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Optimal microchannel design using genetic algorithms †

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Abstract

This paper presents a novel method of optimizing particle-suspended microfluidic channels using genetic algorithms (GAs). The GAs can be used to generate an optimal microchannel design by varying its geometrical parameters. A heuristic simulation can be useful for simulating the emergent behaviors of particles resulting from their interaction with a virtual microchannel environment. At the same time, fitness evaluation enables us to direct evolutions towards an optimized microchannel design. Specifically, this technique can be used to demonstrate its feasibility by optimizing one commercialized product for clinical applications such as the microchannel-type imaging flow cytometry of human erythrocytes. The resulting channel design can also be fabricated and then compared to its counterpart. This result implies that this approach can be potentially beneficial for developing a complex microchannel design in a controlled manner.

Keywords: Genetic algorithm; Design optimization; Microchannel; Microchip flow cytometer

1. Introduction

Partly due to the short history of the lab-on-a-chip industry, design problems have been solved by a trial-and-error method dictated by design specifications as well as guided by the experience and intuition of the designer [1]. However, researchers are continually developing analysis and optimization tools to assist engineers in the laborious design process and to foster creativity in arriving at "the optimal" design. Recently, innovations in the field of optimization tools have emerged with the advent of high-speed computer processors. Optimization techniques offer huge potential for providing automated solutions for complex problems. Upon review of the optimization techniques available in the literature, the genetic algorithm (GA) was selected to stochastically guide the algorithm through the solution space of available designs and to arrive at an evolved one [2-6]. In the literature, the GA is a form of artificial evolution and is a commonly used method for optimization [7-11]. A Darwinian "survival of the fittest" approach has been employed to search for optima in large multidimensional spaces [13, 14]. The GAs enable the creation of virtual entities without requiring an understanding of the procedures or parameters used to generate them. The measure of success and fitness of each individual can then be calculated automatically.

It is convenient to use the biological terms, 'genotype' and 'phenotype' when discussing artificial evolution. A genotype is a coded representation of a possible individual or problem solution. In our simulation, the genotype is a series of design variables for the microchannel geometry. In biological systems, this is usually composed of DNA and also contains instructions on how an organism is developed. The GAs

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typically use populations of genotypes consisting of strings of binary digits or parameters. Those populations are usually read-out for producing phenotypes which are then evaluated according to some fitness criteria before being selectively reproduced. New genotypes can be generated by copying, mutating, and combining the genotypes of the fittest individuals. Thus, this cycle can be repeated while the population ascends to the highest levels of fitness.

In this paper, we present a robust design methodology for optimizing microchannel geometry using the GA, especially for a particle-suspended microfluidic channel. In addition, we introduce a heuristic particle dynamics simulation that can be useful for the fitness evaluation of the GA. Generally, it is too complex to predict fluid dynamics (including solid walls, a liquid flow, and buoyant solid particles inside it). Therefore, we developed a heuristic dynamics simulation based on the object-oriented programming (OOP) paradigm, through which we can perform a simulation based on several simple rules. In addition, this approach can be useful for simulating emergent group behaviors resulting from complex interactions of the particles entangled with those rules [15]. In our simulation, the GA can be used to run in parallel on multiple computers connected via TCP/IP protocols using JAVA and SQL database technology.

We specify a key example for this optimization, i.e., the imaging flow cytometry kit (Digital Bio Technology, Inc.) This system can be used for counting human erythrocytes in a drop of a whole blood sample. Briefly, it can be driven through its single narrow microchannel (6 microns in width, 2 microns in depth) and measured under the bright field. The fluorescence morphology of the blood cells can also be measured by real-time image processing. The readers can be directed to our previous achievements for a more detailed understanding of this system (See the references[16, 17]) Given that the device used carries out visual inspection when the cells are inside a microchannel, the cells should be sparsely distributed between them and should not be close together as such an arrangement would result in erroneous data acquisition [18]. In our experiment, the GA can be used for maximizing the distances between these blood cells as they pass through the microchannel by optimizing its channel geometry. As the device measures qualitative characteristics from the blood cells, the throughput of detection is trivial here; thus, the GA can focus on this single objective. The optimized microchannel design can be fabricated and then compared with its counterpart. This work has been greatly inspired by Karl Sims' virtual creatures for generating virtual environments [19] and by Craig Reynolds' boids for simulating heuristic particle dynamics [15].

2. Materials and methods

2.1 Principle of microchannel design and its optimization

Currently, we are working on optimizing complex microchannel networks with multiple fluid inlets and outlets using the GAs [20]. Toward this end, the genetic representation of the goal design includes directed graph of nodes and connections, each including additional geometry constraint settings. In this study, we aim to focus on optimizing a detailed geometry of a single microchannel suspended with microparticles. The phenotype embodiment of the microchannel design is illustrated in Fig. 1, from which we can see the genetic representation of this design as a series of coordinates denoting all the geometry points (Fig. 1). A phenotype of the microchannel can be automatically generated from this information. From there, a virtual microchannel environment was constructed with appropriate boundary conditions. The details are described in the next section

The evolution of microchannel design commences by first creating an initial population of genotypes. Fig. 1 shows the four types of microchannel design

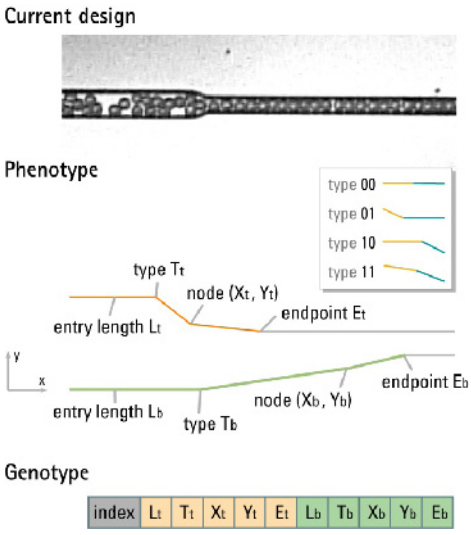

Fig. 1. The genotype and the phenotype of the microchannel design.

used in this study. The creation of the initial population of genotypes comprises of the following two steps:

(1) Random selection of the type of channel; and

(2) Synthesis of a genotype "from scratch" by random generation of dimensions constrained by its type definitions.

The process above must be carried out in order to distribute the probabilities of the creation of all of the types of microchannels. Without step 1, the probability of creating type 11 microchannel is greater than that of the other types of channels. After performing the process mentioned above, the performance of a genotype often referred to as the fitness was evaluated by the heuristic dynamics simulations as discussed in the next section. Giving more probability of selection to high-scored genotypes, they were selected for a subsequent genetic manipulation process. Upon selection of the population of genotypes, we then carried out the genetic manipulation process consisting of two steps. In the first step, the crossover operation recombining the dimensions (genes) of each two selected genotypes (chromosomes) was executed. Various types of crossover operators are found in the literature. For this study, the single point crossover operation was selected for use. The second step in the genetic manipulation process is called mutation in which the dimensions at one or more randomly selected positions of the chromosomes are altered. The mutation process helps overcome the trapping phenomenon at the local maxima. The offspring produced by the genetic manipulation process are the next population to be evaluated, after which the cycle of evolution is repeated until a desired termination criterion is reached. In this work, the criterion was set by the number of evolution cycles (computational runs).

2.2 Heuristic particle dynamics simulation

Heuristic dynamics simulation is used to calculate the movement of particles resulting from their interaction with a virtual microchannel environment. There were several components of the physical simulation that were used in this work: basic heuristic rules for solid body dynamics, numerical integration, collision detection, collision response, and an optional viscous fluid effect based on Poiseulli's fluid flow model for rectangular channel [21-23]. The basic heuristic rules for particles are as follows:

No.1: Particles shall not penetrate each other and shall not pass through walls.

No.2: Without violating the preceding rule, the velocity of a particle is determined by Poiseulli's solution for the fluid velocity filed in a rectangular channel.

No.3: Without violating the above rules, if a preceding particle is slower than a following one, then the following particle shall roll over its preceding one.

Indices for the rules indicate their priorities for the simulations. Poiseulli's solution for the fluid velocity is only briefly summarized here as fluid dynamics simulation is not an important issue in this paper. Nevertheless, we provide a brief background in this section. In a Poiseuille flow, the fluid is driven through a long, straight, and rigid channel by imposing a pressure difference between the two ends of the channel. In our case, the pressure difference was generated by the capillary forces. Originally, Hagen and Poiseuille had studied channels with circular cross-sections because such channels are easy to produce. It is perhaps a surprising fact that no analytical solution is known to the Poiseuille flow problem with a rectangular cross section. We used a Fourier sum representing the solution found in the literature. Boundary conditions for the inlet and outlet flow velocities were approximated by the experiments using existing microchannel products.

Due to the fact that all the particles exist in a single plane constrained by the depth of the microchannel, the simulation was executed in 2D. Fig. 2 shows a snapshot of the dynamics simulation program. As can be seen, the shapes of particles are represented here by simple circles. We have found that circular presentation of the particles reduced the number of collision tests between particles. Pairs whose world-space distances were below their diameters were then tested for penetrations; at the same time,if there were any collisions with a channel boundary, they were also tested. Collision response is accomplished by no. 1 and no. 2 of the heuristic rules mentioned above. Rolling direction for the rule no.2 is determined by comparing y position of the preceding and following particles. Viscous drag effects were ignored since the particles moved passively following the pre-defined velocity fields and there were no velocity discrepancies between solid particles and the liquid flow. This is a simple approximation that does not include dy-

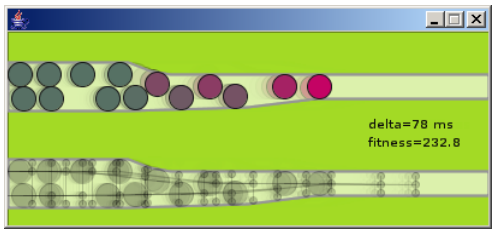

Fig. 2. Visual simulation with processing.

namic pressure variations owing to the existence of particles inside a microchannel, but is still sufficient for simulating heuristically reasonable looking particle dynamics.

The aim of the simulation is not to identify the exact dimensions for the optimized geometry but to produce some guidelines for coming up with enhanced designs by observing their pathways of genetic evolutions. There are possible sources of calculation errors in the numerical integrations, or assumptions such as 2D constraints and rigid body simplifications with no viscous drag effects can result in erroneous conclusions. However, there exists no perfect simulation which replicates natural phenomenon exactly it is, and even if one exists, it would take gigantic calculation loops to simulate such a very simple phenomenon. That is the main reason why we took simple but obvious heuristic rules into account and observed genetic evolutions ruled by this principle. We just need to observe emergent behaviors of particles ruled by heuristic rules and evolution procedures through the genetic algorithms.

The program was coded in the Processing programming language. Processing is an open project initiated by Ben Fry (Broad Institute) and Casey Reas (UCLA Design | Media Arts) [24, 25]. Here, processing was first derived from ideas explored in the Aesthetics and Computation Group at the MIT Media Lab. Processing was chosen because it is a fully object-oriented language and environment based on JAVA technology which can easily implement particles and microchannels as virtual objects. The object-oriented programming (OOP) paradigm is an excellent choice when intuitively simulating real-world phenomenon in a programming language. Moreover, the powerful JAVA networking can help us to easily set up a parallel implementation of the algorithm's massive calculation loops.

2.3 Distributed computing

As previously mentioned, the genetic algorithm

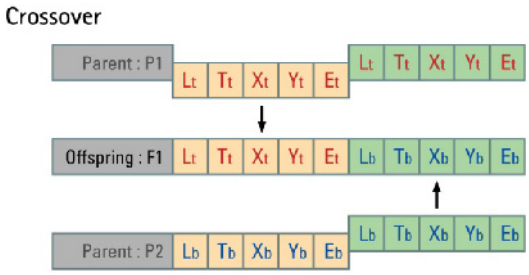

Fig. 3. The single point crossover scheme.

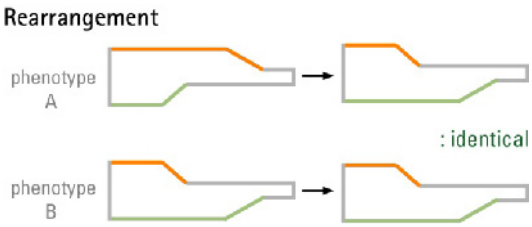

Fig. 4. The scheme for genome rearrangement.

was implemented to run in parallel [26] on multiple computers connected via TCP/IP protocols using JAVA and SQL database technology. A server computer schedules the genetic algorithm process by setting the current population of genotypes in a database and farming them out to the other computers to be fitness tested. Afterwards, it then gathers back the fitness values after they have been determined. The fitness tests are the dominant computational requirement of the system. Performing a fitness test per processor is a simple but effective way to parallel this genetic algorithm, and the overall performance scales quite linearly with the number of processors. Our parallel implementation has several merits in connection with its use of the latest web technologies. First, it was developed as a web applet. This means that anyone who can access the internet through any kinds of web browsers can participate in our project by visiting our web page. Secondly, the program is based on JAVA which means that it can be run on any operating systems including Windows, MAC OS, Solaris, or even on OSs for cellular phones and PDAs.

3. Results and discussion

3.1 Evolution procedures

Considering the minimum geometry resolutions of microfabrication procedures, the design problem was redefined as a simpler version of the 10-mer genotype.

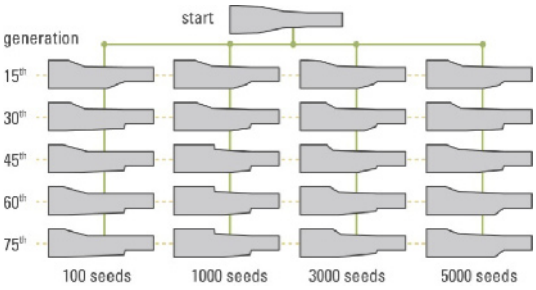

Fig. 5. The evolutionary tree for the microchannel optimization.

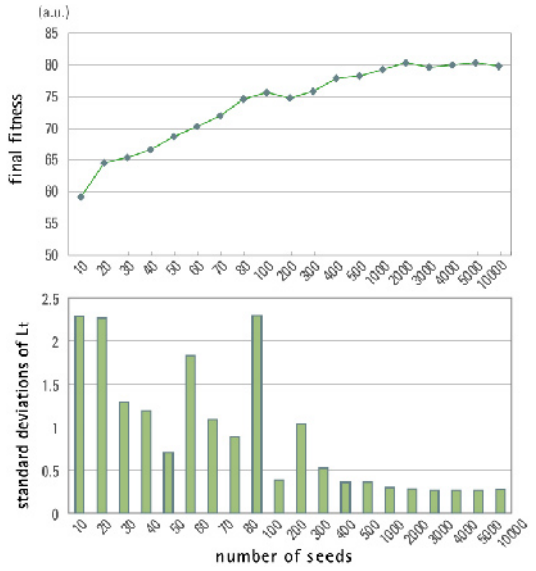

Fig. 6. The average fitness of the individuals of each species (20 species, 5000 populations in each species) and the standard deviation of a design parameter Lt.

The genotype and the phenotype of the microchannel design are illustrated in Fig. 1. Here, the subscript t represents the top side, while the subscript b represents the bottom side of the channel phenotype. Fig. 3 shows the single-point crossover scheme.

During the fitness evaluation, the current genotype under consideration was converted into a regulated form as depicted in Fig. 4. Genotypes were rearranged in a way that the phenotypes had first wedge on the top side and the second wedge on the bottom side. Given that genotypes A and B in Fig. 4 are identical, this procedure is necessary to eliminate the 'saddle point' of the evolution progress.

In order to determine the required number of genomes for the simulation, the evolution was tested with genomes ranging from 10 to 10,000. Each evolution was repeated 10 times in order to examine the deviations between species. The evolutions were performed using five desktop computers for the solvers and a notebook for the scheduler. Evolutions took about three hours when run with 10,000 genomes. Some examples of optimized microchannel morphologies with respect to the number of genomes through the generations are shown in Fig. 5. The average fitness of all species and the standard deviation of a design parameter (Δy of the first segment in this case) between species of each test are plotted in Fig. 6. As depicted in Fig. 6, the fitness and standard deviations are saturated when the number of genomes exceeds 3000. Therefore, to develop reliable design guidelines based on the results of this simulation, we should seed more than 3000 genomes to achieve sufficient fitness while avoiding the evolution results of widely distributed design parameters.

The final evolution was performed using 20 species of 5,000 genomes. The average fitness of the individuals of each species is plotted over 75 generations in Fig. 7. The rate of evolutionary progress was similar for all species. All species took about 30 generations before they reached their plateau, after which the populations of each species converged toward homogeneity. Through the evolution process, the fitness values increased by about 40% compared with their initial values on average. In other words, the distances between particles became about 140% of their initial values in the optimized designs.

The design parameters such as the skewness (difference in the lengths to the ends of wedges) of the nozzle and slopes of the wedge segments were monitored through the evolution processes. Fig. 7 shows the plotted data. By inspecting the evolution procedures, we could extract several important guidelines for the optimized designs. As the evolution converges, microchannel design becomes asymmetric, having the skewness of about twice the diameter of its suspended particles. Eventually all the wedges become type 01 (flat line followed by a slope), and the first wedge of the channel becomes about three times steeper than the second one.

3.2 Fabrication of optimized designs

The erythrocyte deformability test device was fabricated by silicon processing techniques. Using photolithography, the microchannel patterns were etched on a silicon wafer by 2 μm in depth. In the back-side

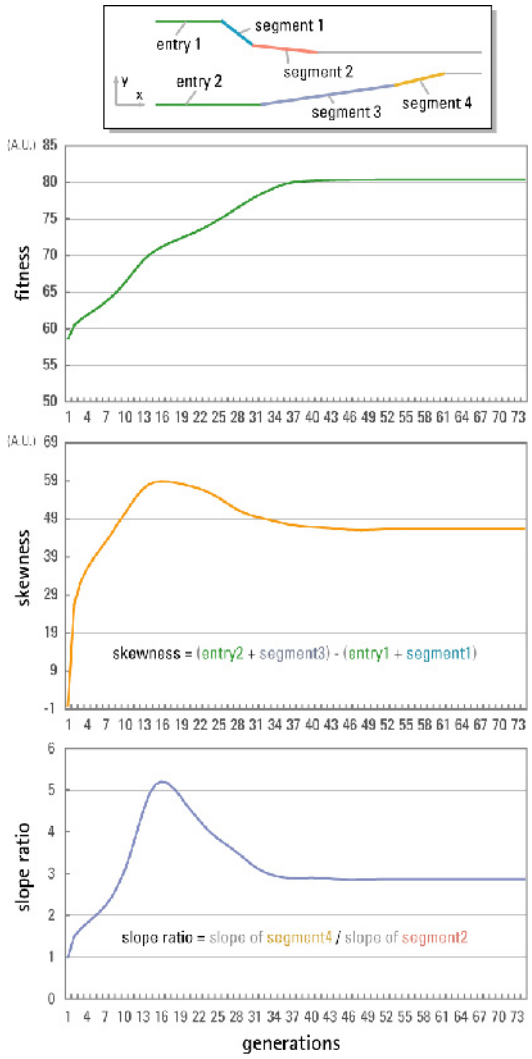

Fig. 7. The fitness and design parameters for the final evolution.

of the patterned wafer, an oxide layer 1 μm in depth was deposited as masking material whose open area holes were etched through the use of an etching solution. Fabricated Si wafer was then bonded with Pyrex glass to make a closed microchannel. The Pyrex glass layer also gave optical clarity to allow direct observation of flowing erythrocytes. Fig. 8 shows the fabricated erythrocyte deformability analysis channel. The microchannels shown in Fig. 8 had the following dimensions: 10 mm long, 5 mm wide and 2 mm deep.

Erythrocytes flowed through both the existing and newly fabricated microchannels. With a single drop of whole blood, the microchannels drove the sample with its capillary forces. The comparison between

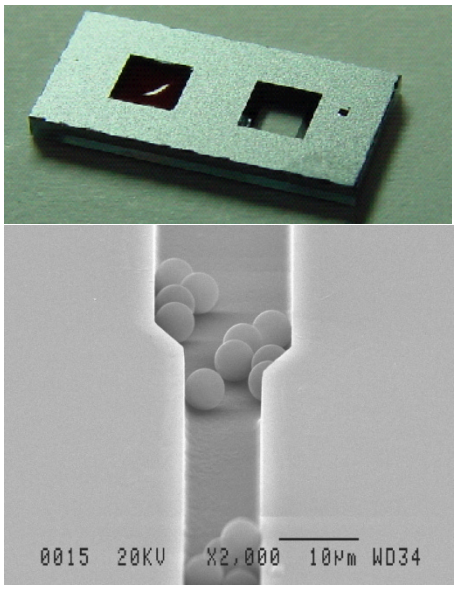

Fig. 8. A fabricated microchip. The left chamber is filled with a drop of blood sample. (thickness: 2.1 um, surface roughness: 30 A).

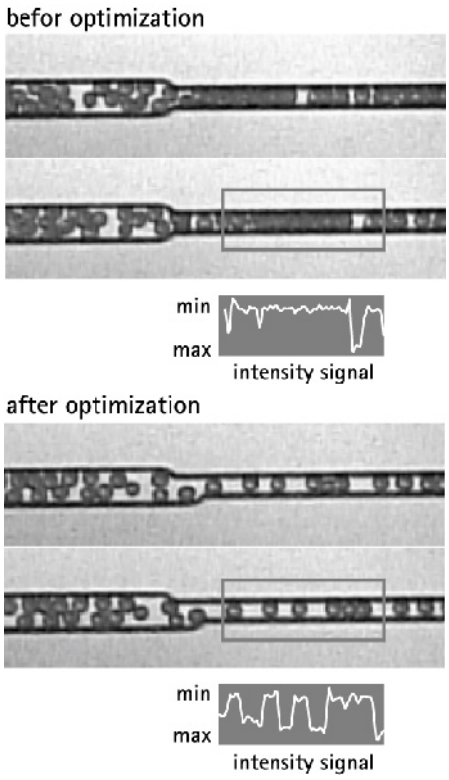

Fig. 9. Erythrocytes passing through the microchannel before and after the optimization with their respective intensity profiles.

these two microchannels clearly proved that the newly fabricated one was enhanced. As in Fig. 9, erythrocytes in the newly fabricated microchannel are more sparsely distributed in the observation channel and do not show any doublets of erythrocytes. In this paper, the design problem was a rather simple one. Nevertheless, we can extend the methodology to more complex design problems. Actually, we are now applying this method to optimize the design of a microchip flow cytometer [27]. Currently, several theories are being considered for calculating the fluidic resistance of the microchannel. The choice of appropriate model is thus important for evaluating the overall fitness of the microchip design. In this paper, we chose a heuristic model for simulating microfluidic phenomena while evaluating the fitness of a microchannel design. This kind of model comes from a top-down way of thinking. Currently, we are developing a new way of simulating microfluidic phenomena by cellular automata (CA) [28]. Cellular automaton, a process with which one can simulate natural phenomena in a bottom-up way, is a discrete model studied in computability theory, mathematics, and theoretical biology.

4. Conclusions

In this paper, we demonstrated that the GA can be potentially beneficial for optimizing the design of a particle suspended microchannel. A heuristic particle dynamics simulation can be useful for the GA-based chip integration as well as a fitness evaluation module. To assess the feasibility of our approach, we also specified a key example for a commercial microchannel product. This effort has led to a significant advance of this channel performance. Moreover, this result implies that our approach can be useful for overcoming several problems that the traditional design methods have encountered. This study may be at the beginning stage of the GAs for microchip channel designs; still, it will be potentially beneficial for designing complex microfluidic networks. By implementing simulations such as microchannel mixing, electro-osmosis and multiphase flows, we expect that this methodology will be applicable to processes involving the handling of various microchannel design problems [29]. We also believe that this approach will enable us to make new breakthroughs, consequently enhancing microchip devices. Furthermore, this can be helpful for overcoming the current challenges of channel design in the industry.

References

[1] D. Figeys and D. Pinto, Lab-on-a-chip: a revolution in biological and medical sciences, *Anal. Chem.* 72 (2000) 330A-335A.

[2] G. Taubes, Computer design meets Darwin, *Science*, 277 (1997) 1931-1932.

[3] T. H. Won, G. H. Hwang et al, Design of FLC for high-angle-of-attack flight using adaptive evolutionary algorithm, *KSME International Journal*, 17 (2) (2003) 187-196.

[4] Y. M. Kong, S. H. Choi et al, Development of integrated evolutionary optimization algorithm and its application to optimum design of ship structures, *Journal of Mechanical Science and Technology*, 22 (2008) 1313-1322.

[5] Y. K. Ahn and Y. C. Kim et al, Optimal design of a squeeze film damper using an enhanced genetic algorithm, *KSME International Journal*, 17 (12) (2003) 1938-1948.

[6] J. Park and S. Song, Optimization of a composite laminated structure by network-based genetic algorithm, *KSME International Journal*, 16 (8) (2002) 1033-1038.

[7] R. J. Hartfield, J. E. Burkhalter et al, Scramjet missile design using genetic algorithms, *Applied Mathematics and Computation*, 174 (2006) 1539-1563.

[8] E. Keedwell and S.-T. Khu, A hybrid genetic algorithm for the design of water distribution networks, *Eng. Applications of Artificial Intelligence*, 18 (2005) 461-472.

[9] D. C. van Leijenhorst, C. B. Lucasius et al, Optical design with the aid of a genetic algorithm, *BioSystems*, 37 (3) (1996) 177-187.

[10] E. Salajegheh and S. Gholizadeh, Optimum design of structures by an improved genetic algorithm and neural networks, *Adv. In Eng. Software*, 36 (2005) 757-767.

[11] V. Kradinov, E. Madenci et al, Application of genetic algorithm for optimum design of bolted composite lap joints, *Composite Structures*, 77 (2) (2007) 148-159.

[12] C. Darwin, *The Origin of Species, New American Library* (1859).

[13] D. E. Goldberg, *Genetic Algorithms in Search, Optimization, and Machine Learning*, *Addison-Wesley,* USA, (1989).

[14] J. H. Holland, *Adaptation in Natural and Artificial Systems*, *University of Michigan Press*, Ann Arbor, USA (1975).
[15] C. W. Reynolds, Flocks, Herds, and Schools: A Distributed Behavioral Model, *Computer Graphics*, 21 (4) (1987) 25-34.
[16] J. Wietzorrek, N. Plesnilal et al, A new multiparameter flow cytometer: optical and electrical cell analysis in combination with video microscopy in flow, *Cytometry*, 35 (1999) 291-301.
[17] F. Kubota, Analysis of red cell and platelet morphology using an imaging-combined flow cytometers, *Clin. Lab. Haem*., 25 (2) (2003) 71-76.
[18] J. Park, S. Chung et al, Asymmetric nozzle structure for particles converging into a highly confined region, *Current Applied Physics*, 6 (2006) 992-995.
[19] K. Sims, Evolving Virtual Creatures, *Computer Graphics (SIGGRAPH'94) Annual Conference Proceedings*, (1994) 43-50.
[20] H. Bang, S. H. Lim et al, Serial dilution microchip for cytotoxicity test, *J. Micromech. Microeng.*, 14 (2004) 1165-1170.
[21] M. E. Staben and R. H. Davis, Particle transport in Poiseuille flow in narrow channels, *Int'l J. Multiphase Flow*, 31 (5) (2005) 529-547.
[22] H. N. Unni and C. Yang, Brownian dynamics simulation and experimental study of colloidal particle deposition in a microchannel flow, *J. Colloid and Interface Science*, 291 (2005) 28-36.
[23] X. Xuan, S. Raghibizadeh et al, Wall effects on electrophoretic motion of spherical polystyrene particles in a rectangular poly (dimethylsiloxane) microchannel, *J. Colloid and Interface Science*, 296 (2) (2006) 743-748.
[24] B. Fry, Ph. D. dissertation, MIT, 2005.
[25] C. Reas, M. S. thesis, MIT, 1996.
[26] O. K. Lim, K. S. Hong et al, Initial Design Domain Reset Method for Genetic Algorithm with Parallel Processing, *KSME International Journal*, 18 (7) (2004) 1121-1130.
[27] J. K. Kim, H. Bang et al, Single-cell manipulation and fluorescence detection in benchtop flow cytometry system with disposable plastic microfluidic chip, *Proceedings of SPIE (The International Society for Optical Engineering),* 4982 (2003) 8-20.
[28] S. Wolfram, Cellular Automata and Complexity: Collected Papers, *Westview Press*, (1994).
[29] H. A. Stone, A. D. Stroock and A. Ajdari, Engineering flows in small devices: Microfluidics towards a lab-on-a-chip, *Annu. Rev. Fluid Mech.*, 36 (2004) 381-411.

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