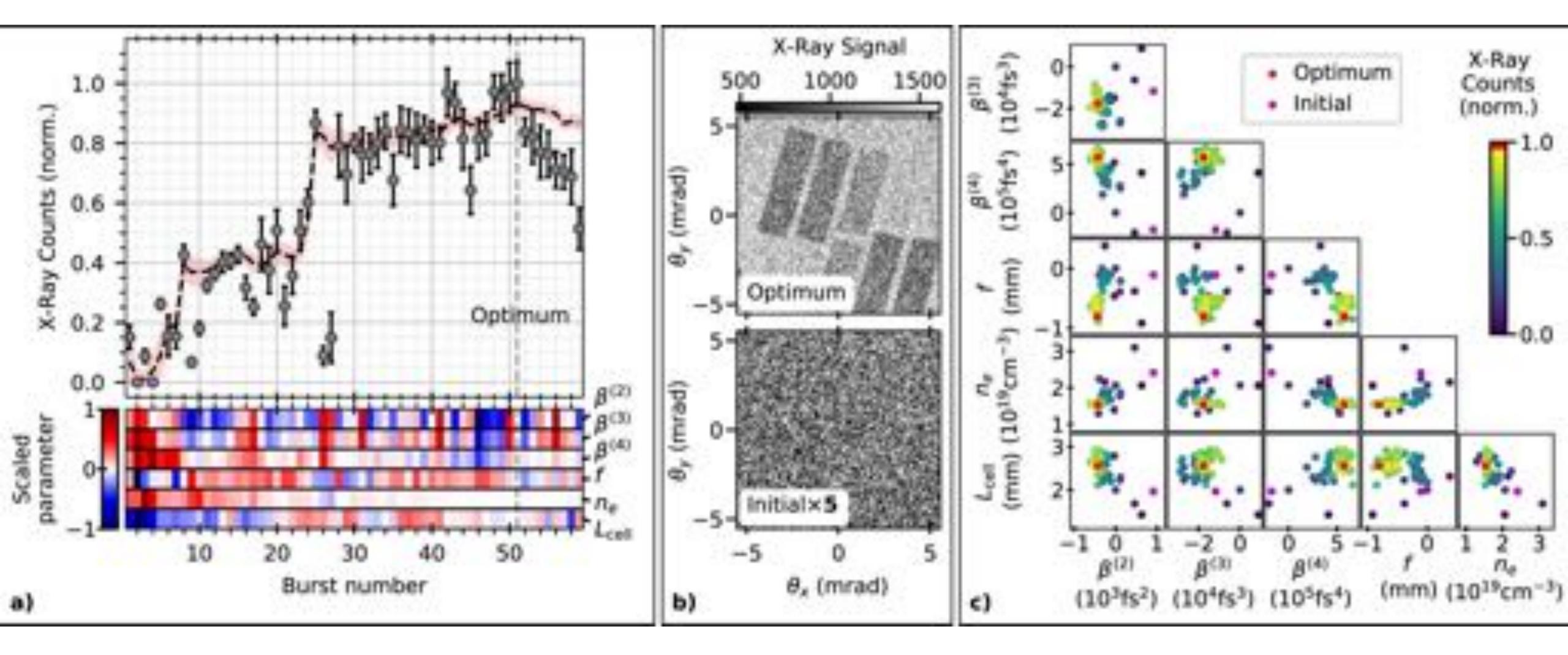




Bayesian optimization

First experimental results in laser-plasma acceleration





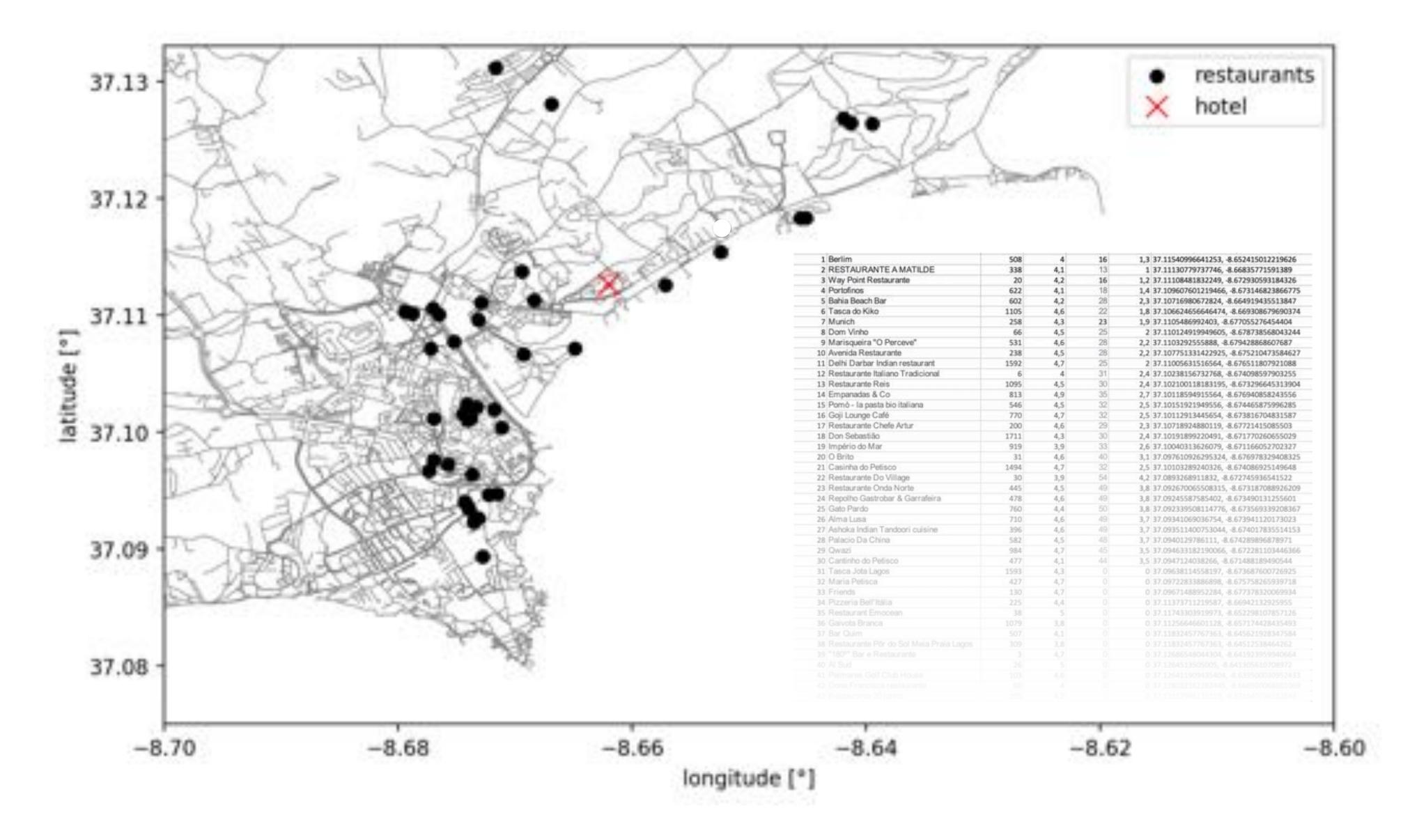


Multi-objective, multi-fidelity

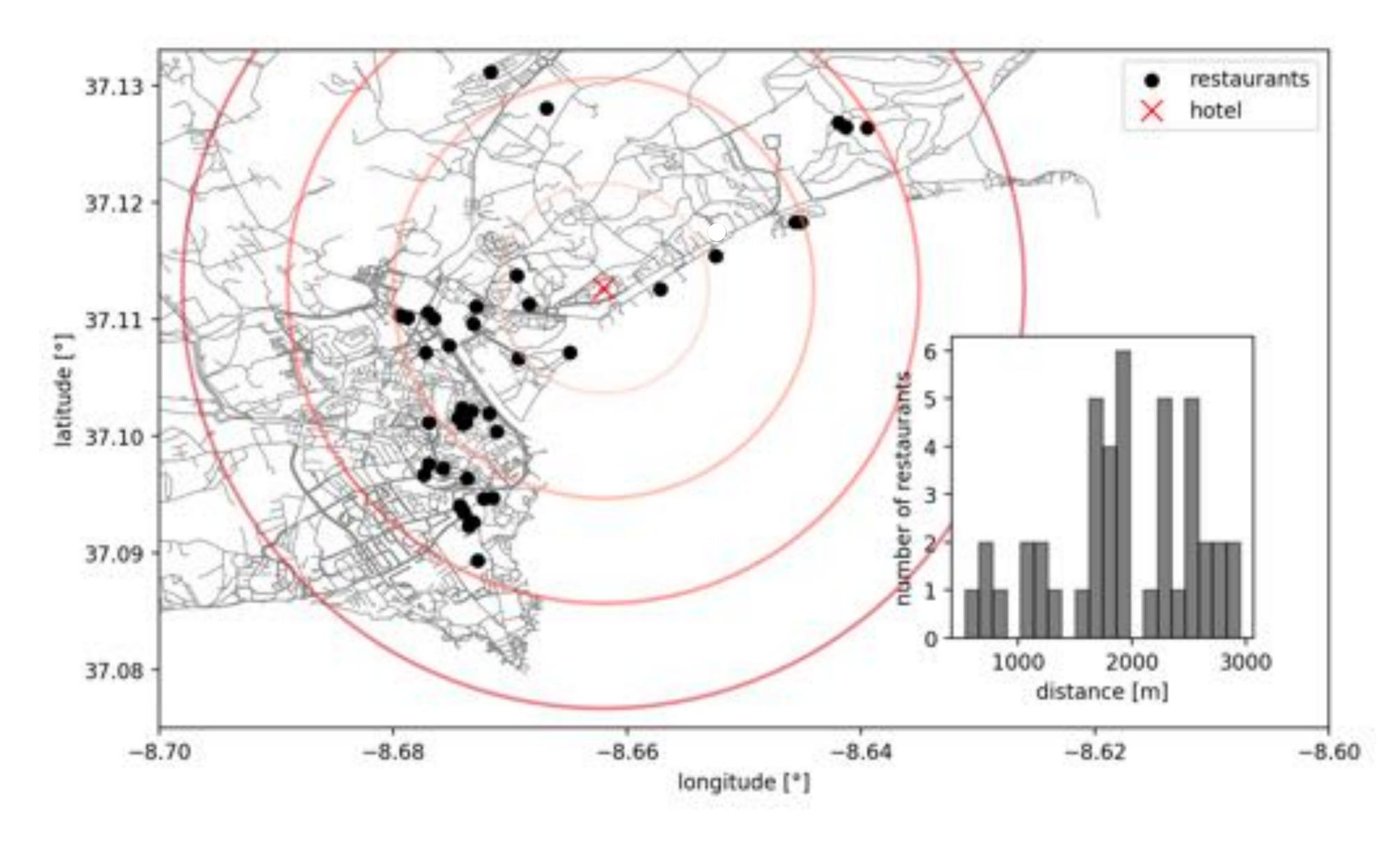
Bayesian optimization



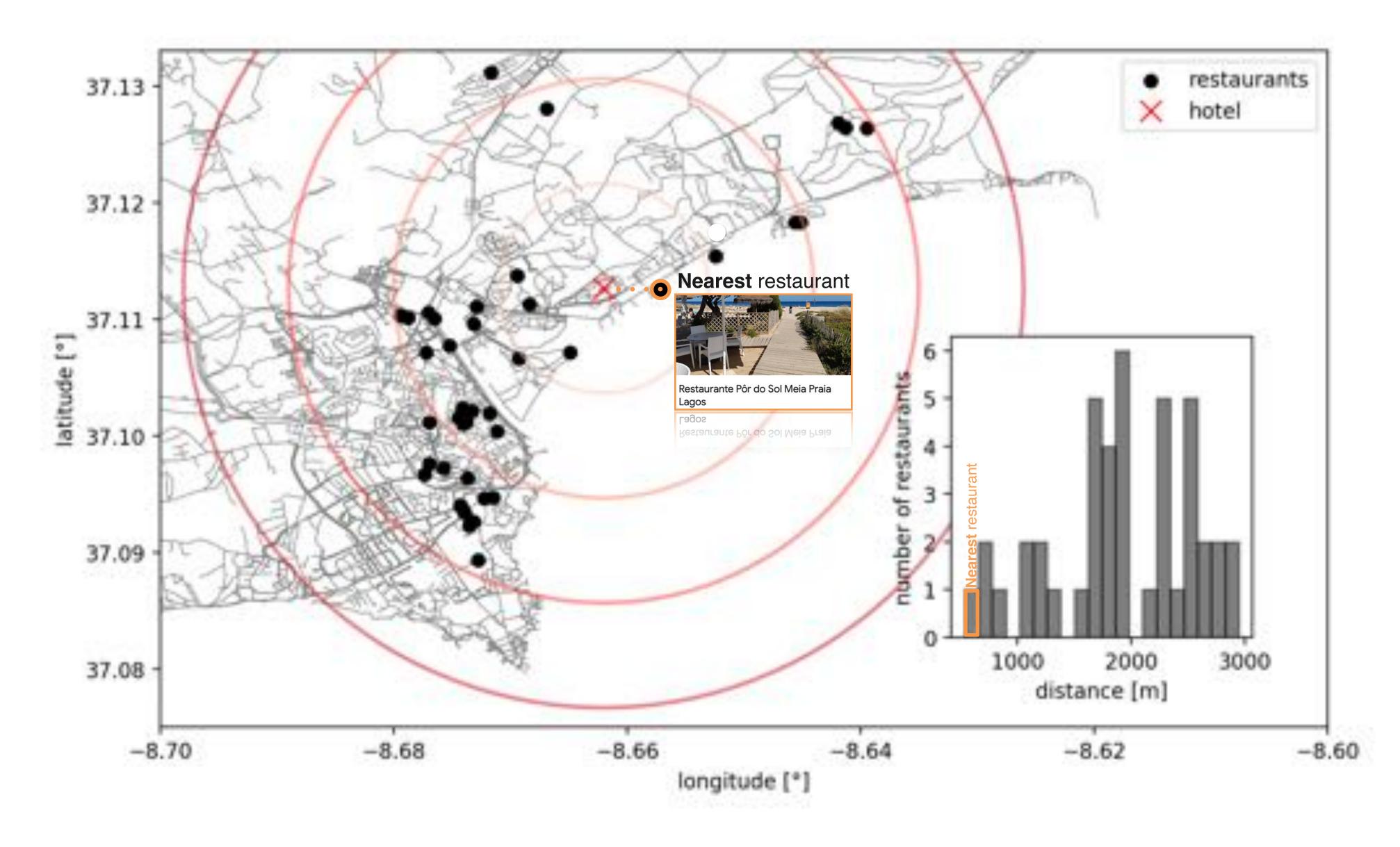




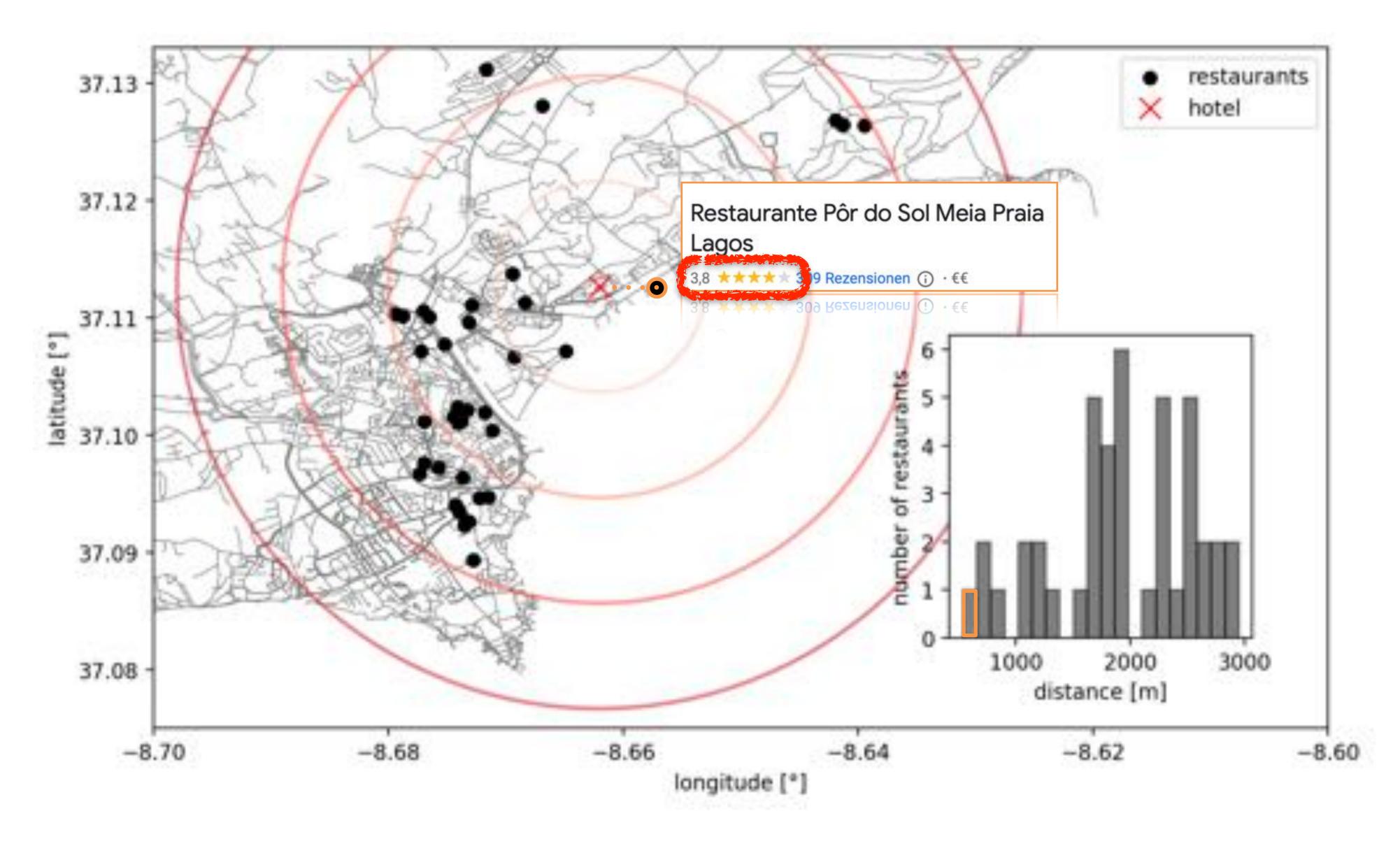




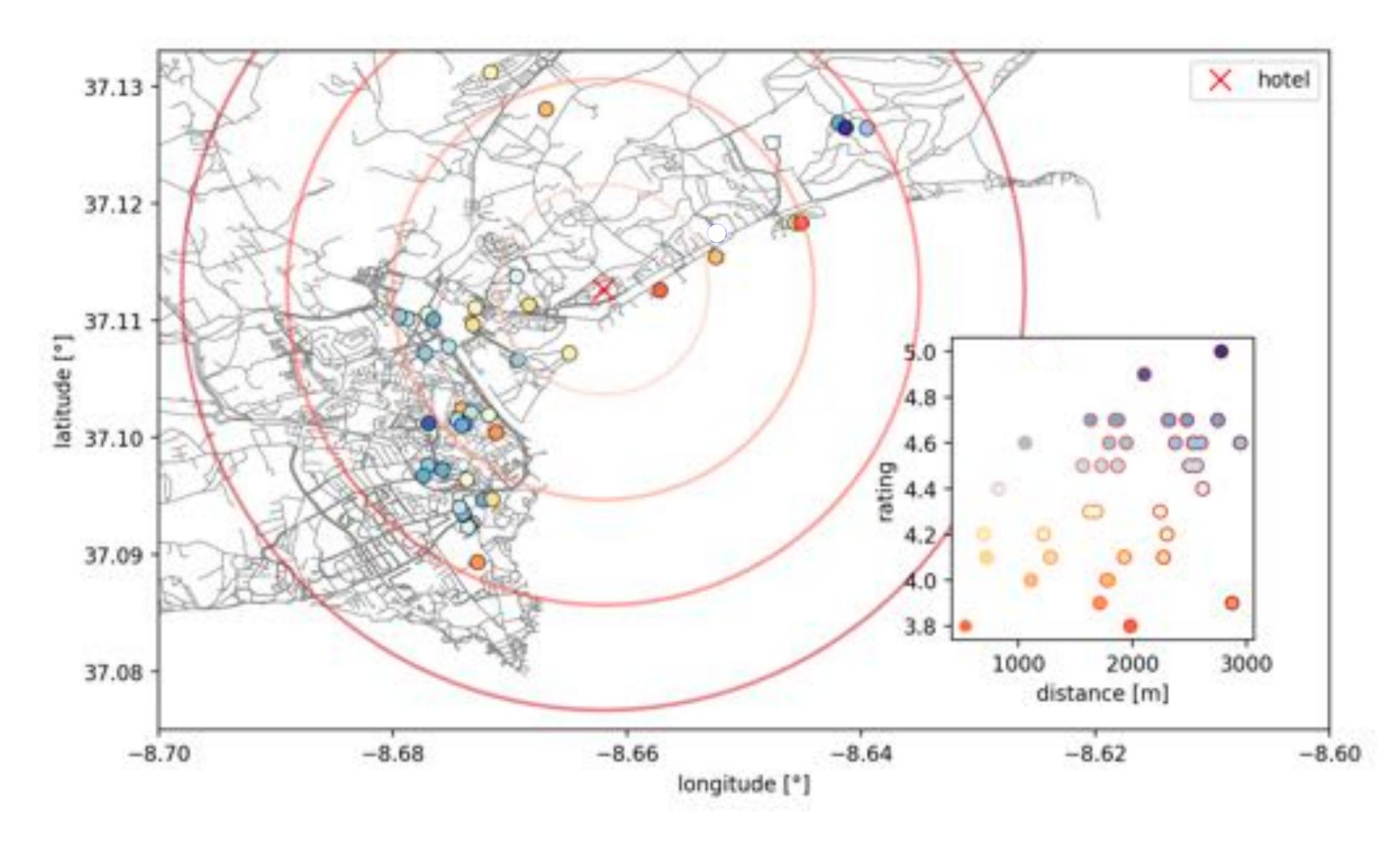




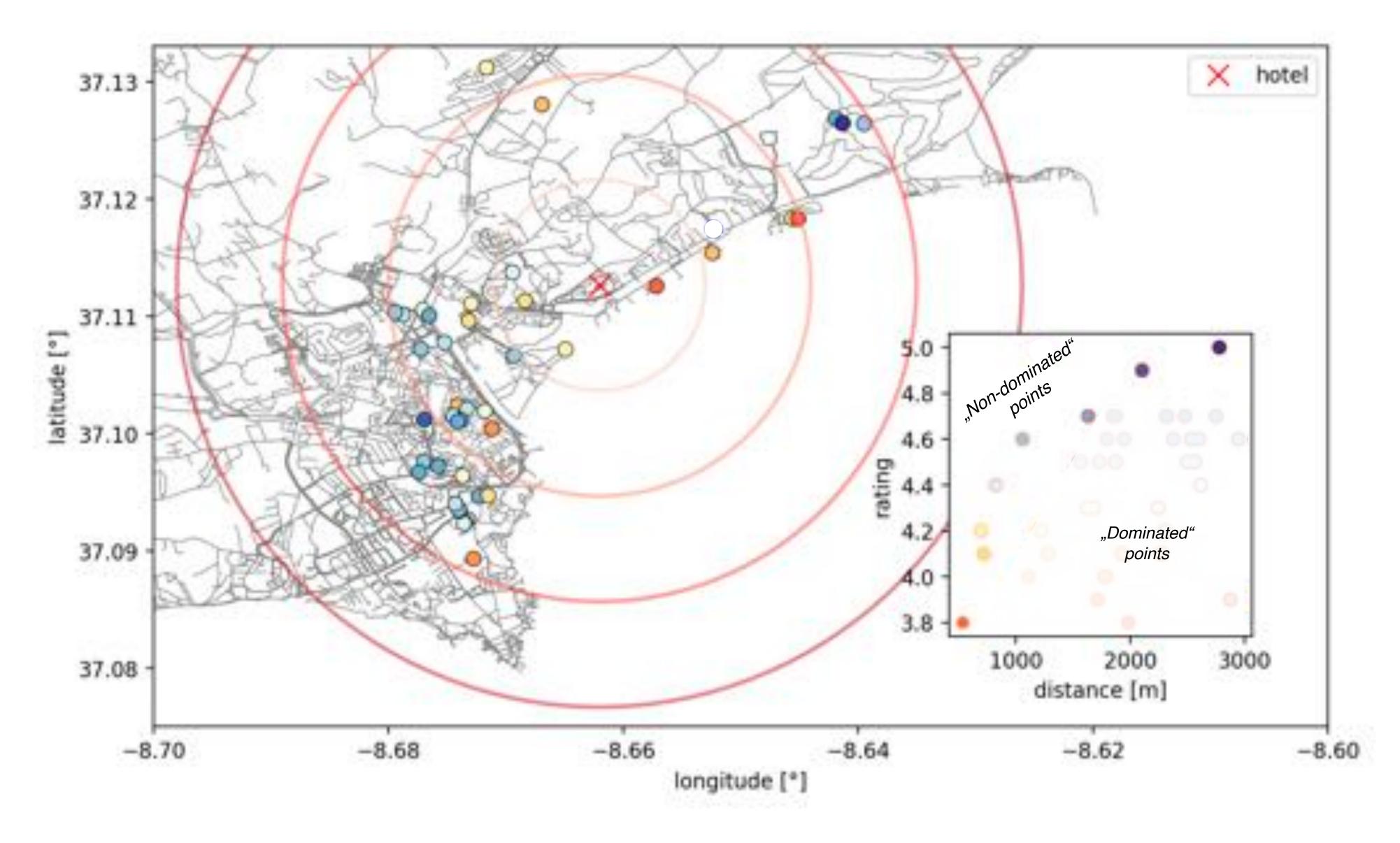






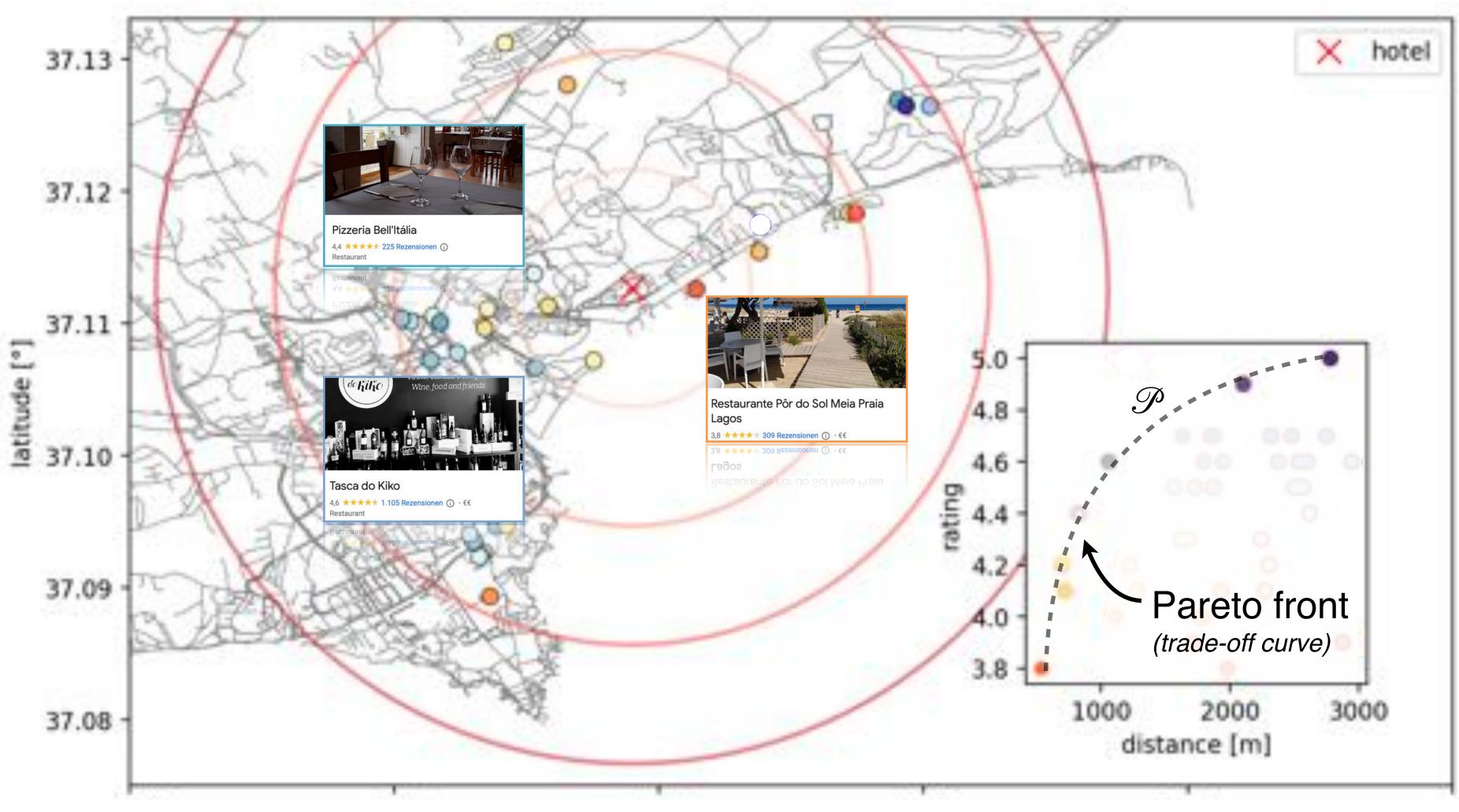






The dinner problem

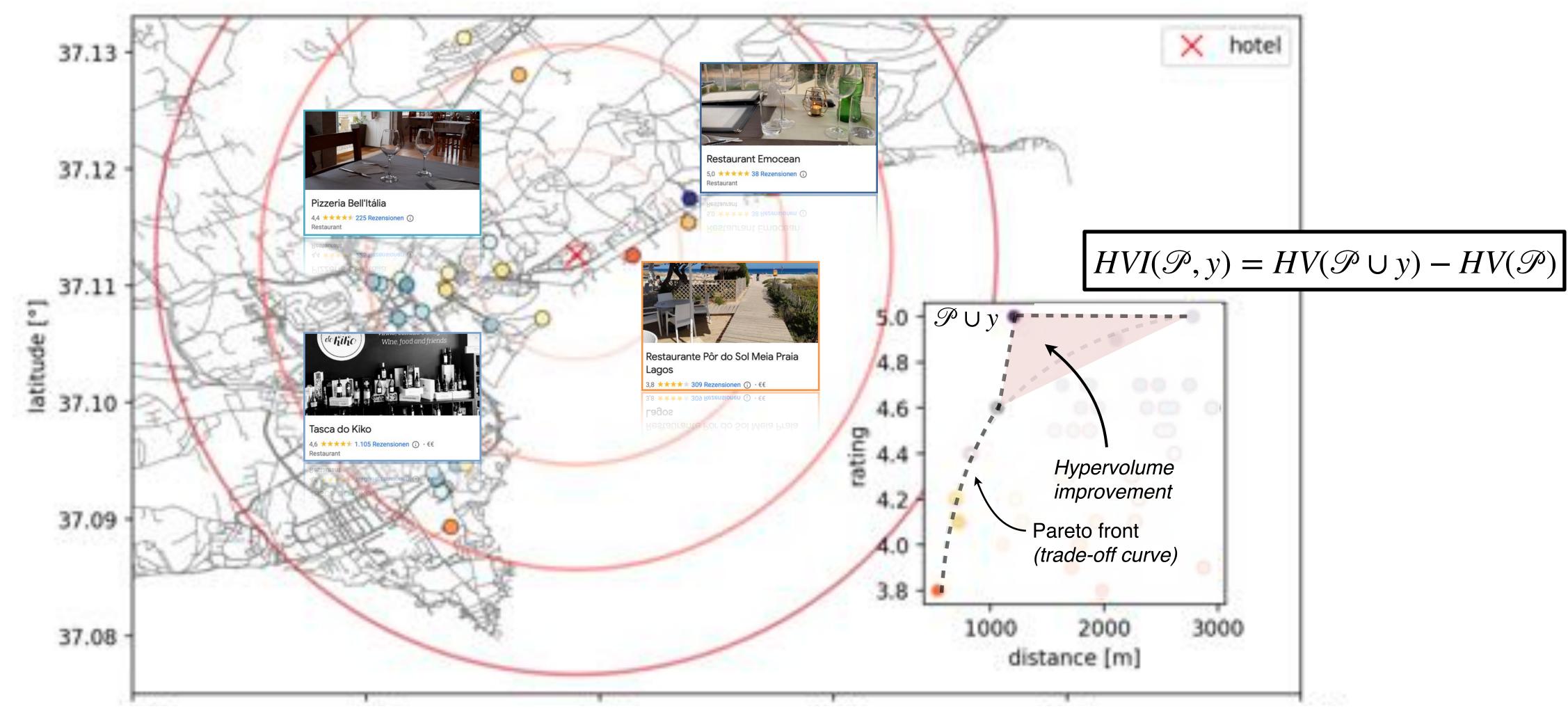




In multi-objective optimization we have multiple (competing) goals with different trade-offs.

The dinner problem

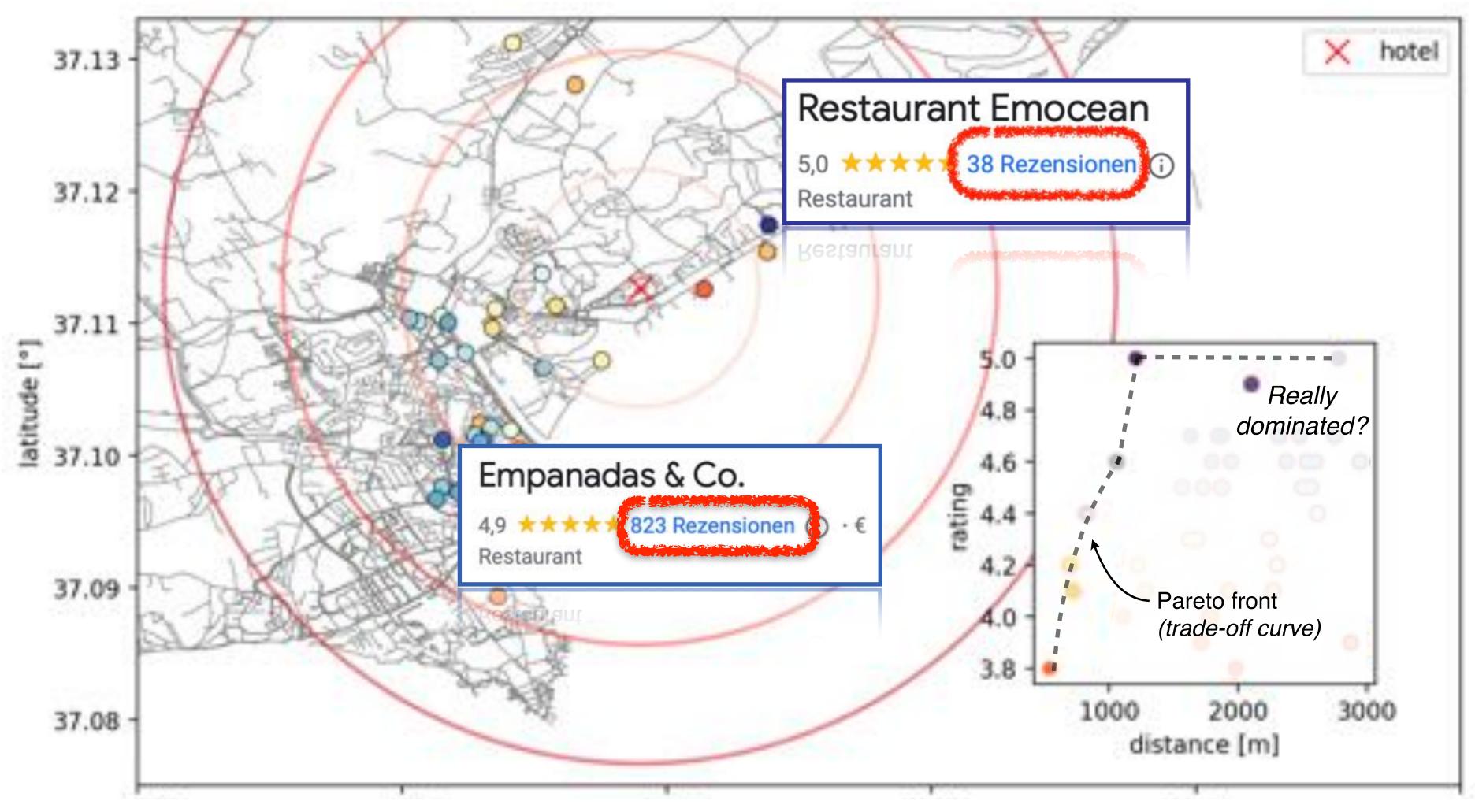




In multi-objective optimization we have multiple (competing) goals with different trade-offs.

Multi-fidelity optimization



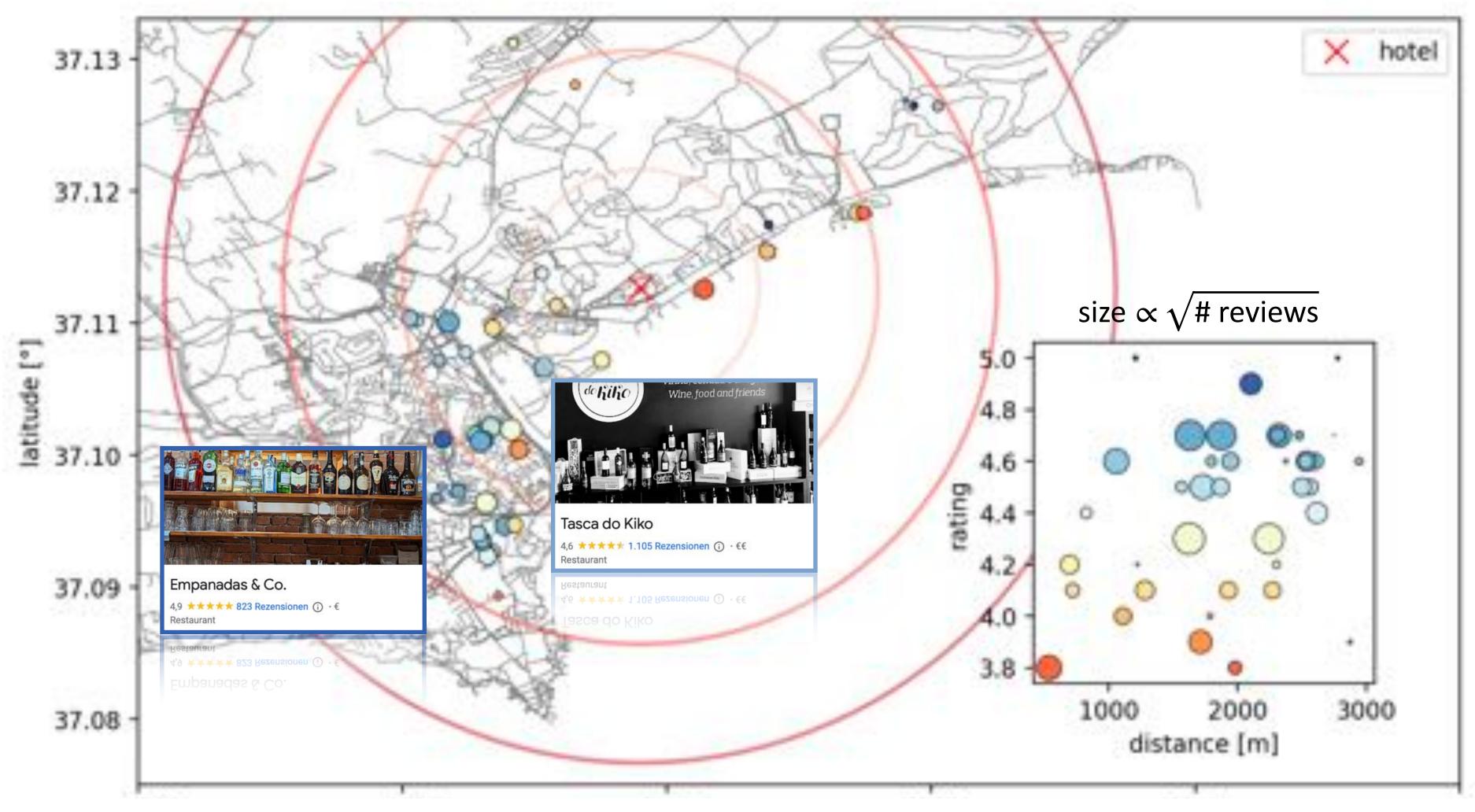


In multi-fidelity optimization we have different confidence in measurements.

Multi-fidelity optimization

The dinner problem





In *multi-fidelity* optimization we have **different confidence in measurements**, thus **spanning another dimension** that represents how much we *trust* the point.

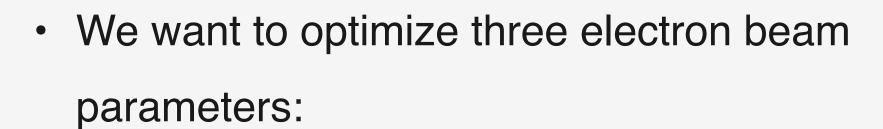


Multi-objective, multi-fidelity

Bayesian optimization

applied to laser-plasma acceleration

Optimization of electron beam properties (FBPIC simulations)



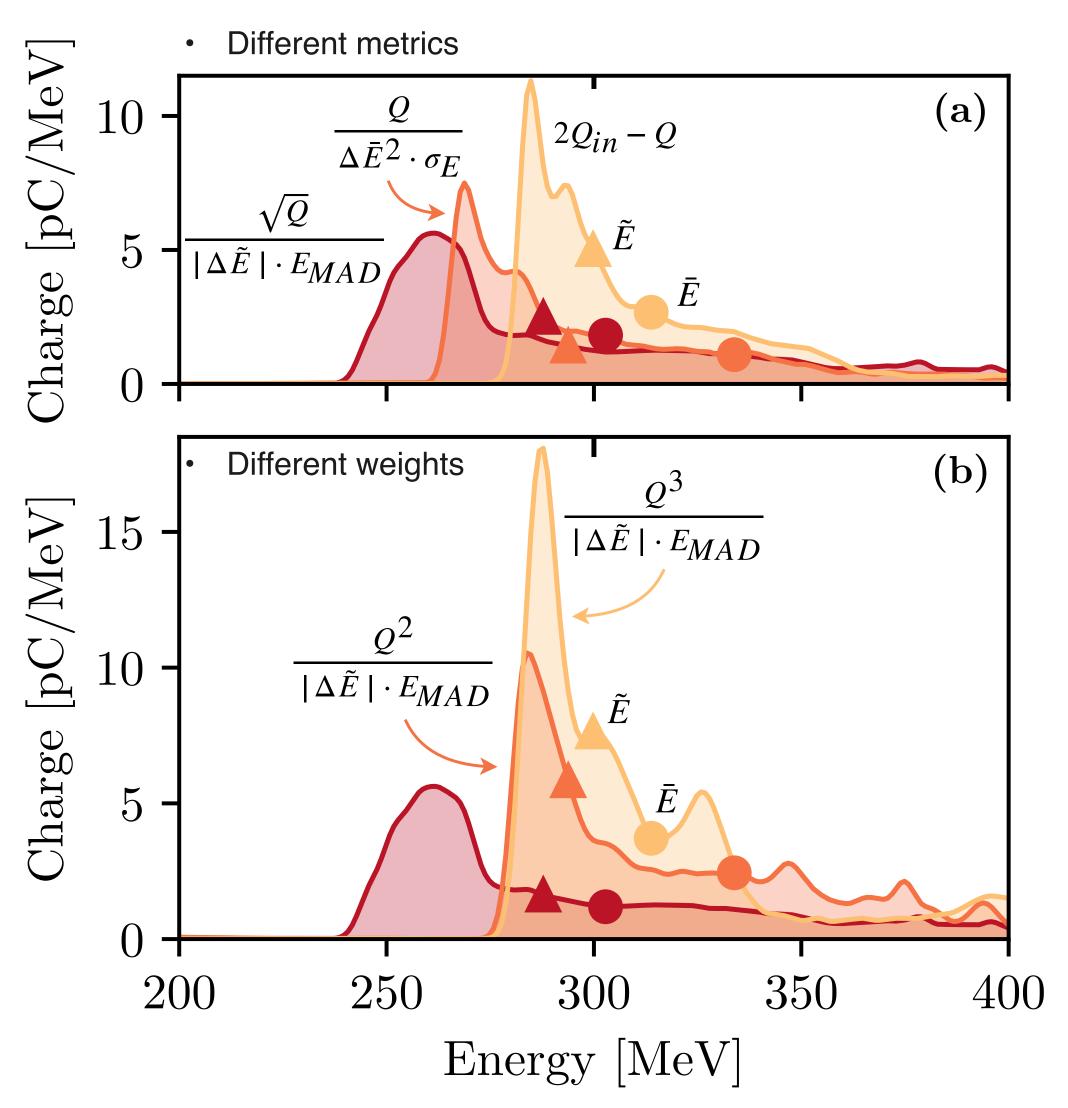
- Charge Q (total charge, charge within FWHM, etc.)
- Bandwidth (standard deviation σ_E , median absolute deviation E_{MAD} , etc.)
- Distance to a target energy $|E_{target} E|$ (using mean energy, median energy, peak energy, etc.)



Optimization of electron beam properties (FBPIC simulations)



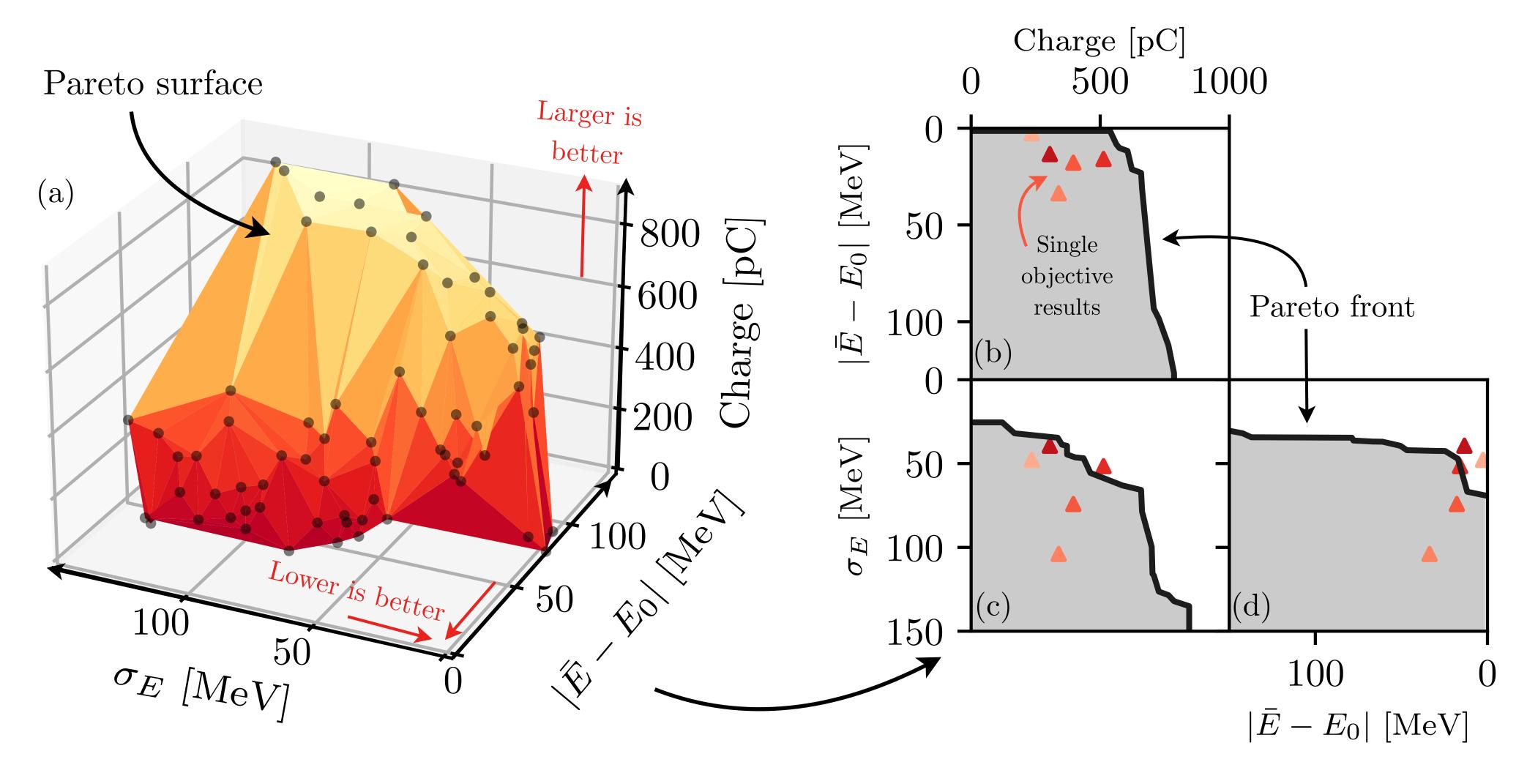
- We want to optimize three electron beam parameters:
 - Charge Q (total charge, charge within FWHM, etc.)
 - Bandwidth (standard deviation σ_E , median absolute deviation E_{MAD} , etc.)
 - Distance to a target energy $|E_{target} E|$ (using mean energy, median energy, peak energy, etc.)
- We can use the simulation resolution as our fidelity, i.e. we trust a high-resolution simulation more than a low-resolution simulation (including low-res gives one order of magnitude speed-up)
- Choosing different metrics or weights for each objective changes the outcome in an a priori unknown way!



• Irshad, F., Karsch, S., & Döpp, A. Multi-objective and multi-fidelity Bayesian optimization of laser-plasma acceleration. *Phys. Rev. Research 5, 013063 (2023)*

Optimization of electron beam properties (FBPIC simulations)





^{1.} Irshad, F., Karsch, S., & Döpp, A. EHVI for simultaneous multi-objective and multi-fidelity optimization. arXiv preprint arXiv:2112.13901 (2021)

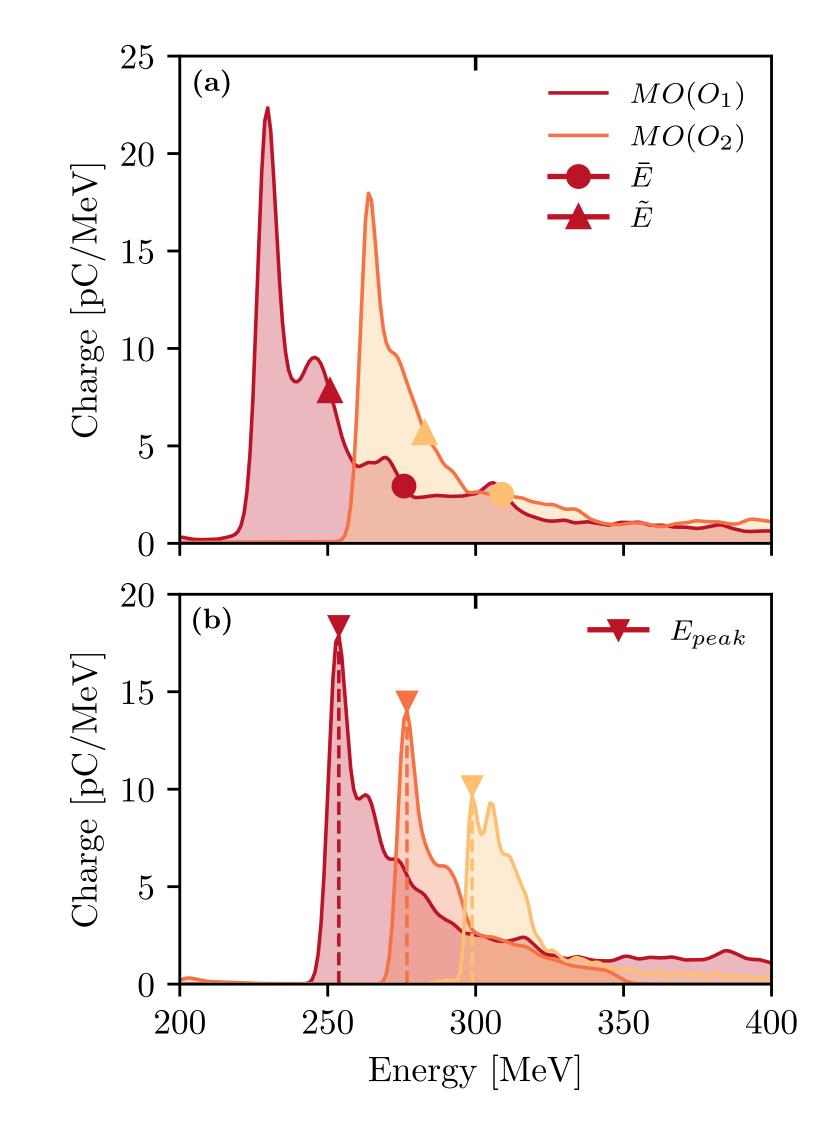
^{2.} Irshad, F., Karsch, S., & Döpp, A. Multi-objective and multi-fidelity Bayesian optimization of laser-plasma acceleration. Phys. Rev. Research 5, 013063 (2023)

Optimization of electron beam properties (FBPIC simulations)

PULSE CALA.

 Once the Pareto-optimal solutions are identified, we can choose from them what kind of beam we want.

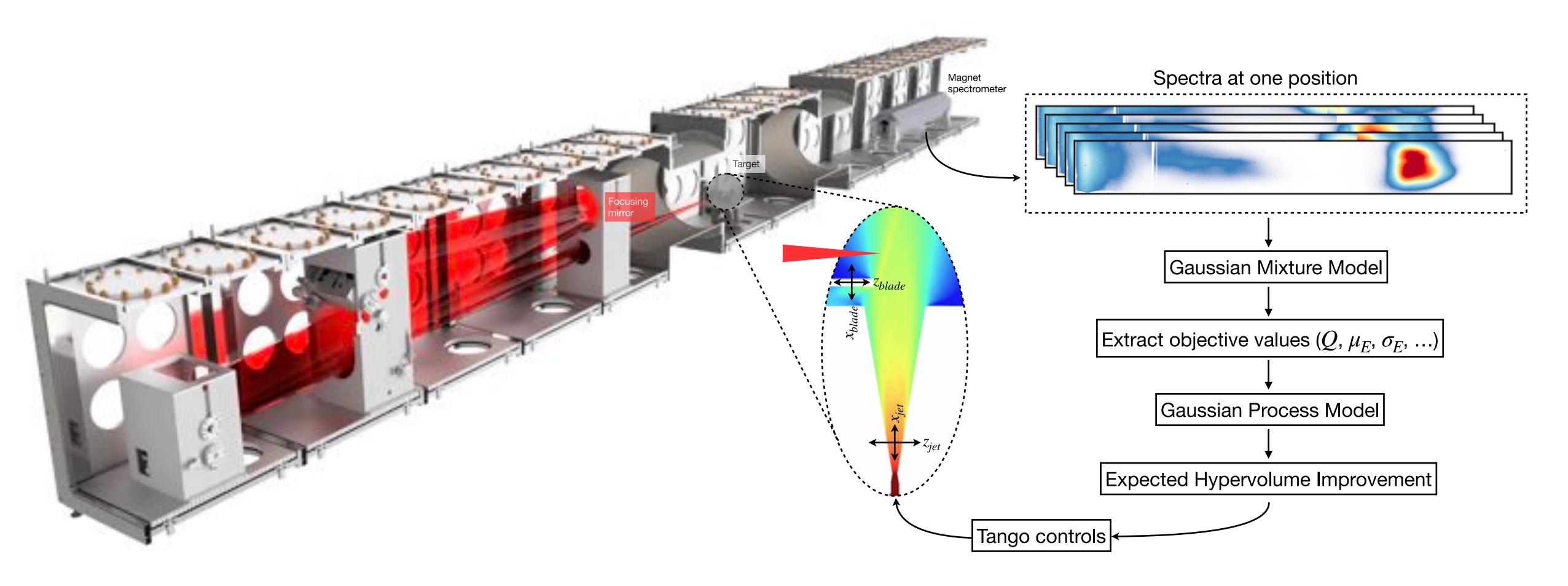
 We can also use the model's data to change parameters a posteriori, e.g. to tune the beam energy.



• Irshad, F., Karsch, S., & Döpp, A. Multi-objective and multi-fidelity Bayesian optimization of laser-plasma acceleration. *Phys. Rev. Research 5, 013063 (2023)*

Optimization of electron beam properties (Experiment)

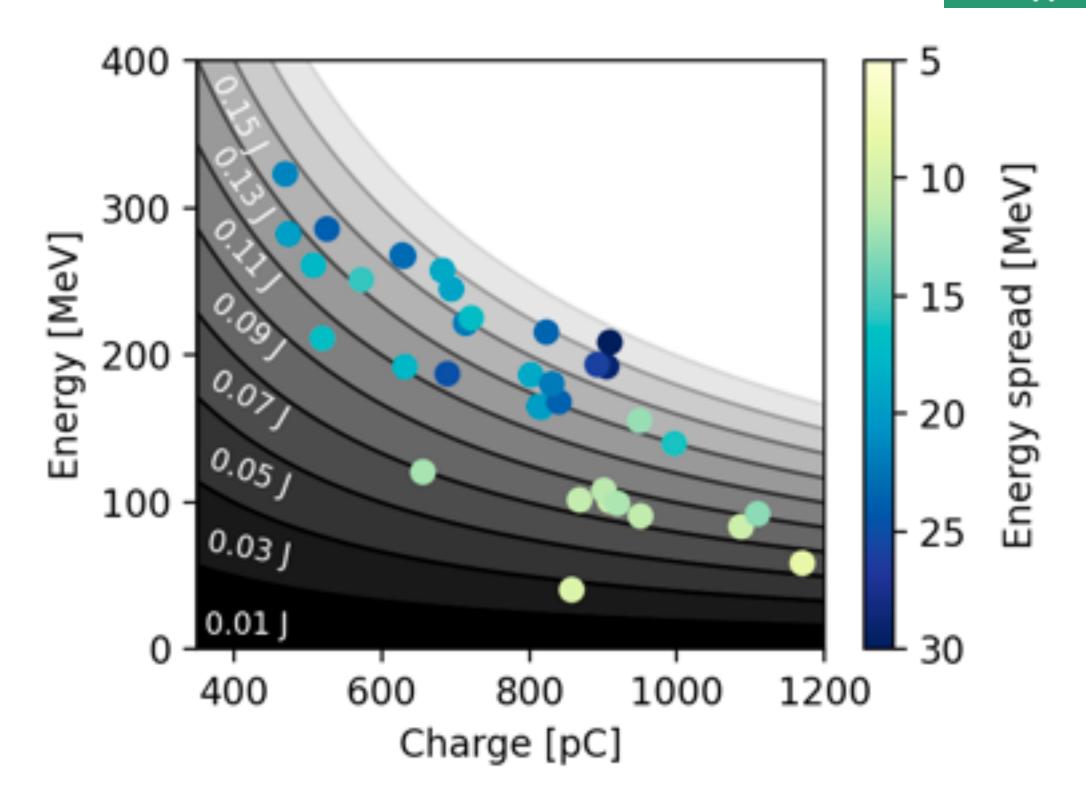




- N. Weiße et al. Tango Controls and Data Pipeline for Petawatt Laser Experiments, HPLSE, 10.1017/hpl.2023.17 (2023)
- F. Irshad, et al. Pareto Optimization of a Laser Wakefield Accelerator (under review)

Optimization of electron beam properties (Experiment)

- Once the Pareto-optimal solutions are identified, we can choose from them what kind of beam we want.
- We observe that many of the Pareto-optimal solutions yield the same laser-to-beam efficiency.



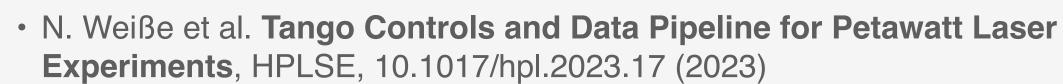


[•] N. Weiße et al. Tango Controls and Data Pipeline for Petawatt Laser Experiments, HPLSE, 10.1017/hpl.2023.17 (2023)

[•] F. Irshad, et al. Pareto Optimization of a Laser Wakefield Accelerator (under review)

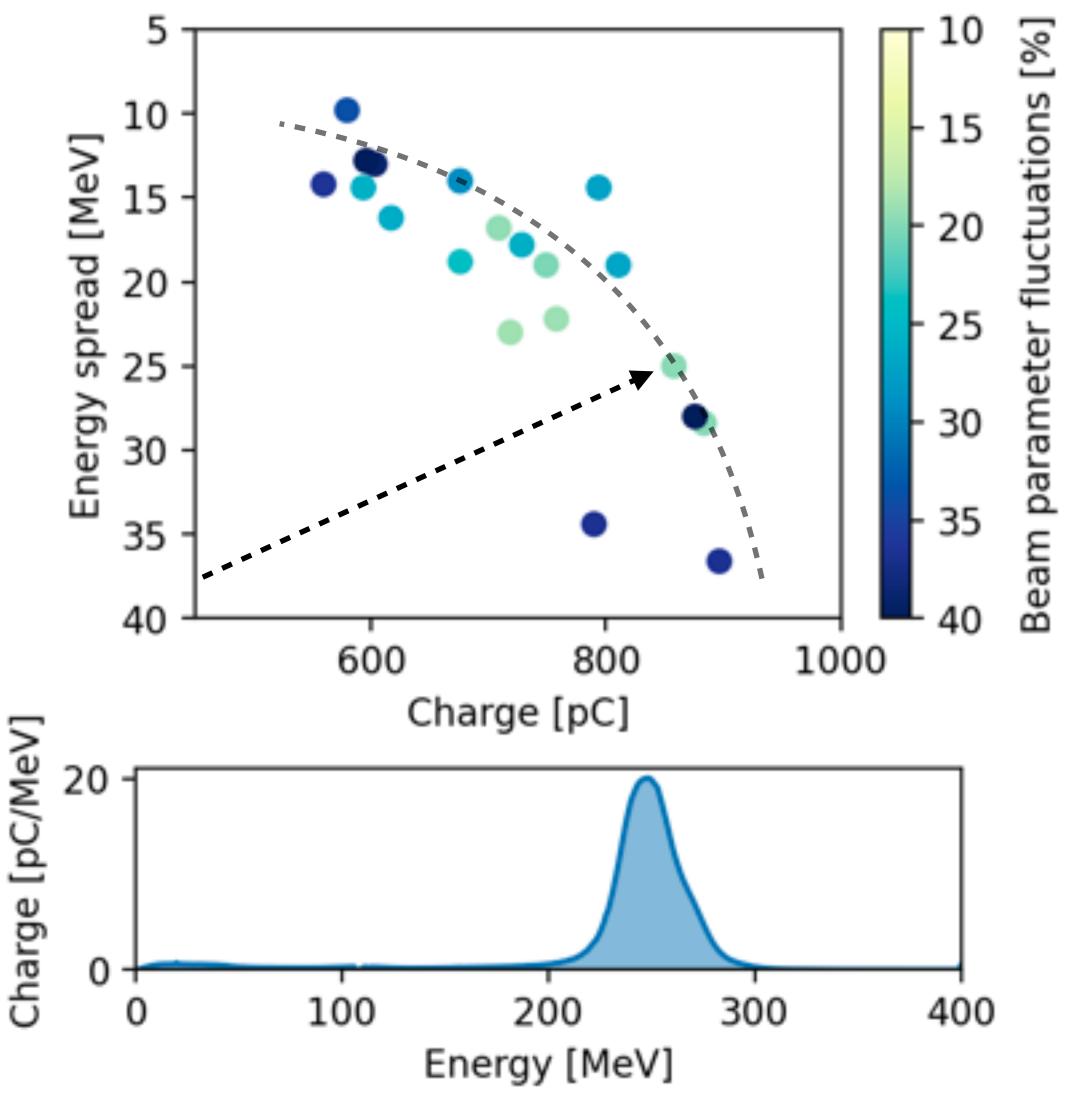
Optimization of electron beam properties (Experiment)

- Once the Pareto-optimal solutions are identified, we can choose from them what kind of beam we want.
- We can select and exploit one particular solution within the Pareto-optimal solutions by fitting $O_{select} = a_1 Q + a_2 \sigma_E + a_3 |E_{target} E|$ such that it is maximized for the selected point.



[•] F. Irshad, et al. Pareto Optimization of a Laser Wakefield Accelerator (under review)





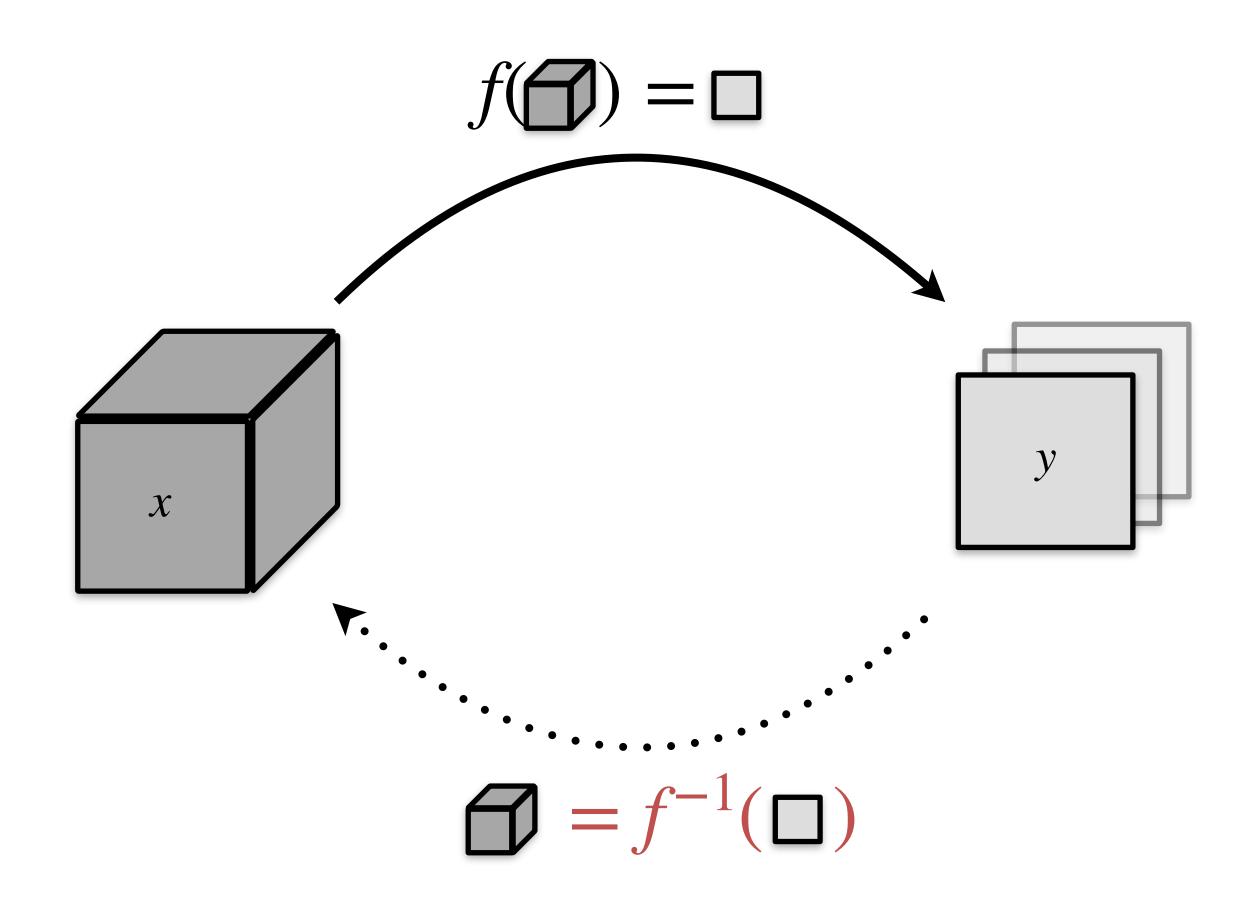


Part 2 Inverse problems

Inverse Problems

Determining cause from effect



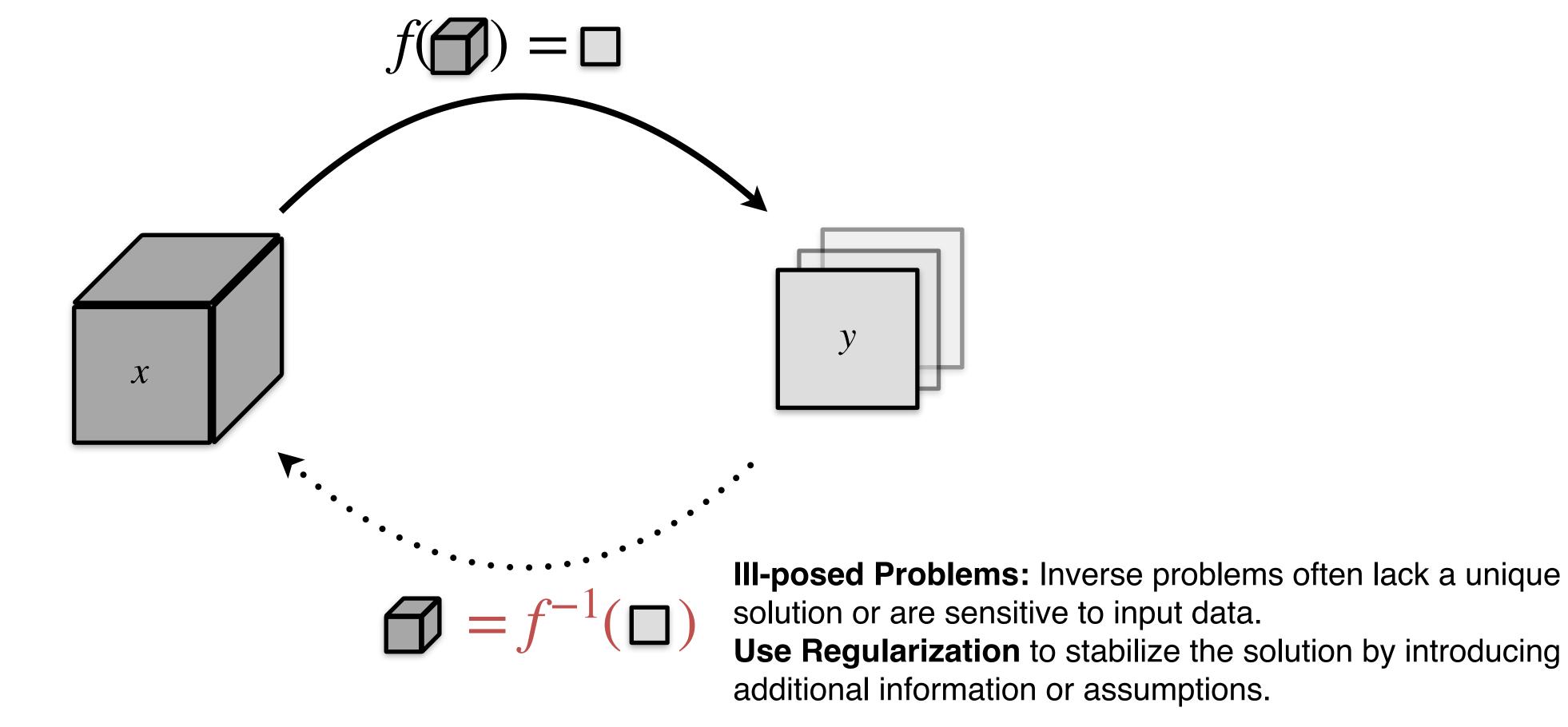


Cause and Effect: Inverse problems involve determining the cause (e.g. 3D structure) from the observed effect (e.g. 2D projections).

Inverse Problems

Determining cause from effect





Cause and Effect: Inverse problems involve determining the cause (e.g. 3D structure) from the observed effect (e.g. 2D projections).

Inverse Problems

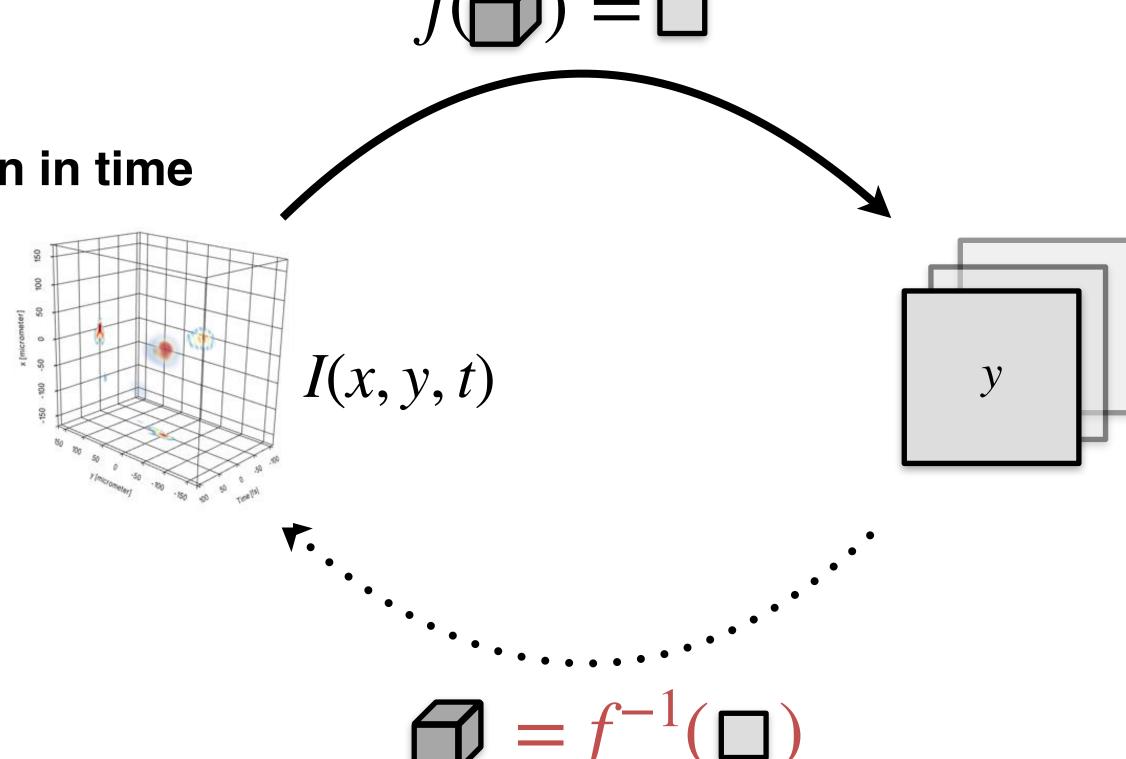
An example



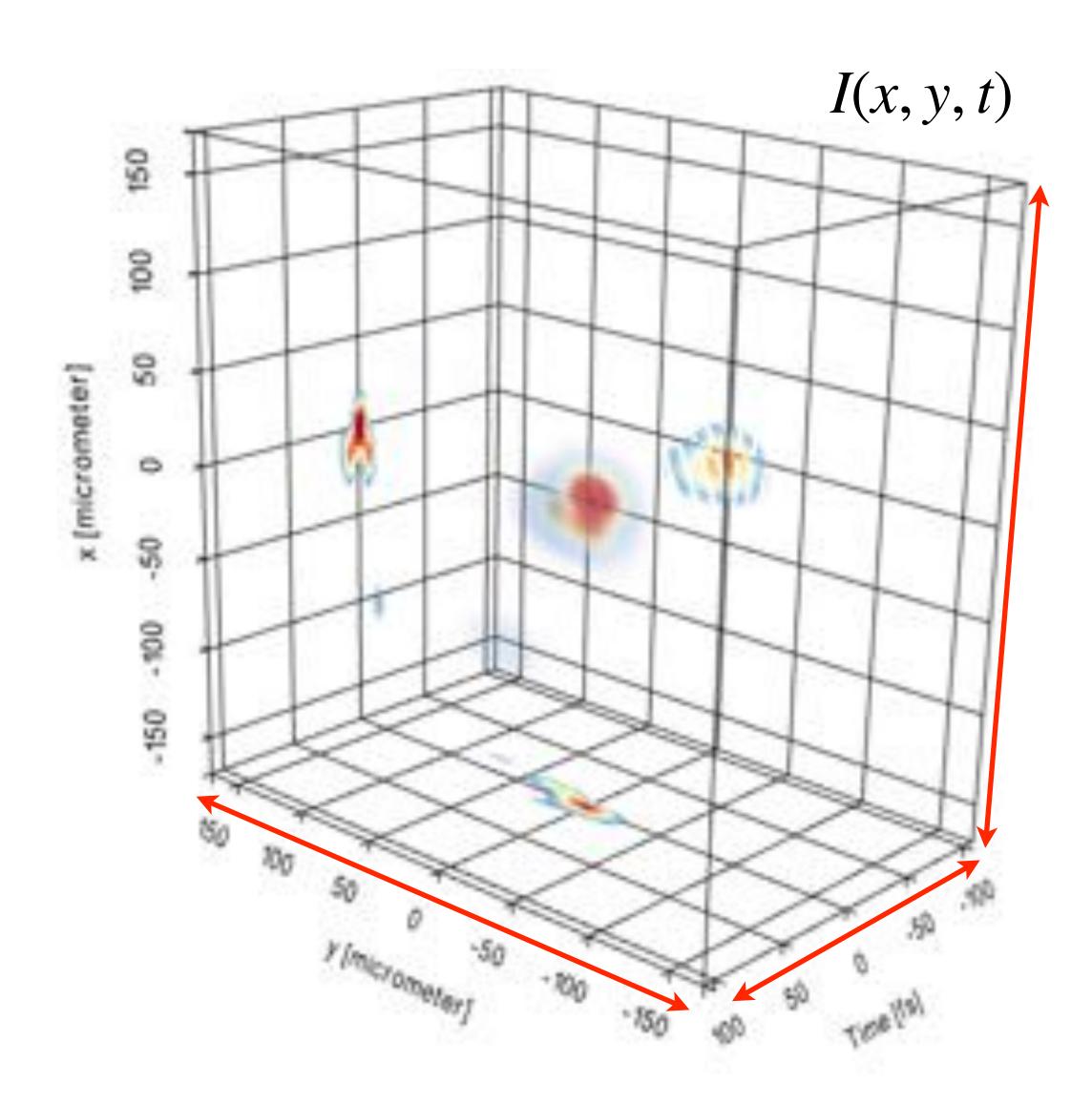
3-D intensity distribution in time

Knowledge necessary for

- Highest peak-intensity
- Accurate simulations
- Spatio-temporal shaping (flying focus etc.)
- •







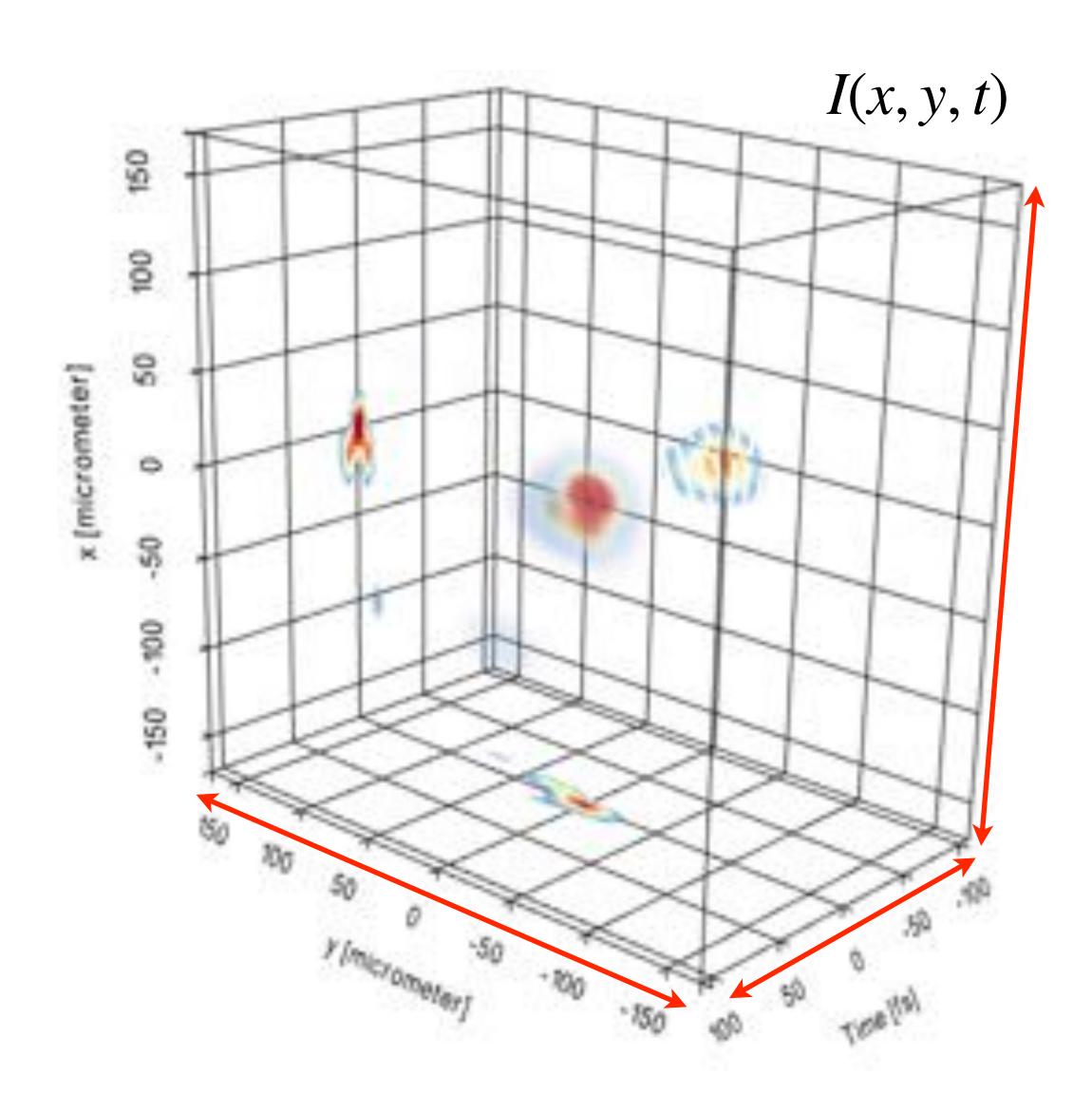
3-D intensity distribution in time

$$n = n_x \times n_y \times n_\lambda \sim 1000 \times 1000 \times 100 = 10^8$$
 voxels

100 million parameters: Need many measurements

Common solution: Fourier transform spectroscopy (INSIGHT, TERMITES) with >1000 2D measurements at 1 MP





3-D intensity distribution in time

$$n = n_x \times n_y \times n_\lambda \sim 1000 \times 1000 \times 100 = 10^8$$
 voxels

100 million parameters: Need many measurements

Common solution: Fourier transform spectroscopy (INSIGHT, TERMITES) with >1000 2D measurements at 1 MP

But are voxels really a good base function choice?

Multi-spectral, modal reconstruction



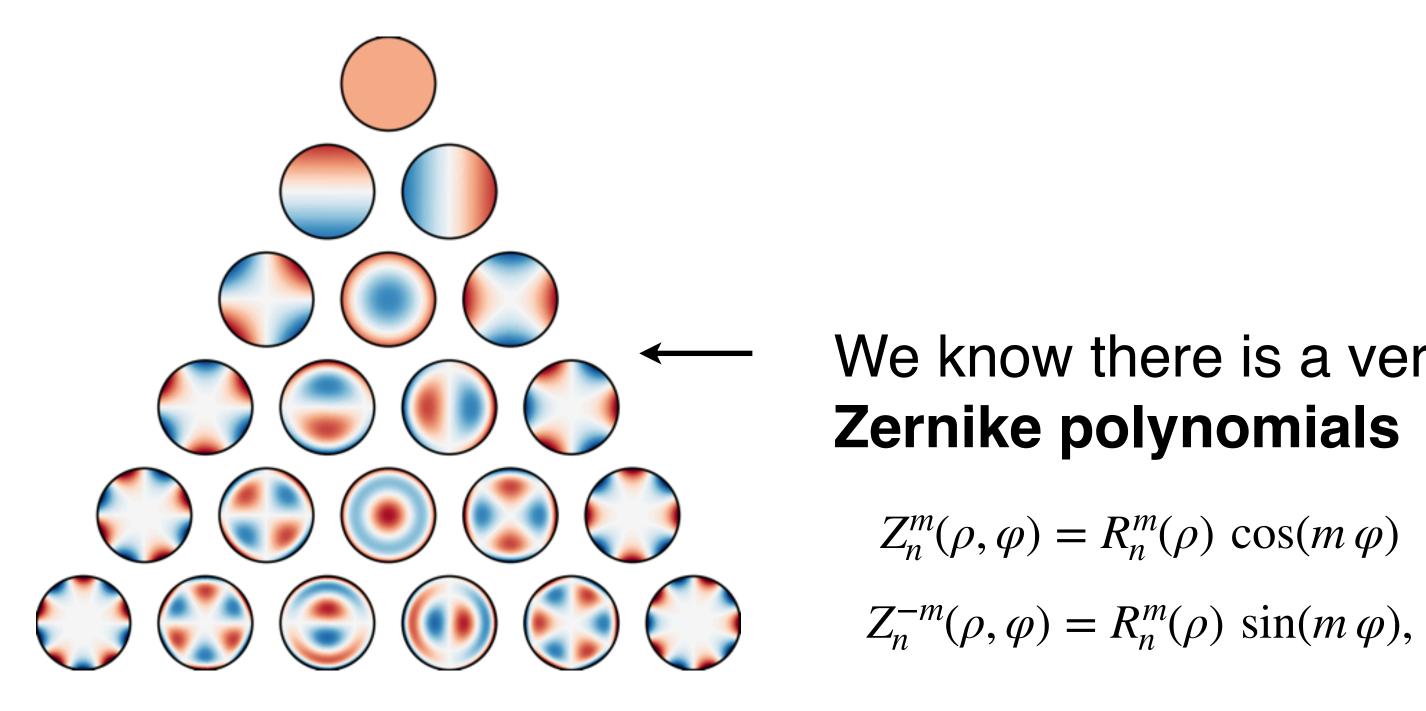
$$I(x, y, t) = \|\mathcal{F}\left[\sqrt{I(x, y, \omega)} \cdot \exp\left(i\Phi(x, y, \omega)\right)\right]\|^{2}$$

This is the important part, describing the focused intensity!

Multi-spectral, modal reconstruction



$$I(x, y, t) = \|\mathscr{F}\left[\sqrt{I(x, y, \omega)} \cdot \exp\left(i\Phi(x, y, \omega)\right)\right]\|^{2}$$



We know there is a very good base to describe phase: Zernike polynomials

$$Z_n^m(\rho, \varphi) = R_n^m(\rho) \cos(m \varphi)$$

$$Z_n^{-m}(\rho,\varphi) = R_n^m(\rho) \sin(m\varphi)$$

Multi-spectral, modal reconstruction

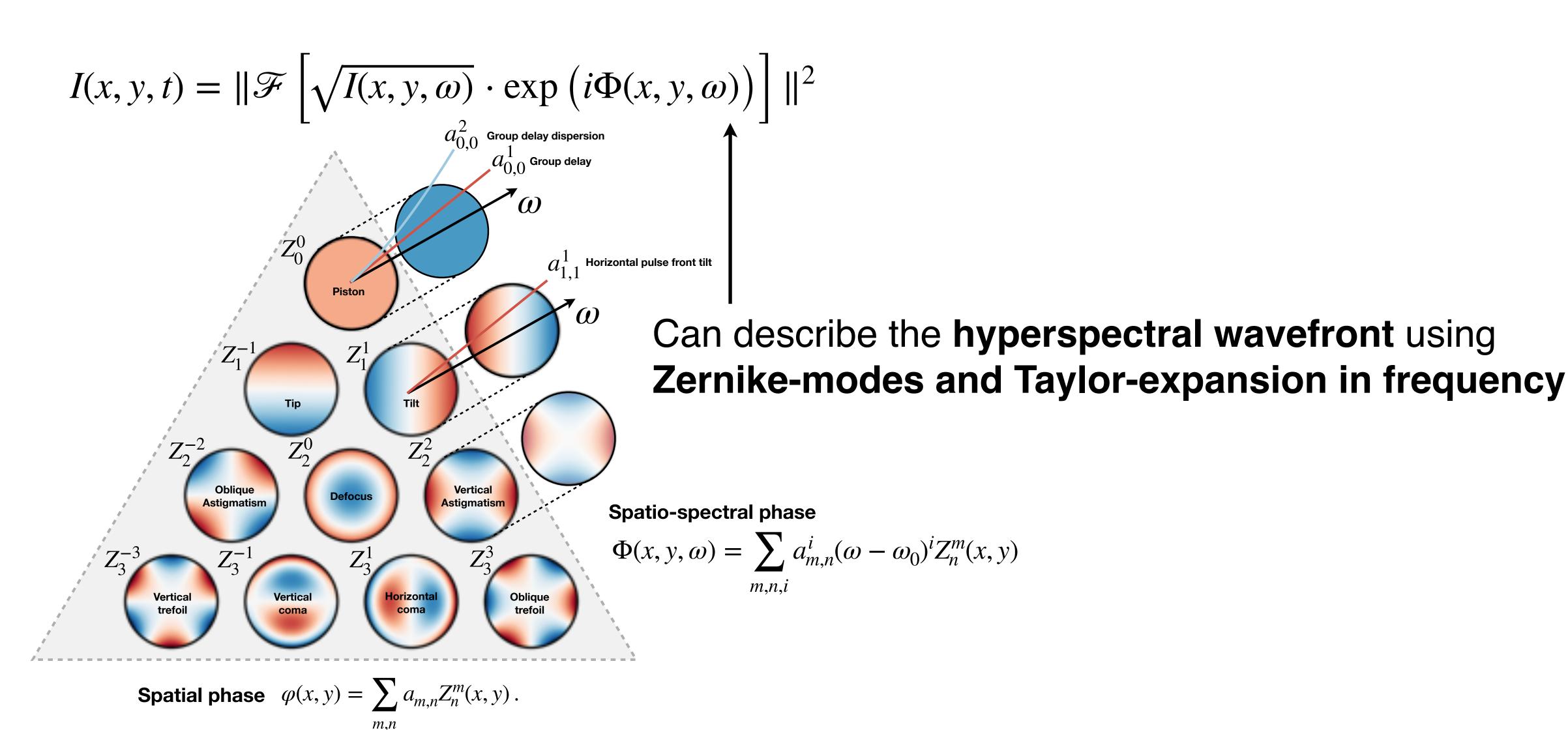


$$I(x, y, t) = \|\mathscr{F}\left[\sqrt{I(x, y, \omega)} \cdot \exp\left(i\Phi(x, y, \omega)\right)\right]\|^2$$

We also know there is a very good way to describe spectral phase: **Taylor expansion** (group delay, group delay dispersion, etc.)

Multi-spectral, modal reconstruction





Multi-spectral, modal reconstruction



$$I(x, y, t) = \|\mathcal{F}\left[\sqrt{I(x, y, \omega)} \cdot \exp\left(i\Phi(x, y, \omega)\right)\right]\|^{2}$$

$$\Phi(x, y, \omega) = \sum_{m, n, i} a_{m, n}^{i} (\omega - \omega_{0})^{i} Z_{n}^{m}(x, y)$$

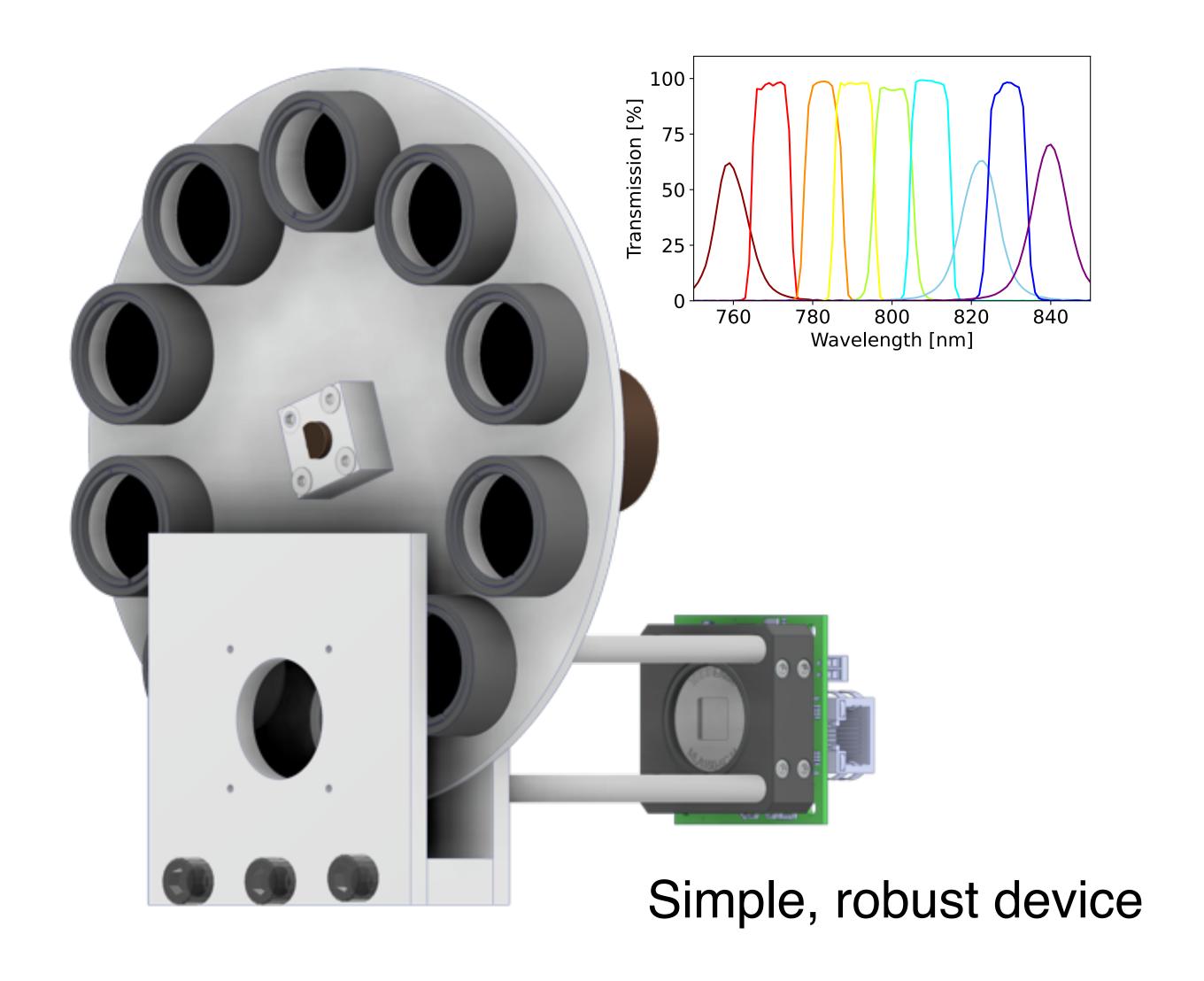
Can describe the hyperspectral wavefront using Zernike-modes and Taylor-expansion in frequency

Instead of > 1,000,000 voxels we only need to reconstruct dominant mode coefficients

Allows us to retrieve spatio-temporal couplings within a few measurements

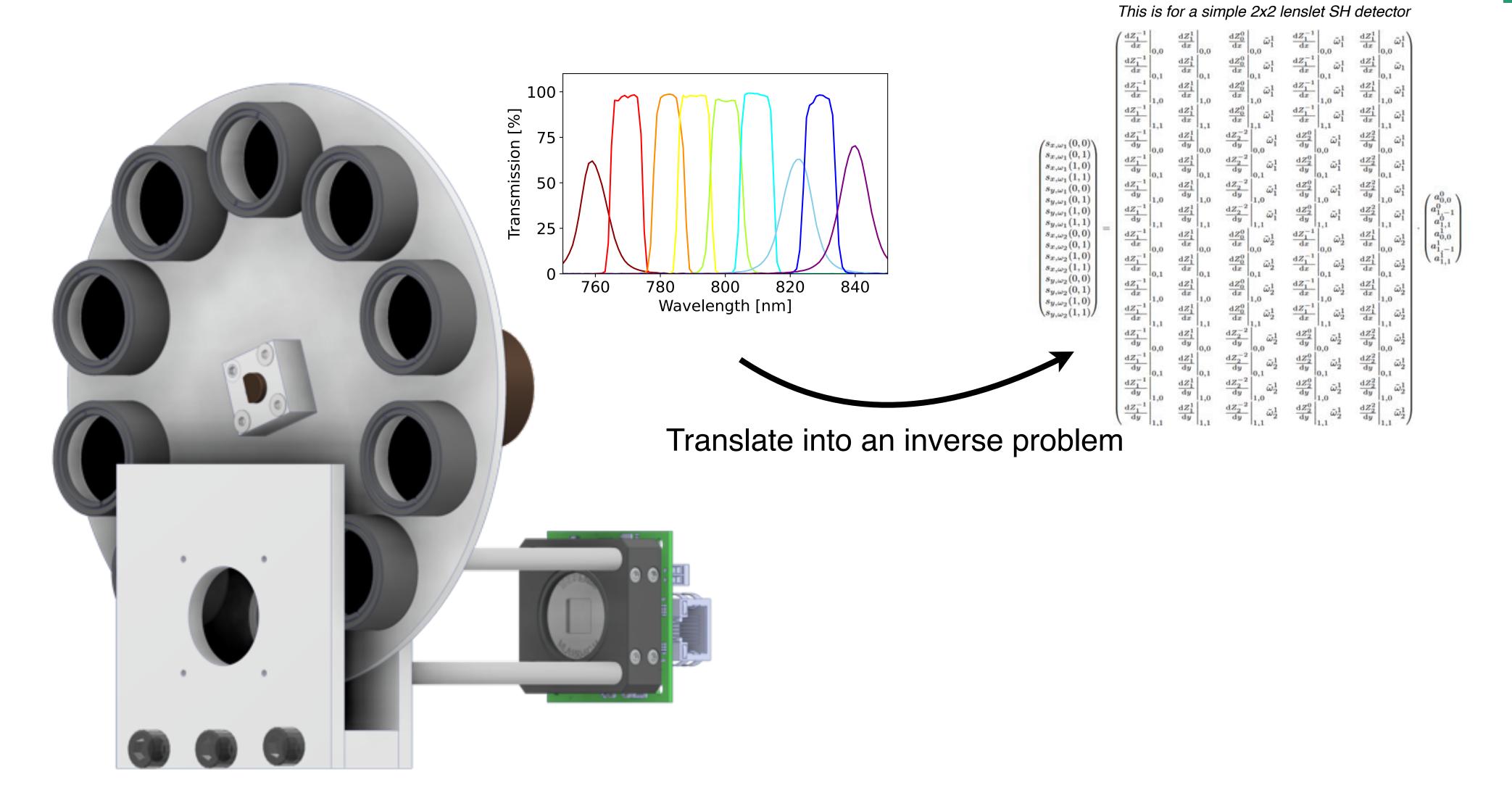
FALCON - Fast Acquisition of Laser Couplings using Narrowband Filters





PULSE

FALCON - Fast Acquisition of Laser Couplings using Narrowband Filters

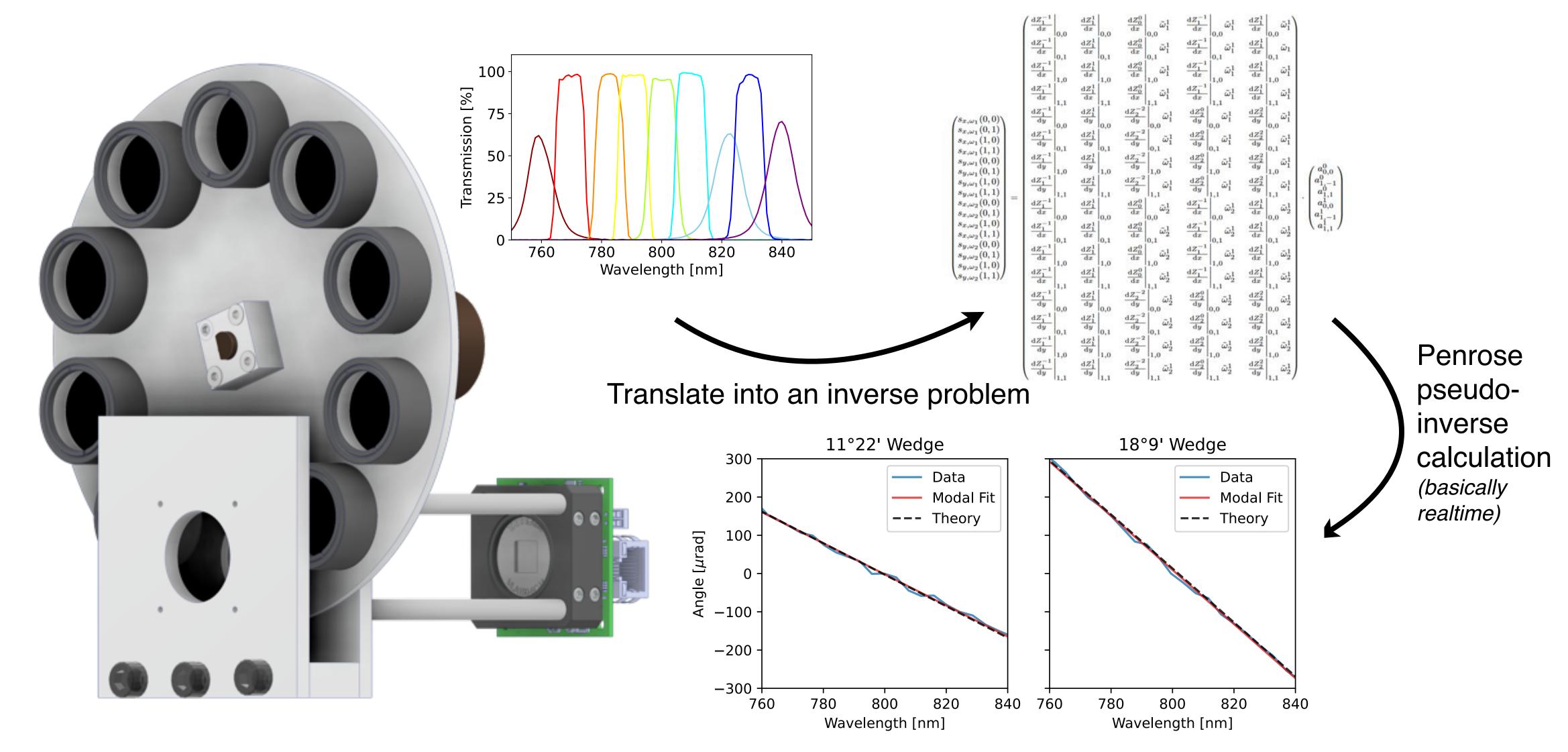


N. Weiße, J. Esslinger et al. Measuring spatial-temporal couplings using modal multi-spectral wavefront reconstruction, Opt. Express 31, 19733-19745 (2023)

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FALCON - Fast Acquisition of Laser Couplings using Narrowband Filters





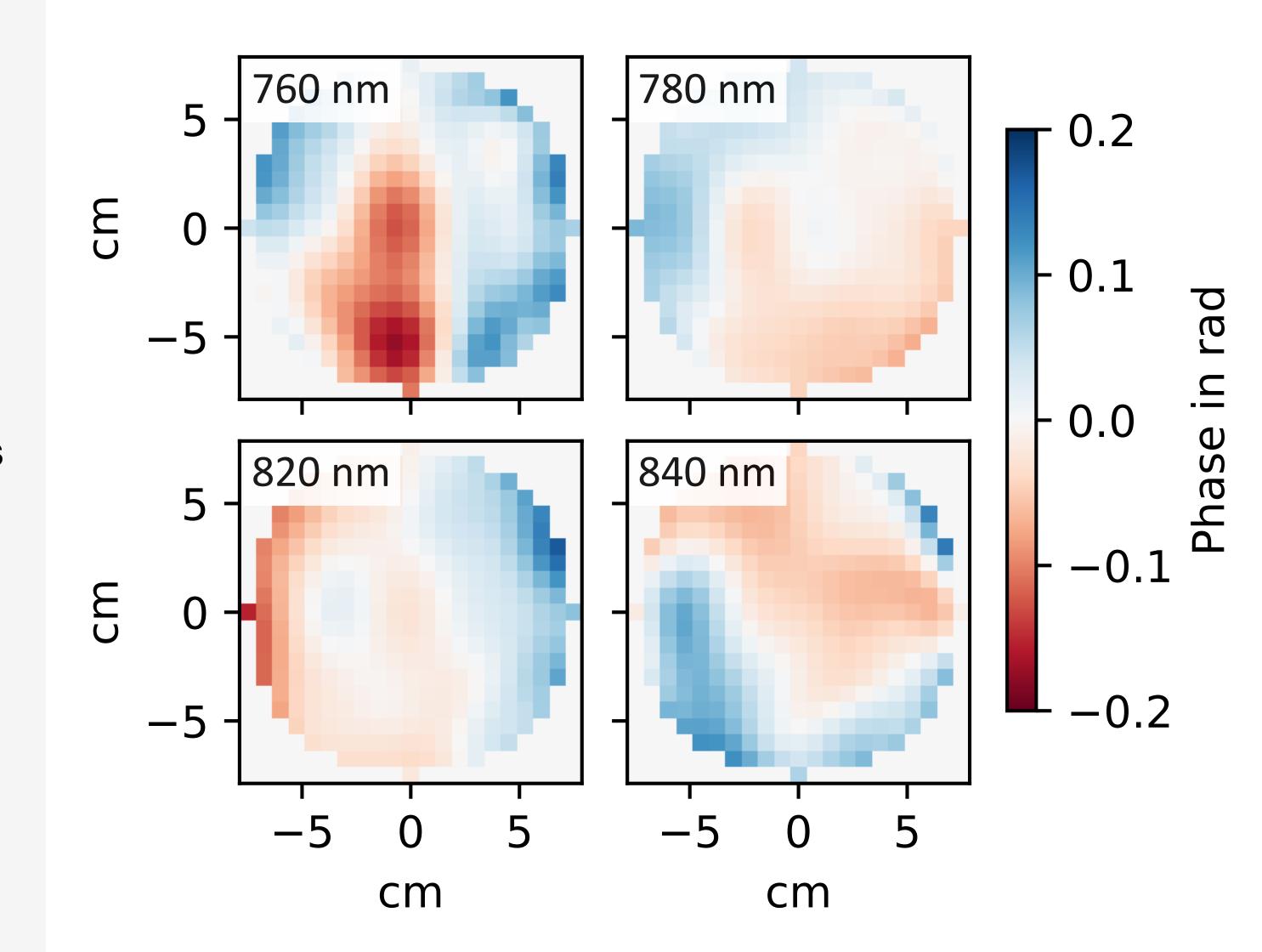
N. Weiße, J. Esslinger et al. Measuring spatial-temporal couplings using modal multi-spectral wavefront reconstruction, Opt. Express 31, 19733-19745 (2023)

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Measurement of STCs of the ATLAS petawatt laser

PULSE CALA.

- Full measurement takes ~ 1 minute
 (9 wavelengths, 5 shots each)
- Measurement shows couplings in ATLAS are
 < λ/10 between 780 820 nm
- FALCON measurement now routinely performed every day after focus measurements



N. Weiße, J. Esslinger et al. Measuring spatial-temporal couplings using modal multi-spectral wavefront reconstruction, Opt. Express 31, 19733-19745 (2023)

Least-squares in Zernike-Taylor basis



Much more robust reconstruction!

Compressed sensing



$$Ax = y \xrightarrow{\text{Minimize}} \arg\min\{\|Ax - y\|^2\}$$

$$\downarrow^{x}$$

$$\downarrow^{\text{Transform to some sparse basis}}$$

$$\text{(e.g. wavelet, PCA, etc.)}$$

$$\arg\min\{\|A\Psi\tilde{x} - y\|^2 + \|\tilde{x}\|_1\}$$

$$\tilde{x}$$
Few coefficients as possible

Deep compressed sensing



$$Ax = y \xrightarrow{\text{Minimize}} \arg\min_{\{\|Ax - y\|^2\}}$$

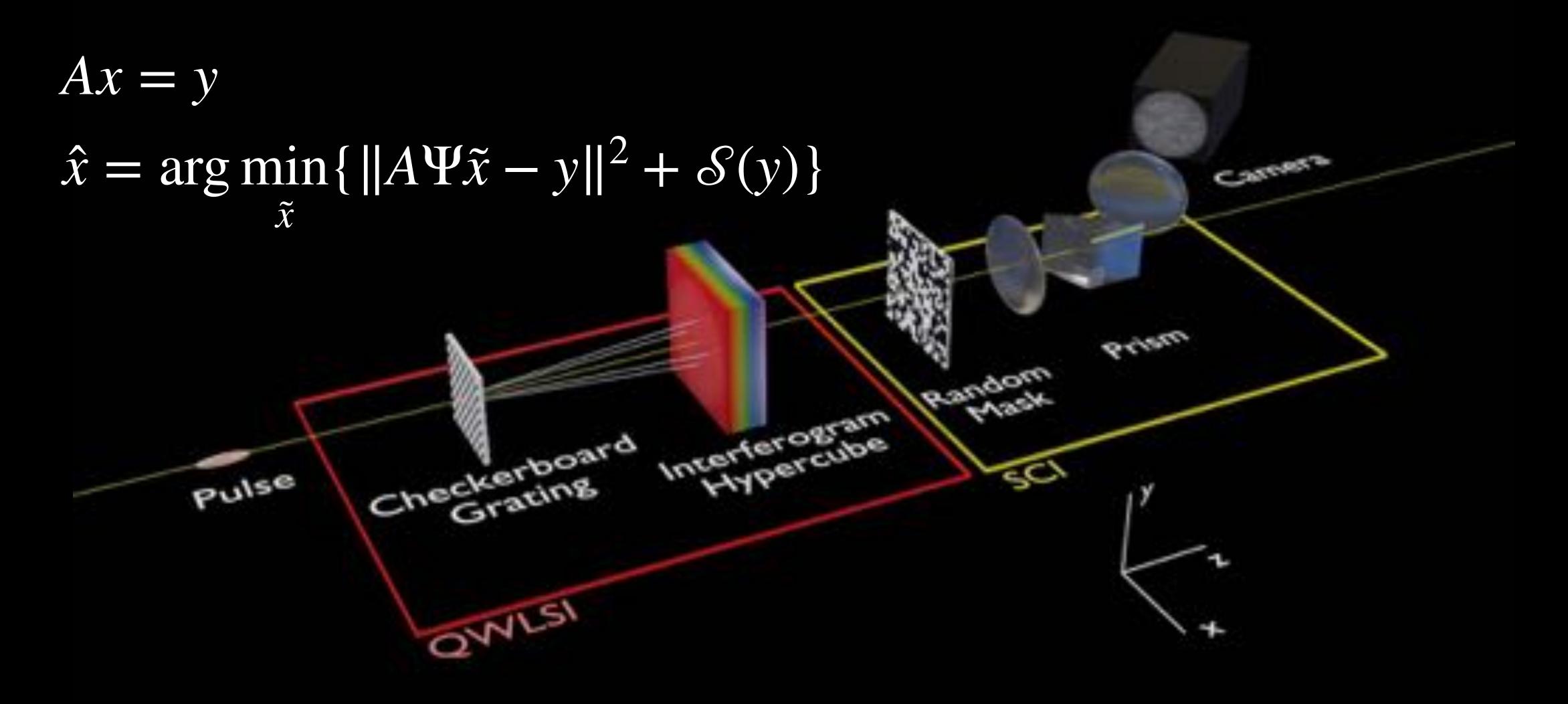
$$\arg\min_{\{(e.g. \text{ wavelet, PCA, etc.})} \arg\min_{\{(e.g. \text{ wavelet, PCA, etc.})}$$

$$\arg\min_{\{(e.g. \text{ wavelet, PCA, etc.})} |A\Psi\tilde{x} - y||^2 + \mathcal{S}(y) \}$$

$$\ker\left(((e.g. \text{ wavelet, PCA, etc.})\right)$$

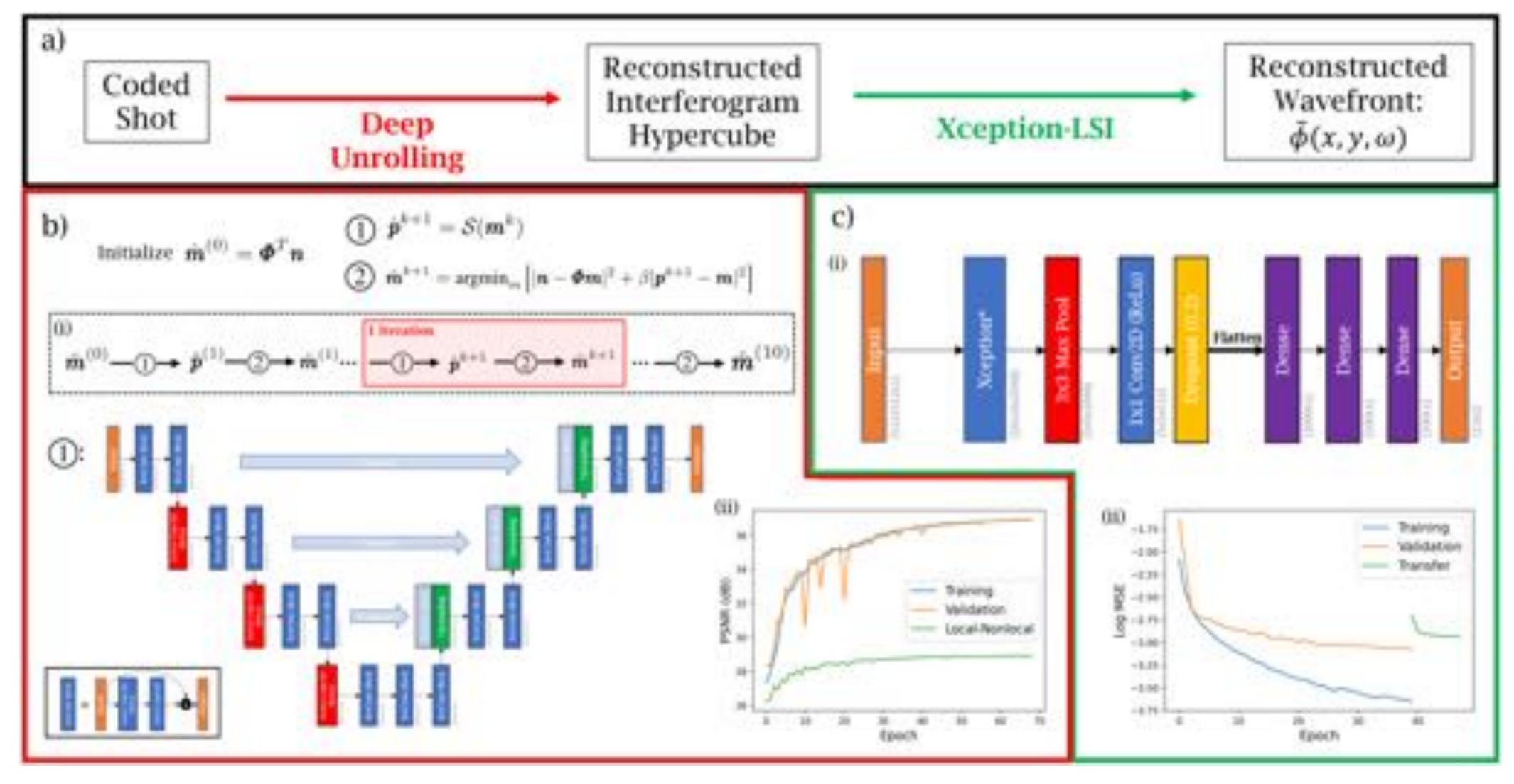
PULSE CALA.

Deep compressed sensing



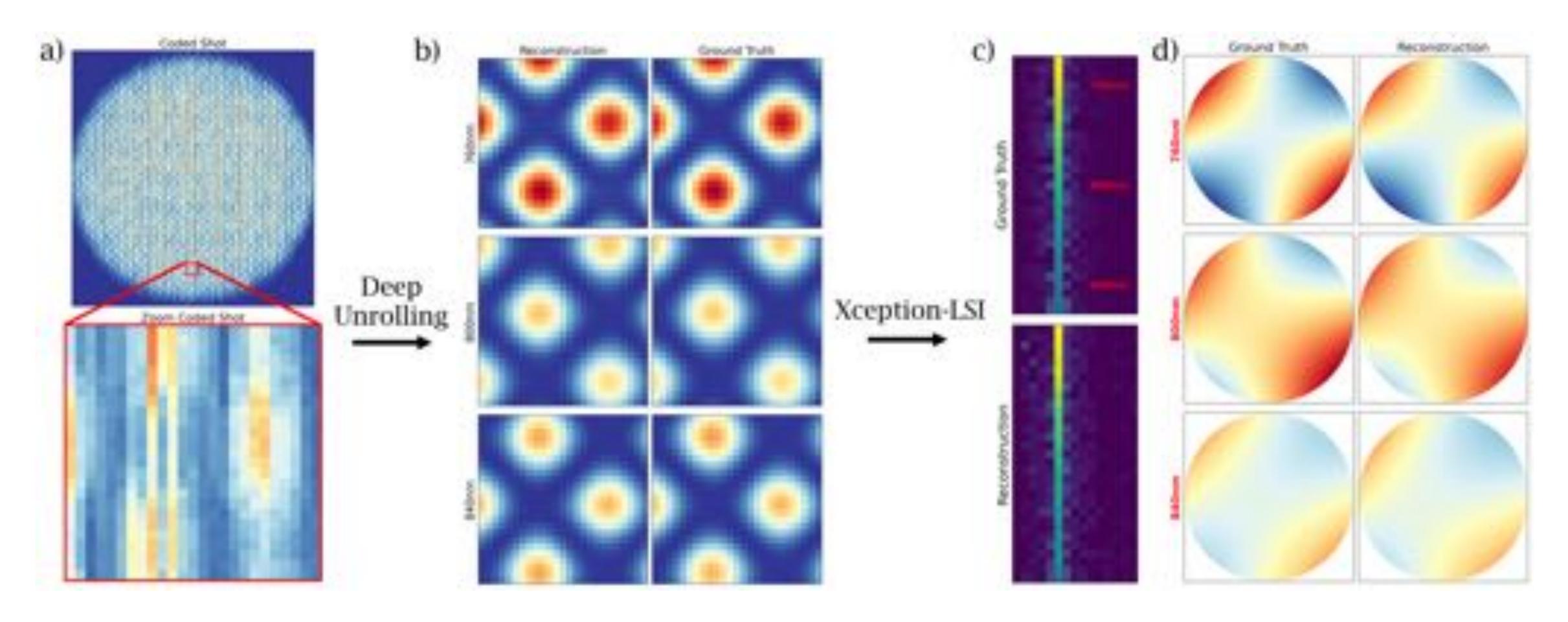
Deep compressed algorithm unrolling





Deep compressed algorithm unrolling

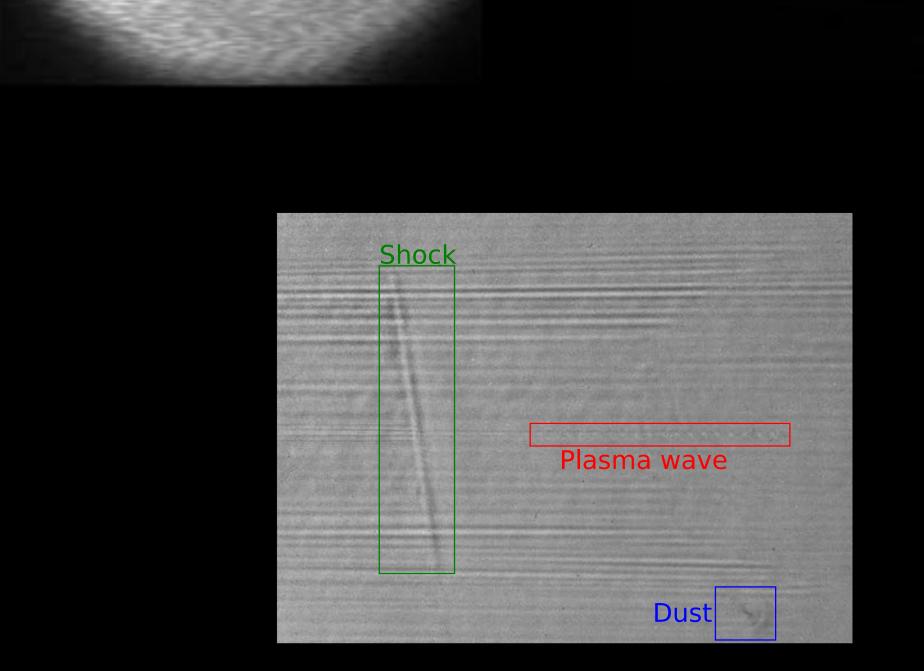




Conclusions and Outlook

- Machine learning is quickly advancing in laserplasma physics community
- Physics-driven developments can improve essential building blocks of machine-learning
- Presented new Bayesian optimization approaches using multiple objectives and fidelities
- Presented new approaches to measuring spatiotemporal couplings; single-shot diagnostic under development
- Many other applications in development, e.g. object detection, etc.







Thank you for your attention!

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