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Extremal Distribution Sorting Algorithm for a CFD Optimization Problem

K.Yano and Y.Kuriyama
Mie University
Gifu University
Japan

1. Introduction

The numerical simulator for fluid analysis based on computational fluid dynamics (CFD) is focused on analyzing the behavior of a fluid around an object, or its thermal hydraulics. CFD is a technique that considers the Navier-Stokes equation and energy conservation law and uses the mass conservation method. With the development of computing power and the price plummet of personal computers, the CFD simulator has become a useful and realistic tool (Stefano et al., 2005). Furthermore, CFD is now used not only for analyzing of the behavior of a fluid but also for optimization of a fluid's shape or flow for improved quality or performance. That said, the optimization with a CFD simulator for improved quality or performance still has many problems. For example, the solution space formed by the solution of optimization using a CFD simulator has become a multimodal space with a lot of local minimums, as shown in Fig. 1. Furthermore, the optimizations for practical use become more complication because these applications require more variables and constraints.

As a method of searching efficiently for a complex solution space, the meta-heuristic algorithm (Pablo, 2003) is a heuristic technique. As an algorithm with the greatest general

Fig. 1. Solution space of CFD optimization problem

versatility, the genetic algorithm (GA) is generally used (Kokolo et al., 2000). However, in cases such as analyzing a problem that has a lot of local solution, the solution that incorporates the general GA is highly likely to derive local solution, and thus it is difficult to derive the global optimized solution. Of course, this problem can be solved by enlarging the number of population members, the number of generations and the mutation evolution; on the other hand, the computational time for one condition was a few minutes and the optimization requires hundreds of repeated computations. Thus the optimization using the CFD simulator needs a lot of time to finish the task.

The purpose of this study was to design a solution search algorithm using fewer populations and generations to derive the optimized solution more efficiently for an optimization problem by using a CFD simulator. Specifically, focusing on an extremal solution in a multimodal space, we propose the Extremal Distribution Sorting Algorithm (EDSA), which searches intensively at the improving point in the nearly extremal solution. The proposed method makes it possible to derive the global optimized solution quickly with few repeated computation. The effectiveness of the proposed method is shown through experiments in actual die-casting plants for deriving the optimum plunger input.

In this study, the design of the Extremal Distribution Sorting Algorithm (EDSA) is described and applied to actual die-casting plant. In section 2, the algorithm of EDSA is indicated. The EDSA are based on GA, a big feature of EDSA is using the approximate curve to search the extreme value. In section 3, the EDSA is applied the actual optimization problem of die-casting plant, and the GA is also applied to compare the performance. Finally, section 4 concludes with the effectiveness of the proposed algorithm.

2. Extremal distribution sorting algorithm

In this study, to derive the optimum solution in a multimodal space in a CFD optimization problem with low calculation frequency, we propose the Extremal Distribution Sorting Algorithm (EDSA). The EDSA distinguishes an progressive area and analyzes the solution space of a CFD optimization problem and the tendency toward the improvement of the solution by using the approximation curve of the evaluation value and the extreme value. An outline of the EDSA is presented in Fig. 2. The possibility of getting into the local minimum is high only when searching for the optimization solution neighbourhood, and all that simply. Therefore, the EDSA searches for the tendency to the improvement of the solution and aims at an efficient optimized calculation by comprehending the distribution of the solution in the entire solution space. In addition, a loop of an optimization group is treated as a generation, the best solution in a generation is treated as an elite, the following optimization group of the present analytical optimization group is treated as a next generation.

3.1 Deriving the extreme value

Though all individuals inside the generation are handled as the next generation candidates in the GA, an excellent individual is analyzed by priority in the EDSA. Thus the n -dimensional CFD optimization problem is replaced with two-dimensional space by the evaluation value and one variable, and the algorithm searches for the tendency to the solution to each variable by repeating the operation n times. First, each extreme value and the neighborhood of the evaluation value and the approximation curve are obtained. When the evaluation value of the CFD simulator is assumed to be $f(x)$, the extreme value cannot

Fig. 2. Extremal distribution sorting algorithm

$$(f(x_{i+1,k}) - f(x_{i,k})) \times (f(x_{i,k}) - f(x_{i-1,k})) < 0 < (f(x_{i,k}) - f(x_{i-1,k})) \quad (1)$$

$$(f(x_{i+1,k}) - f(x_{i,k})) \times (f(x_{i,k}) - f(x_{i-1,k})) < 0, \quad (f(x_{i,k}) - f(x_{i-1,k})) < 0 \quad (2)$$

be derived by the differentiation because it is discontinuous. Therefore, whether k th variables and the i th individual is an extreme value is judged by using the following Equation 1 and Equation 2.

When Equation 1 is filled at the same time, $x_i ; k$ is the maximum value. When Equation 2 is filled at the same time, $x_i ; k$ is the minimum value. When $x_i ; k$ is judged as an extreme value, x_i is preserved as an extreme value. When thinking about the extreme value neighborhood of $x_i ; k$, the minimum unit e_k of the variable is used. Afterwards, the two points $x_i ; k + e_k$ and $x_i ; k - e_k$ that adjoin $x_i ; k$ are substituted for the extreme value. The extreme value and the neighborhood are calculated in the same way for the approximation curve, and the individual is preserved.

3.2 Deriving the approximate curve

The approximation curve of the evaluation value to comprehend the tendency to the solution is derived. It depends on a complex solution space by using the approximation curve, and it searches for the area where the improvement of the solution is expected. The

approximation curve used to search for the solution is derived by the least-squares method, as follows Equation 3, where N : the number of samples, n : the degree of the CFD optimization problem, m : the degree of the approximation curve, x_i ; k : the k th, i th individual, J_i : the evaluation value of i th individual. The degree of the approximation curve m is changed in proportion to the number of samples N . Condition m is that 5th dimensions are assumed to be the maximum degree in this study.

$$\begin{pmatrix} N & \sum_{i=0}^N x_{i,k} & \sum_{i=0}^N x_{i,k}^2 & \cdots & \sum_{i=0}^N x_{i,k}^m \\ \sum_{i=0}^N x_{i,k} & \sum_{i=0}^N x_{i,k}^2 & \sum_{i=0}^N x_{i,k}^3 & \cdots & \sum_{i=0}^N x_{i,k}^{m+1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sum_{i=0}^N x_{i,k}^m & \sum_{i=0}^N x_{i,k}^{m+1} & \sum_{i=0}^N x_{i,k}^{m+2} & \cdots & \sum_{i=0}^N x_{i,k}^{2m} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{pmatrix} = \begin{pmatrix} \sum_{i=0}^N y_i \\ \sum_{i=0}^N x_{i,k} \cdot J_i \\ \vdots \\ \sum_{i=0}^N x_{i,k}^m \cdot J_i \end{pmatrix} \quad (3)$$

3.3 Election of the next generation individual

After deriving the extreme value of the CFD simulator from the evaluation value and the approximation curve, the next generation's candidates are elected based on those tendencies. Note that the approximation curve is not a curve that passes the extreme value that actually exists. There is a possibility that the extreme value is not more excellent than an actual evaluated value because the approximation curve is composed of the value of the guess. Naturally, the opposite possibility can exist, too. Then, only the individual to which the improvement of the solution is expected and the individual with a higher evaluation value are left as election candidate. And, the parents of the next generation are elected from among these candidates. The parents are elected based on the extreme value of the evaluation value. First, a set of the individual with a bad extreme value and its neighborhood is assumed to be X_b . A set of the penalty X_p is also listed it based on X_b to exclude the next generation's candidates. Moreover, an individual that doesn't fill the restriction is added to X_p . Next, a set of the individual with a good extreme value and its neighborhood is assumed to be X_g . Note that if the extreme value whose evaluation value is larger than the mean value of the maximum value $\bar{f}(x_g)$,

$$f(x_g) > \bar{f}(x_g) \quad (4)$$

only the extreme value that fills Equation 4 is preserved as a set of candidate X_c , which makes an inquiry into X_p . If there is a corresponding individual to X_p in X_c , it is excluded from X_c . The conceptual diagram of the above operation is shown in Fig.3.

In addition, the candidate's exclusion is done based on the following conditions. When you compare the extreme value of the approximation curve with that of the evaluation value, the latter is preserved by priority because it is dependable. A good extreme value of the evaluation value is assumed to be x_g . In addition, only the individual that fills Equation 4 is made a candidate x_c from among x_g . A bad extreme value of the evaluation value is assumed to be x_b , and its neighborhood is assumed to be x_{g+e} , x_{b+e} . A good extreme value of the approximation curve is assumed to be x_{Ag} , and a bad extreme value of the approximation curve is assumed to be x_{Ab} , and the neighborhood is assumed to be x_{Ag+e} , x_{Ab+e} . Candidates are chosen based on the following condition:

Fig. 3. The individual selection

$$x_c > x_b > x_{g+e} > x_{Ag} > x_{b+e} > x_{Ab} > x_{Ag+e} > x_{Ab+e} \tag{5}$$

Candidates are preserved as x_n based on Equation 5. The best solution in a generation is added to the candidate as the elite to continue the improvement of the solution. Finally, these candidates are preserved as the parents of the next generation individual x_n .

3.4 Simplex crossover

The parents individual that generates the next generation individual is elected from X_n . The roulette selection is applied to the election method. The roulette selection is the method of selecting the individual according to the selection rate corresponding to the evaluation value. The probability P_i that a certain individual is selected is expressed in Equation 6.

$$P_i = \frac{f(x_i)}{\sum_{j=1}^{N_g} f(x_j)} \tag{6}$$

In the use of Equation 6 and simplex crossover (SPX), next generation individuals are generated. The conceptual diagram of SPX is shown in Fig.4. SPX is a crossover method for a real-coded genetic algorithm (RCGA)(Shigeyoshi et al. 1999). The RCGA uses the crossover method for treating not the variable as bit strings but the real vectors. Especially, it is an effective crossover method for solving a continuous optimization problem, and it is an effective way to consider the dependence among

Fig. 4. Simplex crossover

variables. Moreover, information on the parents individual can be easily passed on to the child individual (Isao et al. 1997). The RCGA has several kinds of crossover methods. In the proposal algorithm, in spite of the dependence among variables or the scale problem, SPX is employed to deal with any optimization problems. Moreover, the n dimensional CFD optimization problem is replaced with two-dimension space by the evaluation value and one variable. The individual with the extreme value of each variable is distinguished. Therefore, other values of the variables can be operated as crossover while maintaining the value of a variable that became an extreme value.

The procedure of SPX is as follows. When the intended CFD optimization problem is R_n , $n+1$ th parents $P \vec{x}_0, \dots, P \vec{x}_n$ are elected from Xn according to Equation 6. Next, the barycentric position G is derived based on the parents.

$$\bar{G} = \frac{1}{n+1} \sum_{i=1}^k \overrightarrow{Px_i} \quad (7)$$

The range of formation of the next generation is decided based on G , and the next generation individual is generated by using the uniform random number.

$$\vec{p}_0 = \bar{G} + \varepsilon(\overrightarrow{Px_0} - \bar{G}) \quad (8)$$

$$\vec{c}_0 = \vec{0} \quad (9)$$

$$\vec{p}_j = \bar{G} + \varepsilon(\overrightarrow{Px_j} - \bar{G}) \quad (10)$$

$$\vec{c}_j = r_{j-1}(\overrightarrow{P_{j-1}} - \vec{p}_j + \vec{c}_{j-1}), \quad (j = 1, \dots, n) \quad (11)$$

Note that r_{j-1} is calculated from the uniform random number $u(0,1)$ in section $[0,1]$.

$$r_{j-1} = (u(0,1))^{\frac{1}{j+1}} \quad (12)$$

And, the next generation C_x is the following equation.

$$\vec{c_0} = \vec{x_n} + \vec{C_n}$$

(13)

When the relation between the number of individuals in generation N and the degree of the CFD optimization problem k is $N > k$, the selection of the parents and the generation of the next generation individuals are repeated until the number of individuals reaches N . And, if the restriction is not filled or does not conform to penalty lists X_p , the next generation individual is not preserved.

3. Application to Die-casting

3.1 Evaluation of air entrapment

Our fluid analysis software was a 3D fluid calculation program using calculus of finite differences for treating a wide range of flows from an incompressible flow to a flow accompanied by an adjustable surface, flow accounting for compaction, and flow accompanied by solidification. The free surface is calculated by the Volume Of Fluid(VOF). The geometric for a complex obstacle is recognized by Fractional Area Volume Obstacle Representation(FAVOR). Fig.5 shows an overview of the mesh setting, and Table 1 shows the parameters of the mesh setting which was used by past study(Ken'ichi et al. 2008).

Fig. 5. Mesh setting for CFD simulation

	Cell size	Number of cell
X-direction	0.004	20
Y-direction	0.002~0.006	132
Z-direction	0.0022~0.0035	29
Total number of cell		76,560

Table 1. Mesh parameter

As seen in Fig.5, the sleeve is symmetrical to the X axis. Thus, the analyzing area is set as only a one-sided model to reduce the analyzing time to, only about ten minutes. Table 1 shows the minimum settings to do calculations quickly and accurately, and the mesh parameter is set so that the rough mesh is used around the start point of the sleeve because the velocity is low and the fluid is stable in the section. On the other hand, the fine mesh is

used around the end point of the sleeve because the breaks of the wave at an early stage of filling cause dispersion by collision with the sprue core in the section. In this study, the plunger tip was flat, and we used hot working die steels (SKD61) for the die, sleeve, and plunger. Aluminum alloy of ADC12 is assumed as the molten metal. Table 2 shows the fluid properties of ADC12. We set the die temperature during pouring to 110 to 150°C (steady state) and the molten metal temperature in the melting furnace to 660 to 680°C. We used Yushiro AZ7150W as a parting agent.

Density of fluid	2700 kg/m ³
Viscosity of fluid	0.0030 Pa•s
Specific heat	1100J/(kg•K)
Thermal conductivity	100.5 W(m•K)
Initial temperature	653.15 K

Table 2 . Fluid properties of ADC12

Using the fluid analysis software to determine the air entrapment amount in molten metal caused by plunger movement in the sleeve, we calculated the air entrapment amount on the liquid surface assuming that a turbulent eddy surface, i.e., turbulent strength exceeds gravity and we analyzed stabilization of surface tension and the range of liquid elements lifted on the free surface. V_a : air entrapment column fraction, F_f :fluid volume fraction, and V_f :cell volume fraction (ratio of an obstacle area to a fluid area) calculated by fluid analysis software in each mesh cell are multiplied by the column of each mesh cell and summed. Equation 14 calculates air entrapment amount $a(t)$.

$$a(t) = \sum_{k=1}^n V_{ak} F_{fk} V_{fk} V_{ck}$$

(14)

where V_c is the volume of a mesh cell and n the total of mesh cells. In experiments, we could not strictly measure the air entrapment amount caused by actual plunger movement, and it is difficult to evaluate $a(t)$, so we used air entrapment amount $a(t_{fill})$ at the completion of filling the sleeve ($t=t_{fill}$)resulting from analysis with index A representing the ease of air entrapment. We fixed acceleration at 0.05 m and changed low velocity v_l from 0.20 to 0.60 m every 0.01 m/s to analyze air entrapment until sleeve filling. Simulation confirmed the break of an initial wave and scattering due to collision the break of an initial wave and

Fig. 6. Simulation result of $v_l = 0.50$ m/s

scattering due to collision with the sprue core at 0.37 m/s or more (Fig.5). Air surrounded by the sleeve wall, plunger, and molten metal was also confirmed at $t = 0.66$ s. These phenomena are expressed as "air shutting". Even if velocity is decelerated to less than or equal to 0.23 m/s, however, a big wave is generated by reclusion between the return wave and plunger (Fig.6 ($v_l=0.21$ m/s)) and air shutting is also generated by molten metal. This implies that low-velocity projection alone cannot prevent air entrapment and suppress product defects.

Fig. 7. Simulation result of $v_l=0.21$ m/s

3.2 Setting the cost function

The actual casting plants can be control the multistep velocity, and the velocity pattern, which has five phases, is derived from past studies. Thus, in this study the velocity is set by v_1, v_2, v_3 , and the acceleration distance is set by x_1, x_2 . The plunger velocity is expressed as shown in Fig.8, where x_{fill} is filling position which is a constant value. The optimization problem was defined with a cost function equivalent to the sum of the weighted quantity of air entrainment and the weighted filling time, as shown in Equation 15,

minimize : $J = w_a A(v_i(t), x) + w_t t_f(v_i(t), x) + K_p + A_{shut}$ (15)

Fig. 8. Die-casting simulation model

$$\begin{aligned}
 \text{subject to : } & 0.02 \leq v_i \leq 0.60 & (i = 1 \sim 3) \\
 & 0.02 \leq x_i \leq 0.35 & (i = 1 \sim 2) \\
 & 0 \leq t_{\text{fill}} \leq 0.35 \\
 & A_{\text{shut}} \leq 2.0
 \end{aligned} \tag{16}$$

where A is the quantity of air entrainment, t_{fill} is the filling time, x is the acceleration distance, and $w_a = 1.0$ and $w_t = 0.1$ are the weighting factors, where K_p is the penalty. Each time the penalty conditions shown in Equation 16 hold, the penalty $K_p = 108$, which is big enough to avoid the penalty conditions, will be added to satisfy the specifications. And A_{shut} is the volume of trapped air to avoid air surrounded by the sleeve wall, plunger, and molten metal when the plunger injection is switched from low speed to high speed. A_{shut} is defined as shown in Fig.9.

Three parameters are introduced to calculate the quantity of air shutting.

- D_1 : Volume/opening column of fluid in the Y cross section.
- D_2 : Threshold of air entrapment amount.
- D_3 : Calculation time step.

We used fluid analysis of t were each time interval specified by D_3 to output the cell column fraction and the fraction of fluid for calculating the filling per sleeve cross section.

We calculated the space volume at the back where the fraction of fluid is behind $D_1 \times 100\%$ for the cross section and defined the maximum space volume as the amount of air shutting A_{shut} m³. If plunger velocity input is designed to enable the air entrapment amount to be decreased using this simulator, good results will be obtained in actual projection experiments.

Fig. 9. The relationship of the air entrapment to velocity and switching position by using the CFD simulator

3.3 Optimum result of die-casting

The parameters for the EDSA are shown in Table 3, and the parameters for the GA to be compared with the EDSA are shown in Table 4, where the initial population is the same for each algorithm, allowing us to calculate under the same conditions.

Parameter	Numerics
Number of generation	60
Number of population	30
Number of elite preservation	2
Order of fitting curve	5

Table 3. Parameters for EDSA

Parameter	Numerics
Number of generation	60
Number of population	30
Number of elite preservation	1
Crossover fraction	0.80
Mutation fraction	0.01

Table 4. Parameter for GA

The results of calculating using the EDSA and the GA are shown in Fig.10. Fig.11 shows the process of calculating. The result of the optimization shown in Table 5, the GA has good convergence at the early stage. However, the GA is stopped at the early stage, and finally the solution converges by the 31st generation. The reason is that the solution fell into the spot of a local solution. The results show that the GA can't be used to derive the optimum solution without an enormous amount of calculation.

On the other hand, the EDSA took a long time until convergence, but it is continued to calculate at the maximum generation, and compared with the GA, the solution derived by using the EDSA is better than the solution derived by using the GA. Based on these results, we conclude that the proposed method can derive the optimized solution with few repeated computations.

3.4 Verification by experiment

Experiments for an actual die-casting plant were performed with the obtained optimum velocity input derived using the EDSA and the GA. The plunger velocity used in the experiment is shown in Table 6. The result of the blister examination is shown in Fig.12. Fig.12 is the total area of the air bubble that appeared on the test piece surface after the blister examination is shown.

Parameter	EDSA	GA
Cost function	0.3441	0.4622
Air entrainment	0.1682	0.2737
Filling time	1.76 s	1.89 s
Optimum termination	41	19

Table 5. Performance comparison sample

Fig. 10. Optimization result of EDSA and GA

Fig. 11. Optimization process of EDSA

The amount of air entrainment by the CFD simulator is also indicated in Fig.12 for comparison. As seen in the Fig.12, there is a significant difference in the amount of air

entrainment between the experimental result and the simulation result. However, seen from the relative scale, the amount of air entrainment using the EDSA is better than that resulting from using the GA. From the results of the amount of air entrainment by the CFD simulator and experimental result, the amount of air entrainment using the EDSA is better than that resulting from using the GA.

EDSA	Time s	Velocity m/s	Position m
1	1.23	0.26	0.160
2	1.34	0.50	0.200
3	1.76	0.29	0.367

GA	Time s	Velocity m/s	Position m
1	1.32	0.22	0.145
2	1.62	0.44	0.245
3	1.87	0.56	0.367

Table 6. Calculated optimum plunger velocity by using EDSA and GA

Fig. 14. Experimentant results and simulation results.

4. Conclusion

The purpose of this study was to design a search algorithm that used smaller number of populations and a generation that can derive the optimized solution more efficiently for an optimization problem using a CFD simulator. Specifically, focusing on the extremal solution in the multimodal space, we proposed the Extremal Distribution Sorting Algorithm (EDSA), which searches intensively for the improvement point in the nearly extremal solution. The proposed method makes it possible to derive the global optimized solution quickly with few repeated computations. The effectiveness of the proposed method is shown through experiments in actual die-casting plants for deriving the optimum plunger input. The proposed method can derive the optimized solution with few repeated computation. Finally, the effectiveness of the proposed method was clarified by experimental results, which showed that the amount of air entrainment by using the EDSA was better than that resulting from using the GA.

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Search Algorithms and Applications

Edited by Prof. Nashat Mansour

ISBN 978-953-307-156-5

Hard cover, 494 pages

Publisher InTech

Published online 26, April, 2011

Published in print edition April, 2011

Search algorithms aim to find solutions or objects with specified properties and constraints in a large solution search space or among a collection of objects. A solution can be a set of value assignments to variables that will satisfy the constraints or a sub-structure of a given discrete structure. In addition, there are search algorithms, mostly probabilistic, that are designed for the prospective quantum computer. This book demonstrates the wide applicability of search algorithms for the purpose of developing useful and practical solutions to problems that arise in a variety of problem domains. Although it is targeted to a wide group of readers: researchers, graduate students, and practitioners, it does not offer an exhaustive coverage of search algorithms and applications. The chapters are organized into three parts: Population-based and quantum search algorithms, Search algorithms for image and video processing, and Search algorithms for engineering applications.

How to reference

In order to correctly reference this scholarly work, feel free to copy and paste the following:

K.Yano and Y.Kuriyama (2011). Extremal Distribution Sorting Algorithm for a CFD Optimization Problem, Search Algorithms and Applications, Prof. Nashat Mansour (Ed.), ISBN: 978-953-307-156-5, InTech, Available from: <http://www.intechopen.com/books/search-algorithms-and-applications/extremal-distribution-sorting-algorithm-for-a-cfd-optimization-problem>

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51000 Rijeka, Croatia
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Phone: +86-21-62489820
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