Bayesian Optimisation Guided PIC Simulations for EPAC

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1 Introduction

Experimental Area 1 at the Extreme Photonics Applications Centre (EPAC) will predominantly be used for electron acceleration in underdense plasmas. A mixture of permanent magnet and electromagnetic quadrupoles will be used to collect and transport electrons from the source to the application area or to diagnostics. To aid the design of the magnetic beamline, Particle-In-Cell (PIC) simulations have been performed to generate realistic electron beam outputs from the EPAC laser wakefield accelerator.

2 Bayesian Optimisation of PIC Simulations

Simulations were performed using FBPIC [1]. FBPIC uses a quasi-cylindrical coordinate system which allows faster computational times than full 3D algorithms, without loss of accuracy in a close to cylindrically symmetric system. This improved computational time means simulations can take minutes/hours rather than days, so many iterations can be performed to quantify a parameter space. The vast parameter space dealt with in laser-plasma interactions means detailed grid scans still require a prohibitive amount of time to perform. Machine learning techniques, such as Bayesian optimisation [2], can be used to more quickly evaluate a parameter space given a specified objective. The method used here is similar to Ref. [3]. Figure 1 shows the process used for Bayesian optimisation. First, an objective function is defined. This is the value that is maximised/minimised in this process. Next, several simulations are run at random points within the chosen parameter space to train the surrogate model, which gives an estimate of the objective function over the parameter space. Gaussian process regression [4] is used here to generate this model. Once we have a rudimentary model of the parameter space, we use an acquisition function to find the next set of parameters to trial. Expected improvement is used here, which considers both the probability that a given point in the parameter space will give a better evaluation of the objective function than previous evaluations, and the expected magnitude of the increase when computing the next value to trial [2]. Once simulation at this point in the parameter space has been performed, the surrogate model can be updated and the acquisition function can give a new set of parameters to trial. Through many iterations, something close to the maximum of the objective function can be found within the parameter space. This can be found with far fewer iterations than with a grid scan, as the guided optimisation approach leads to fewer evaluations performed at far from optimal parameters.

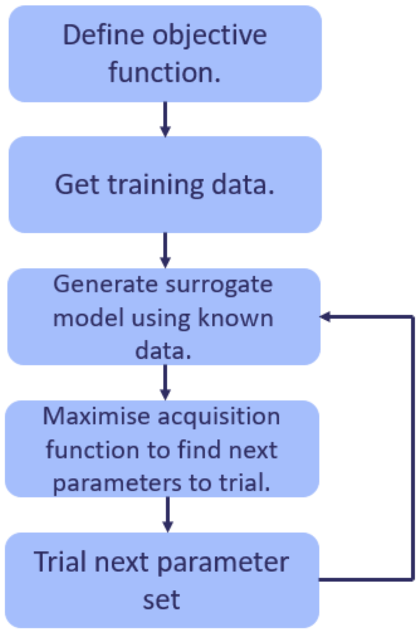

Figure 1: Flow chart for Bayesian optimisation.

Using this process, a simulated laser wakefield accelerator was optimised to produce high brightness, 1 GeV electron beams. The simulated laser replicated the EPAC laser expected day 1 parameters: an energy of 20 J, a duration of 30 fs and a spot $1/\mathrm{e}^2$ radius of 60 μm. A dual-stage, trapezoidal gas density profile was chosen to limit injection to the small, mixed gas nitrogen in helium injector region, before the helium accelerator region, as in figure 2. The objective function quantified the electron brightness by

$$B = \frac{Q}{\epsilon_x \epsilon_y \sigma_t \sigma_e} \quad (1)$$

where ϵ is the rms normalised emittance, σ_t is the bunch duration and σ_e is the energy spread. The objective function weighted this against a penalty function which rewards proximity to 1 GeV.

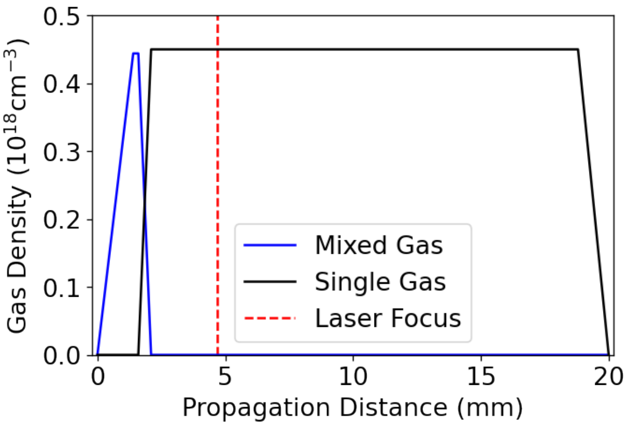

Figure 2: Gas density profile simulated. Optimised laser focal plane plotted as red line.

3 Results

Using the PIC simulation setup described above, the parameter space consisting of the following parameters was explored: laser energy, laser focal plane, accelerator region length, accelerator region gas density, injector region gas density and injector region nitrogen concentration. Over 300 iterations (20 training, 280 with optimiser), the objective function is plotted in figure 3. Large gains can be seen in the first 150 iterations, after which only marginal improvements are seen. The optimised parameter were:

1. Laser energy = 19.3 J.
2. Laser focal plane = 4.7 mm (red line in figure 2).
3. Accelerator region length = 16.7 mm.
4. Accelerator region gas density = $0.45 \times 10^{18}\mathrm{cm}^{-3}$.
5. Injector region gas density = $0.37 \times 10^{18}\mathrm{cm}^{-3}$.
6. Injector region nitrogen concentration = 5.9 %.

The longitudinal phase space of the optimised electron bunch is plotted in figure 4. The bunch has a median energy of 1 GeV, with an rms energy spread of 0.6 % and a charge of 25 pC. The emittance in the laser polarisation direction is 4.2 mm.mrad and 1.3 mm.mrad in the orthogonal direction. The divergence in the laser polarisation direction is 1.6 mrad and 0.9 mrad in the orthogonal direction. The 6D brightness of the optimised bunch is 3.2×10^{14} A/m^2/0.1% bandwidth. This bunch has been fed into magnetic tracking simulations for design of the EPAC electron beam transport.

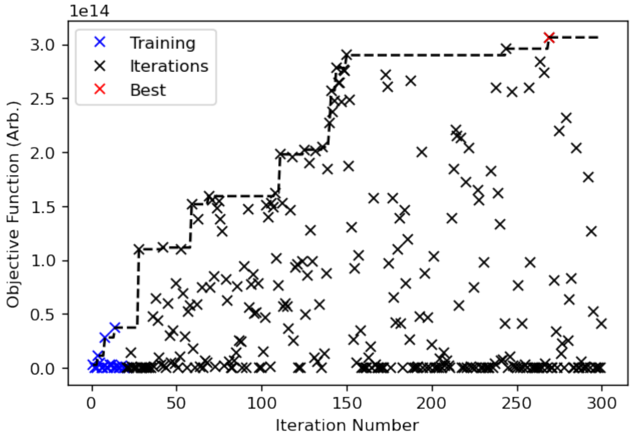

Figure 3: Objective function plotted against iteration number for a PIC simulation optimisation run.

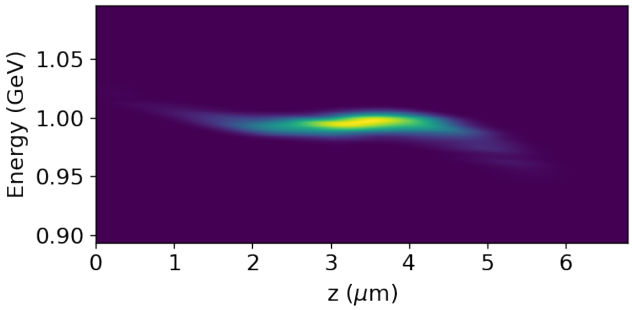

Figure 4: The longitudinal phase space of the optimised electron bunch.

4 Conclusion and Outlook

Bayesian optimisation guided PIC simulations have been performed to generate a high quality, 1 GeV electron bunch, which can be used to inform electron transport beamline design. This could be further optimised by exploring the effect of other parameters, such as laser chirp. Realism of the simulation can be increased once gas targets capable of generating a similar density profile to the one simulated have been designed, modelled and characterised. The final goal in this simulation campaign is to have a catalogue of realistic simulated electron outputs with different energies and optimised for different objectives, which can be used to aid experimental design at EPAC.

References

[1] Rémi Lehe et al. A spectral, quasi-cylindrical and dispersion-free Particle-In-Cell algorithm. *Computer Physics Communications* **203**, (2016), pp. 66–82.

[2] Donald R Jones, Matthias Schonlau, and William J Welch. Efficient Global Optimization of Expensive Black-Box Functions. *Journal of Global Optimization* **13,** (4 1998), pp. 455–492.

[3] Sören Jalas et al. Bayesian Optimization of a Laser-Plasma Accelerator. *Phys. Rev. Lett.* **126,** (10 2021), p. 104801.

[4] Carl Edward Rasmussen and C K I Williams. *Gaussian processes for machine learning.; The MIT Press: Cambridge, USA*. 2006.