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Modular microfluidic design automation using machine learning

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Modular Microfluidic Design Automation Using Machine Learning

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1 INTRODUCTION

Microfluidics is the science of handling liquids inside sub-millimeter microchannels at nano-liter and pico-liter scales. This volume reduction enables increased resolution, sensitivity, and throughput, while, reducing the reagent cost significantly [1, 11]. These advantages make microfluidic devices to be ideal substitutes for bench-top and robotic liquid handling in numerous life science applications, specifically, synthetic biology where there is a need for low-cost, automated, and high-throughput platforms [3]. Despite the need, implementing microfluidic platforms in the life science research work-flow is an exception rather than being the norm [8, 10]. This can be attributed to the high cost of fabricating microfluidic devices and a lack of microfluidic design automation tools that can design a microfluidic geometry based on the desired performance [6]. As a result, designing a microfluidic device that delivers an expected performance is an iterative, time-consuming, and costly process [2]. To address this, we previously described a low-cost and accessible micro-milling technique to fabricate microfluidic devices in less than an hour while costing less than $10 [7]. However, still designing a microfluidic device that performs as expected is an iterative and in-efficient process. Therefore, microfluidic design automation tools that are able to design a microfluidic geometry and provide the necessary flow conditions and fluid properties that would deliver a user-specified performance is with great importance. We propose a modular design automation tool, called DAFD, that is able to design a microfluidic device based on user-specified performance and constraints. DAFD uses machine learning to generate accurate predictive models, and then exploits these models to provide a design automation platform. DAFD can be implemented in many microfluidic applications such as droplet generation [4], high-throughput sorting, and micro-mixing.

2 A MODULAR DESIGN AUTOMATION TOOL

DAFD can be divided into two sections. First a forward predictive model that is built by choosing the most accurate algorithm from the built-in machine learning algorithms. Once an accurate model is identified by the user, this model is able to predict the performance of the systems if the inputs are given. Second, the reverse model (i.e., design automation tool) that allows the user to specify the desired performance and get the required inputs in return, as shown in Fig. 1.

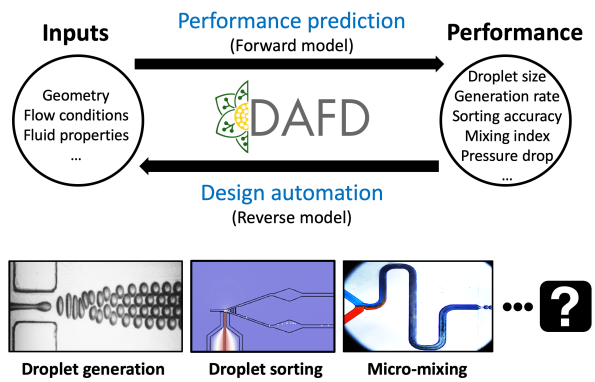

Figure 1: DAFD, relies on a forward predictive model that relates the inputs of the system to its performance. Using this predictive model the design automation tool can then provide the required inputs to achieve a user-specified desired performance. This open-source tool allows researchers to train design automation tools on different microfluidic components such as droplet generators and droplet sorters.

Performance prediction

Machine learning techniques enable system behavior prediction and have advanced several fields from biology to cyber-physical systems [9]. With the introduction of low-cost microfluidic fabrication in recent years, large design spaces previously only explored using numerical simulations [12], can now be studied experimentally in a time- and cost-efficient manner [5]. Therefore, machine learning algorithms can now be trained on large and reliable experimental data-sets to generate accurate predictive models for different microfluidic modules. Several built-in machine learning algorithms are included in DAFD and the user can pick the most accurate model for the experimental data of any given microfluidic, as shown in Fig. 2.

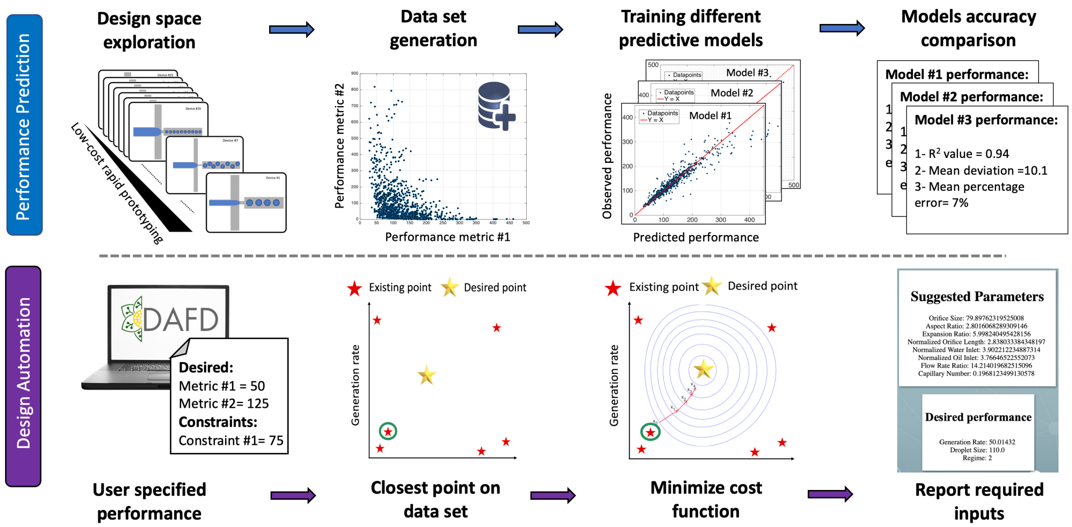

Figure 2: Large experimental datasets can now be generated using low-cost micromilling. Once a dataset is generated, several built-in machine learning algorithms (neural networks, random forest, support vector regression, nearest data-point, etc.) can be trained on the dataset to develop an accurate predictive model. The reverse model exploits the predictive model, dataset, and gradient descent to provide the required inputs for the desired performance. Thus, eliminating the need for design iterations.

Design automation

Once an accurate predictive model is generated, DAFD workflow allows the user to specify the desired performance and constraints. As shown in Fig. 2, the algorithm starts with finding a point on the data-set that is closest to the specified performance. Then, by defining a cost function Eq. (1) and using gradient descent the cost function is minimized until the desired performance is reached and the inputs that resulted in that performance are reported.

$$F(x) = \sum_{i=1}^{n} (P_{i,d} - P_{i,x})^2 \tag{1}$$

where $F(x)$ is the cost function, $P_{i,d}$ is the i_{th} desired performance metric, and $P_{i,X}$ is the i_{th} current performance.

3 CONCLUSION AND FUTURE WORK

DAFD is a modular design automation tool for microfluidics that enables researchers to design microfluidic devices by specifying the desired performance. Thus, lowering the barrier to entry to microfluidics for life science groups with limited knowledge of microfluidics. DAFD allows for experimental researchers with limited knowledge of machine learning to build design automation tools by training DAFD forward models on an input-performance data-set of any microfluidic component through an open-source codebase.

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