Batch Bayesian optimization of attosecond X-ray bursts

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What is attosecond?

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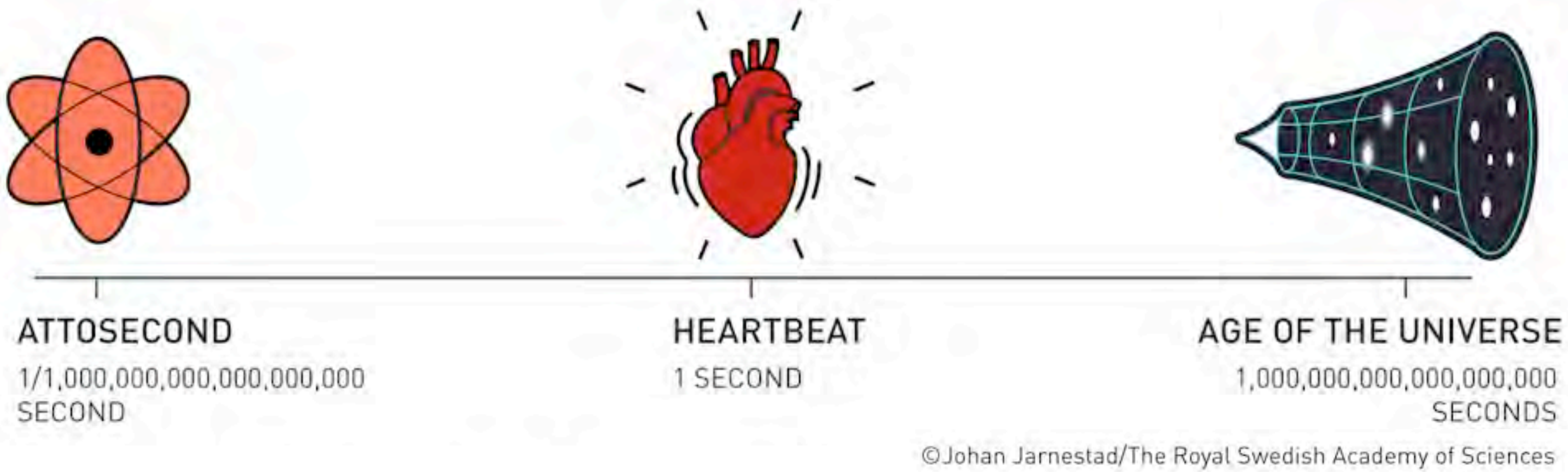
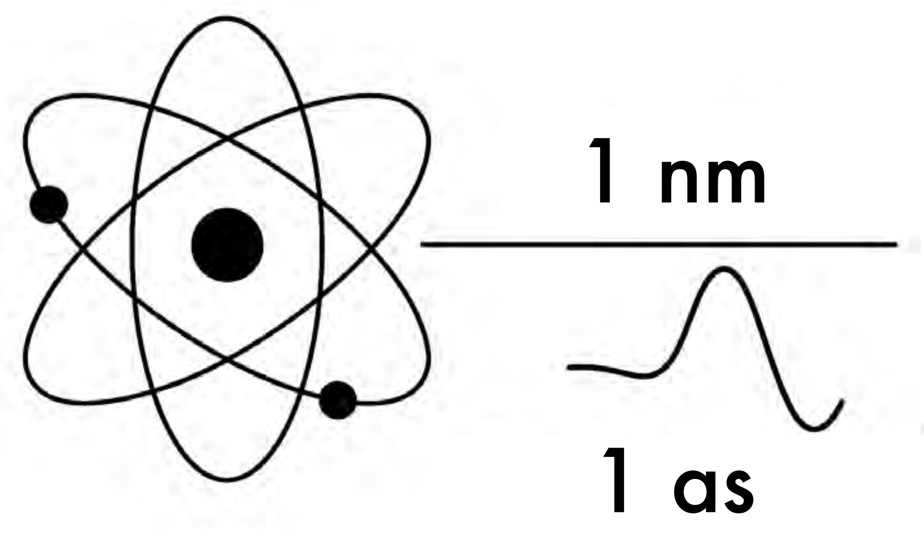


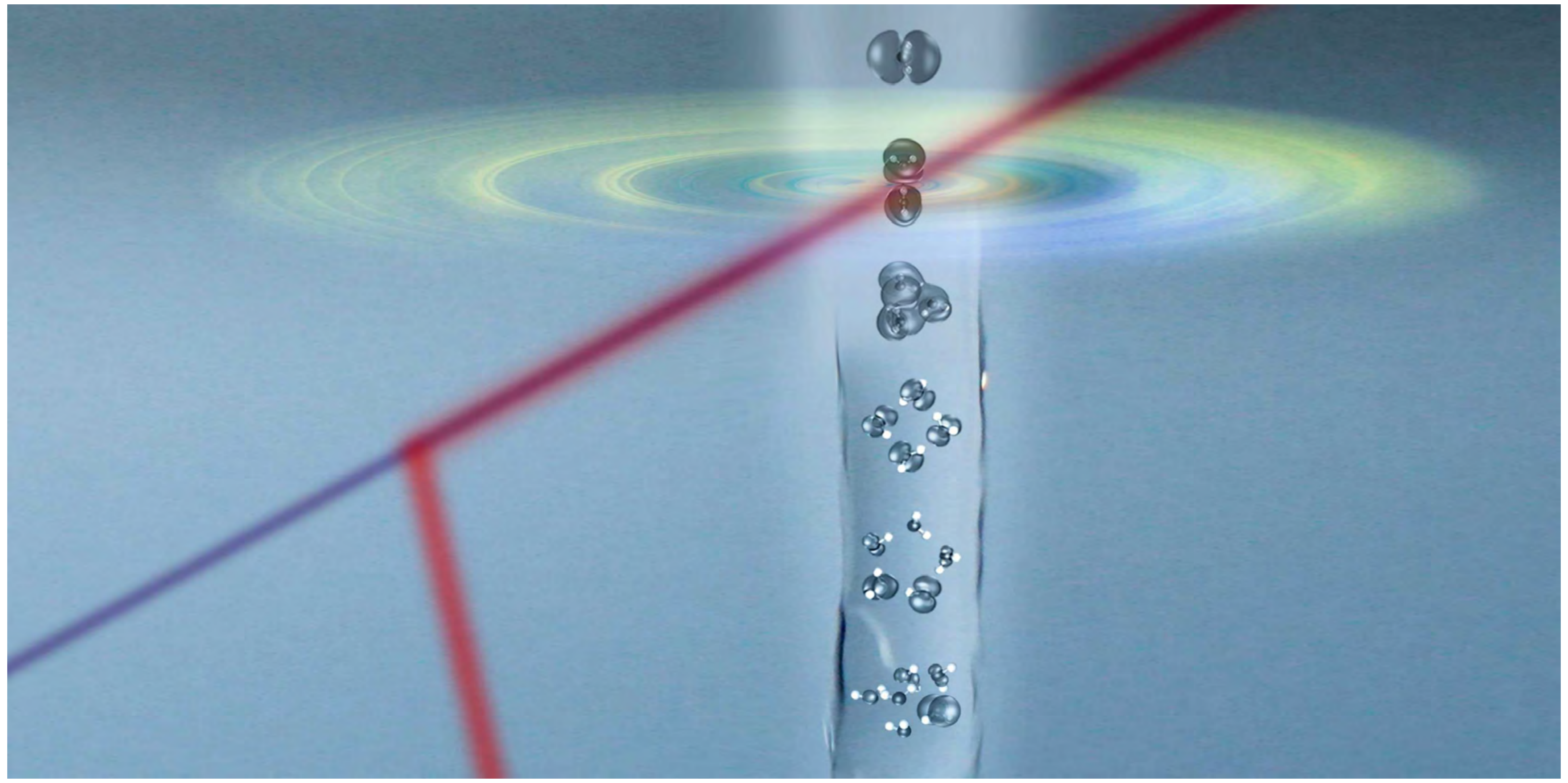
SHORTEST PULSE EVER CREATED AND MEASURED: 43 as

T. Gaumnitz et al. *Opt. Express* 25, 27506-27518 (2017)

Why attosecond light sources?

- Probing matter on scales of electron motion in atoms
- Timing and controlling ionization dynamics
- Probing ultrafast light–matter interactions, ...





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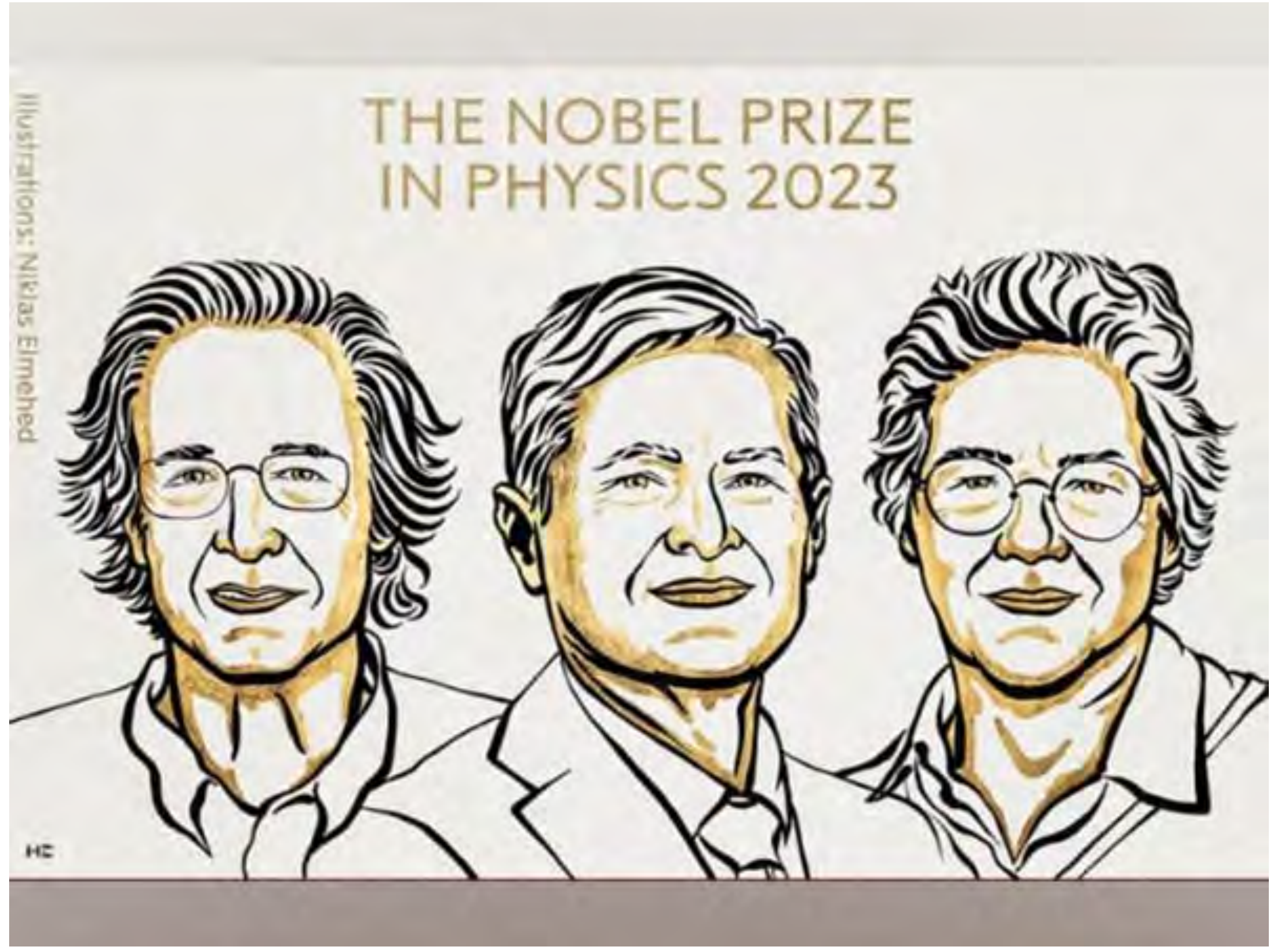

Niklas Elmehed © Nobel Prize Outreach

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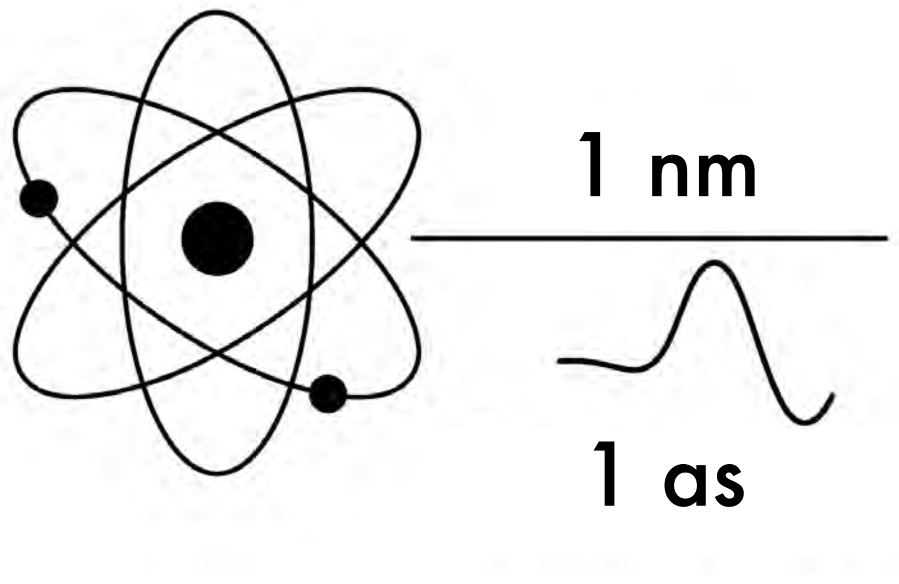

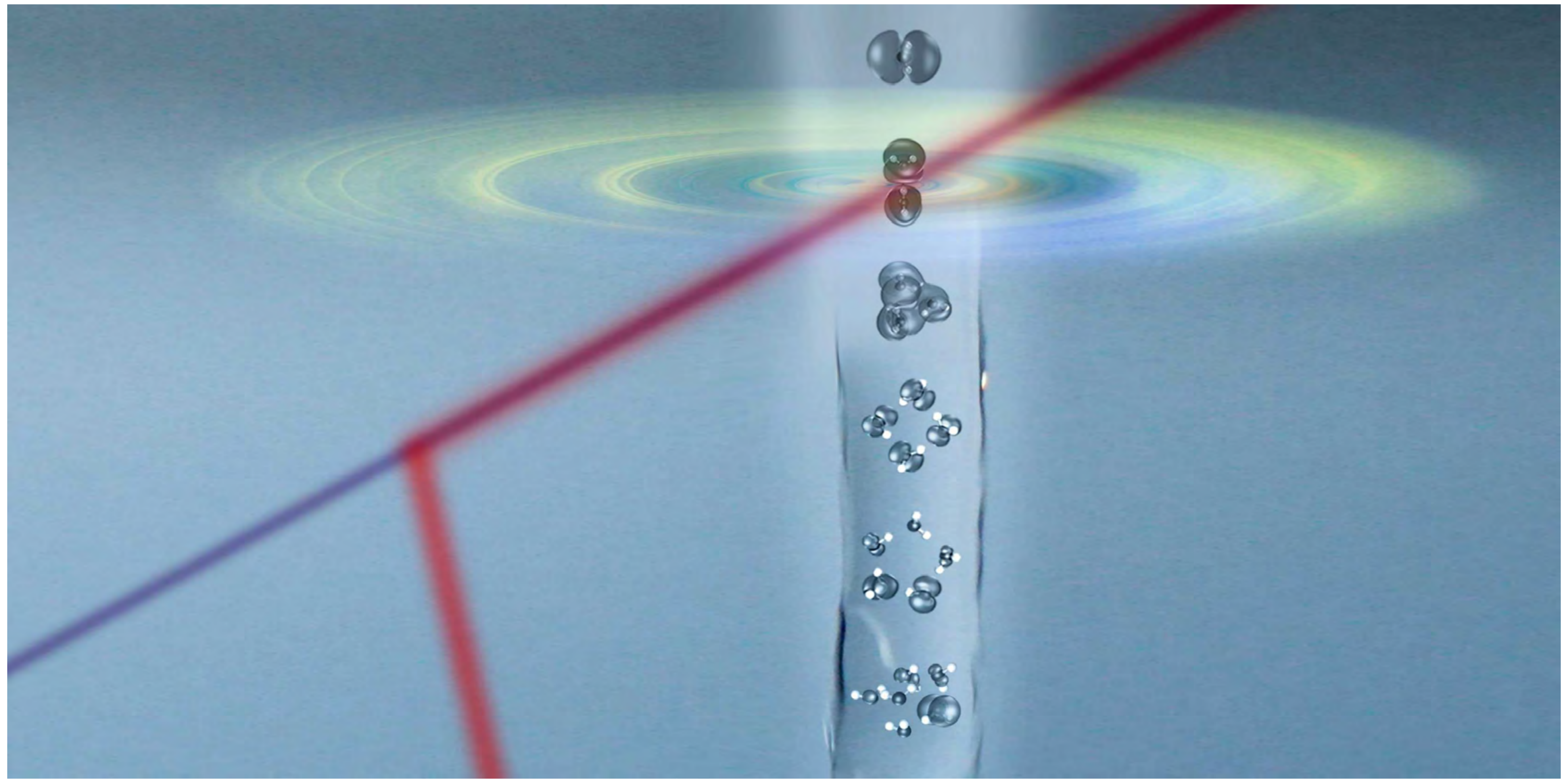

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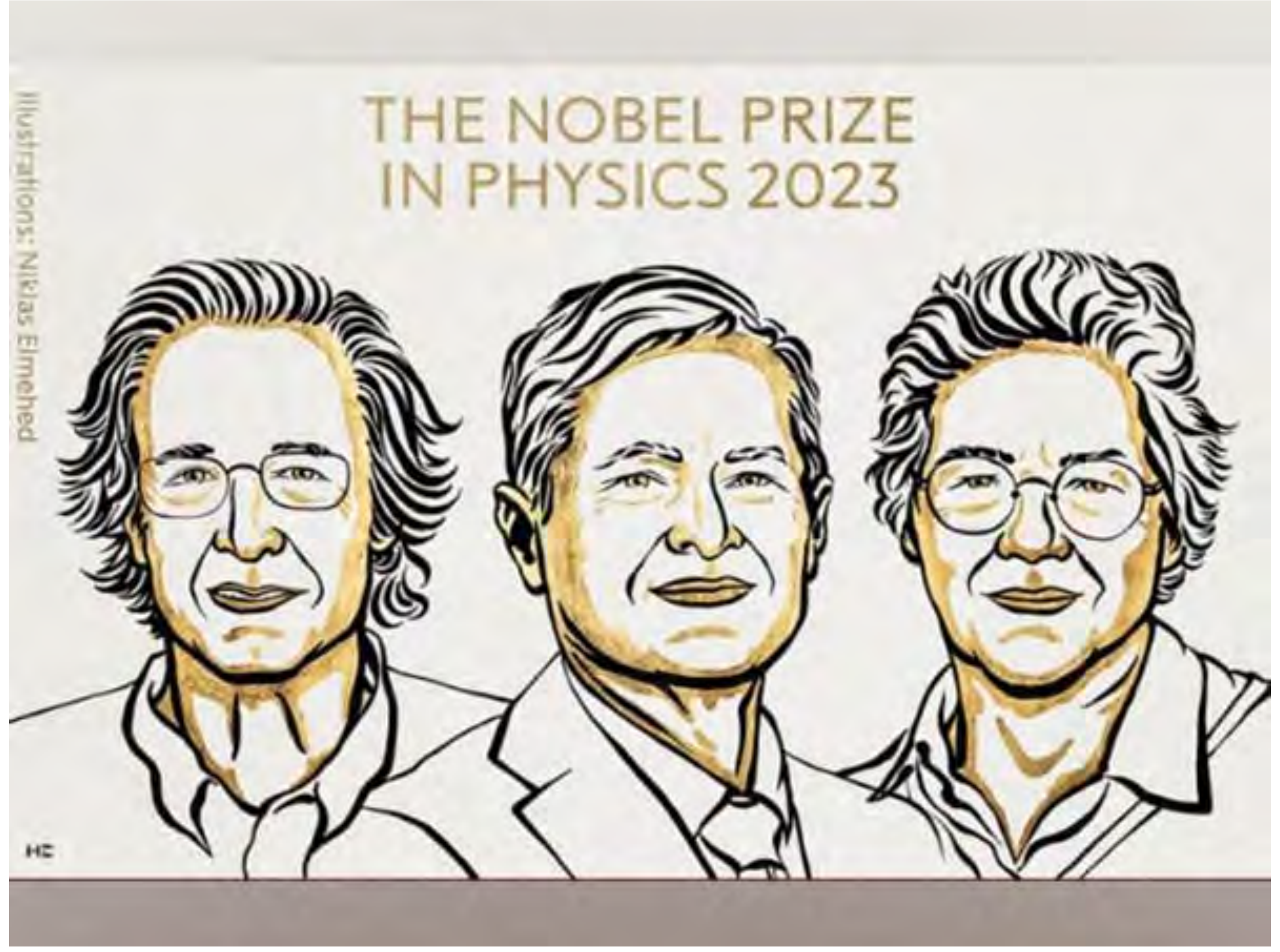

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Attosecond bursts are typically generated in gases with femtosecond infrared laser light.

Laser wakefield acceleration can be also utilized to produce attosecond bursts in plasma

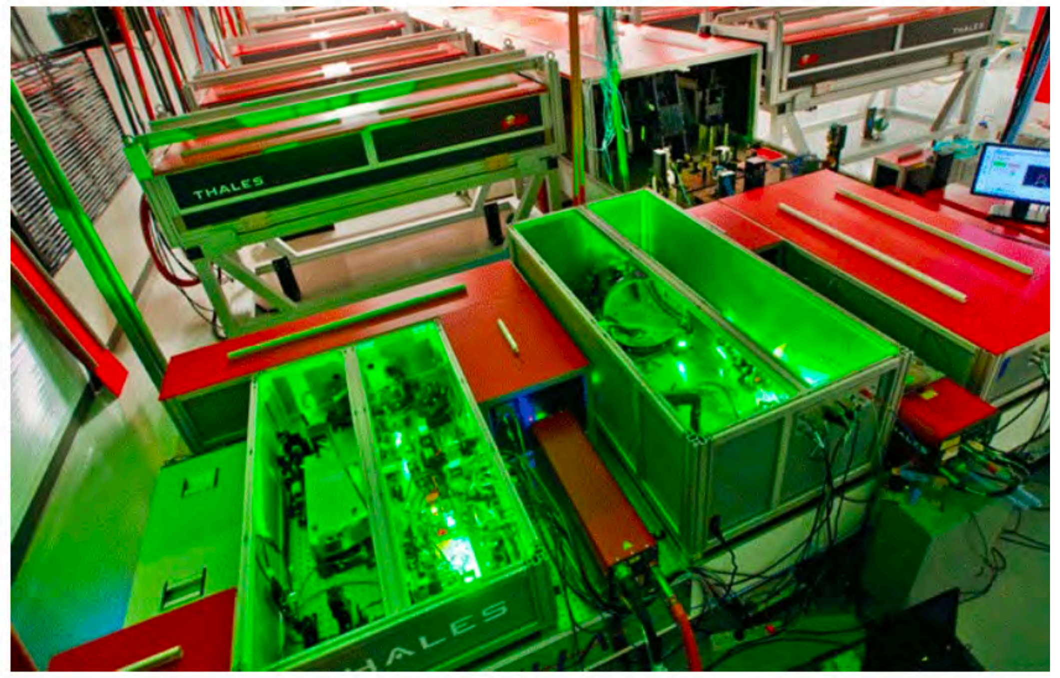
- Laser wakefield accelerator is a very **compact particle** (electron) **accelerator**
- Acceleration happens in **PLASMA**= ionized state of matter containing charged particles

CONVENTIONAL ACCELERATOR

Picture credit: DAVID PARKER / SCIENCE PHOTO LIBRARY

1000x SMALLER!

LASER ACCELERATOR



Picture credit: Berkeley Lab

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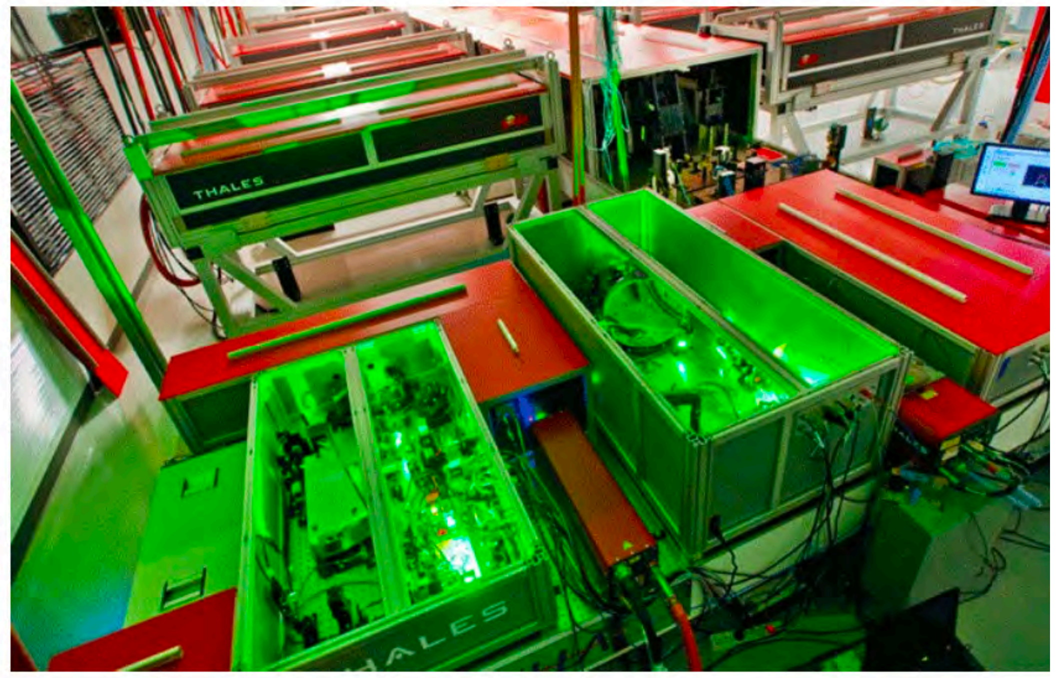

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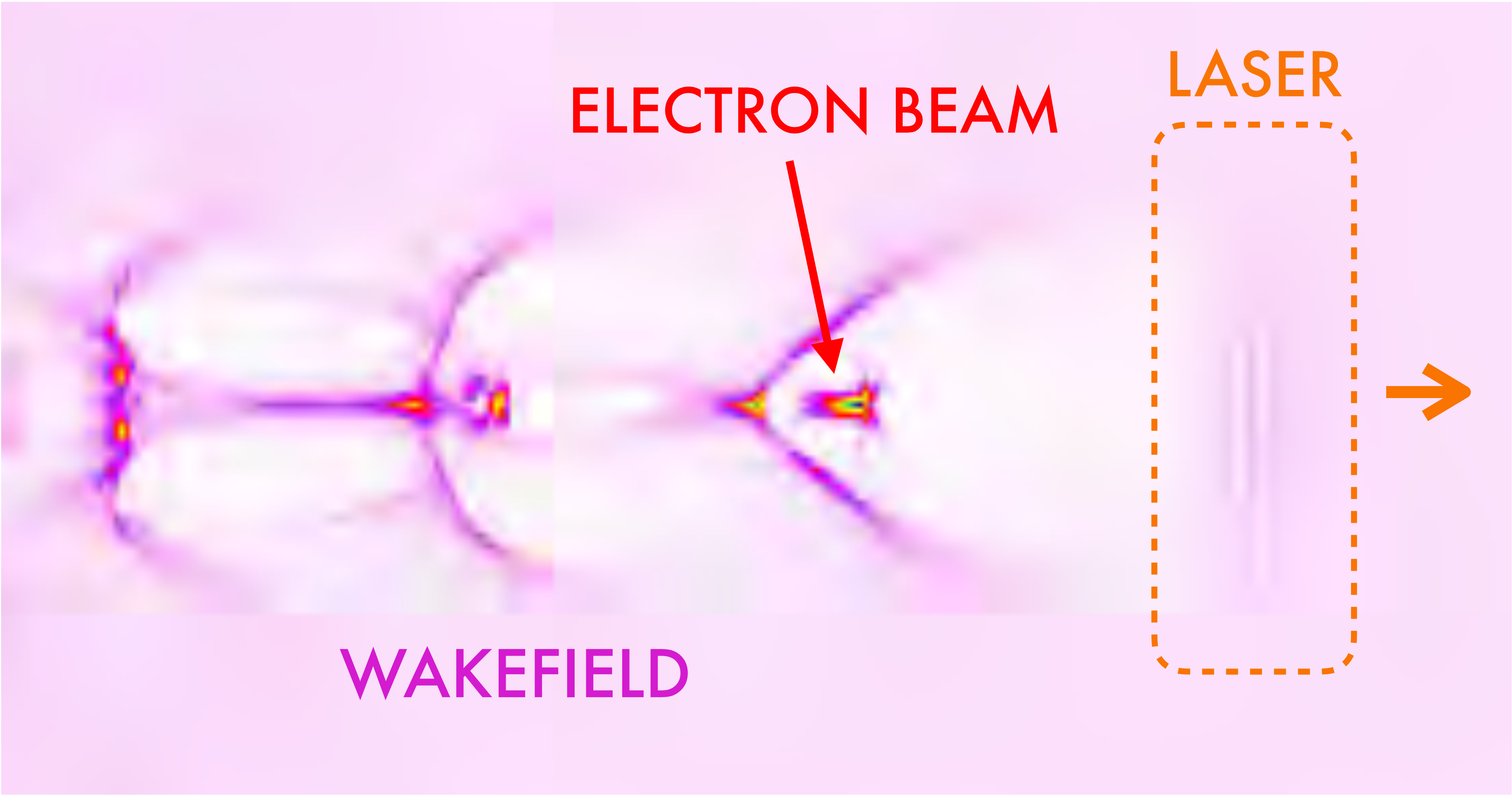
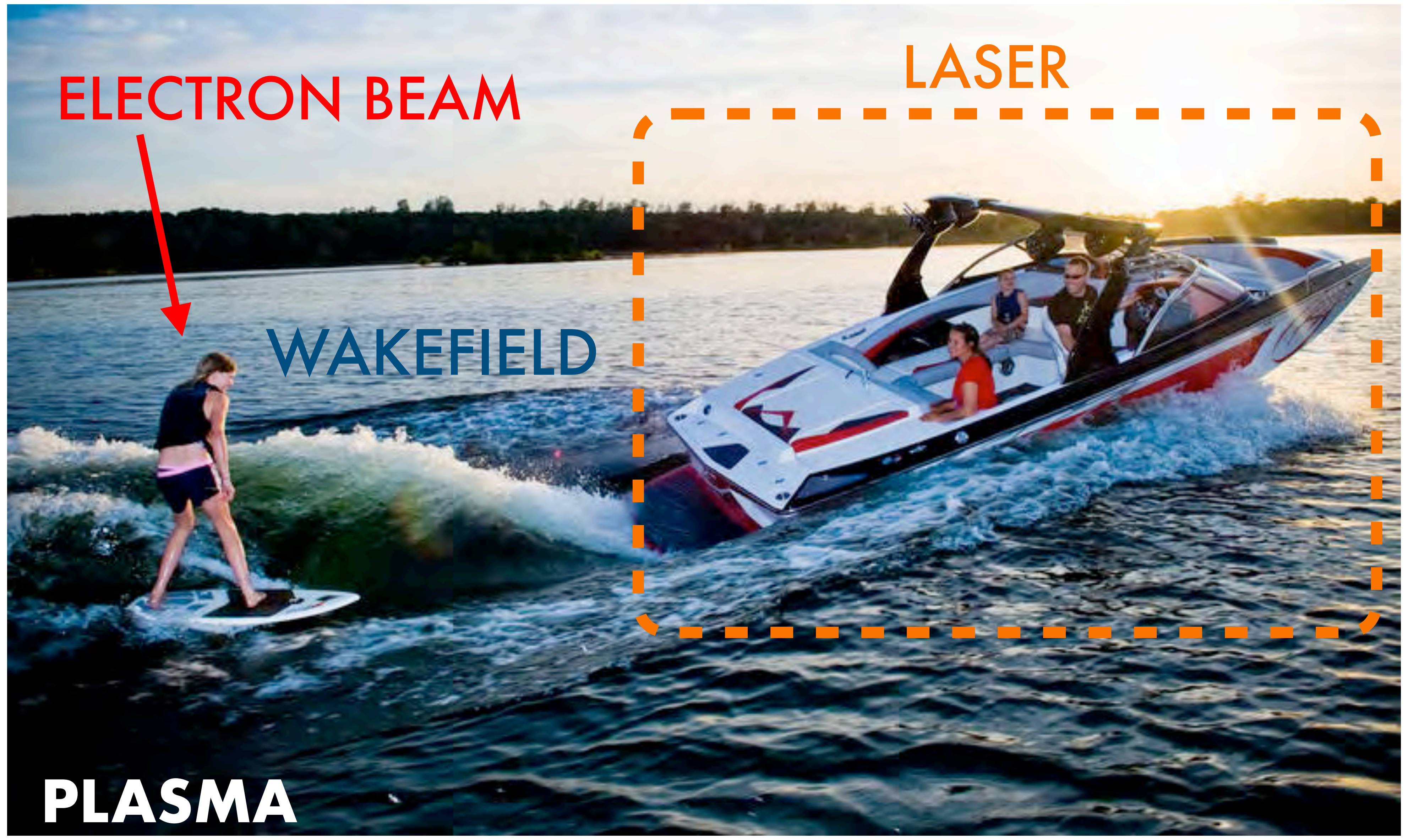
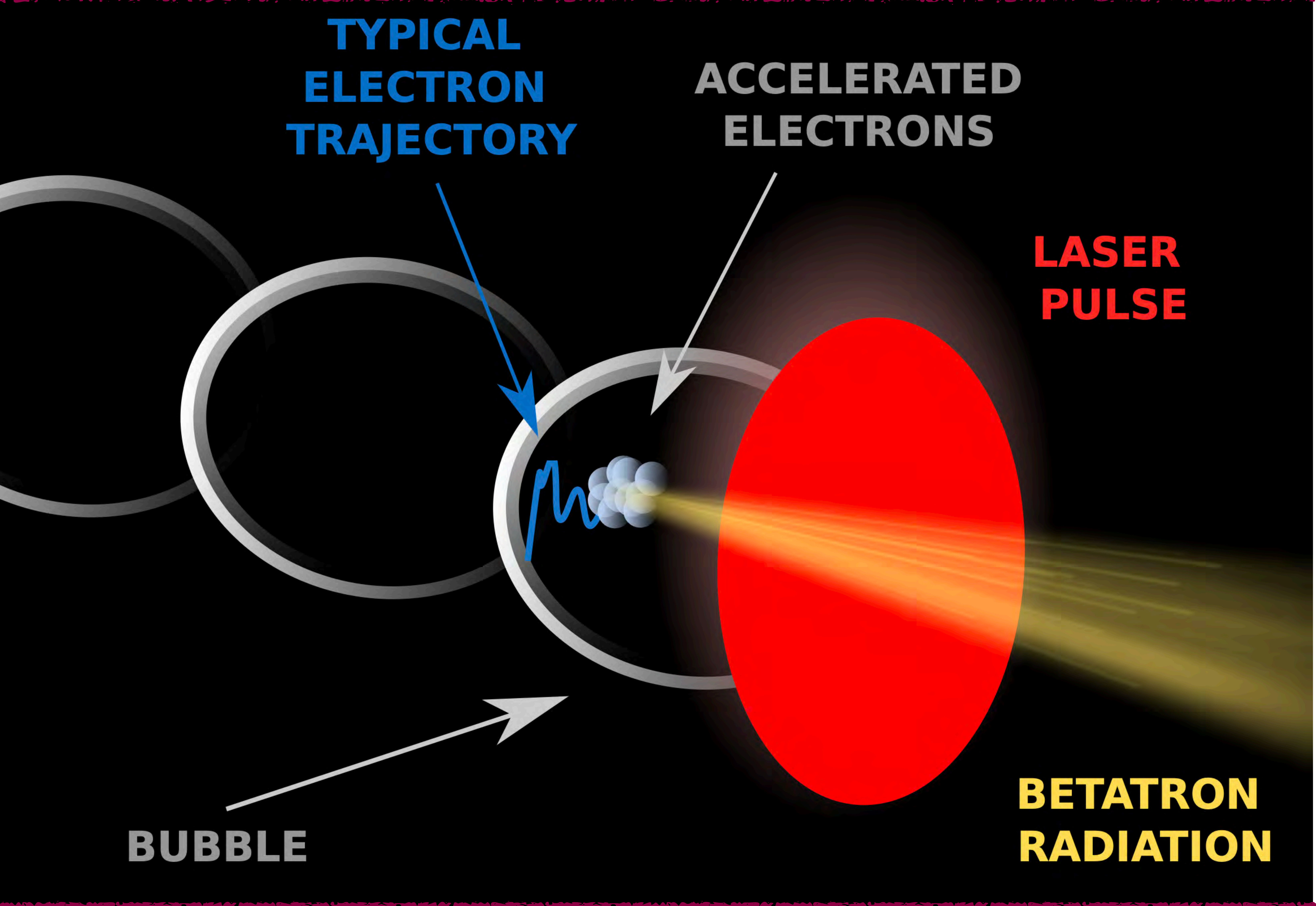


PLASMA ELECTRON DENSITY



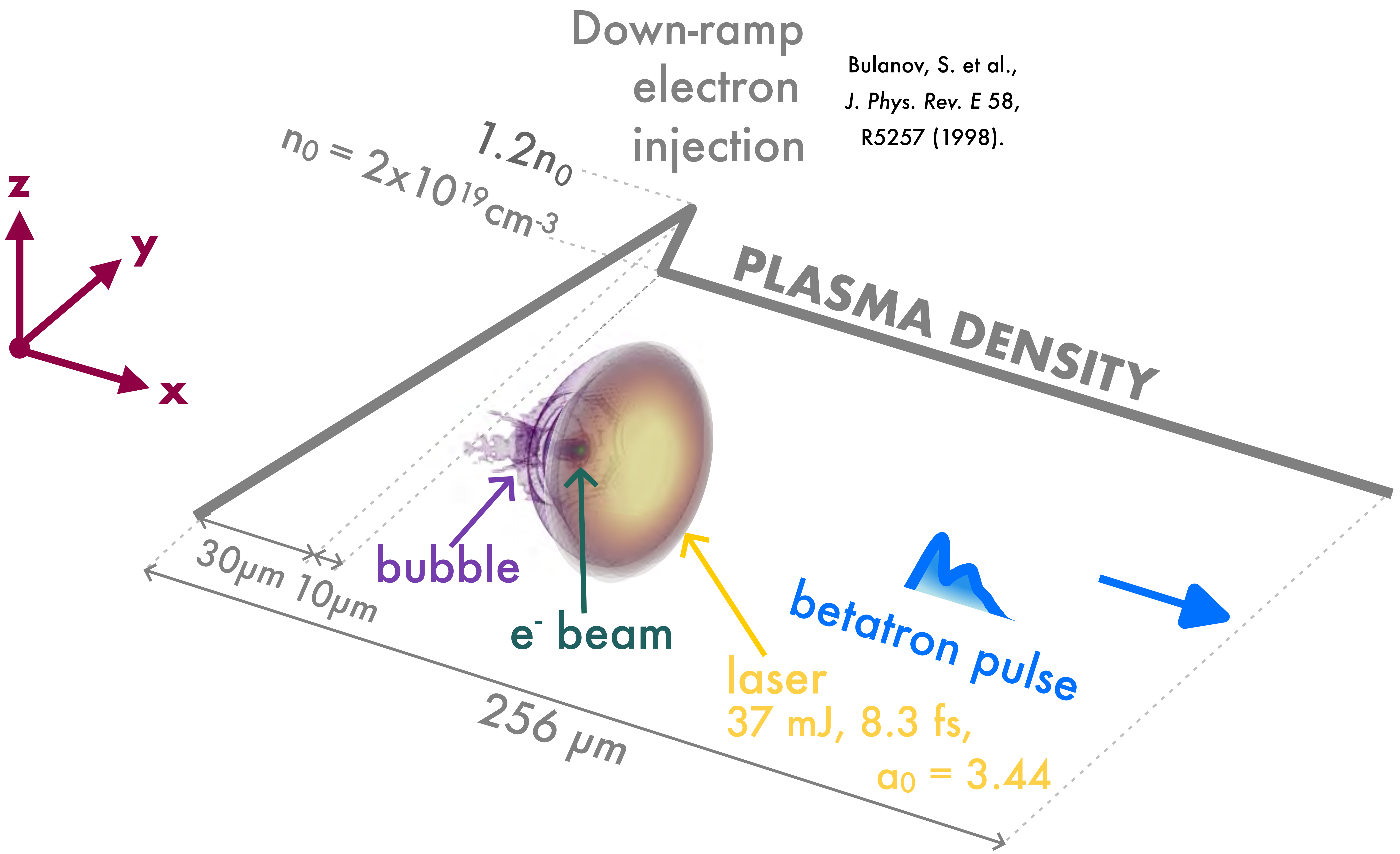
Picture credit: https://www.precision-performance.com/blog/wakesurfing–how-to-get-started-9429

Electron oscillations in laser wakefield generate X-ray "betatron" bursts



- Electrons undergo **transverse oscillations**
- They produce **femtosecond (10^{-15} s) X-ray betatron radiation bursts**
- **Simulations** have shown that the durations can be **decreased down to atttoseconds (10^{-18} s)**
- Applications would benefit from the **increase of the radiation gain**

We tailor the properties of a density spike in simulations to enhance attosecond betatron radiation



Bulanov, S. et al., *J. Phys. Rev. E* 58, R5257 (1998).

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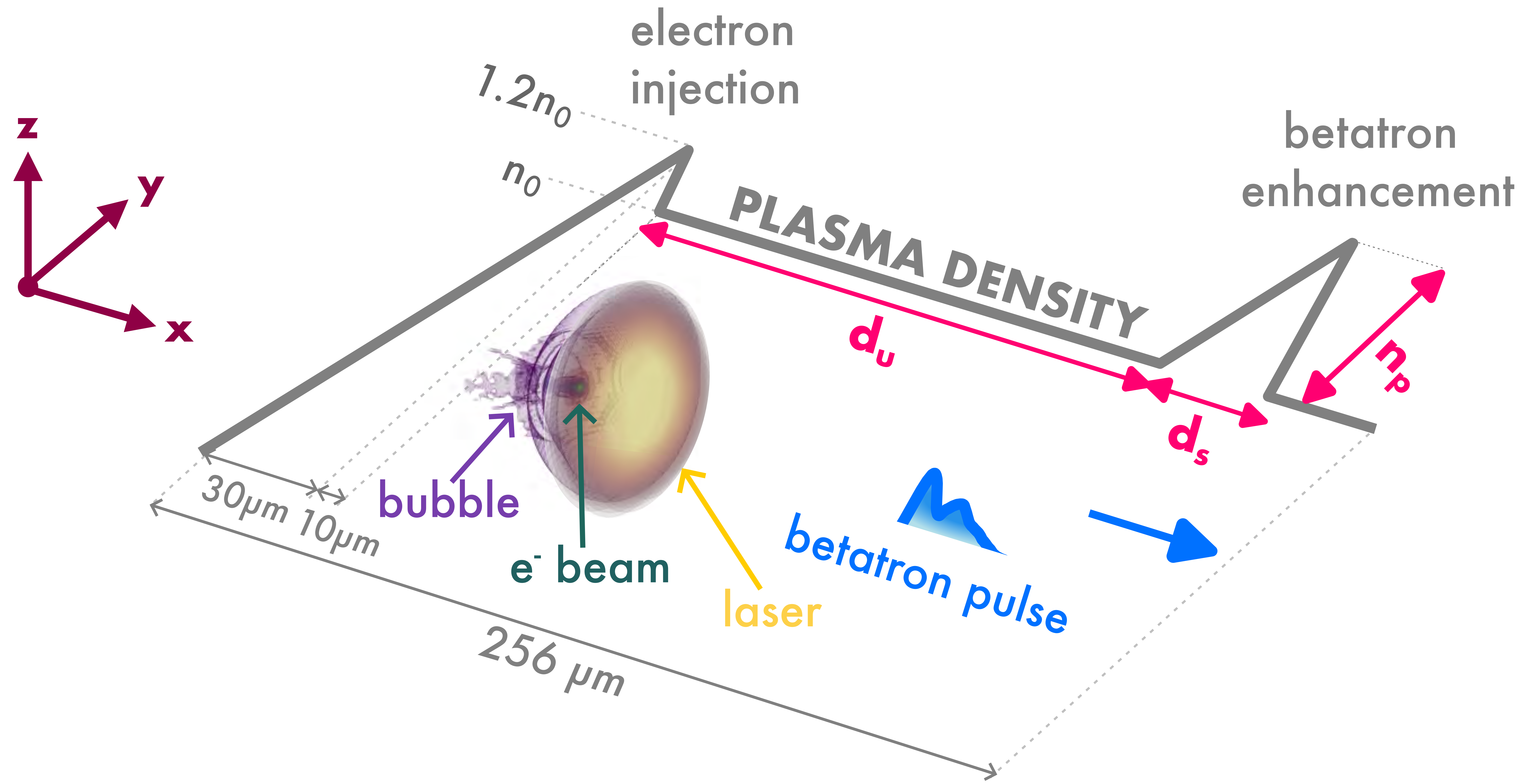

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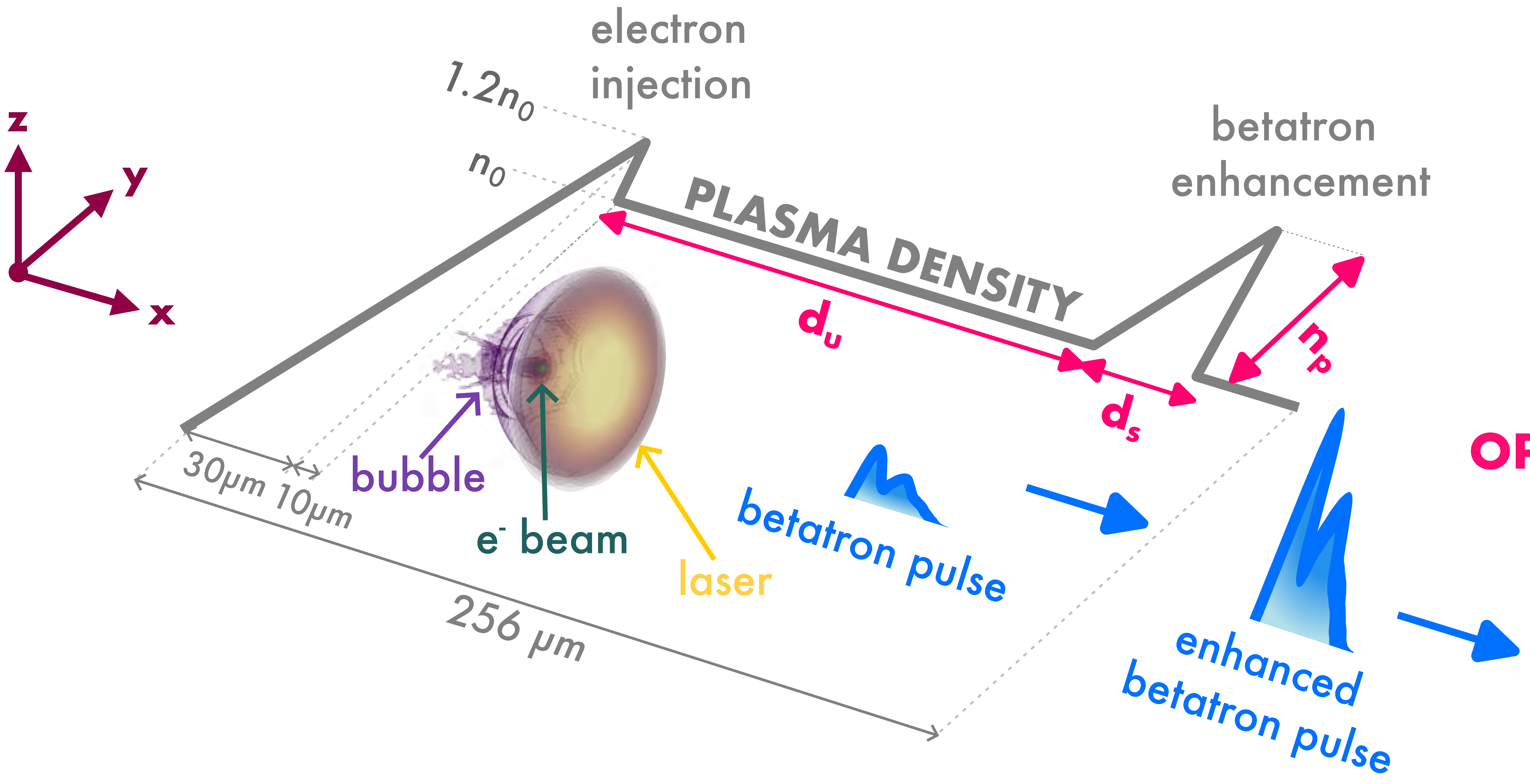
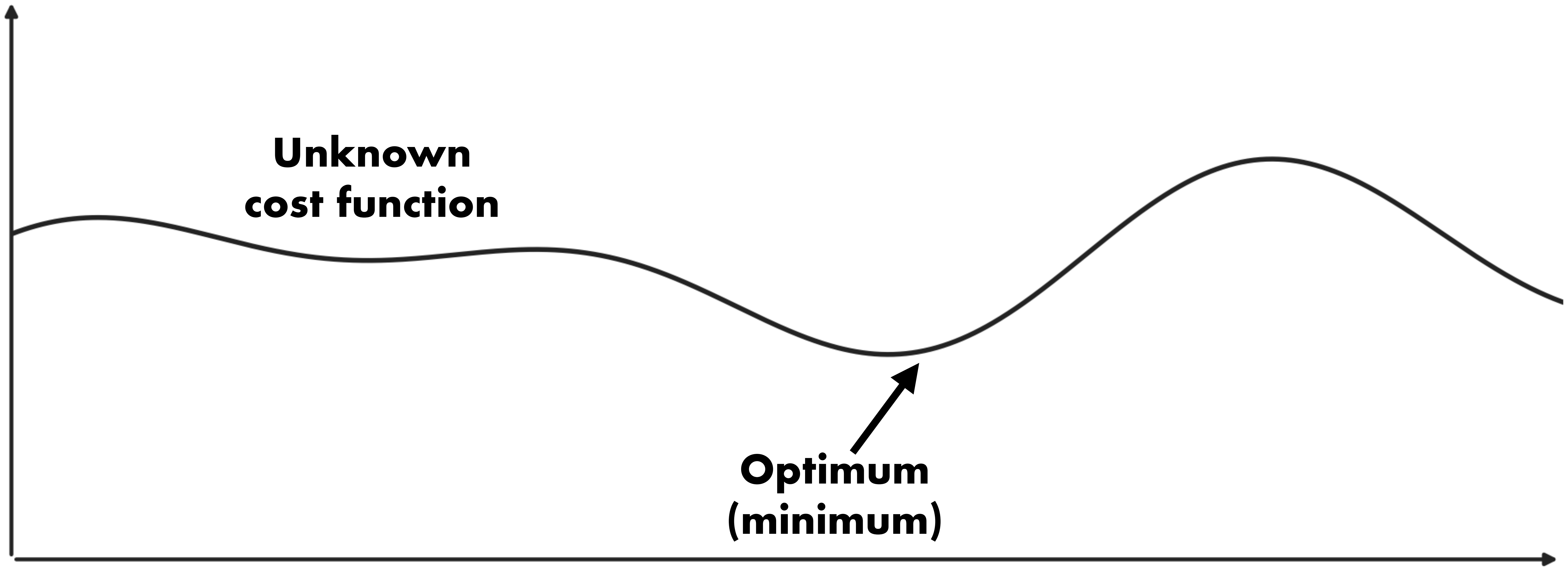


BATCH BAYESIAN OPTIMIZATION

Bayesian optimization can search for optimum of black-box functions under limited evaluations

- **The objective cost function is modeled** with limited number of evaluations **by a surrogate model.**
- To find the optimum, **a next point where the cost is evaluated is picked** (explore↔exploit).



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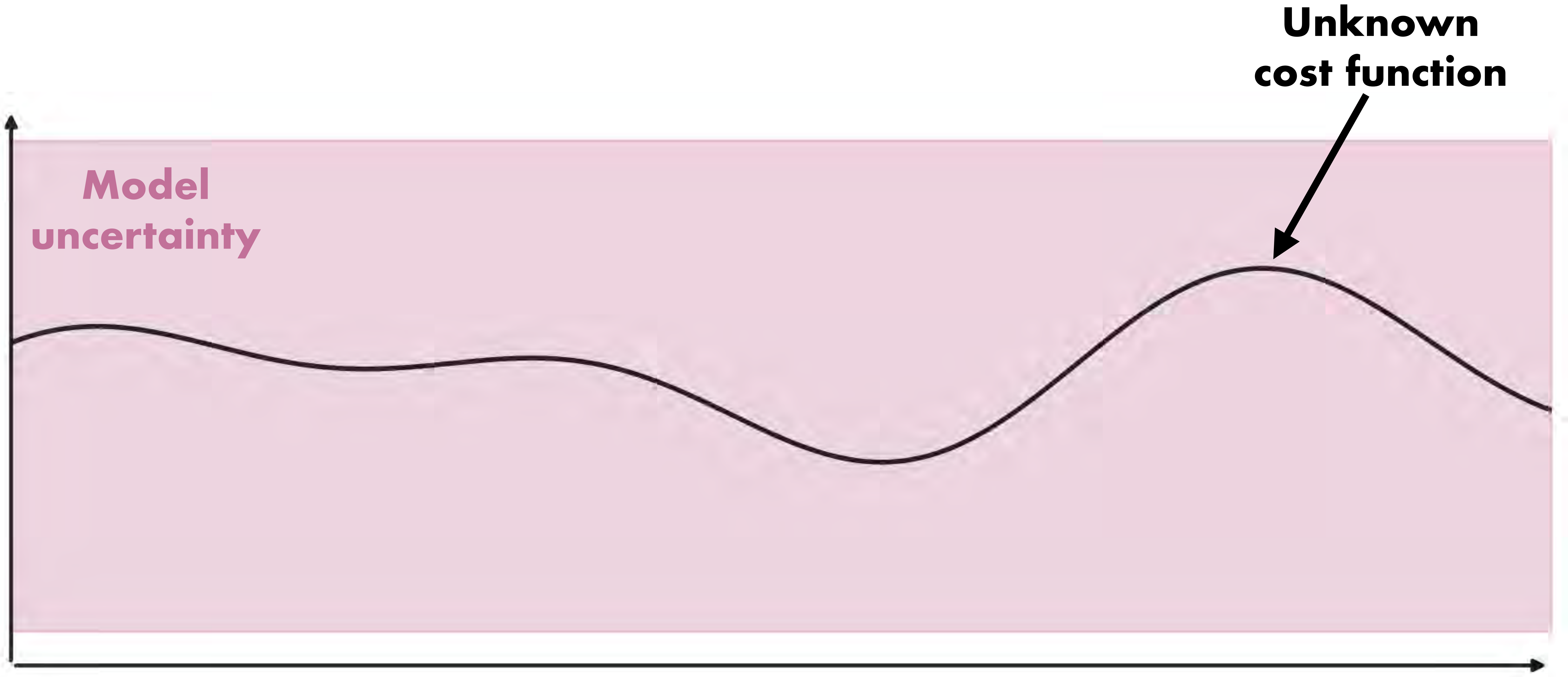

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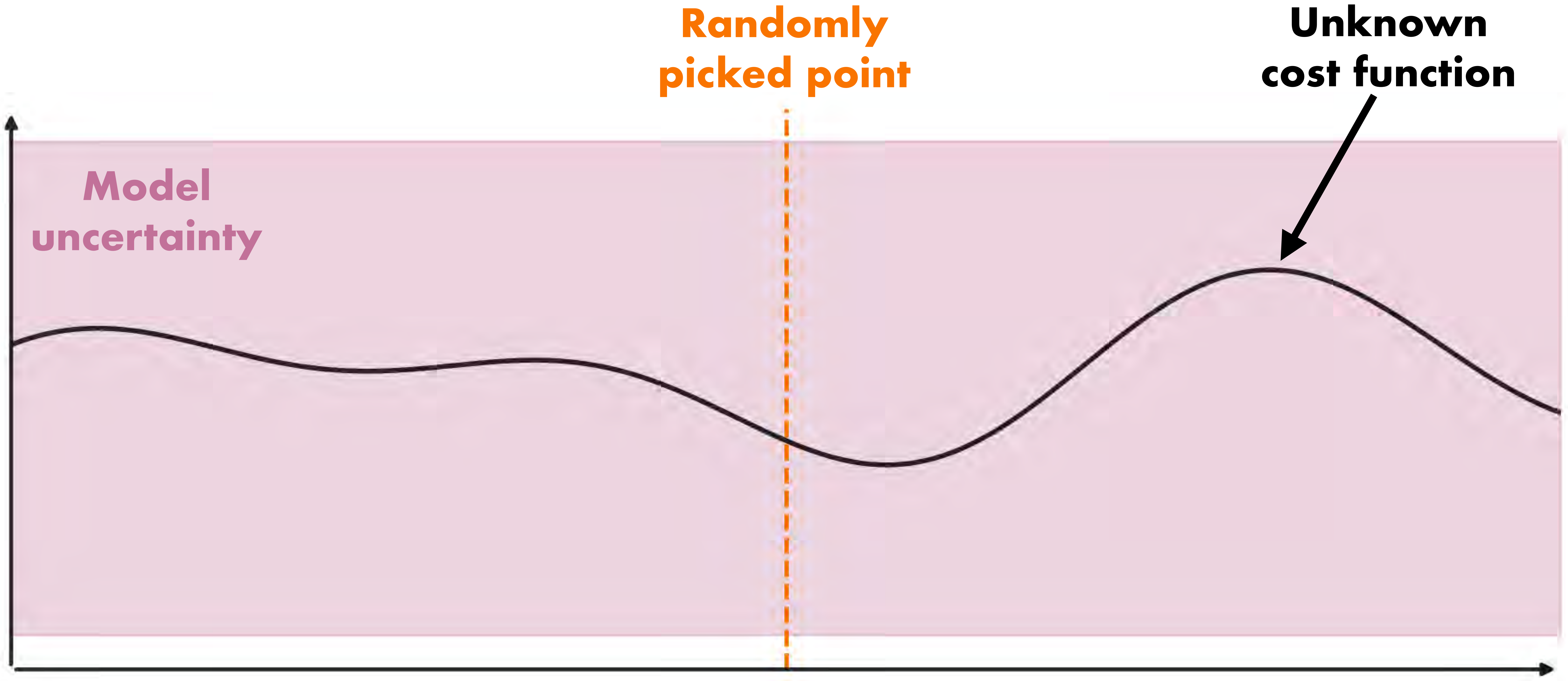

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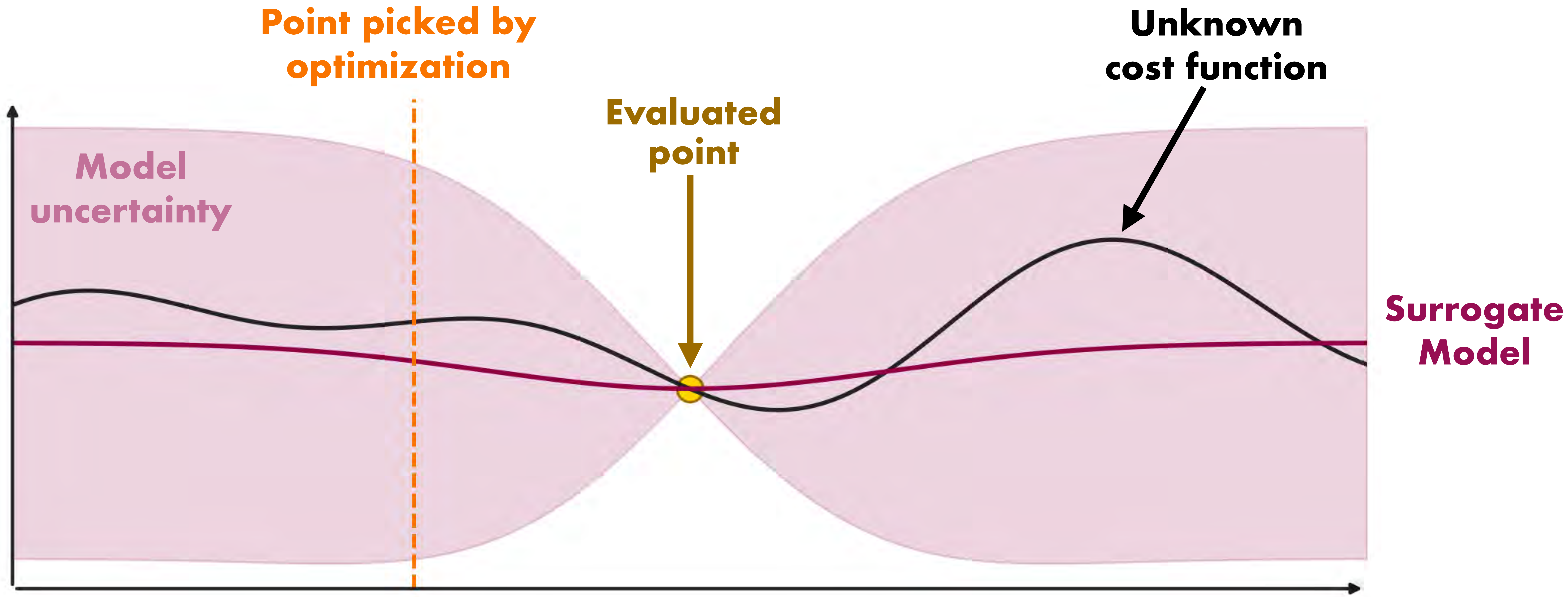

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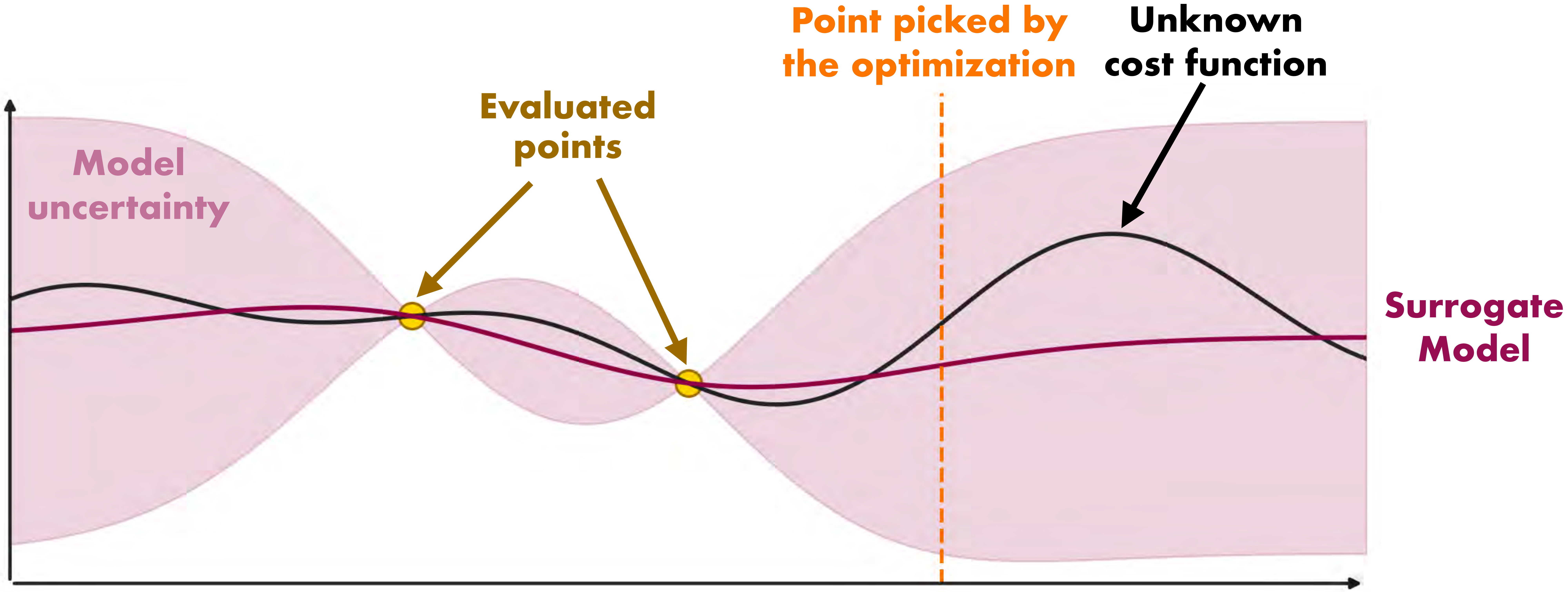

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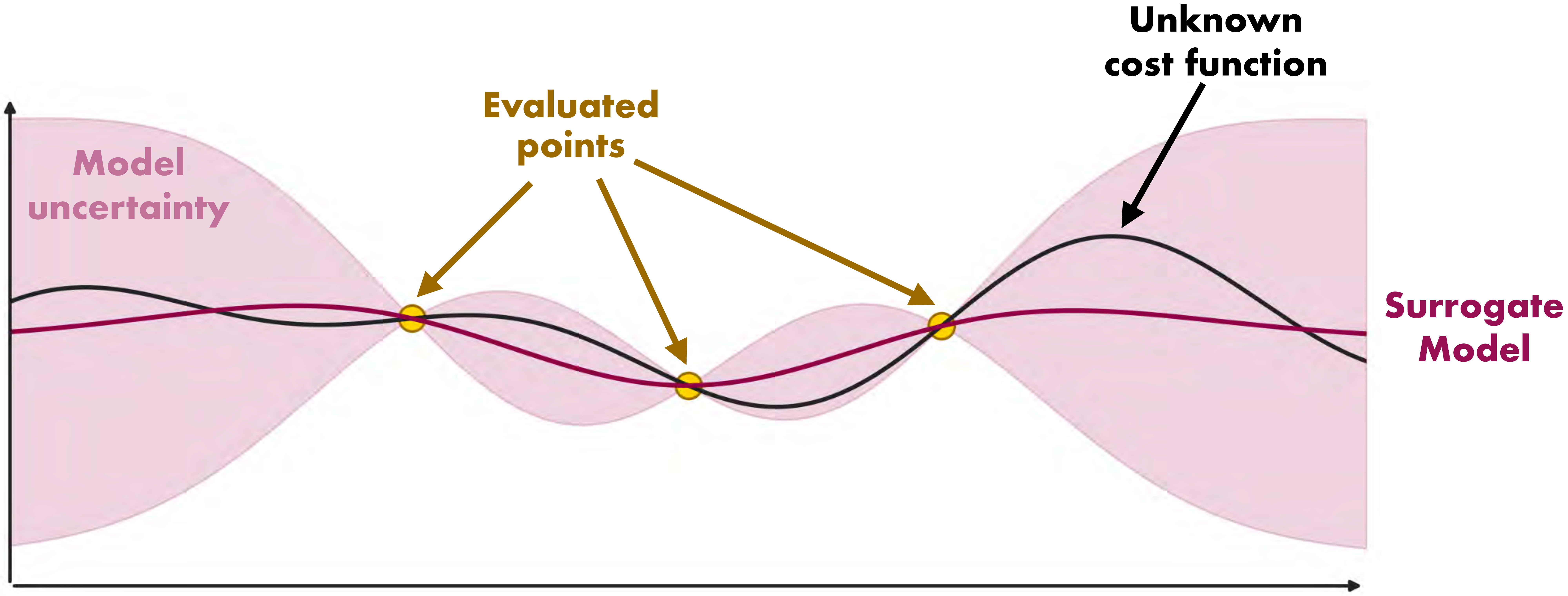
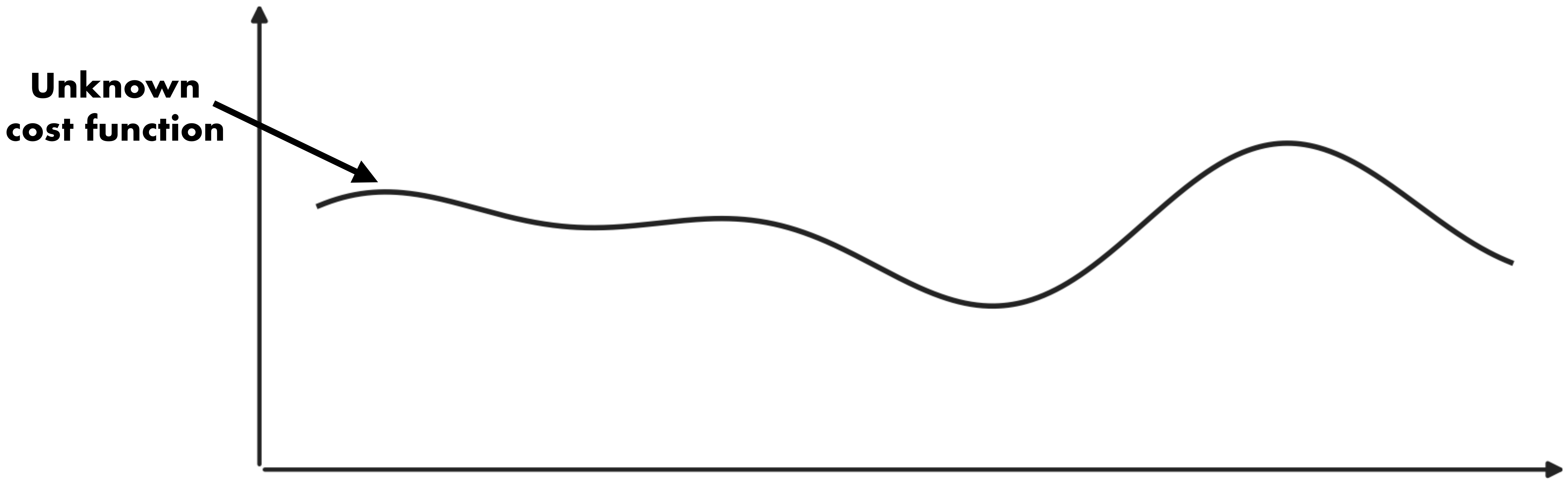


BATCH Bayesian optimization evaluates several points at once

- **Several next points (batch) are picked** via the acquisition.



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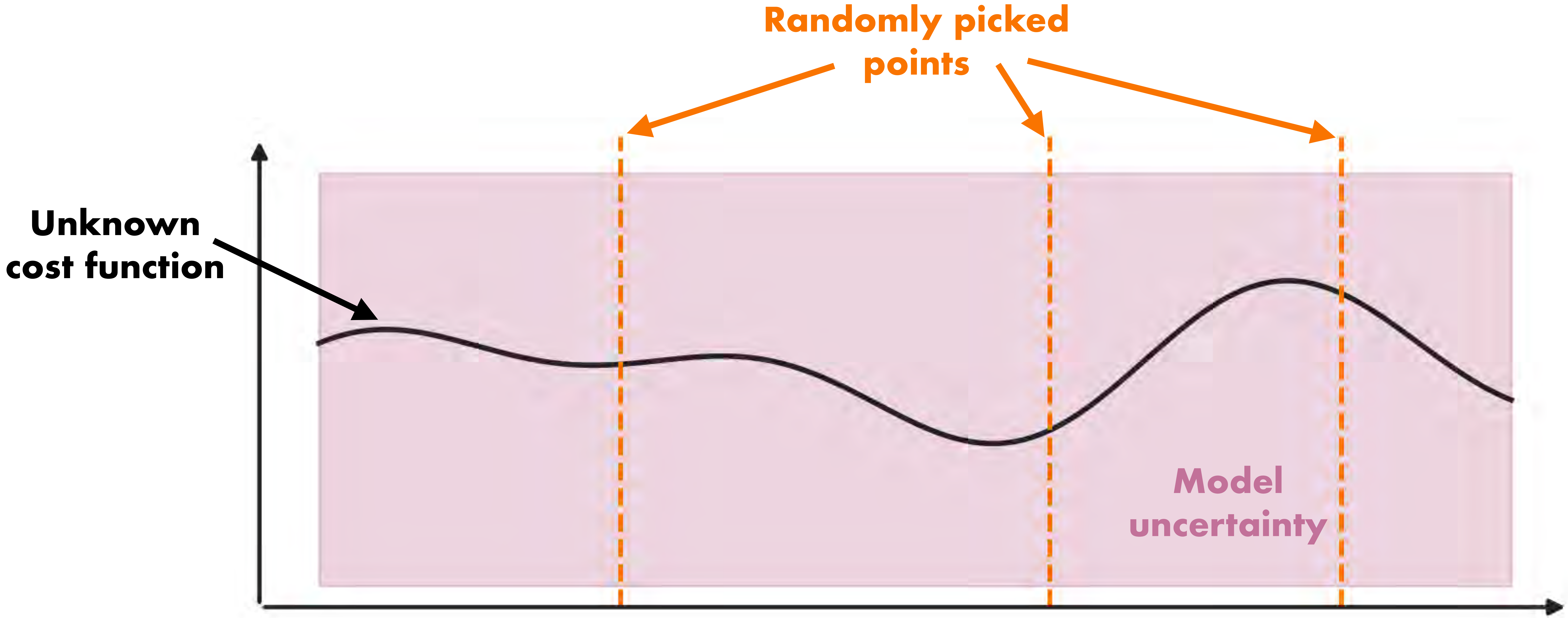

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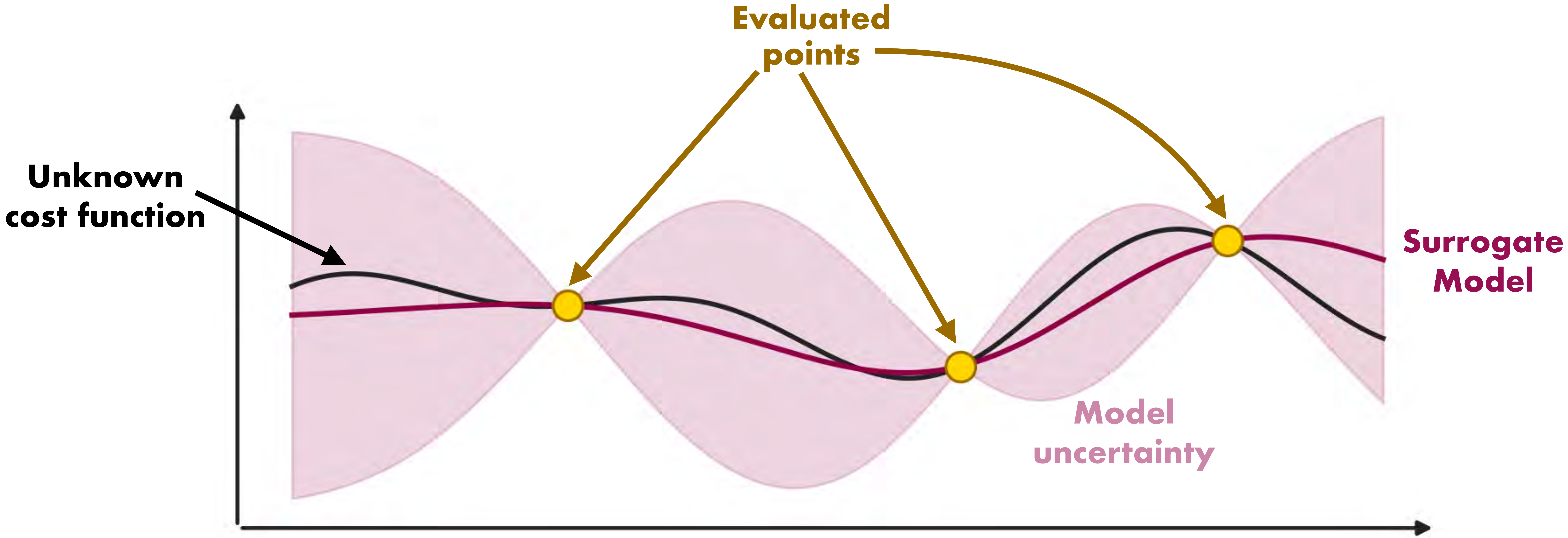

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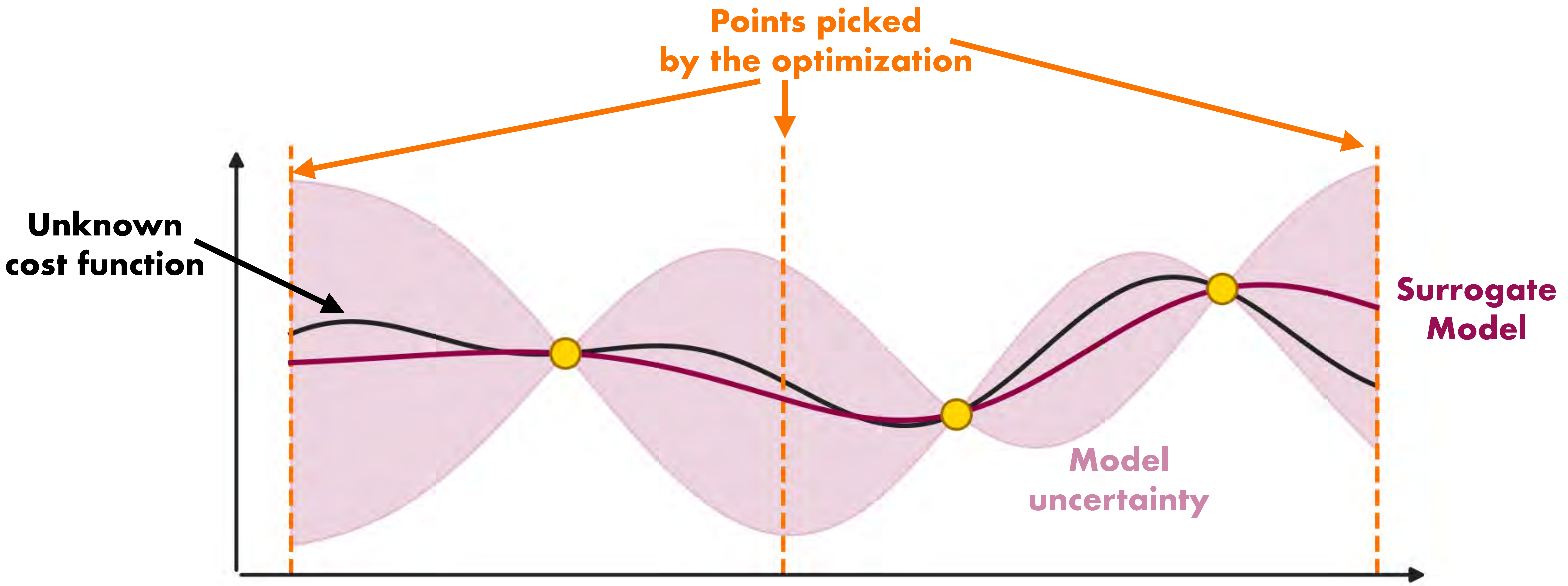

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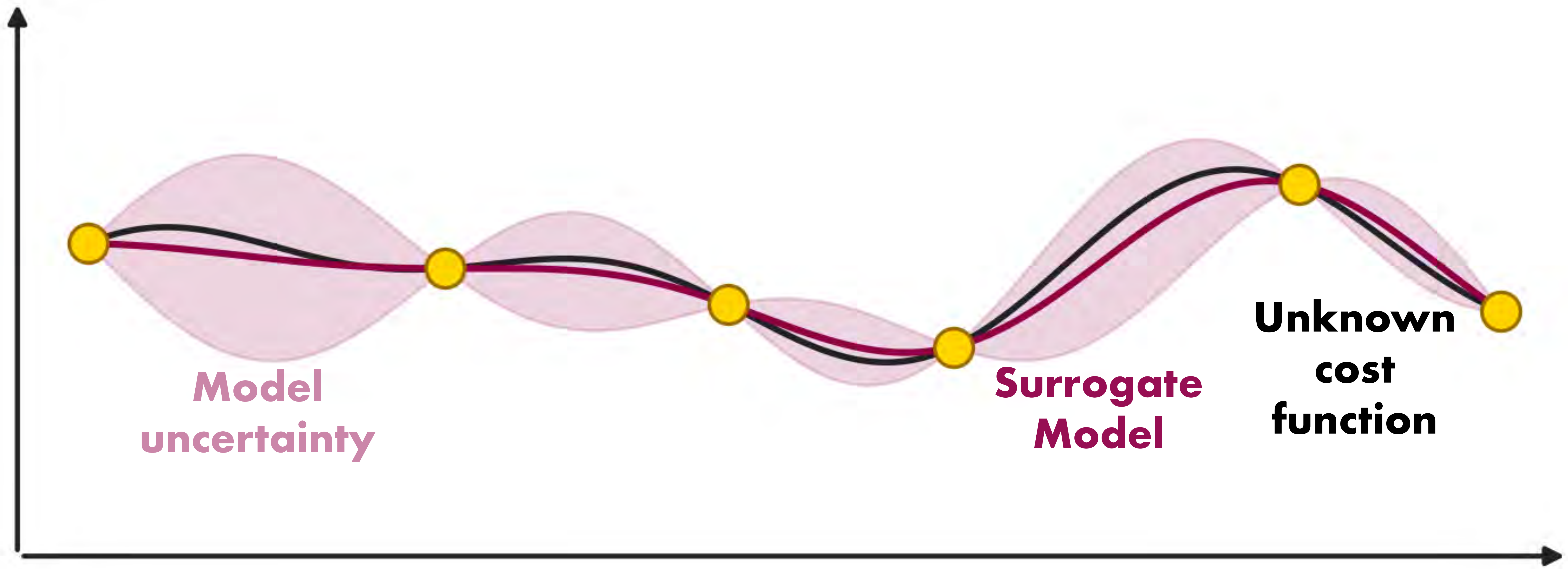

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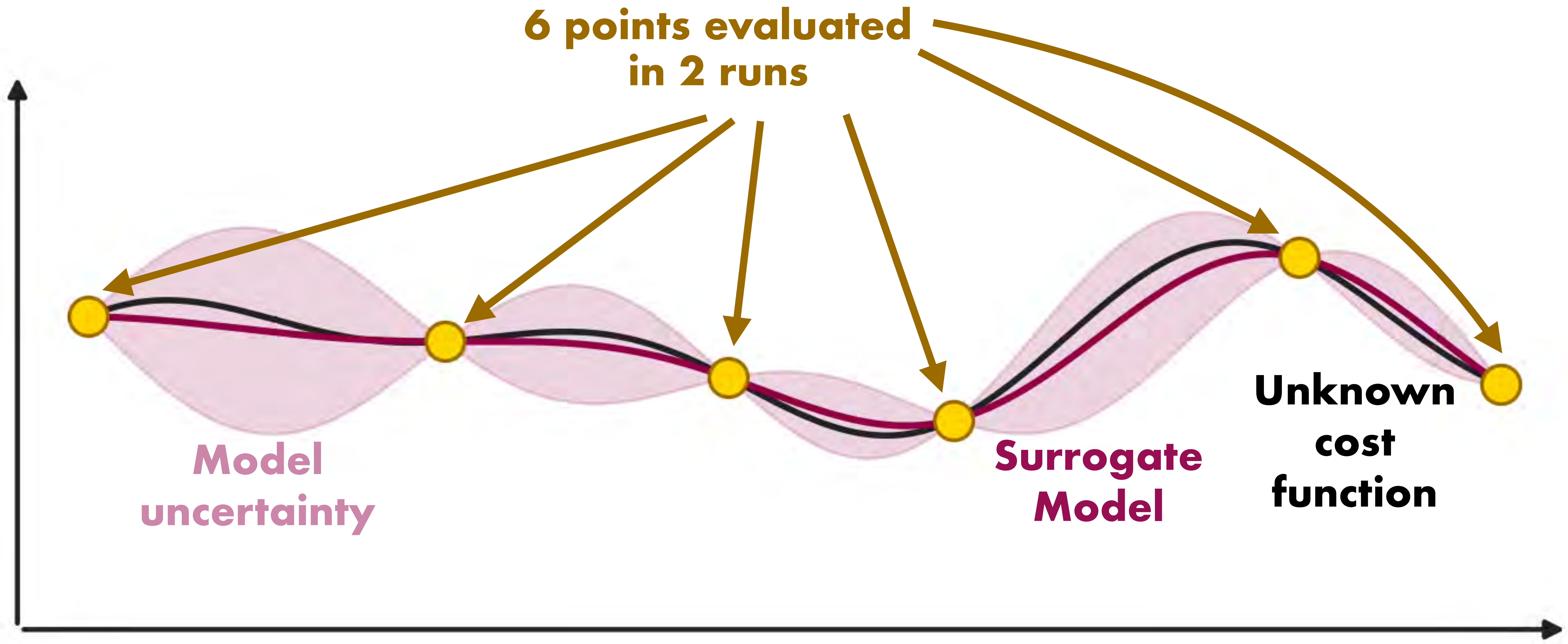

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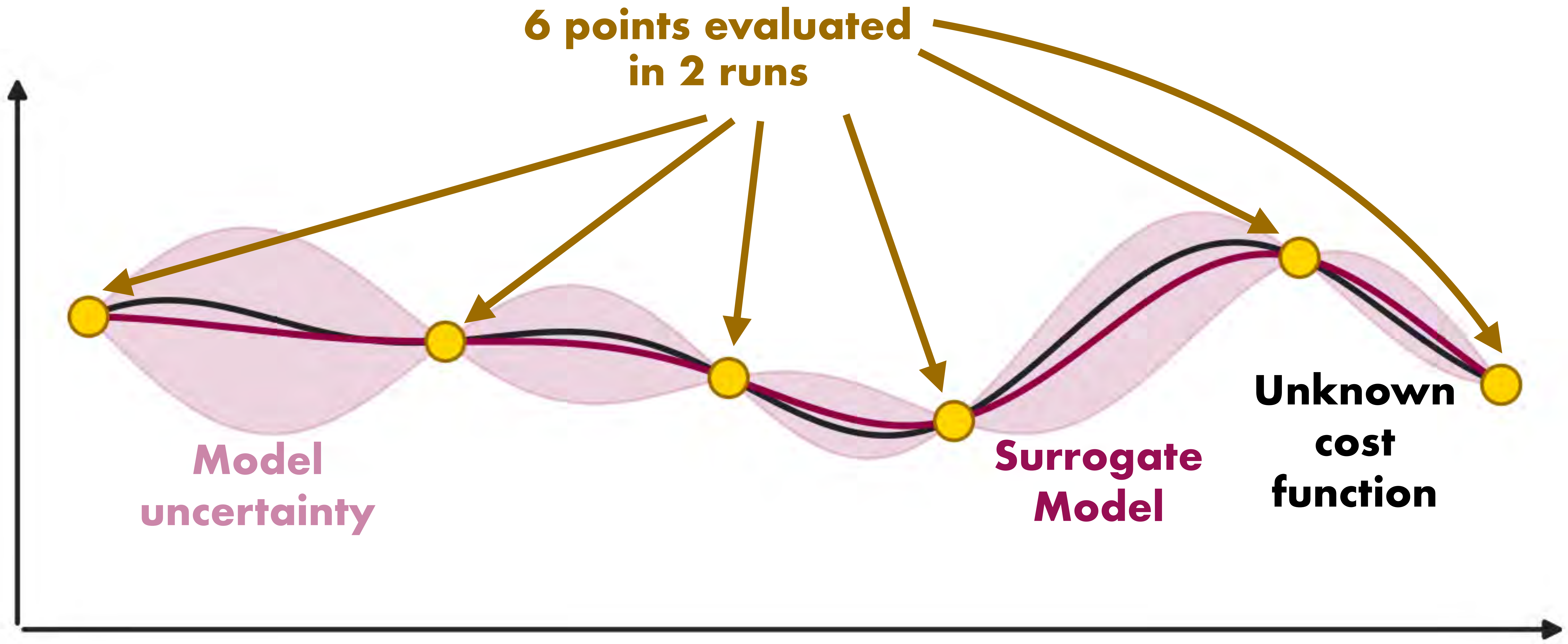
POSSIBLY FASTER THAN SEQUENTIAL BAYESIAN OPTIMIZATION!

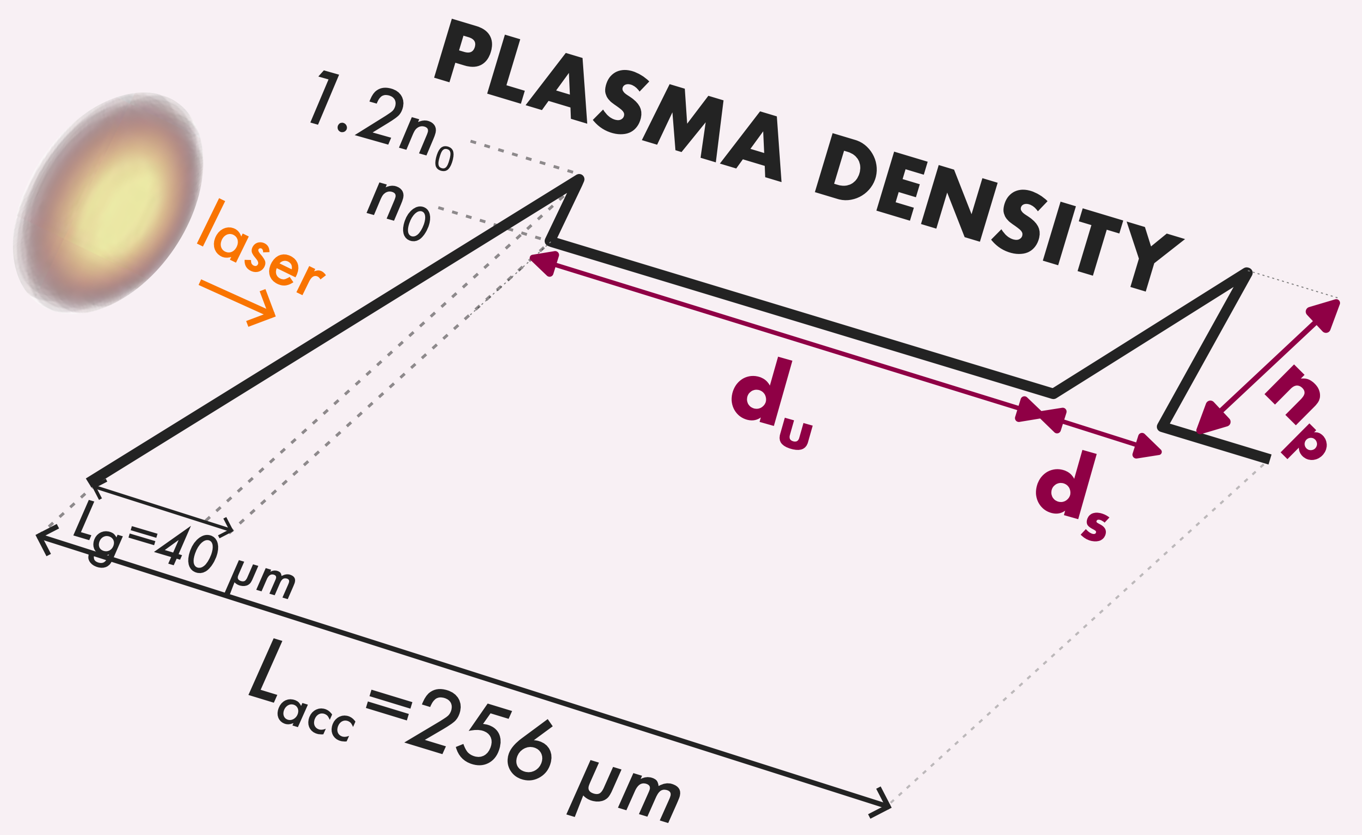


The attosecond betatron peak radiation was optimized, with penalty for long durations

INPUT: PLASMA SPIKE PARAMETERS

- **Spike position d_u** $\in [0, L_{acc} - L_g - 5\ \mu m]$
- **Spike length d_s** $\in [5\ \mu m, L_{acc} - L_g]$
- **Density peak n_p** $\in (1, 4n_0]$

$$d_u + d_s + L_g \leq L_{acc}$$



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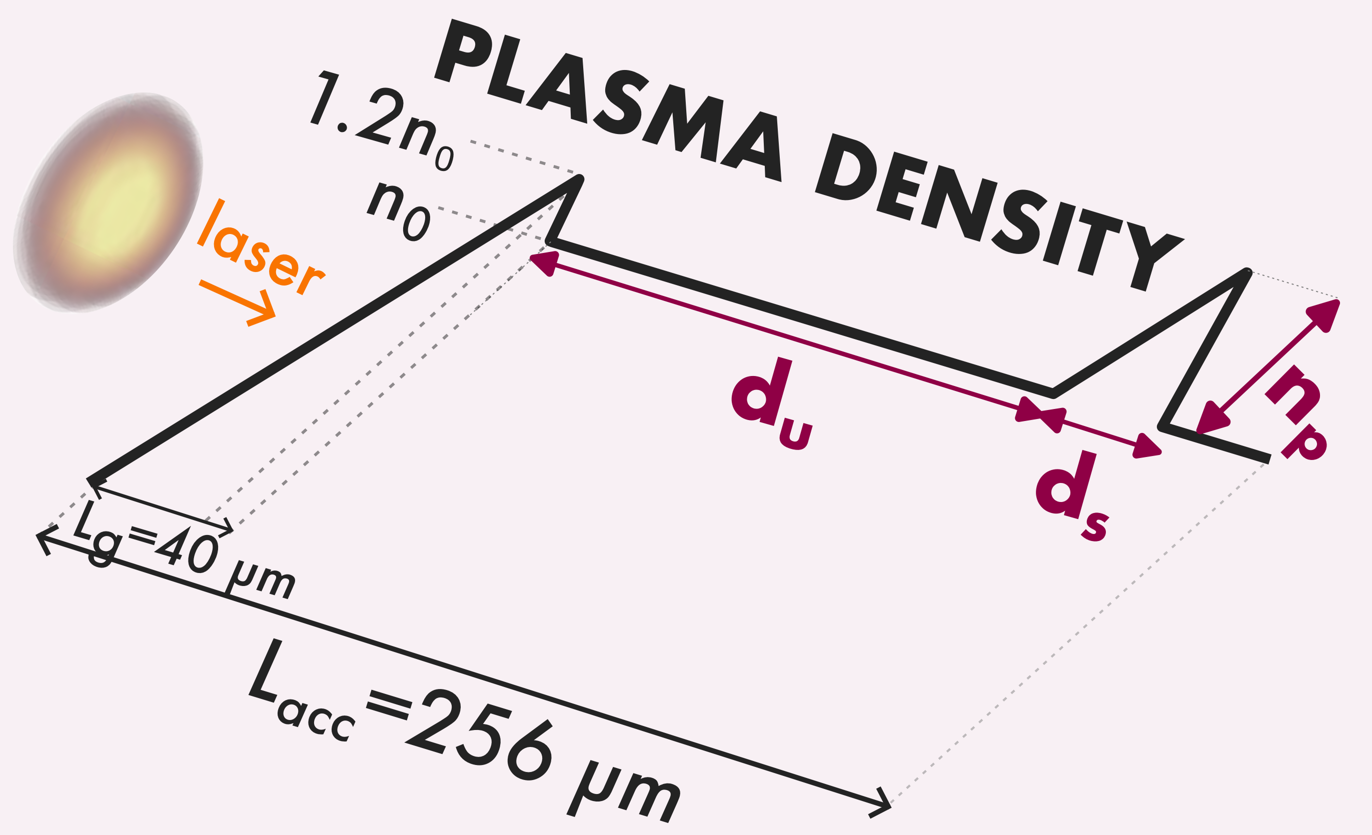
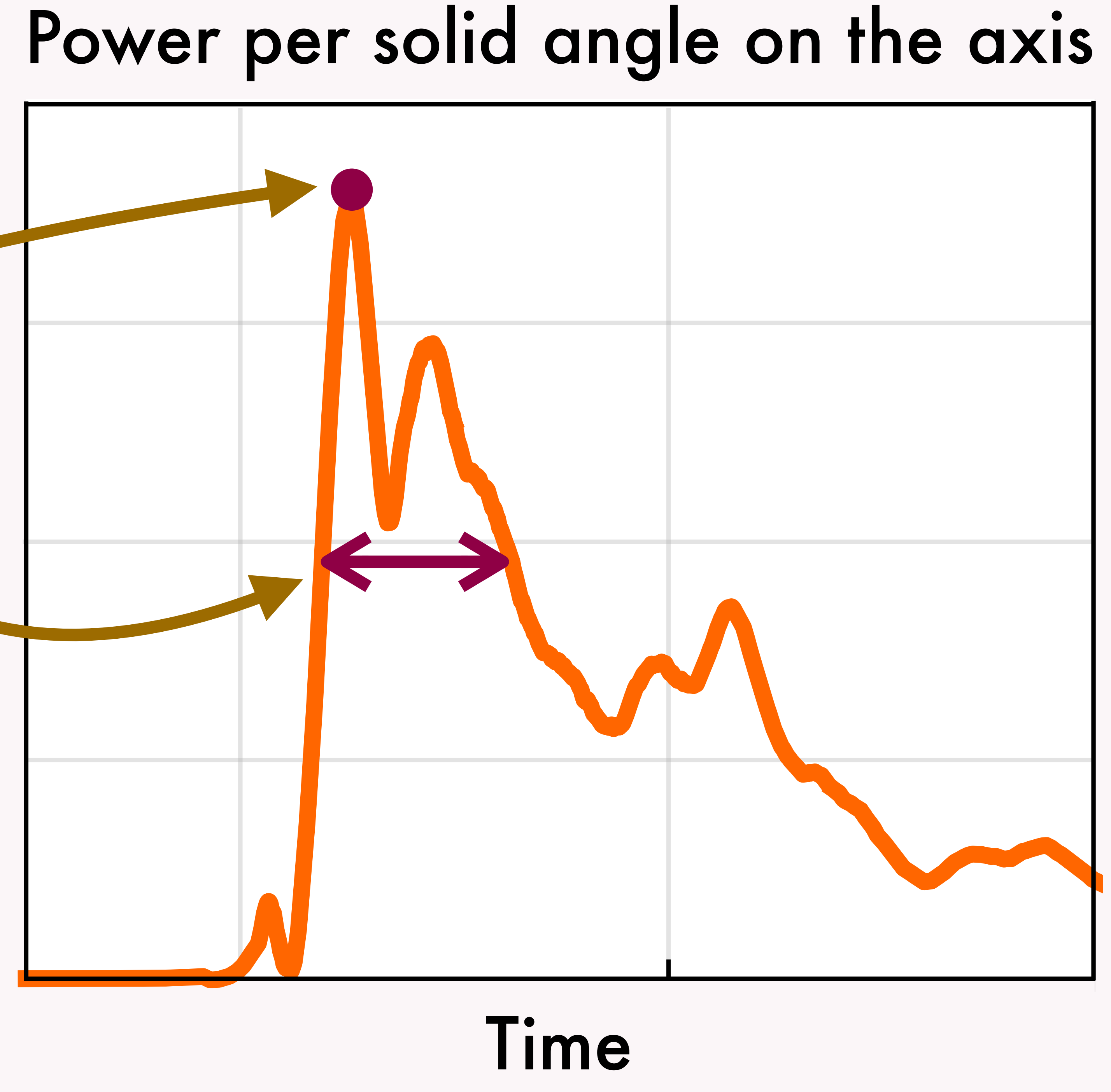


→

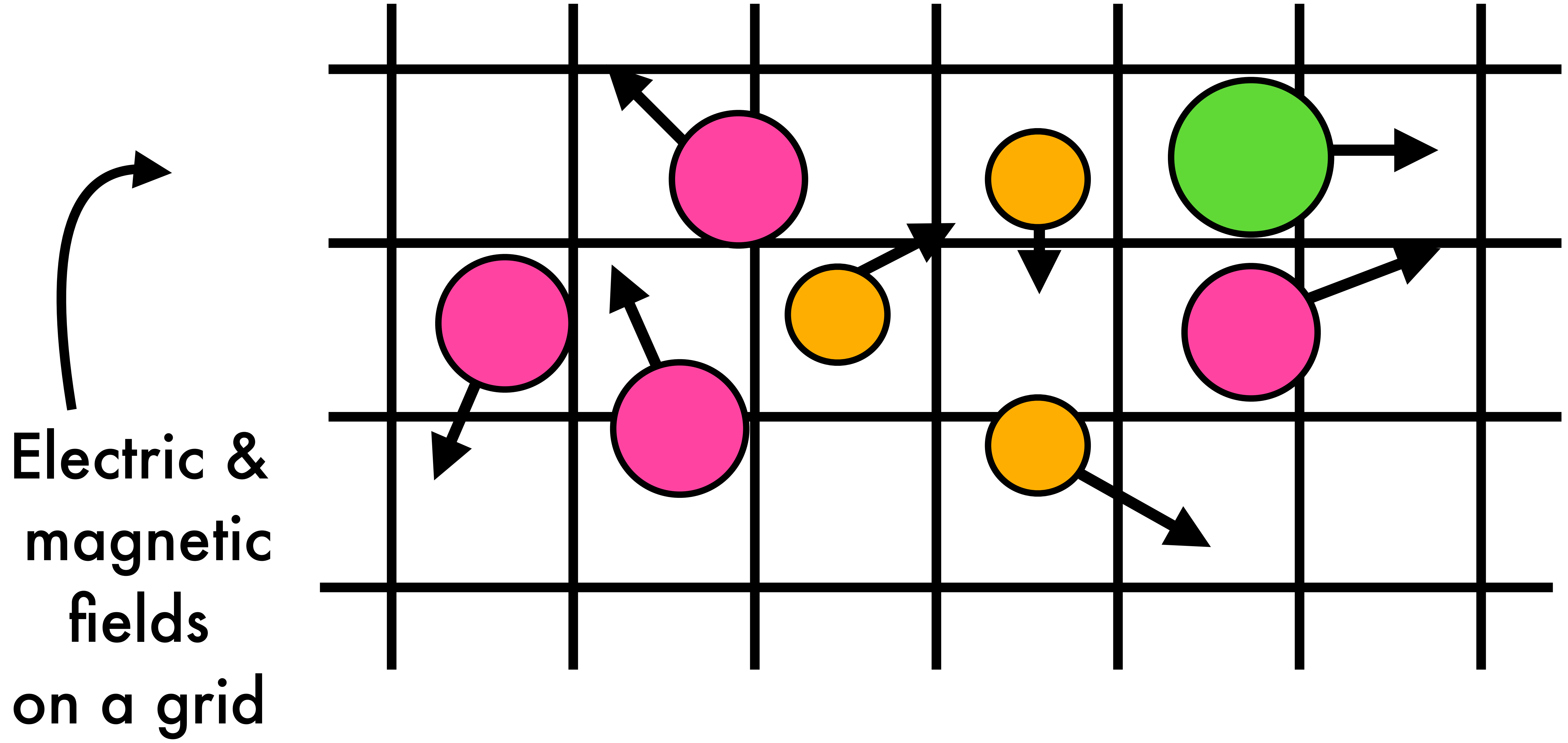
MINIMIZE THE COST FUNCTION C ENHANCE RADIATION PEAK

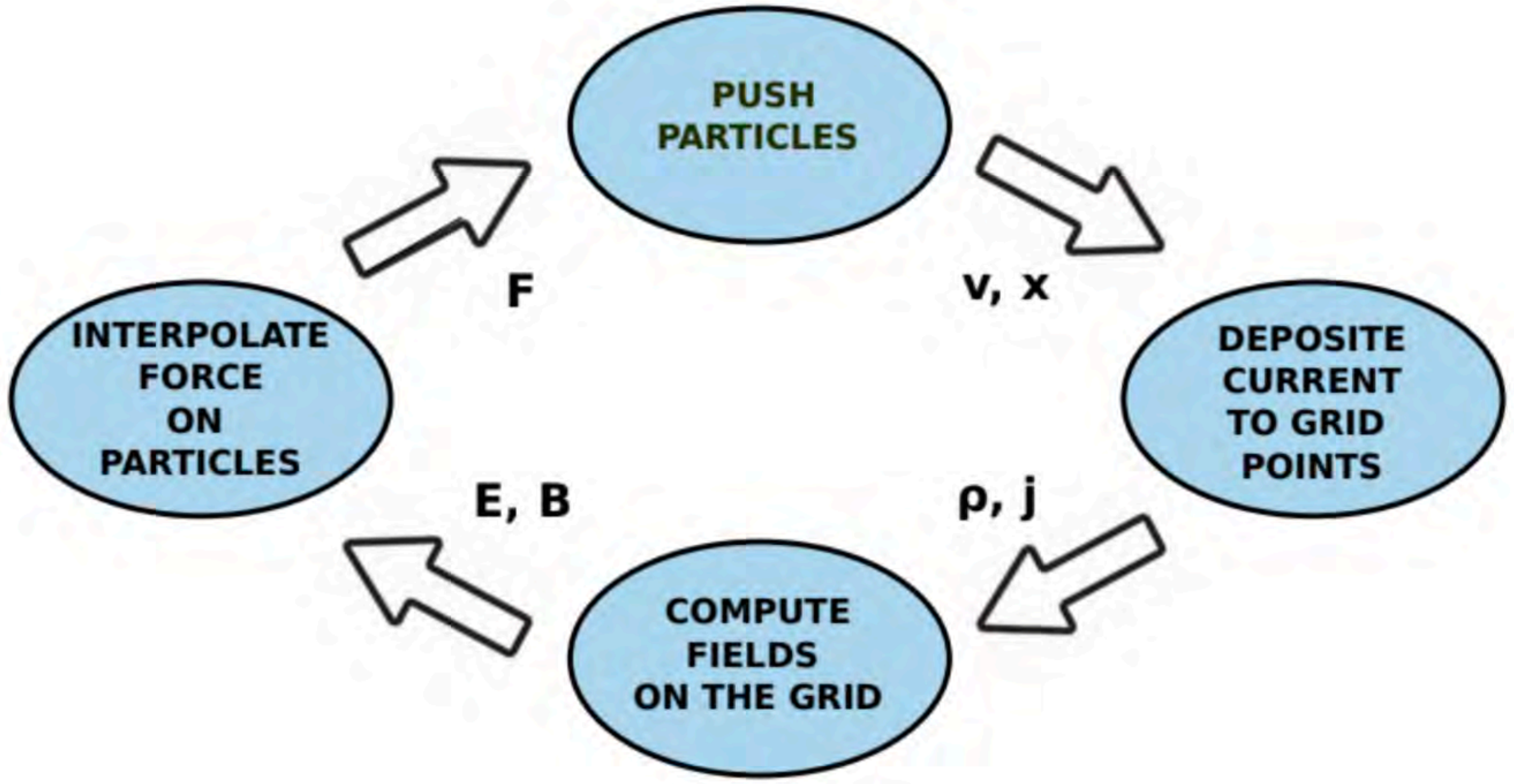
$C(P_\beta, \tau_\beta) = -\ P_\beta\ /\ \tau_\beta$



Particle-in-cell simulations of laser plasma-interaction

- **Particle-in-Cell (PIC)** is a computational method to model systems of moving charged particles.
- It tracks **macroparticles** (= many real particles).
- The electric and magnetic fields are calculated on a grid, particles move freely in space.





Optimization cycles were carried out in three steps

REPEAT

1 **Particle-in-cell:** to calculate **electron trajectories**
Running a parallel batch with varying spike properties d_u, d_s, n_p

1 simulation on Dardel: parallel, 8 nodes, walltime ~ 1.5 hours

Smilei)

Derouillat, Julien, et al. *Computer Physics Communications* 222 (2018): 351-373.

2 **Radiation code:** to compute **radiation emitted by electrons** in far field, to obtain power peak P_β on the axis and duration τ_β

1 simulation on Dardel: serial, 1 node, walltime: ~ 0.5 hours

FIKA code available on GitHub

FIKA

3 **Batch Bayesian optimization** updated the model & selected new points for Particle-in-Cell input

Optimize spectrum peak over betatron duration

OPTIMIZATION →

Suggest new points for the next batch of 8-10 PIC simulations

Secondmind

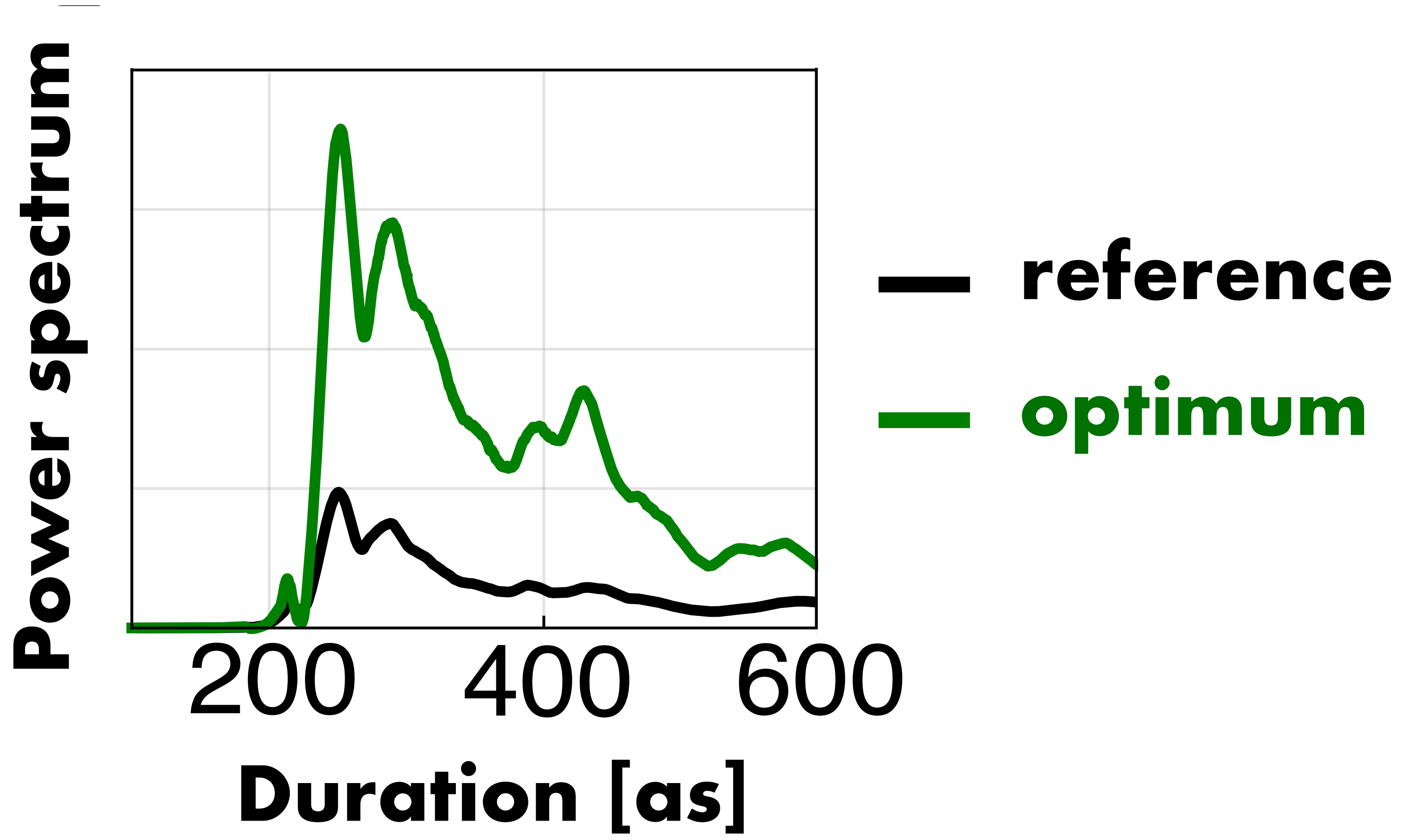
$C(P_\beta, \tau_\beta) = - P_\beta / \tau_\beta$

{Spike position d_u, spike length d_s, density peak n_p}

Performed on a personal computer, negligible time

High-density short spikes placed closely to the end of the acceleration lead to improvement over the reference case

- The model converged after 5 iterations (=5 batches)
- 43 PIC simulations in total
- Batches of 9, 8, 8, 8, 10 simulations



Reference
NO SPIKE
0.43 GWsr-1
81 as

→

Optimum
$\{d_u, d_s, n_p\}$={147 μm, 5 μm, 3.9n_0}
1.57 GWsr-1
92 as

>350% increase at radiation peak
only 14% in duration compared to reference

Summary

- **Attosecond X-ray bursts offer unprecedented temporal resolution,** allowing the probing of processes occurring on the electron timescale inside atoms.

- We investigate **a new type of source** of attosecond bursts coming from a **laser-based electron accelerator** via kinetic particle-in-cell simulations.

- The source was optimized with **batch Bayesian optimization**. The radiation peak increased by almost 4 times.

- In ongoing work, we examine the optimization performance and explore alternative cost-function designs.

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Acknowledgment

This project received funding from the Knut and Alice Wallenberg Foundation (Grants No. KAW 2020.0111 and 2023.0249). The computations were enabled by resources provided by the National Academic Infrastructure for Supercomputing in Sweden (NAISS), partially funded by the Swedish Research Council through grant agreement No. 2022-06725.