Study of Error Propagation in Free Surface Simulations

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***Abstract* - In numerical simulations, a great deal of effort has been made to control errors so as to guarantee the correctness of numerical simulations. Moreover, errors may propagate along meshes, and a slight error might amplified during the propagation which deteriorate the overall accuracy at last. Therefore, to study the characteristic of error propagation along the mesh is essential for the success of the simulation. General source of error in simulations include discretization error, truncation error, etc. However, in free surface simulations, such as bubble in the water, vessel with blood, the most significant error source is the correctness of the surface point position, which would result in a series of errors such as the error of boundary condition, the error of discretization, etc. In this paper, the influence of the error caused by two misplaced surface points are studied based on previous results of one misplaced point. The results show that factors which would influence the final result caused by one point wrong displacement are still important for two points cases. Furthermore, the error of each cell caused by two wrong displacement points is the superposition of the influence of each wrong displaced point, and the final result after two points movement can be predicted by the result caused by only one point movement.**

Keywords - Error propagation; Discretization error; Free surface

I. INTRODUCTION

The control of the error is important to guarantee the success and accuracy of numerical simulations. General errors in numerical simulations include round-off error, truncation error, discretization error etc. Previous researches have made a great effort to study these influence factors. However, for free surface simulations [1, 2], such as vessel with blood, bubble in the water etc. The wrong or improper position of free surface point is usually the largest error source. First of all, it would bring in discretization error because of wrong or improper position accordingly. What is more, the boundary condition may become incorrect (for cases with dynamic boundary condition such as extrusion simulations) which further results in failures of free surface simulations.

Besides the error caused by wrong or improper position of free surface point, the propagation of the error along the mesh is also important for simulations. Some errors would spread outwards which lead to failure of the simulation finally, while others may have little influence on the accuracy of the solution in important areas. Therefore, discovering the characteristic of error propagation along the mesh is vital in controlling the error and guaranteeing the success of the simulation.

Previous research have found out that mesh quality measurements, such as the aspect ratio (the ratio of cell length to cell width), skew and distortion, would influence the solution accuracy [3-5]. Moreover, discretization schemes and difference methods [6] would also influence the accuracy of the solution. However, these individual indicators could not explain how they would affect the simulation result from local area to the whole domain. General methods used to investigate error propagation include matrix-based method and model-based method. Matrix-based method predicts the error of the final solution by investigating the characters of linearized equations [7]. Though it could predict the threshold of solution error well, it is difficult to describe the propagation process of the error. Model-based method builds up models to depict the propagation action of the error [8]. The difficulty is that there is no general error propagation model for complex cases at present. There might be no models existed for some applications.

Based on error propagation model method, our previous work [9] have investigated the characteristic of error propagation caused by one surface point movement in FVM systems for pipe flow like case. However, for a real problem, there are usually several wrong displaced points, and all these misplaced points would have an influence on each cells. How would multiple misplaced pints interact with each other and have an effect on other cells is still a mystery. Based on the previous work, this paper further investigates the effects of two wrong displaced surface points for three basic arithmetic operators (first time derivative, the convection term, the Laplacian term) so as to build up error propagation models for multiple error sources. The contributions of this paper are as follows:

* We built up two-point error propagation models based on one-point error propagation models we have built before. Based on two-point error propagation models, we predict all possible situations caused by two wrong displaced surface points for three basic arithmetic operators.

* To evaluate the effectiveness of two-point error propagation models, we designed experiments which cover all possible predicted solutions. According to experimental results, the errors of each cell caused by two wrong displaced points really can be considered as the superposition of the influence of each wrong displaced points.

The rest of this paper is organized as follows. An brief

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overview of error model and the result of one point error propagation models are given in Section II. Descriptions of two points error propagation model are presented in Section III in detail. Experiments are introduced in Section IV. Literature review in detail is reported in Section V. Conclusions are drawn in the last section.

II. OVERVIEW

This section gives a brief review of the error model and one point error propagation models proposed before.

A. Error model

For free surface problems, the position of the surface point is of significant importance to the correctness of simulation results. Wrong surface point position could be caused by hardware fault or software fault (improper surface adjustment algorithm). It would firstly lead to a different discretization value. Furthermore, for cases with a dynamic boundary condition, such as extrusion simulations, the boundary conditions is no more accurate if the position of the surface is not correct. These errors would change the elements in the linearized equations and result in incorrect solutions. After that, the incorrect solution might further move the surface point to a position far away from the correct position according to the surface adjustment algorithm which finally leads to the failure of the simulation. In this paper, surface grids is manually moved for producing the initial error source so as to investigate the influence of wrong displaced surface points.

B. One point error propagation models

In this section, One point error propagation models established in our previous work are reviewed. We discovered the characteristics of error propagation in physical simulations. Such simulations are always governed by various controlling equations. One of the most notable equations is the momentum equation which is given as

$$\rho(\frac{\partial u}{\partial t} + u \cdot \nabla u) - \beta \Delta u = c \qquad (1)$$

where ρ is the liquid dense, u is the velocity, t is the time, β is the viscosity and c can be a constant force. Three items in the left side of the equation are time derivative term, convection term and Laplacian term, respectively. Without loss of generality, the constant c is set positive.

Errors are introduced by manually moving the surface grids outwards and inwards. For the case of simplicity, the research object is flows in a straight pipe (see Fig. 1), and only one surface point is misplaced along vertical direction (see Fig. 2).

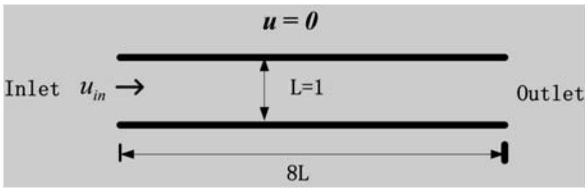


Fig.1 Pipe flow configurations

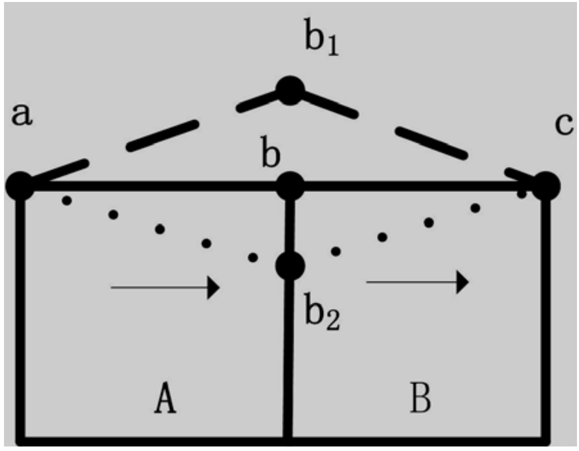


Fig.2 One point at the surface is displaced

Three basic terms mentioned above with various difference methods and various mesh parameters (mainly aspect ratio) based on FVM are investigated in previous work. The conclusions can be drawn as follows

* In terms of the first time derivative term, it would not spatially propagate the error, which means only cells connected to the moved surface point might be influenced. With Euler difference method, moving the grid outwards would lead to a decrease of the velocity nearby and vice versa.

* The convection term would arouse spatial error propagation. If the flow in the pipe is uniform, only cells in the varied boundary layer may be affected by the moved surface point. Moving the grid outwards would lead to a decrease of concentration of its left cell (cell A in Fig. 2) and an increase of its right cell (cell B in Fig. 2). The concentration of boundary layer cells after cell B would also increase. The condition of boundary layer cells before cell A is related to the difference method.

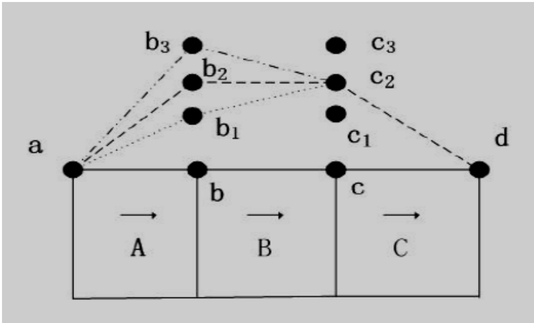
* The Laplacian term would cause the error propagate along all directions. Moving the grid downwards would lead to a decrease of velocity. It would be complex when the grid is moving outwards. If the surface point moved a long distant and the cell owned a small aspect ratio (e.g. small than four), the velocity of the cell connected to the displaced points would decrease, while the velocity would increase for other cells. Otherwise, the velocity of all the cells would increase.

More details could be seen in [9].

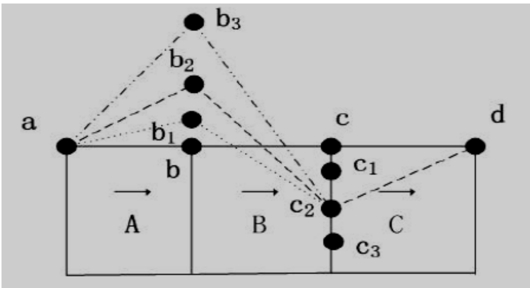
III. TWO POINTS ERROR PROPAGATION MODEL

A. Error propagation model for two points

The conditions for two misplaced points are more complex. In this paper, two points with wrong positions are connected together. Without loss of generality, the condition of all two points moved outwards (see Fig. 3(a)) and one point outwards the other inwards (see Fig. 3(b)) are analyzed.



(a) Two points moved outwards



(b) One point moved outwards and the other one moved inwards

Fig.3 Conditions of two misplaced points

Suppose the misplaced points are individual error sources, and then the influence of two wrong displaced points could be regarded as the superposition of the influence of each wrong displaced point. It can be written as

$$E_k = \lambda E_{bk} + \gamma E_{ck} \quad (2)$$

where E_k represents the error of cell k, E_{bk} and E_{ck} represent the error of cell k caused by the movement of surface point b and point c, respectively. λ and γ are positive coefficients. According to Eq. 2, the final solution after two points movement can be predicted by the result caused by only one point movement obtained before.

B. Prediction for time derivative term

The equation is written as $du/dt = c$. The solution after the surface point is moved is given as below (see [9])

$$u_P^n = c^n \Delta t + (u_P V)^o / V^n \quad (3)$$

where n and o represent current time step and previous time step respectively. u_P is the velocity of cell P and V is the cell volume. It can be seen from Eq. 3 that the velocity is only related to the cell volume no matter how many surface points are moved. As long as the cell volume is increased, the velocity of the corresponding cell would decrease and vice versa (Note previous velocity u_P^o is considered as non-zero here).

The possible results could also be predicted by Eq. 2. Taking cell B in Fig. 3 as an example. If two points are all moved outwards, E_{bB} and E_{cB} should be all negative, then E_B must be negative which indicates the velocity of cell B must be decreased. In terms of the condition that one point is moved outwards and the other one is moved inwards, E_{bB} is negative while E_{cB} is positive. Then the error of cell B E_B could be positive, negative or zero. This conclusion is in accord with theoretical analyses. For the case of simplicity, P, N and Z are used to represent positive, negative and zero respectively in the following sections.

C. Prediction for the convection term

A typical equation including the convection term can be written as $\nabla \cdot (U\alpha) = c$, Where α could be regarded as the concentration. The flow is imposed as uniform flow along the pipe, and the velocity at the inflow keeps constant. It can be known that the solution is related to the difference method. Therefore, the prediction should be classified as using central difference method and using upwind difference method.

When two points are all moved upwards (see Fig. 3(a)), with upwind difference method, The errors of cell A, B and C caused by the movement of point b and c, which are symbolized as E_b and E_c , are (N,P,P) and (Z,N,P) respectively. According to Eq. 2, the final results of cell A, B and C could be (N,N,P) and (N,P,P). Zero error is usually not considered as a special state in this paper unless it is easy to obtain in some specific conditions. In terms of using central difference method, the errors of these three related cells caused by two misplaced surface points are (N,P,P) and (P,N,P), respectively. Besides the same possible solution (N,N,P) and (N,P,P), there could be a new possible solution (P,N,P). There seemingly exits a possible solution (P,P,P), however, it is impossible in fact with a further analysis. E_b and E_c can be further formalized as (-mx,x,z) and (ny,-y,k). where x, z, y, k are positive error values, and m and n are corresponding positive coefficients. If the final solution is (P,P,P), it requires $-\lambda mx + \gamma ny > 0$ and $\lambda x + \gamma y > 0$. Namely $(n/m)\gamma y > \lambda x > \gamma y$. That is to say it should satisfy $n > m$. The solution after only one point is moved outwards (supposing it is point c) is shown in Table Ⅰ. It can be seen that n approximately equals one. m can be calculated through the error of cell B and cell C which approaches 200. Thus, the solution of (P,P,P) would never appear.

TABLE I CONCENTRATION AFTER ONLY POINT C IS MOVED OUTWARDS WITH CENTRAL DIFFERENCE METHOD

Solutions	A	B	C
α^o	4.9	5	5
α^n	5.09545	4.80407	5.00083
Error	0.19545	-0.19593	0.00083

TABLE II POSSIBLE SOLUTIONS OF CELL A, B, C FOR THE CONVECTION TERM AFTER TWO POINTS ARE MOVED

Points position	Difference method	E_b	E_c	Possible solutions
(O,O)	UM	(N,P,P)	(Z,N,P)	(N,N,P) (N,P,P)
(O,O)	CM	(N,P,P)	(P,N,P)	(N,N,P), (N,P,P), (P,N,P)
(O, I)	UM	(N,P,P)	(Z,P,N)	(N,P,P), (N,P,N), (N,P,Z)
(O, I)	CM	(N,P,P)	(N,P,N)	(N,P,P), (N,P,N), (N,P,Z)

If point b is moved outwards and point c is moved inwards (see Fig. 3(b)), similar to the analysis described above, E_b and E_c are (N,P,P) and (Z,P,N) for the upwind difference method, and (N,P,P) and (N,P,N) for the central difference method, then the possible final solutions are (N,P,P), (N,P,N) and (N,P,Z), no matter what kind of difference methods are used.

All possible solutions of cell A, B, C after two points are moved are summarized in Table Ⅱ. where O and I represent the point is moved outwards and inwards. UM and CM represent upwind difference method and central difference method respectively.

F. Prediction for the Laplacian term

The Laplace operator is constructed as $-\nabla \cdot (\nabla u) = c$. Mesh parameters (aspect ratio) have a significant influence on the final solutions. The distance of the movement is also of great importance. Using similar analysis method with Eq. 2, the possible solutions can also be predicted.

TABLE III E_b AND E_c WHEN TWO POINTS ARE ALL MOVED OUTWARDS WITH CELL ASPECT RATIO 1

Solutions	Distance	A (10^{-3})	B (10^{-3})	C (10^{-3})
E_b	0.02	0.069	0.069	0.026
E_c	1	0.687	3.367	-3.367

In the condition of all points are moved outwards, if the grid is moved outwards with a long distance and the aspect ratio is not large (e.g. small than 4), E_b and E_c are (N,N,P) and (P,N,N). Otherwise, E_b and E_c can only be (P,P,P). Therefore, there are four possible combination schemes including (P,P,P)+(P,P,P), (P,P,P)+(P,N,N),(N,N,P)+(P,P,P) and (N,N,P)+(P,N,N). The possible final solutions could be (P,P,P), (N,N,N), (N,N,P), (P,N,N), (N,P,P) and (P,P,N). Note there is no possibility to obtain (P,N,P). This is because the degree of each cell influenced by the moved points is different according to the distant between the error source and the cell. Taking the combination plan (P,P,P)+(P,N,N) as an example. The error E_b and E_c when two points are all moved outwards with cell aspect ratio 1 are shown in Table Ⅲ. Where the item 'distance' means the distance of the point moved, and the unit is the times of the cell length. It can be seen from the table that $E_{bB} > E_{bC}$ while $E_{cB} > E_{cC}$. Thus, according to Eq. 2, $E_B = \lambda E_{bB} + \gamma E_{cB}$ would always larger than $E_C = \lambda E_{bC} + \gamma E_{cC}$, which means the situation of (P,N,P) would never appear.

In terms of one point is moved outwards and the other is moved inwards, E_b is (N,N,P) in the condition of a long distance movement and a small aspect ratio, while it is (P,P,P) in other conditions. E_c is always (N,N,N). The two possible fixed plans are (N,N,P)+(N,N,N) and (P,P,P)+(N,N,N). Thus, the final solutions are possibly be (P,P,P), (N,N,P), (P,N,N), (N,N,N) and (P,P,N).

All possible solutions for the case of two moved surface points are summarized in Table Ⅳ. Where Cd_1 represent the condition that the point is moved with a long distance and the cell aspect ratio is small, Cd_2 represent other conditions besides Cd_1, and Cd_3 stand for any conditions.

TABLE IV POSSIBLE SOLUTIONS OF CELL A, B, C FOR THE LAPLACIAN TERM AFTER TWO POINTS ARE MOVED

Points position	Point b	Point c	E_b	E_c	Possible solutions
(O,O)	Cd_1	Cd_1	(N,N,P)	(P,N,N)	(N,N,P), (P,N,N), (N,N,N)
(O,O)	Cd_1	Cd_2	(N,N,P)	(P,P,P)	(N,N,P), (P,P,P), (N,P,P)
(O,O)	Cd_2	Cd_1	(P,P,P)	(P,N,N)	(P,P,P), (P,N,N), (P,P,N)
(O,O)	Cd_2	Cd_2	(P,P,P)	(P,P,P)	(P,P,P)
(O, I)	Cd_1	Cd_3	(N,N,P)	(N,N,N)	(P,P,P), (N,N,N), (P,P,N), (P,N,N), (N,N,P)
(O, I)	Cd_2	Cd_3	(P,P,P)	(N,N,N)	(P,P,P), (N,N,N), (P,P,N), (P,N,N)

IV. EXPERIMENTS

Research plans and simulation configurations are similar to the previous research in [9]. The fluid is flowing in a straight pipe (see Fig. 1). Two middle points (x=4 and x=4.05) at the upper wall are moved up and down along the vertical direction manually (see Fig. 3) as the initial error source. Only the conditions that two points are all moved up and one point is moved up while the other point is moved down are analysed as typical examples. Various combination schemes with different amplitude of point movement are tested to obtain possible solutions desired. More detailed initial conditions of the flow would be described in each subsection below. A steady state with the original mesh is obtained at time 1 as the correct solution. Then the middle points are moved and the reference data is obtained at time 10. Without loss of generality, the constant c is taken as 1 in the simulations. Without specification, the mesh used in the simulation is 160*20. All experiments are implemented in OpenFOAM, which is an open source FVM-based CFD simulation tool [10].

A. Error propagation analysis of the first time derivative term

The uniform flow begins from 1 m/s. As the velocity would grow up gradually and no steady state exist during the simulation, the error of a cell is chosen as the difference between it is now and it should be without the move of surface points at time 10 (actually the value of other cells which are not connected to the moved points could be regarded as the correct solution). The variation of cell B under different combination schemes are shown in Table Ⅴ. It can be seen that the error of cell B is closely related to the volume of the cell as demonstrated in Sec. D. An increase of the volume would result in a decrease of the velocity and vice versa. The result also matches the prediction mentioned in Sec. D.

TABLE Ⅴ SOLUTIONS OF CELL B UNDER DIFFERENT COMBINATION SCHEMES

Points position	Point b	Point c	E_B
(O,O)	0.02	0.02	-0.0196
(O, I)	0.02	-0.01	-0.005
(O, I)	0.02	-0.02	0
(O, I)	0.02	-0.04	0.0101

B. Error propagation analysis of the convection term

The uniform flow with 1 m/s constant speed is used in this section. α at the inlet is keeping fixed (the concentration is set as 1) as a constant source. Solutions with central difference method are listed in Table Ⅵ (the results are off to one significant figures). The result shows that every possible solutions predicted in Sec. E can actually be obtained, which again validates the effectiveness of Eq. 2. Experiments with upwind difference method are also implemented, but they are not listed in the paper as they are relatively more simple.

TABLE VI SOLUTIONS OF CONVECTION TERM WITH CENTRAL DIFFERENCE METHOD

Points position	Point b	Point c	(E_A, E_B, E_C)
(O,O)	0.02	0.02	(0.002,-0.2,0.002)
(O,O)	1	0.001	(-5,-0.06,0.05)
(O,O)	5	1	(-8,0.1,0.3)
(O,I)	0.02	0.02	(-0.4,0.2,0)
(O,I)	0.02	0.001	(-0.3,0.1,0.0005)
(O,I)	0.001	0.02	(-0.3,0.2,-0.0005)

C. Error propagation analysis of the Laplacian term

As the variation for experiments with large cell aspect ratio is too simple, only solutions with aspect ratio equals to one are listed in Table Ⅶ (the results are off to one significant figures). All the possible solutions for the conditions that two surface points are moved outwards and the first point is moved outwards while the second point is moved inwards predicted in Sec. F are obtained. The results demonstrate that Eq. 2 works well for equations with Laplacian term too.

TABLE VII SOLUTIONS OF LAPLACIAN TERM WITH ASPECT RATIO EQUALS TO ONE

Points position	Point b	Point c	(E_A, E_B, E_C) (10^{-3})
(O,O)	0.02	0.02	(0.1,0.1,0.1)
(O,O)	1	1	(-1,-2,-1)
(O,O)	1	0.02	(-3,-3,0.7)
(O,O)	0.02	1	(0.7,-3,-3)
(O,O)	0.5	0.2	(-0.1,0.1,1)
(O,O)	0.2	0.5	(1,0.1,-0.1)
(O,I)	0.02	0.02	(0.04,-0.01,-0.05)
(O,I)	0.02	0.01	(0.05,0.03,-0.01)
(O,I)	0.02	0.002	(0.07,0.06,0.02)
(O,I)	0.8	0.8	(-5,-7,-5)
(O,I)	0.8	0.002	(-2,-2,0.7)

V. RELATED WORK

There are usually two methods to investigate the characteristics of the error propagation, matrix-based method [4, 7] and model-based method [8, 9]. Matrix-based method stands from the perspective of mathematics and predicts the error of the final solution through numerical analysis. Actually this method turned out to investigate the linearized equation Ax = b. The error generated during discretization and the error caused by the change of boundary condition would in fact result in a slight error in A and b. The deviation of the final solution would closely depend on the properties of the matrix. This method could be used to tackle with most of the problems, and an accurate error limit prediction of the final solution could be obtained. However, it could not describe the characteristics of error propagation in a clear way. Thus, it could not propose any advices to control the propagation of the error.

On the contrary, Model-based method builds up models to describe the propagation of errors intuitively. For instance, when simulating physical issues with LBM, according to the basic theory of particle collision, an error would only influence surrounding cells in one time step. This characteristic could be used for fault tolerance to design low-overhead soft error detection mechanisms [8]. It can be seen that model-based method could directly reveal the law of error propagation in meshes and guide the control of the error so as to guarantee the success of the simulation. However, error propagation characters in simulations with discretization methods like FVM are quite different from those with LBM, one error in any position probably pollutes all other cells immediately. [9] proposed three models for each of three basic arithmetic operators (first time derivative, the convection term, the Laplacian term) in FVM systems. However, there is only one misplaced point in the simulation, and it can not reveal the characters when multiple misplaced points interacting with each other.

VI. CONLUSION

In this paper, the characteristics of error propagation in the mesh caused by two adjacent misplaced points are investigated. Experiments were implemented separately for three basic arithmetic operators (first time derivative, the convection term, the Laplacian term). The results showed that factors ever considered in one point error propagation models would also influence the final solution in the conditions of two misplaced points. What is more, the error of the cell caused by two wrong displacement points is the superposition of the influence of each misplaced point, and the final result after two points are moved can be predicted by the result caused by only one point movement according to proposed formula Eq. 2. This formula may shed light on characters of error propagation for multiple error sources, namely linear superposition. More characteristics may be discovered with further study in the future so as to control the error in simulations.

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REFERENCES

[1] Tukovic, Z. and H. Jasak, "A moving mesh finite volume interface tracking method for surface tension dominated interfacial fluid flow". Computers & Fluids, 55: p. 70-84. 2012.

[2] Sommerfeld, M. and S. Decker, "State of the Art and Future Trends in CFD Simulation of Stirred Vessel Hydrodynamics". Chemical Engineering & Technology, 27(3): p. 215–224. 2004.

[3] Baker, T.J. "Deformation and quality measures for tetrahedral meshes". in European Congress on Computational Methods in Applied Siences and Engineering, Barcelone. 2000.

[4] Gargallo-Peiró, A., et al., "Defining Quality Measures for Validation and Generation of High-Order Tetrahedral Meshes". Proceedings of the 22nd International Meshing Roundtable, p. 109-126. 2014.

[5] Parthasarathy, V.N., C.M. Graichen, and A.F. Hathaway, "A comparison of tetrahedron quality measures". Finite Elements in Analysis and Design, 15(3): p. 255-261. 1994.

[6] Diskin, B. and J.L. Thomas, "Effects of Mesh Irregularities on Accuracy of Finite-Volume Discretization Schemes". 2012.

[7] Freitag, L.A. and P.M. Knupp. "Tetrahedral element shape optimization via the Jacobian determinant and condition number". in IMR. 1999.

[8] Xiaoguang, R., et al., "GS-DMR: Low-overhead soft error detection scheme for stencil-based computation". Parallel Computing, 41(0): p. 50-65. 2015.

[9] Yu, C., et al. "Study of Error Propagation in Mesh Caused by Surface Point Movement in FVM Systems". in ICECEE. 2015.

[10] Jasak, H., "OpenFOAM: Open source CFD in research and industry". International Journal of Naval Architecture and Ocean Engineering, 1(2): p. 89-94. 2009.