Generative Design of Microfluidic Channel Geometry Using Evolutionary Approach

Nikolay O. Nikitin
ITMO University
Saint Petersburg, Russia
nnikitin@itmo.ru

Alexander Hvatov
ITMO University
Saint Petersburg, Russia
alex_hvatov@itmo.ru

Iana S. Polonskaia
ITMO University
Saint Petersburg, Russia
ispolonskaia@itmo.ru

Anna V. Kalyuzhnaya
ITMO University
Saint Petersburg, Russia

Georgii V. Grigorev
Tsinghua University, (TBSI)
Shenzhen, China

Xiaohao Wang
Tsinghua University, (SIGS)
Shenzhen, China

Xiang Qian
Tsinghua University, (SIGS)
Shenzhen, China

ABSTRACT

In this paper, we propose the evolutionary approach for the generative design of microfluidic channel geometry. Sets of candidate solutions for geometry of single cell analysis devices can be used to simplify the decision-making process for micro-devices design. The algorithmic core is based on continuous optimization of coordinates of a polygons set. The proposed approach is validated experimentally with the fabricated microfluidic device. The experiments confirm the correctness and effectiveness of the proposed methods.

CCS CONCEPTS

• **Theory of computation → Evolutionary algorithms**; • **Applied computing → Physics**.

KEYWORDS

evolutionary algorithm, generative design, microfluidics, single cell analysis

ACM Reference Format:
Nikolay O. Nikitin, Alexander Hvatov, Iana S. Polonskaia, Anna V. Kalyuzhnaya, Georgii V. Grigorev, Xiaohao Wang, and Xiang Qian. 2021. Generative Design of Microfluidic Channel Geometry Using Evolutionary Approach. In *2021 Genetic and Evolutionary Computation Conference Companion (GECCO '21 Companion), July 10–14, 2021, Lille, France.* ACM, New York, NY, USA, 2 pages. https://doi.org/10.1145/3449726.3462740

1 INTRODUCTION

In the paper, we present the solution for the automated design of microfluidic geometry with fluid-structure interactions based on evolutionary algorithms. Although the problem of wet optimization seems to be well established and its solutions focus mainly on methods of topology optimization [6], there are a few limitations for the approach. The major limitation is due to local solutions of gradient-based algorithms in the topology optimization approach which can not provide a range of possible solutions with close goodness of fit values. This becomes critical for problems with hidden, unformulated requirements.

In this case, the local solution of the gradient-based algorithm is not sufficient. Instead, we can provide a number of high-quality solutions that can be used by the particular field experts to choose the best solution taking into account all the requirements which were not integrated into the optimization algorithm. This situation is typical for engineering tasks that contain high-precision manufacturing. One of the promising applications of generative approaches is the design of microfluidic channel geometry like blood cell traps for single cell analysis [3]. At the stage of manufacturing, micro-engineers usually have to correct the geometry of a device to make its fabrication possible. In case micro-engineers have the opportunity to choose the optimal geometry without its manual correction, they save much time and resources. For the creation of diverse solutions for microfluidic structures, we propose an evolutionary approach. Evolutionary algorithms are widely used for the related tasks as a single solution or as a hybrid method [1]. As an example of fluid-related evolutionary algorithms application for the generative design, the optimization of breakwaters structure [5] can be used. However, the microfluidic design has its own task-related specificity that should be taken into account in the algorithm.

GECCO '21 Companion, July 10–14, 2021, Lille, France

ACM ISBN 978-1-4503-8351-6/21/07.
https://doi.org/10.1145/3449726.3462740

2 EVOLUTIONARY GENERATIVE APPROACH

The generative approach for the design of microfluidic topology is implemented using a genetic algorithm. The channel geometry of the proposed approach is described in Fig. 1.

To modify the polygons included in the channel geometry, the custom mutation and crossover operators were implemented. Also, a set of constraints was added: self-intersection constraint, inter-polygon distance constraint, as well as restrictions for velocity in the simulated flow field (see Fig. 1). The tournament selection is used to improve the quality of constraint-handling.

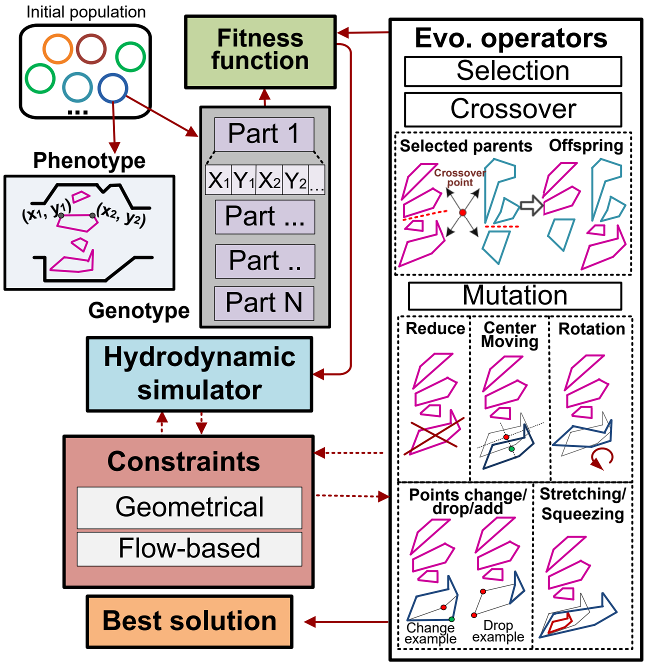

Figure 1: The scheme of evolutionary approach for the design of microfluidic geometry and an example of problem-specific evolutionary operators.

The numerical simulation of the liquid flow around the channel obstacles is a computationally expensive task. For this reason, the implementation of the evolutionary operators was parallelized. Each attempt to generate a new channel geometry or modify the existing one, as well as validation of the structural constraints is performed in a separate process. Then the pool of processes is starting. After the computations end, the simulation-based constraints are evaluated for each individual. However, the parallelization of the fluid flow simulation is the responsibility of the simulation tool.

3 EXPERIMENTAL ANALYSIS

As a case study, we use the design problem of micro hydrodynamic traps with a unique feature to trap red blood cells in the flow channels by keeping it suspended to allow fluidic flows [4]. The existing design methods in this field are based mostly on expert-developed heuristics [2].

The fitness function is evaluated as a ratio of speed inside the cell trap and outside it. The flow velocity field is simulated using COMSOL Multiphysics 5.6 with Python API. Different optimization approaches are applied: random search as a baseline and the proposed evolutionary approach. The size of the population is 100 individuals, and the probabilities of crossover and mutation are 0.6 and 0.4. The results of the experimental studies are compared in Fig. 2. Evolutionary optimization allows obtaining better solutions than a random search. It confirms the conceptual correctness of the implemented prototype.

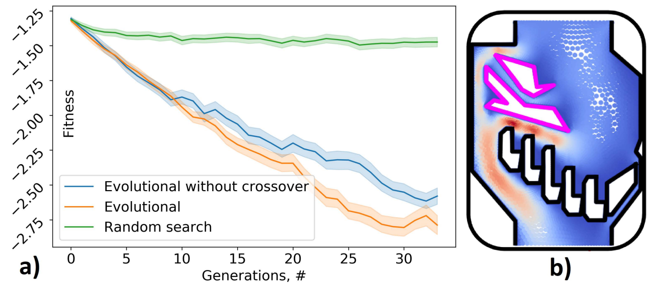

Figure 2: a) The convergence of the fitness function for the baseline (random search) and implemented evolutionary approach (with and without crossover). The population size is 300 individuals. The intervals represent the variability of the solutions in the populations; b) The simulation results for the best-found solution configuration. The pink polygons are the dynamic part of the solution.

4 CONCLUSIONS AND FUTURE DEVELOPMENTS

In the paper, we propose the approach for generative design based on continuous evolution optimization. Despite this approach is already applied for the practical tasks of the design of the microfluidic geometries, further improvement of this approach is possible and desirable.

The promising direction to improve it is the iterative involvement of the generative neural networks (GAN) to the generation of the initial assumptions with higher quality. Also, the convolutional neural networks (CNN) can be applied to conduct the sensitivity analysis of the candidate configurations in order to determine the most promising location for the polygons. Finally, the use of the gradient-based methods for the fine-tuning of the best solutions allows combining the advantages of topology optimization and evolutionary generative design.

5 ACKNOWLEDGMENTS

This research is partially supported by The Russian Scientific Foundation, Agreement #19-11-00326. We are grateful to Tsinghua University (TBSI/SIGS) for provided experimental data.

REFERENCES

[1] Ms Trupti Bhoskar, Mr Omkar K Kulkarni, Mr Ninad K Kulkarni, Ms Sujata L Patekar, GM Kakandikar, and VM Nandedkar. 2015. Genetic algorithm and its applications to mechanical engineering: A review. *Materials Today: Proceedings* 2, 4-5 (2015), 2624–2630.

[2] Allan Guan, Aditi Shenoy, Richard Smith, and Zhenyu Li. 2015. Streamline based design guideline for deterministic microfluidic hydrodynamic single cell traps. *Biomicrofluidics* 9, 2 (2015), 024103.

[3] Da-Han Kuan, Chia-Chien Wu, Wei-Yu Su, and Nien-Tsu Huang. 2018. A microfluidic device for simultaneous extraction of plasma, red blood cells, and on-chip white blood cell trapping. *Scientific reports* 8, 1 (2018), 1–9.

[4] Vigneswaran Narayanamurthy, Sairam Nagarajan, Fahmi Samsuri, TM Sridhar, et al. 2017. Microfluidic hydrodynamic trapping for single cell analysis: mechanisms, methods and applications. *Analytical Methods* 9, 25 (2017), 3751–3772.

[5] Nikolay O Nikitin, Iana S Polonskaia, Anna V Kalyuzhnaya, and Alexander V Boukhanovsky. 2020. The multi-objective optimisation of breakwaters using evolutionary approach. *arXiv preprint arXiv:2004.03010* (2020).

[6] Ole Sigmund and Kurt Maute. 2013. Topology optimization approaches. *Structural and Multidisciplinary Optimization* 48, 6 (2013), 1031–1055.