GPJet: Physics-Informed Machine Learning of E-jet Printing Dynamics

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Abstract

We present GPJet, a Bayesian learning framework that is capable of …

(revolutionizing Melt Electro-Writing (MEW), an additive manufacturing technology with wide range of applications in biomanufacturing, energy storage technology etc. One of the greatest challenges is accurate real time metrology of features characterizing the jet, and therefore the process. Another is the difficulty in control and optimization of the process due to its multiparametric nature. GPJet addresses both of these issues. It consists of a Computer Vision module capable of performing real time object detection and metrology, and a Bayesian Optimization module to automatically minimize the jet's lag distance by altering collector's speed. Most notably, Bayesian Optimization can contribute in both process and computational optimization. Implementation and adaptation of Bayesian Optimization and machine learning in general, into additive manufacturing techniques, could lead to more efficient printing, by enabling better informed, data-driven parameter tuning.)

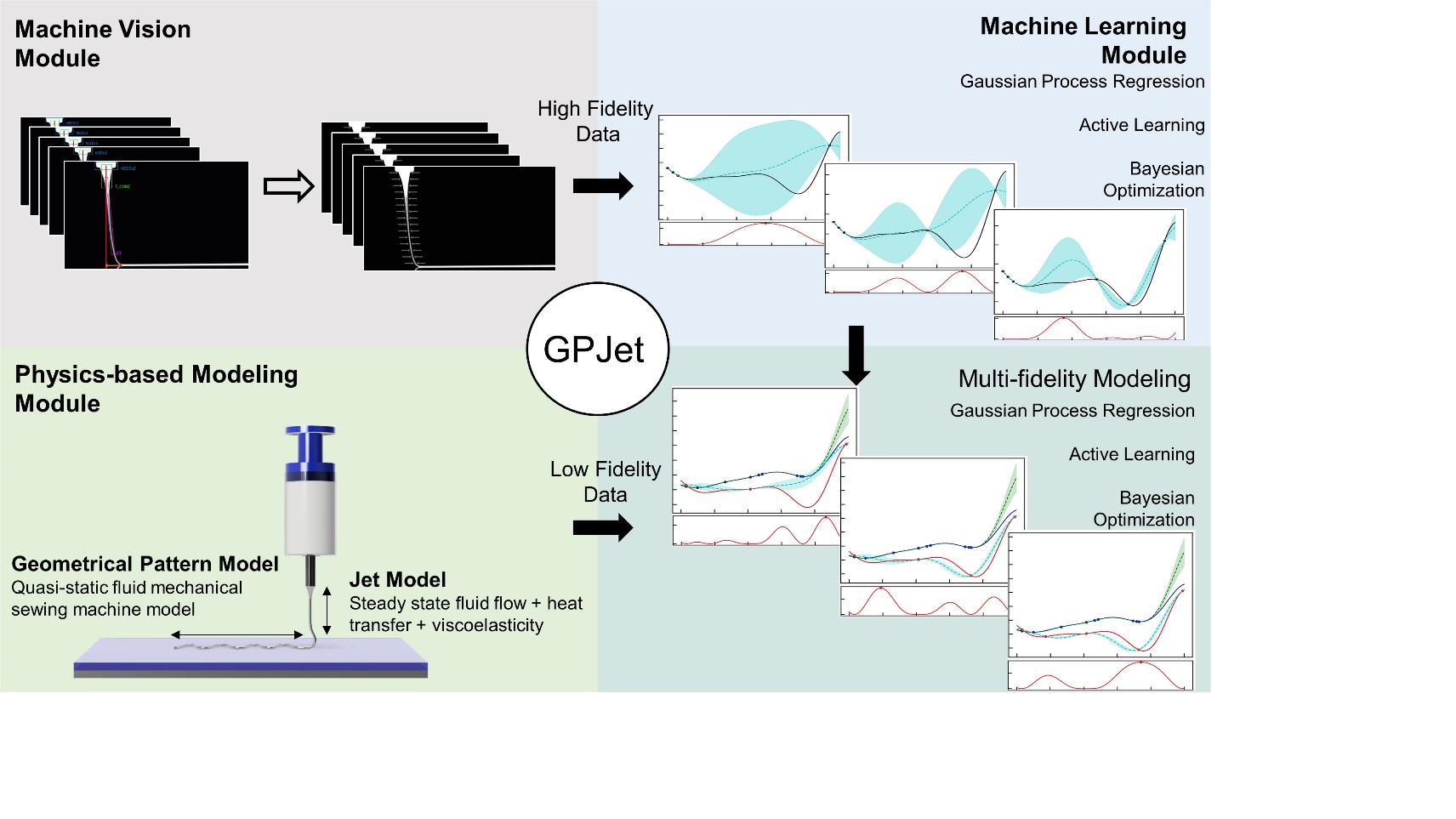
# Introduction

The programmable assembly of functional inks in two- and three-dimensions dimensions using computer numerically controlled (CNC) machines coupled with printing technologies has revolutionized the way we design and fabricate physical objects. Scientists, engineers, designers and makers have at their disposal a wide palette of extrudable inks to process. This toolset allows them to provide material solutions with cellular architectures and feature resolutions spanning nm to cm scale1. With these attributes at hand, extrusion-based additive manufacturing (AM) technologies, often referred as direct ink writing or 3D printing, are transforming fields such as healthcare, robotics, electronics and sustainability 2,3.

While the potential of 3D printing is celebrated very often in scientific journals and in the media, there is a “secret” that practitioners and companies of 3D printing, do not stress out. This under-reported reality entails the extensive experimentation and manual labor required to achieve expected end-part properties and reproducible process outcomes. Every time a new ink needs to be processed or a machine is moved to another location with different ambient conditions, trial and error approaches are being followed to optimize the printing process. These practices have led to desktop and industrial machines that are rigid and never “learn”. Only the user learns, leading to the creation of experienced "super users" at the expense of an enormous degree of individual process engineering.



**Figure 1: Electrohydrodynamics Jet Printing Process.** Solution electrospinning (SES) vs. melt electrospinning (MES). The main differentiating feature between the two processes is the extent of the jet instabilities that arise from the electrostatic forces acting at the polymer jet-air interface. For MES, the chaotic jet regime is limited close to the grounded collector plate due to the high viscosity and dielectric properties of the pure polymer melt. b Direct melt electrowriting (MEW) and its operating principle.



**Figure 2:The GPJet Pipeline Framework.** A Physics-informed Bayesian Machine Learning framework comprised by three different modules: a) the Machine Vision module, which takes as an input timeseries video focusing on the polymer jet in the free flow regime and performs extraction of high-fidelity jet features in real-time based on an automated image processing workflow b) the Physics-based Modeling Module, which and c) the Machine Learning module, which takes as an input high fidelity experimental data from the Machine Vison module and low fidelity modeling data from the and performs a series of data-driven tasks to learn the jet dynamics.

**E-jet printing**. A notable example of such a family of extrusion- AM technologies are the electrohydrodynamics-based additive manufacturing technologies, also known as E-jet printing. this is traditionally achieved by “scanning” the space, often on a simple Cartesian grid. Selecting a scanning strategy implies picking a scan resolution without knowing the model function, which will unequivocally lead to inaccuracies and inefficiencies. When the parameter space is high-dimensional, an approach based on intuition is often used, i.e., manually selecting measurements, assessing trends and patterns in the data, and selecting follow-up measurements. With increasing dimensionality of the parameter space, this method quickly fails to efficiently explore the space and becomes prone to bias. Needless to say, the human brain is generally poorly equipped for high-dimensional pattern recognition

**Data-Driven Approaches in Additive Manufacturing.**

……. Artificial intelligence and machine learning are transforming many areas of experimental science. While most techniques focus on analyzing “big data” sets, which are comprised of redundant information, i.e. information that is not strictly needed to define the model confidently, collecting smaller but information-rich data sets has become equally important. Brute-force data collection leads to tremendous inefficiencies in the utilization of

**Proposed Solution.**

…….

Overall, the main contributions of this paper are as follows:

This paper is organized as follows: First, we introduce….. Second, we …… Third, we……

# GPJet: The Physics-Informed Machine Learning Pipeline

To demonstrate the ability of learning the physics of EHD Jet printing processes in a data-driven way, we first developed a computer vision workflow, hereafter denoted as the Machine Vision module. The Machine Vision module allows us to probe and measure the jet dynamics. The jet metrology capability serves as a feature extraction step of high-fidelity data that inform the Machine Learning module of GPJet framework (see **Figure 2**).

The module is validated by a previously published dataset of time series video data [ADD CITATION]. The dataset is acquired by a conventional camera with 50 fps and a field of view spanning the area between the needle tip and the grounded collector of a melt electrowriting system. MEW constitutes an ideal testbed for demonstrating the capabilities and the flexibility of our GPJet framework. The highly dynamic nature of the process and the multiple user-controlled independent process parameters, pose several challenges. These challenges are reflected to the following fundamental question that we tried to address during the development of GPJet:

In the context of this paper, high-fidelity observations are referred to the jet features extracted by the machine vision module, whose experimental and computational cost aims to be minimized and low-fidelity observations are referred to data points that can be easily obtained with minimum cost by a numerical model that is not an absolutely accurate approximation of reality.

“Could we come up with a data-driven framework that allows both real time process monitoring and metrology with conventional low-cost cameras?” If yes, such a framework would give us the ability to actively learn the dynamics of the process in an online self-calibrating scenario.

# Results

## 3.1 Learning Jet Dynamics from Videos

As a first goal we set out to tackle the challenge of real-time process monitoring and jet metrology. To demonstrate the highly dynamic nature of the process, we plot overlaid video frames showing the jet hitting a stationary collector (**Figure 3a**). We chose to plot frames with a time step equal to 0.2 sec since the electrostatic nature of the process and the viscoelasticity of the molten jet cause instabilities of a significantly smaller time scale (~0.02 sec) and result to jet topologies that are indistinguishable with a naked eye. This provided a starting point for setting a goal related to the computational efficiency of the machine vision module for real time performance. Since the camera acquisition time was equal to 0.02 sec (50 fps), we proceeded with the goal to maintain computational processing time equal or smaller than that.

To accomplish this, we started by dividing the computer vision workflow in specific algorithmic tasks and implemented a sequential code version. We continued by systematically profiling the code, identifying the computationally expensive tasks, and then gradually parallelizing the code to reduce computational processing time. This led to 3 different code implementations of the machine vision module: a) the sequential, b) the concurrent and the c) parallel, with the last one achieving real-time performance. The results of the profiling experiments are shown in **Figure 3b**, where all the tasks are plotted along with their respective processing time for the three different code implementations.

Specifically, the machine vision tasks per frame are the following:

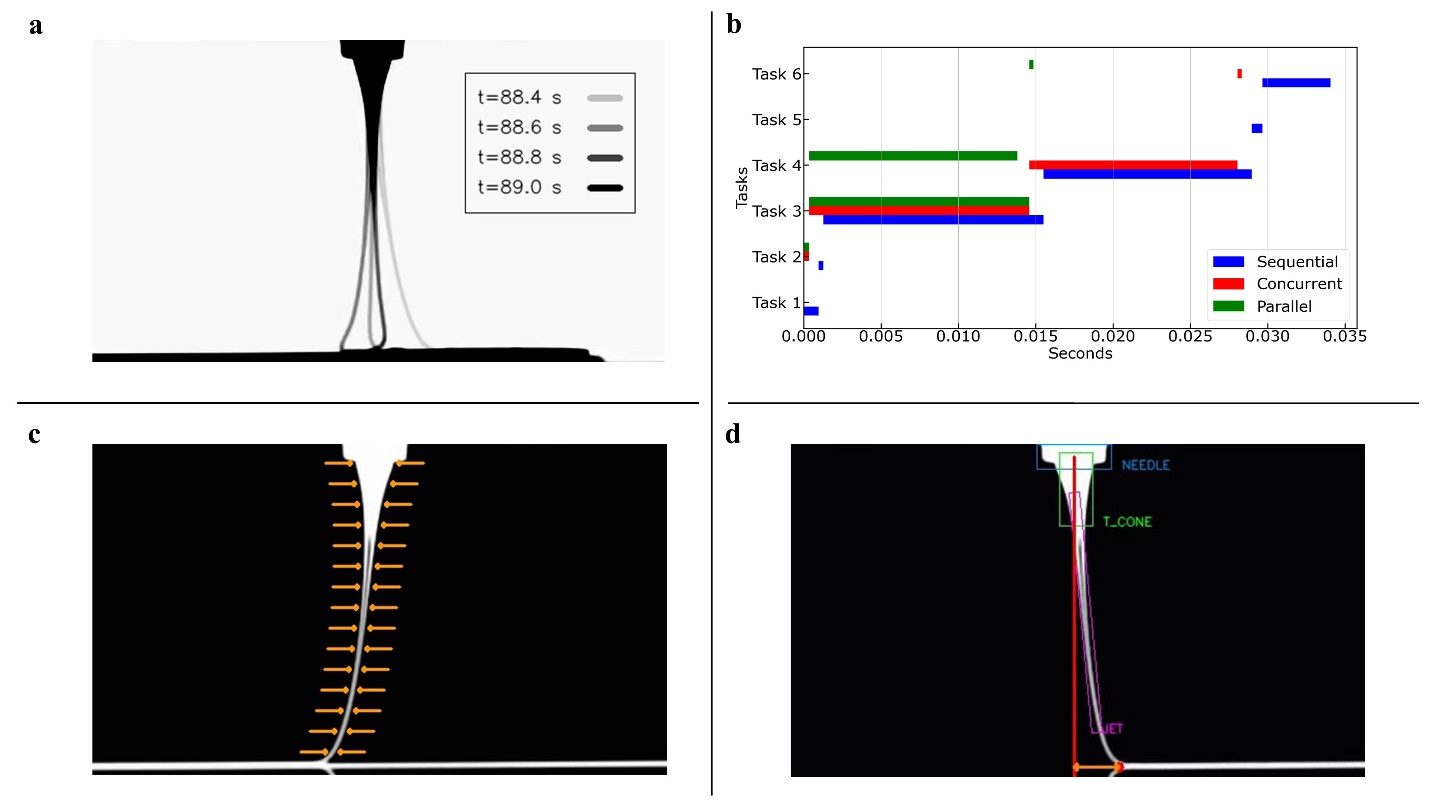
Task 1: Read new video frame.

Task 2: Process the frame to reverse background color.

Task 3: Edge-based feature extraction and data storage.

Task 4: Object-based feature extraction and data storage.

Task 5: Show processed video output.



**Figure 3: Machine Vision Module. a)** Process dynamics and its scale. **b)** Profiling experiments for different code implementations. **c)** Edge-based feature extraction methodology (Task 3 in Figure 3b). **d)** Object-based feature extraction methodology (Task 4 in Figure 3b).

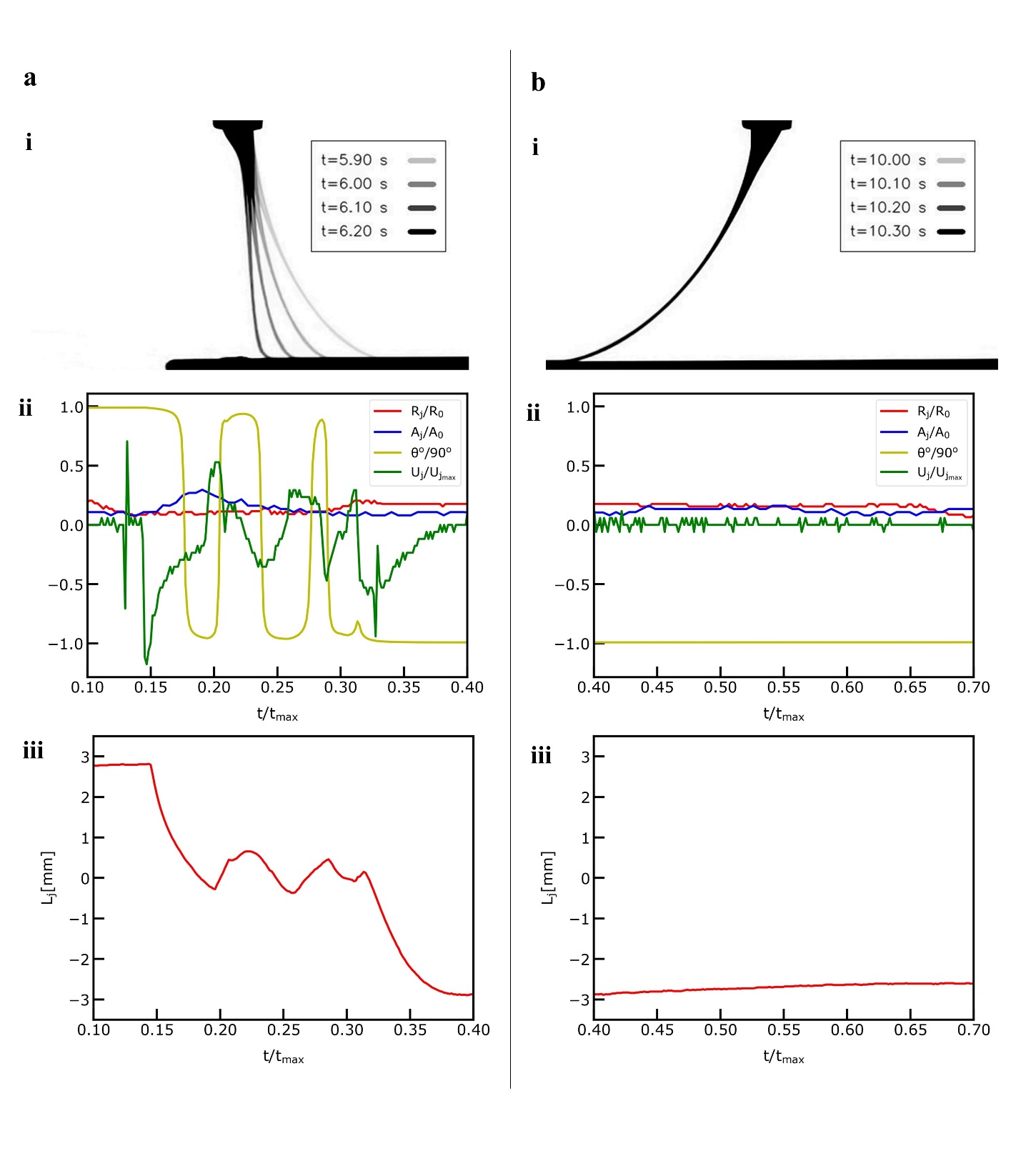
Task 6: Save video output.

Profiling the sequential code version reveals that an average time of 0.033 sec. is needed to perform the whole machine vision workflow per frame with the most expensive task being the one that performs edge-based feature extraction across the jet length (**Figure 3c**). To alleviate this source of computational cost, we employed a multithreading strategy for the concurrent code version that led to a modest improvement of 0.005 sec.

Multithreading is implementing software to perform two or more tasks in a concurrent manner within the same application. Multithreading employs multiple threads to perform each task with no limitation in the number of threads that can be used [10]. We learned that multithreading on one hand can reduce processing time of I/O bound tasks almost to zero, but on the other hand does not improve processing time of CPU bound tasks, such as Task 3 and Task 4, which are the most expensive.

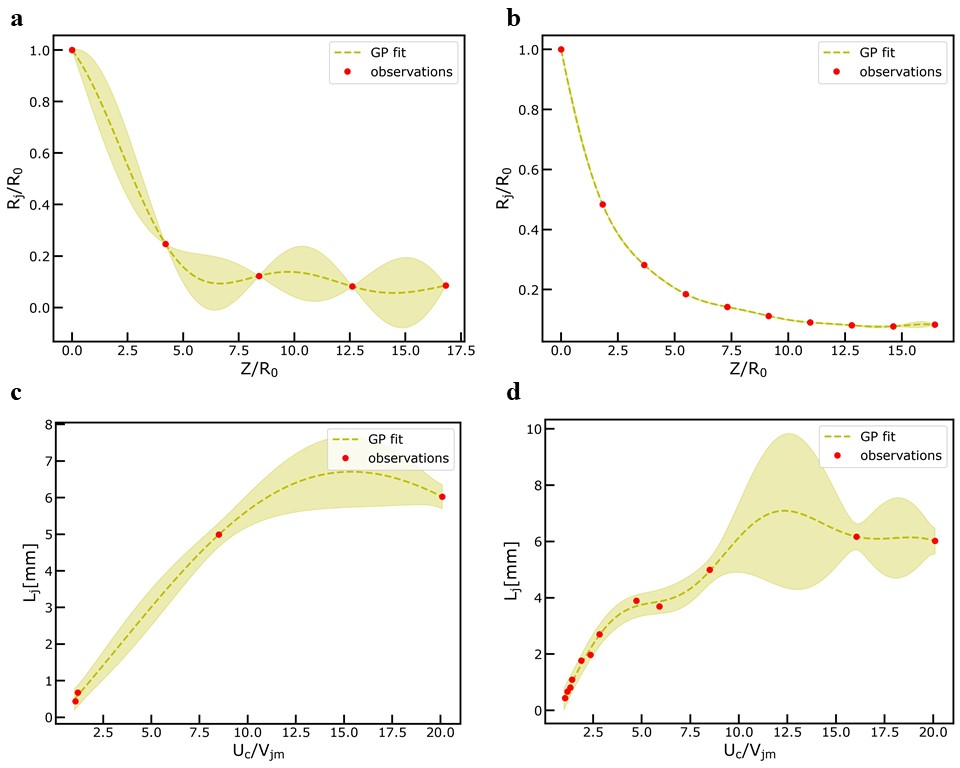
To further reduce processing time, we augmented the concurrent version with a multiprocessing strategy that led to the parallel code version. Multiprocessing systems have multiple processors running at the same time. Therefore, different tasks of an application can be run in different processors in a parallel manner. This capability considerably accelerates program performance. The limitation of this strategy is related to the fact that the number of processes that can be employed must be less or equal the number of processors (CPU cores) of the device [10]. Finally, by employing

multithreading for I/O bound tasks (Task 1, Task 5 and Task 6) and multiprocessing for CPU bound tasks (Task 3, Task 4), we were able to achieve real-time process monitoring and jet metrology with processing time up to 0.014 sec.



**Figure 4: Jet Metrology with the Machine Vision Module. a)** The extracted features during the deceleration-acceleration phase of the printing process. **i)** Overlayed video frames demonstrating the dynamics during the deceleration-acceleration phase and normalized jet length point of interest () denoted with red color. **ii)** Normalized jet radius (), Normalized jet area (), Normalized jet angles () and Normalized jet velocity () at the denoted point of interest plotted against the normalized time () during the deceleration-acceleration phase. **iii)** Jet lag distance plotted against the normalized time () during the deceleration-acceleration phase. **b)** The extracted features during the steady speed phase pf the printing process**. i)** Overlayed video frames demonstrating the dynamics during the steady speed phase. **ii)** Normalized jet radius (), Normalized jet area (), Normalized jet angles () and Normalized jet velocity () at the denoted point of interest plotted against the normalized time () during the steady speed phase. **iii)** Jet lag distance plotted against the normalized time () during the steady speed phase.

**Figure 5**: **Results of Gaussian Process Modeling Regression Tasks**. **a**) fitting normalized () jet radius observation data (n=5) obtained from the computer vision metrology module of the GPJet framework at specific z axis coordinates along the normalized jet length (). **b**)fitting normalized jet radius using a higher number of observation data (n=10) compared to the previous case (a). **c**)fitting lag distance () observation data (n=3) obtained from the computer vision metrology module of the GPJet framework for specific speed ratios (). **d**) fitting lag distance using all available observation data (n=12). For non-normalized quantities units are in SI. Filled contours represent uncertainty bounds (95% confidence intervals (CIs)).



Instrumented with the capability to perform jet feature extraction in real-time, we then focused on quantifying process dynamics relevant features. With the edge-based feature extraction algorithm, which is described in detail in sub-section 5.2 under the Methods section, we were able to measure the jet diameter profile, the area of the whole jet, the angle between the vertical line that connects the nozzle tip with the collector, and different points across the length of the jet profile and finally the translational jet speed at different points across the length of the jet profile. The high content spatiotemporal results are plotted in **Figure … of the Supplementary Information demonstrating** the breadth of information of the machine vision module and the fact that the jet point right above the collector undergoes a highly fluctuating behavior that will direct affect printing quality.

We present the jet metrology results for two distinct phases during the printing process in **Figure 4ai-ii** and **Figure 4bi-ii** focusing on the jet point right above the collector, hereafter after denoted as point of interest. With the object-based feature extraction algorithm which is described in detail in sub-section 5.2 under the Methods section, we were able to detect key objects in the field of view such the needle tip, the Taylor cone, which is defined as the jet area between the needle tip outlet and the jet point 2Ro away from the needle tip, the remaining jet and the collector. In this way, we were able to measure the Lag distance, defined as the distance between the point of interest and the projection of the middle point of the nozzle tip outlet to the collector. All detected objects are denoted graphically in **Figure 3d**, which shows the video output after Task 4 during the computer vision workflow.

As a next step, we asked how we could leverage the extracted features to learn the dynamics of the process in the most efficient data-driven way both with respect to experimental and computational cost. To address this question, we developed several Bayesian learning techniques, hereafter denoted as the Machine Learning module of the GPJet framework. The Machine Learning module takes as input the extracted high-fidelity data and initially uses Gaussian Processes (GPs) to approximate the function describing the relationship between a) the jet radius profile and the nozzle tip to collector distance and b) the Lag distance and the ratio of the collector speed over the jet speed at the point of interest.

Gaussian process regression (GPR) is a robust statistical, non- parametric technique for function approximation with kernel machines. GPR provides the important advantages of uncertainty quantification, the ability to perform well with small datasets and the capability to easily include domain-aware physics-based models in the deployed kernels.

To learn how the jet radius profile evolves over the tip to collector distance, we chose radial basis functions (RBF) as the kernel approximator and performed GPR. We trained the model under 2 different scenarios with n=5 observations and n=10 observations chosen at equally spaced points along the jet length for the 1st and 2nd scenario, respectively. It is important to mention that the machine vision module provides n = 93 observations along the jet length. The results are shown in **Figure 5a** and **Figure 5b** for the two different training scenarios. GPs can approximate the jet radius profile evolution with just n = 10 observations showcasing the efficiency of our data-driven approach with respect to computational cost.

To learn the function describing the relationship between the Lag distance and the ratio of the collector speed over the jet speed at the point of interest, we employ the same modeling strategy as before. Similarly, we set up two different training scenarios with n=4 observations and n=12 observations, respectively. Please note here that the number of high-fidelity observations at our disposal is constrained by our previously published experimental dataset (see sub-section 5.1 under the Methods section), where videos were acquired only at 12 different speed ratio settings. The results are shown in **Figure 5c** and **Figure 5d** for the two different training scenarios. While in the 1st training scenario, GPR provides a smooth function approximation, the prediction’s error from the experimental ground truth quantified by the Root Mean Square Error (RMSE), is significantly higher compared to the 2nd training scenario (**see Figure xxxx in Supplementary Info**). As a result, the function describing the relationship under question, is hard to approximate due to the high variability of the Lag distance caused by the jet instabilities close to the collector.



**Figure 6**: **Results of** **Multifidelity Modeling Regression Tasks. a**) fitting normalized high fidelity observation data (n=6, red color) of jet radius () and low fidelity model data obtained from the computer vision metrology module of the GPJet framework and from the multi-physics model, respectively, at specific z axis coordinates along the normalized jet length () and comparing the results with a simple GP fit using the same number of high fidelity observation data. **b**) fitting a higher number of normalized high fidelity observation data (n=7, red color) of jet radius () and low fidelity model data obtained from the computer vision metrology module of the GPJet framework and from the multi-physics model, respectively, at specific z axis coordinates along the normalized jet length () and comparing the results with a simple GP fit using the same number of high fidelity observation data.

Collectively, our lightweight machine vison module informing the GPR capabilities of the machine learning module with high-fidelity observations demonstrate that we can learn the dynamics of the process. Specifically, GPJet demonstrates excellent performance with respect to the prediction of jet radius profile evolution for a small amount of high-fidelity observations n = 10. Furthermore, GPJet demonstrates good performance for the available number of high-fidelity observations with respect to the Lag distance behavior at different collector speed settings.

## 3.2 Learning Jet Dynamics from Videos & Physics

As a next step, we focused on exploring how we could further reduce the number of high-fidelity observations without losing the predictive capability of GPR with respect to the jet radius profile evolution. To accomplish that, we augmented the high-fidelity observations obtained by the machine vision module with low-fidelity observations obtained in a principled manner by a multiphysics model. The multiphysics model capture the electrohydrodynamics, the heat transfer and viscoelastic constitutive material behavior of the molten jet in 1D across the needle tip to collector distance. The mathematical formulation and numeric implementation of the model are described in detail in sub-section 5.3 under the Methods sections.

We set up our data-driven scheme with two fidelities corresponding to two different kernel machines integrated in one multi-fidelity kernel, in which the correlation between the 2 kernels is encoded as a linear relationship. In other words, we constrain the prior knowledge during GPR with process physics-relevant knowledge, resulting to a physics-informed posterior prediction that needs much less high-fidelity observations.

We trained the multi-fidelity model under 2 different scenarios with n=6 high-fidelity observations and n=7 high-fidelity observations, respectively. For both scenarios the number of low-fidelity observations was kept to a number equal to 32 and equally spaced points across the jet length. For the 1st scenario n=6 equally spaced points were chosen across the jet length depicted in the jet schematic of the **Figure 6a** (upper-left). The results are shown in **Figure 6a-i** and **Figure 6a-ii.** In **Figure 6a-i,** we plot the multi-fidelity GPR predictions for the low and high-fidelity observations respectively. In **Figure 6a-ii**, we plot the predictions of the multi-fidelity GPR in high-fidelity observations together with the predictions of a simple GP in high-fidelity observations. Both plots demonstrate that we can learn the jet radius profile much better using 2 different fidelities compared to using only 1 fidelity for the same number of high-fidelity observations. Our results, point out that we lose predictive accuracy for the Taylor cone area (below the needle tip outlet) This phenomenon was expected due to that the fact that similar behavior was observed when the multiphysics model was tested and informed the strategy of the 2nd scenario, where we chose 7 high-fidelity observations with the additional point being in the Taylor cone area. The results are shown in **Figure 6b-i** and **Figure 6b-ii** demonstrating that we have managed to further reduce the required number of high-fidelity observations need to be extracted by the machine vision module without compromising predictive accuracy.

## 3.3 Active Learning of Jet Dynamics

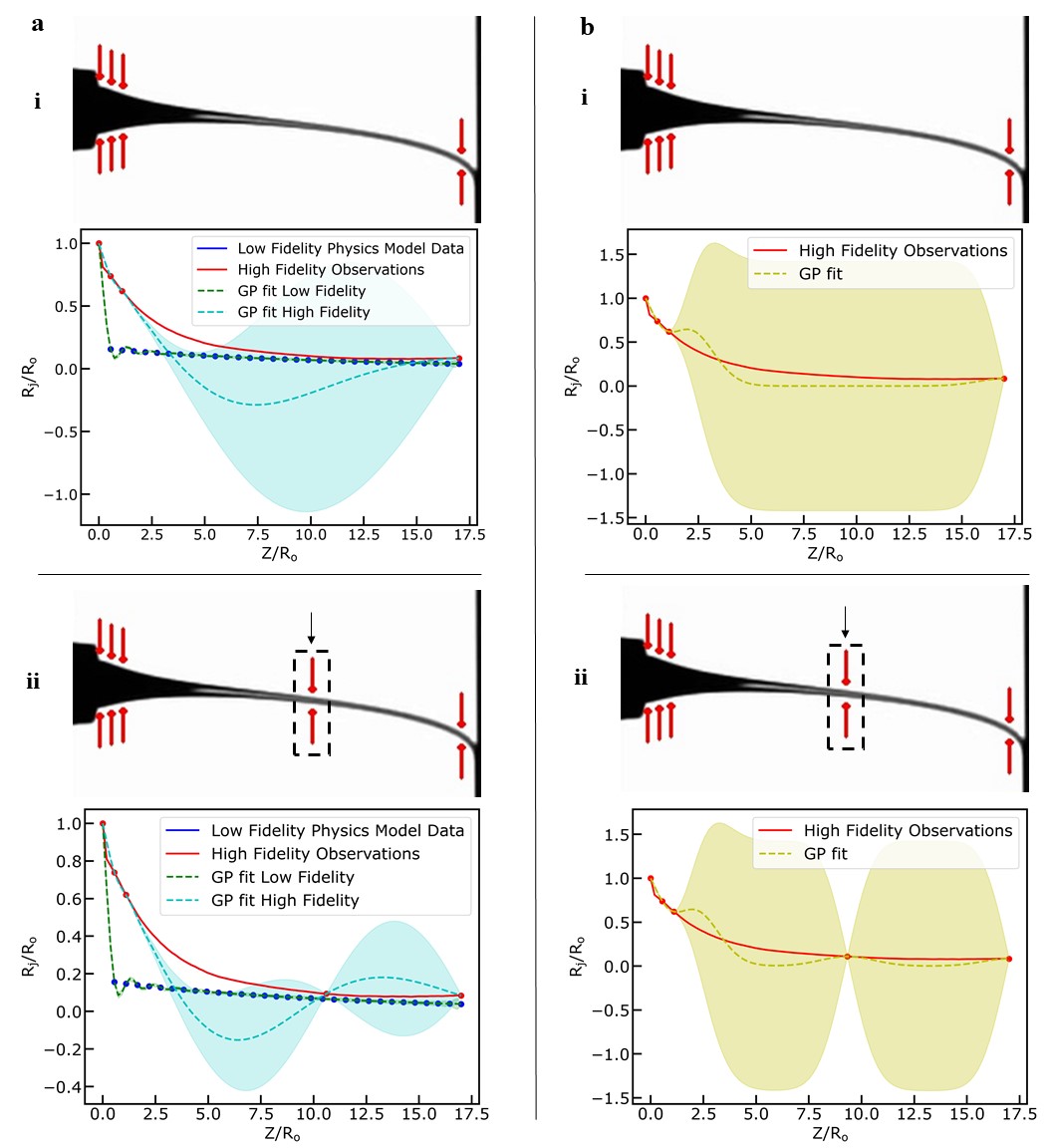
Up to now, we demonstrated that GPJet, is a robust tool for passive learning of jet dynamics. By “passive”, we mean that given a high-fidelity dataset provided by the Machine Vision module and augmented by low-fidelity data provided by the Physics-based module, the GPR capabilities of the Machine Learning module can model the function that mathematically represents the relation between the jet radius and the needle tip to collector distance. In addition to that, we employed the same strategy without low fidelity data, to model the function describing the highly dynamic relationship between the Lag distance and the ratio of the collector speed and the jet velocity at the point of interest.

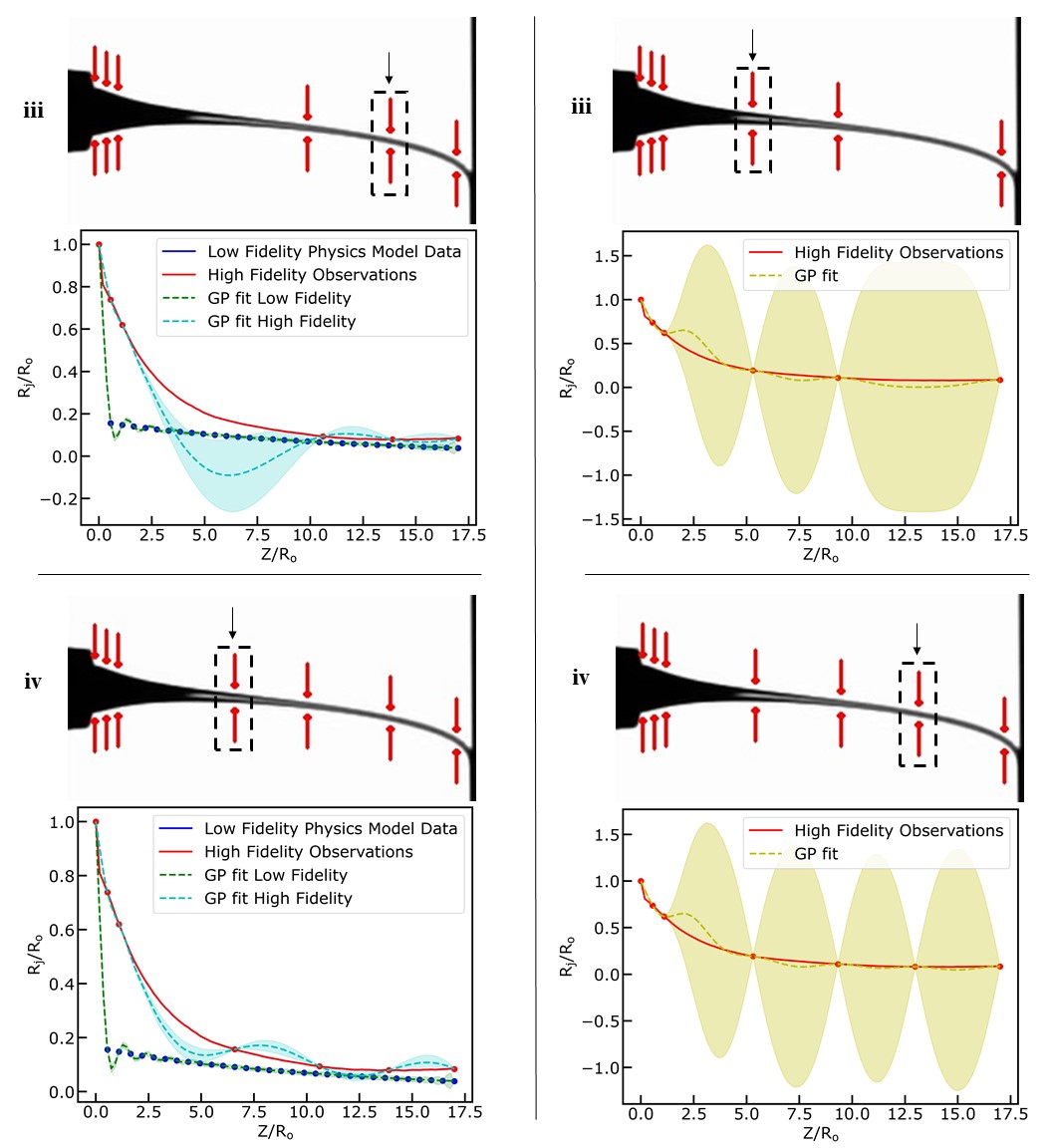
In this section, we asked the questions of whether we could actively choose data points across jet length for which to observe the outputs to accurately model the underlying function describing the jet dynamics with respect to the extracted jet features. To accomplish that, we deploy a virtual MEW machine, whose dynamic range is defined by the available dataset, and we run simulation experiments to demonstrate if we can learn the underlying functions in an active manner as quickly and accurately as possible.

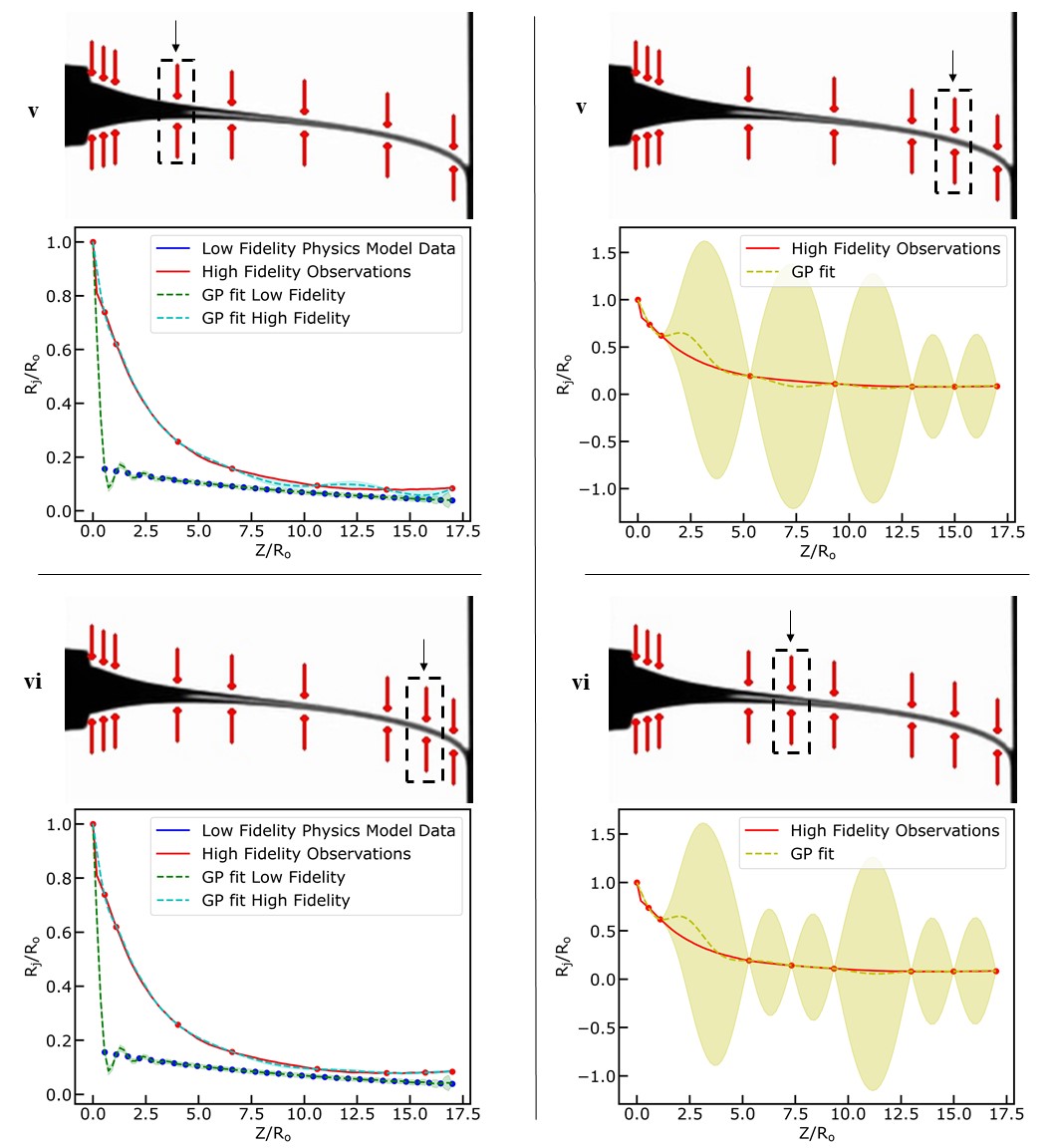
To accomplish that, we set up an exploration scenario, a set-up closely related to optimal experimental design scenarios as it equates to adaptively selecting the input spatial points across the jet length based on what is already known about the function describing the jet radius profile and where knowledge can be improved. We run active learning in both the multi-fidelity GP and simple GP for the jet radius profile evolution. The results are shown in **Figure 7**. To systematically, compare the performance of the two different models, we chose the same initial training points (**Figure7a-i** and **Figure7b-i**) and the same number of iterations during each training phase. For each iteration (**Figure 7a(i-vi)** and **Figure 7b(i-vi)**), we graphically show, on the processed video frame the adaptively selected point across the jet length and below that the modeling results. The adaptive selection is based on a purely exploratory acquisition function that steers the point selection towards the area of least knowledge quantified by the uncertainty output of the modeling step. The results demonstrate that we can learn actively and in a purely exploratory scenario accurately and fast the underlying function. Each iteration phase for the multi-fidelity (MFD) GPs and simple GPs lasts around ~ 0.5 seconds leading to a total learning time equal to 3 sec. Lastly, we extract performance metrics to compare the active learning between the multi-fidelity and simple GP model (see Figure X in Supplementary info). The results demonstrate that active learning on the MFD model is significantly faster (**Figure Xa)** with more confidence about the predictions since the model’s prior assumptions are constrained by domain-aware data.

Then, we employ the same strategy to actively learn the function describing the relation between the Lag distance and the speed ratio (put symbol) in an exploration scenario. The results are shown in **Figure 8**. The virtual MEW machine performs remarkably well in the prescribed experimental simulation. It starts by randomly selecting one speed ratio equal to 5 (see **Figure 8-a**) and after 4 additional iterations (see **Figure 8-a-b-c-d**), the underlying function is effectively approximated. Performance metrics (see Figure X in Supplementary info) demonstrate that the underlying function can be learned fast in an active manner and provide predictions with higher confidence compared to the passive learning approach and specifically after training the GP with all the available high-fidelity observations.

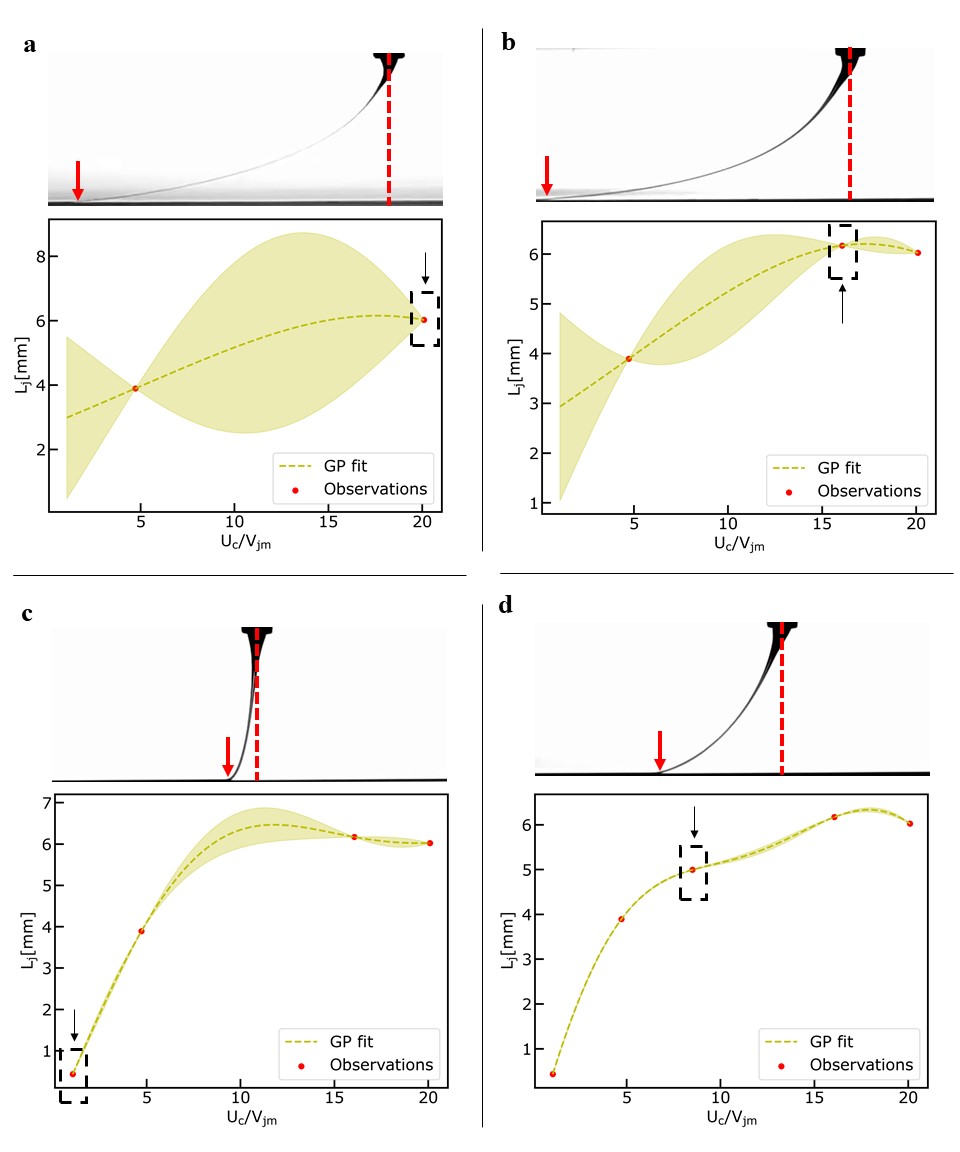
Finally, we set out to address the following question. Can the virtual MEW machine find the speed ratio corresponding to the minimum Lag distance in an autonomous way? Autonomy in this paper instance, refers to the machine’s ability to self-drive measurements of an experiment. Some initial parameters, such as the parameters to explore and their corresponding ranges constrained by the dataset, is defined by the user beforehand. Instead of us learning the relation between the Lag distance and the speed ratio and afterwards calibrating the machine hyperparameters, we aim to demonstrate a self-calibrating scenario. To achieve that we employ an exploitation-exploration scenario in the spirit of Bayesian optimization**.** It is called exploration–exploitation as scenarios where the output of the underlying function must be optimized require us to both sample uncertain areas to acquire more knowledge about the function (exploration) as well as sampling input points that are likely to produce low outputs given the current knowledge of the function (exploitation).The virtual MEW machine performs remarkably well in the prescribed experimental simulation. It starts again by randomly selecting a speed ratio equal to (see **Figure 9-a**) and after 2 additional iterations (see **Figure 9-a-c**) the speed ratio corresponding to the minimum Lag distance has been reached. This speed ratio is close to 1, as expected from the mechanical sewing machine model, which is described in detail in sub-section 5.4 under the Methods section.



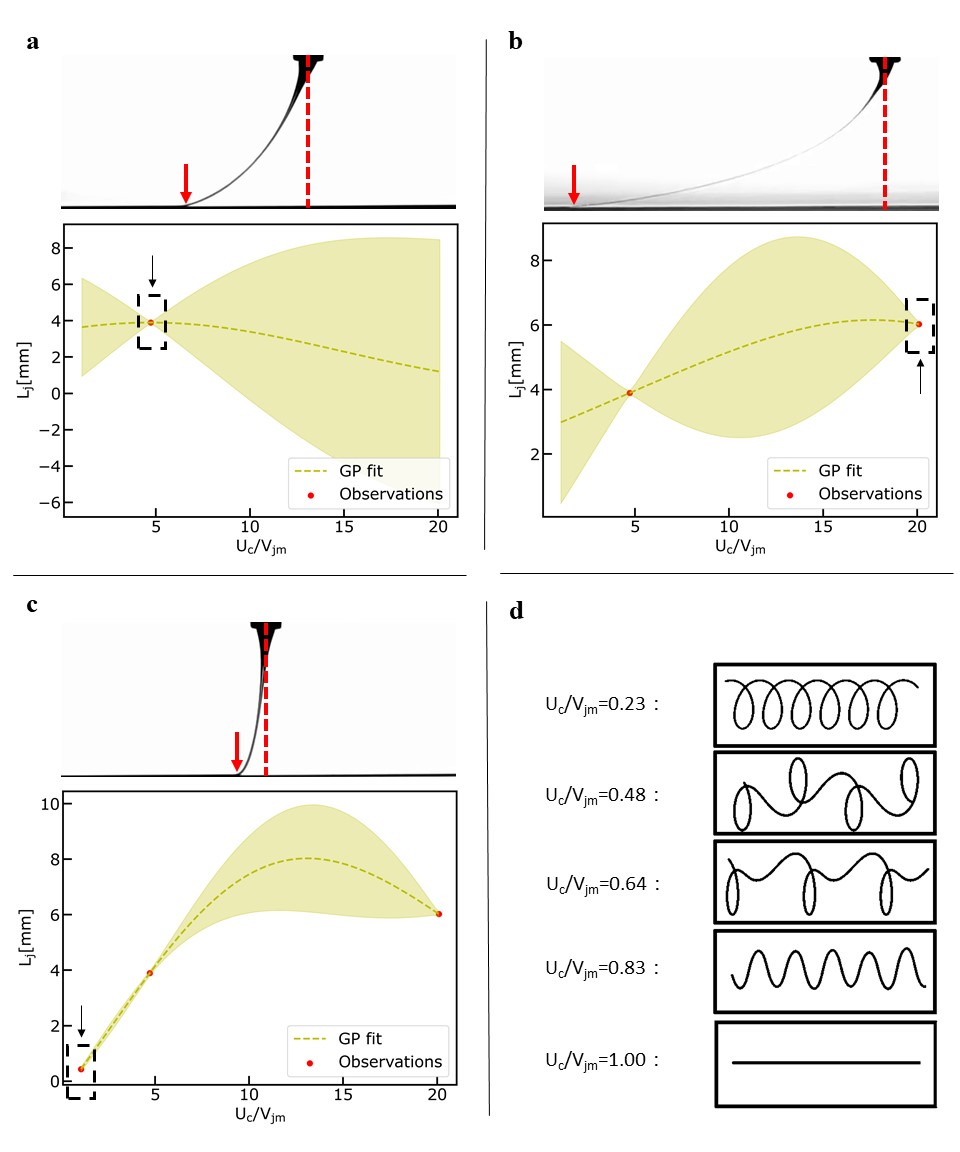




**Figure 7: Results of Active Learning on Multifidelity Modeling Task. a**) exploring the design space using Active Learning to fit a Multifidelity Gaussian Process to normalized high fidelity observation data (red color) of jet radius () and low fidelity model data obtained from the computer vision metrology module of the GPJet framework and from the multi-physics model, respectively, at specific z axis coordinates along the normalized jet length () ( **i – vi** denote the iterations of the active learning algorithm until it meets termination criteria). **b**) exploring the design space using Active Learning to fit a Gaussian Process to normalized high fidelity observation data (red color) of jet radius () obtained from the computer vision metrology module of the GPJet framework at specific z axis coordinates along the normalized jet length () ( **i – vi** denote the iterations of the active learning algorithm until it meets termination criteria).



**Figure 8: Results of Exploring the Design Space Task.** Exploring the design space using active learning tofit a Gaussian Process Model to lag distance () observation data obtained from the computer vision metrology module of the GPJet framework for specific speed ratios (). **a-d)** Iterations of the active learning algorithm until it meets termination criteria.



**Figure 9: Results of Bayesian Optimization Task.** Performing Bayesian Optimization to find the minimum lag-distance () by fitting a Gaussian Process Model to lag distance () observation data obtained from the computer vision metrology module of the GPJet framework for specific speed ratios (). **a-c)** Iterations of the Bayesian optimization algorithm until it meets termination criteria. **d)** For speed ratios less than one ( the process is unstable, no straight line is formed, instead the translated coiling, alternating loops, W patterns and meanders patterns are formed, therefore no lag distance () observation data can be obtained from the computer vision metrology module of the GPJet framework.

BO validates the initial hypothesis formed by universality about mechanical sewing machine model

# Conclusions

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that quantifying process dynamics extracting key enables to map their relationship with user-controlled independent process parameters. The key features of interest are the jet profile diameter and the lag distance

extracted features of interest and the user-controlled, tunable independent process parameters.

The optimization goal is dual from []: to achieve steady Taylor cone jet in the free flow regime and minimum lag distance to avhieve direct writing. It is important to mention that for the community of MEW it took almost a decade to understand that through trial & error and … (look my job package) Edisonian approach. With such a tool in ourt hands and advancement of data-driven approaches, we can have self calibrating printers that could learn the mappin between this and that to achivge the previously mentioned objective. IN csuch a self-calivbrating scenario you would have 2 scanarions: a) off learning and b) online leaerning. In both case, the user would need minimum amount of data to minimize computational cost.

To achieve , we use GPs and we describe noe now Figure 4. The 1st question that we aim to address is to what is the minimum amount of observations d needed in order to learn and predict the jet profile radius and learn the mapping between the jet and the speed ratio. Talk more about PSO

# Methods

## 5.1 Dataset

Video S1 and Video S2 published by P. Dalton [5] were chosen as the dataset to be used for this paper. As described a Sony Alpha 7 (Sony Corp. Japan) digital camera was used with a Nikon ED 200 mm lens (Nikon Corp. Japan). 1080 p resolution videos of the nozzle, jet and collector were taken at 50 frames per second. Process hyperparameters were set to 8 m s-2 and 500 m s-3 maximal stage acceleration and jerk, a 22G nozzle was used, polymer temperature was set to 87 o C and the voltage to the collector was set to -1.5kV, while the voltage to the nozzle was set to +5.75kV.

For Video S1 air pressure feeding the nozzle was set to 1.2 bar and the distance between nozzle and collector was set to 3.5mm with a standard deviation 0.1mm. Collector’s speeds tested in Video S1 were 191.25 mm s-1, 212.5 mm s-1, 255 mm s-1, 340 mm s-1, 510 mm s-1, 850 mm s-1, 1530 mm s-1 and 2890 mm s-1.

For Video S2 air pressure feeding the nozzle was set to 2.4 bar and the distance between nozzle and collector was set to 4.5mm with a standard deviation 0.1mm. Collector's speeds tested in Video S2 were 292.5 mm s-1, 520 mm s-1, 1300 mm s-1 and 4420 mm s-1.

First, videos were split based on the collector speed setting. Second, video frames were cropped to remove redundant pixels that would result to increased processing time. For real time video processing the user would need to specify the region of interest in the frame, so that we can crop it and dispose of needless information, as well as the position of the nozzle, the collector, and a factor, which represents the length of the Taylor cone depended on the nozzle's diameter.

## 5.2 Machine Vision Module

**Jet Metrology.** For the implementation of the Jet Metrology algorithm Python 3.8 was used, along with the python bindings of the OpenCV library, which enables as to read and process video data. The Jet Metrology algorithm consists of two sub-algorithms. The first is the Object Segmentation and Detection algorithm. The second is the Features Extraction algorithm.

The first sub-algorithm segments the needle tip, the Taylor cone, the jet and the deposited fiber on the collector. In addition to that, the algorithm attempts to find the jet's deposition point on the collector. Finally, the segmented objects of interest are plotted for the user to visually inspect the output and assess the performance of the algorithm. To detect the objects of interest in each video frame we use the very much alike meanshift [6] and camshift algorithms [REFERENCES].

The meanshift algorithm is based on a statistical concept directly related to clustering techniques. Similar to other clustering algorithms, the meanshift algorithm scans the whole frame for high concentration of pixels of the same color. The main difference between the meanshift and the camshift algorithms is that the camshift algorithm has the capability to adjust, so that the tracking box can change its size and direction, to better correlate to the movements of the tracked object. The meanshift and camshift algorithm are useful tools to employ for object tracking. Also, unlike neural networks and other machine learning methods of object detection, these algorithms can be immediately implemented and deployed without the need to train a model with numerous labeled images. Instead, the algorithm takes as an input the initial color of the object, that needs to be detected, and then it tracks it throughout the rest of the video. On the other hand, using color as a primary method of identification, neither of the two algorithms can identify objects based on specific shapes and features, which makes them significantly less powerful than other methods. Furthermore, objects varying in color on a large scale and complex or noisy backgrounds can make object detection and tracking problematic. As a result, the meanshift and camshift algorithms work best under controlled environments.

The first step is to reverse the image so that the objects of interest are white and the background black. The next step is to apply a multi color mask to segment them, and then to change the image color-space from BGR to HSV. Finally, the meanshift algorithm is applied to detect the needle and the Taylor cone, since there is barely any significant movement to them, and the camshift algorithm to detect and track the jet.

To find the deposition point, the algorithm needs to know the collector's position. Then, it creates a window around the collector, crops the region of interest from the frame and processes that instead of the whole frame. The built-in function used to find the deposition point is the *cv2.goodFeaturesToTrack*. This function finds the most prominent corner in our region of interest by calculating eigen-values, as described in [9].

Finally, by subtracting the deposition point from the nozzle's position (center of blue rectangle in Figure 2c), we get the lag distance, which is depicted with a two-ways orange arrow in **Figure 3**.

The second sub-algorithm is the one responsible for extracting all the jet features that are relevant to the process dynamics. These features are the diameter, areas, and angles of the jet as we move along the z-axis. Another important feature is the velocity of each jet's point along the x-axis relatively to the nozzle's position. To get all those features we follow a pretty much straightforward procedure. The algorithm takes three inputs, the first is the current video frame. The second input is the calibration factor (), which is a correlation between distance units (mm) and pixels. The last one is the stride. The stride indicates every how many pixels along the z-axis we perform computations. Using a too small stride would lead to more precise calculations but would tremendously rise the computation time. On the other hand, using a too large stride would lead to shorter computation times but there is danger to lose important information.

The first step is to change frame's color-space from RGB to grayscale, so that the Canny edge detection algorithm can be applied. The parameters of the Canny edge detector are [threshold\_1, threshold\_2] and were specified in a semiautomatic way, using trackbars while performing edge detection to other video samples. After this procedure they were set to 150 and 255 respectively. After performing Canny edge detection, we read the first row of pixels in our canny-frame, which now is an array of 0 and 255. If Canny algorithm has been performed correctly when we read this row of pixels from left to right, the first time we encounter a 255 should be the left edge () of our jet. Likewise, the first time we encounter a 255, while reading the row of pixels from right to the left, should be the right edge () of our jet. By subtracting those two pixels' indexes and multiplying with the calibration factor we get the diameter of the jet at this position in the z-axis, which is equal to .

|  |  |
| --- | --- |
|  | (1) |
|  | (2) |

Those indexes are also stored in two variables () so that they can be used to calculate the jet angles as we move down the z-axis.

Then we repeat the procedure for every 'stride' rows. After finding the left () and right () edges and calculating the diameter, the area and angles can be calculated as:

|  |  |
| --- | --- |
|  | (3) |
|  | (4) |
|  | (5) |

The are then updated with the values.

After accessing all frame's rows, the algorithm returns arrays containing all the quantified Diameters, Areas, Right Boundaries, Angles left and Angles right. The same procedure is applied to all frames. Right Boundaries are important because by subtracting the right edges of two consecutive frames we can calculate the jet's velocity on the x-axis.

## 5.3 Multiphysics Model

The importance of accurately extracting jet properties is signified by the numerous studies on predicting the jet stable region diameter, through mathematical modeling. Among those is the model proposed by Zhmayev et al. [11], which is developed by fully coupling the conservation of mass, momentum, charge and energy equations with a constitutive model and the electric field equations at the steady state. Same as most models, this one also utilizes the thin filament approximation to obtain a simpler and more tractable solution. This assumption is possible by appropriately averaging the model variables across the radial direction. In addition, the charge and electric field equations are simplified, under the assumption of low electrical conductivity, as compared to the governing equations for isothermal simulations presented by Carroll and Joo [12].

Also, the conservation of energy relation and a non-isothermal constitutive model were added to extend to non-isothermal situations. The resulting governing equations after being nondimensionalized are:

|  |  |  |
| --- | --- | --- |
| Continuity: |  | (6) |
| Momentum: |  | (7) |
| Charge: |  | (8) |
| Electric field: |  | (9) |
| Energy: |  | (10) |
| Constitutive: |  | (11) |

The system of equations can be reduced to a set of five coupled first order ordinary differential equations (ODEs). Boundary Conditions are required, in order to proceed to numerical analysis.

|  |  |
| --- | --- |
|  | (12) |
|  | (13) |
|  | (14) |
|  | (15) |
|  | (16) |

|  |  |
| --- | --- |
| Property | Value |
| Zero-shear-rate (at ) () |  |
| Relaxation time (at ) () |  |
| Activation energy of flow () |  |
| Density () |  |
| Heat capacity () |  |
| Thermal conductivity () |  |
| Electrical conductivity () |  |
| Surface tension () |  |
| Ratio of solvent to zero-shear-rate viscosity () |  |
| Mobility factor () |  |
| Dielectric constant ratio () |  |

|  |  |
| --- | --- |
| Parameter | Value |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |

The model was implemented in Python. While true properties and parameters of the material are not provided the ones used in [13] for PCL were used. As referred in [12], [13] the model slightly underpredicts the jet radius while in the Taylor cone area, but when the jet is stabilized, it accurately predicts it's radius. Knowing this, even if the volumetric flowrate () is not provided with the dataset, a Particle Swarm Optimization (PSO) algorithm was also implemented to find the for which the predicted jet's radius better fits the computer vision observations.

## 5.4 Geometrical Model

Lag distance is a highly important parameter regarding the quality of the process outcome. Specifically, for some collector speeds, the jet falls onto the moving collector in a way reminiscent of a sewing machine, generating a rich variety of periodic patterns, such as meanders, W patterns, alternating loops and translated coiling. P. T. Brun et al. [14] proposed a quasistatic geometrical model, consisting of three coupled ordinary differential equations for the radial deflection, the orientation and the curvature of the path of the jet's contact point with the collector, capable of reconstructing the patterns observed experimentally while successfully calculated the bifurcation threshold of different patterns. It was also discovered that the jet/collector velocity ratio () was the key factor for pattern variation.

According to this geometrical model, the deposited trace on the collector is a combination of the obit of the contact point (when collector's speed is equal to zero the jet creates coiling patters with radius and the movement of the collector.

|  |  |
| --- | --- |
|  | (17) |

where is the deposited trace, is the arc-length, is time, is the contact point at time , is the direction of the collector's speed, is the time that the contact point moves together with the collector. Differentiating and moving from Cartesian to Polar coordinates ( denote the poler coordinates of the contact point ), and considering the curvature at the bottom of the jet, we get the system of ODEs:

|  |  |
| --- | --- |
|  | (18) |
|  | (19) |
|  | (20) |

This geometrical model was implemented in Python and varying the dimensionless parameter from 0 to 1 as suggested, the orbit and the deposited trace can be reconstructed. Verifying the results from [14], the critical velocity at which the straight pattern appears is , which means . for speed ratios the process is highly unstable, forming the translated coiling, alternating loops, W patterns and meanders when the speed ratios are 0.25, 0.5, 0.65, 0.85, respectively.

## 5.5 Gaussian Process Regression

Gaussian Process Regression is a nonparametric stochastic process with strong probabilistic fundaments [17][24]. GPR is a supervised machine learning technique, which predicts a probability distribution based on Bayesian theory unlike other machine learning algorithms that give deterministic predictions. The idea behind GPR is that the posterior probability can be modified based on a prior probability, given a new observation. Those characteristics give reliability to the prediction from a probabilistic point of view, while providing more wholesome information regarding the prediction. Assuming there is a dataset available, consisting of input-output pairs of observations that are generated by an unknown model

|  |  |
| --- | --- |
|  | (21) |

can be completely determined by a mean and a covariance function

|  |  |
| --- | --- |
|  | (22) |
|  | (23) |

GPR aims to learn the mapping between the set of input variables and the unknown model given the set of observations . To map this correlation is typically assigned a GP prior.

Gaussian Processes (GPs) are powerful modelling frameworks incorporating a variety of kernels. A Gaussian Process is a collection of random variables, any finite number of which have a joint Gaussian distribution [17].

|  |  |
| --- | --- |
|  | (24) |

, where is a kernel function with a set of trainable hyperparameters . The kernel defines a symmetric-positive covariance matrix , which reflects the prior available knowledge on the function to be approximated. Furthermore, kernel's eigenvalues define a reproducing kernel Hilbert space, that determines the class of functions within approximation capacity of the predictive GP posterior mean [17].

Hyper-parameters are trained by maximizing the marginal log-likelihood of the model [17].

|  |  |
| --- | --- |
|  | (25) |

Assuming a Gaussian likelihood and using the Sherman-Morrison-Woodbury formula [17] the expression for the posterior distribution is tractable and can be used to perform prediction given a new output for a new input .

|  |  |
| --- | --- |
|  | (26) |
|  | (27) |
|  | (28) |

, where . As referenced before prediction consists of a mean, computed using the posterior mean , and an uncertainty term, computed using the posterior variance .

## 5.6 Multi-fidelity Gaussian Process Regression

The GPR framework, presented above, can be extended to construct probabilistic models able to take into account numerous information sources of different fidelity levels [24]. Supposing that s levels of information source are available, the input, output data pairs can be organized by increasing fidelity as . So, denotes the output of the most accurate and expensive to evaluate model, while denotes the output of the cheapest and least accurate model to evaluate. Assuming that only two models are available, a high-fidelity model and a low fidelity model. Then, the high-fidelity model can be defined as a scaled sum of the low fidelity model plus an error term:

|  |  |
| --- | --- |
|  | (29) |

, where is a scaling constant quantifying the correlation between the two models and denotes another GP which models the bias term for the high-fidelity data.

A numerically efficient recursive inference scheme can then be constructed, by replacing the GP prior with the GP posterior  of the previous inference level, while assuming that the corresponding experimental design sets have a nested structure. This implies that the training inputs of higher fidelity model needs to be a subset of the training inputs of the low fidelity model. This scheme is matching totally the Gaussian posterior distribution predicted by the fully coupled scheme [24], only now the inference problem is essential decoupled into two GPR problems, yielding the Multifidelity posterior distribution with a predictive mean and variance at each level [29].

|  |  |
| --- | --- |
|  | (30) |
|  | (31) |
|  | (32) |
|  | (33) |

, where denote the number of training points from the high and low fidelity models, respectively.

## 5.7 Active Learning

Let's assume again that observations are available where and the next point to be evaluated needs to be considered. The question that arises is if there is a more informed way to pick those points when evaluation is expensive to perform, rather than randomly picking those.

This is achieved through an acquisition function . The role of the acquisition function is to guide the search for the optimum. They are defined in a way such that high acquisition values to correspond to potentially high (if maximization is the optimization goal) or low values (if minimization is the optimization goal) of the unknown model , great uncertainty or even combination of those. Maximizing the acquisition function is used to select the next point to evaluate the function at. So, goal is to sample at .

Every acquisition function depends from or a combination of the both. The scale at which it depends on each one of those defines its exploration, exploitation tradeoff. When exploring, points where the GP variance is large should be chosen. When exploiting, points where the GP mean is closest to optimization goal should be chosen. Many acquisition functions are available, some of them are:

|  |  |  |
| --- | --- | --- |
| Variance |  | Purely exploration, makes sure, that we learn the function  everywhere on x to a similar level of absolute error. |
| Probability of Improvement | is the normal cumulative distribution function | Selects the point most likely to offer an improvement of at least but is extremely sensitive to the choice of the target. |
| Expected Improvement | where  is the normal probability distribution function | Similar to PI but takes into account the magnitude  of the improvement a point can potentially yield as well |
| Lower Confidence Bound |  | Selects points  for evaluation based on the lower uncertainty bound |

After sampling and evaluating , GP regression is performed to fit to the new point as well. Then the process repeats itself until termination criteria are met, such as a maximum number of iterations, a minimum or maximum value is reached, or uncertainty is below an allowed value.

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