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Mesh–Order Independence in CFD Simulation

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ABSTRACT Accuracy and performance are key issues for CFD simulation. How to meet the specific accuracy requirements, as well as the optimal simulation performance, is always the research hotspot. This paper presents a general theory of Mesh–Order Independence that is used to guide the configuration of two of the most critical control parameters in a concrete CFD simulation process: grid spacing and discretization order. A concept of optimal mesh–order independent pair which can meet both accuracy and performance requirements at the same time is proposed and analyzed. To find the optimal Mesh–order independent pair, the Mesh–Order Independence is applied to high order FEM simulation, and the specific process and key technologies are detailed. Test and results of two benchmark cases, the Laplace equation and the Helmholtz equation, show that the Mesh–order theory proposed in this paper provides an important guidance for the grid spacing selection and discretization order configuration in practical simulation, especially in the case of high precision requirements. Specifically, only 6 pre-runs with low discretization orders and coarse meshes are needed for the both cases to have a prediction accuracy of more than 70%.

INDEX TERMS Mesh–Order independence, grid spacing, discretization order, high-order FEM, CFD.

I. INTRODUCTION

As an emerging interdisciplinary, computational fluids dynamics (CFD) uses numerical methods and computer simulations to solve real physical, biological, and chemical problems [1], [2]. In addition to its low cost and high efficiency, CFD also outperforms the traditional experimental methods for its flexibility and adjustability. For example, in order to observe the phenomena under different physical conditions in the simulation of flow over airfoils, it generally only needs to adjust the relevant parameters in the CFD codes such as the initial conditions and boundary conditions. To obtain more credible results, the increase of accuracy-related parameters such as the density of the grid and the degree of discretization are generally effective. However, the flexibility of CFD simulation is subject to some constraints and limitations in practical applications, simulation performance, for example.

The contradictory relationship between performance and accuracy in CFD simulations poses a significant challenge to parameter configurations. In order to improve the simulation accuracy, the common way is to increase the grid density for low-order simulation methods. However, it is not possible for the users to refine the grid indefinitely because the cost of

CFD simulation increases synchronously with the refinement of the grid, which in turn affects the efficiency of CFD simulation. For low-order methods, the most commonly used method to determine the optimal mesh for simulation is mesh independent study [3], [4]. Simulations are performed on at least three different meshes, and the numerical errors are estimated. The coarsest mesh on which the simulation results meet the certain constraints, such as the prescribe accuracy, is selected as the final optimal mesh.

With the development of high-order methods, high-efficiency and high-accuracy CFD simulation has become a hot topic [5], [6]. A high-order method is a method with a third order or higher accuracy of spatial discretization, which has a faster convergence rate than a low-order method. Over the past two decades, researchers have proposed a variety of high-order discretization schemes, such as high-order continuous finite element method (FEM) [7], high order finite difference method (FDM) [8], and ENO/WENO based high-order finite volume method (FVM) [9]. High-order simulation provides the possibility of high-efficiency solutions and high-accuracy solutions, as well as the challenge of the parameter configurations, because the variable control parameters include both the grid density and discretization order. For instance, to improve the accuracy of high-order simulation, one can either refine the grid or increase the

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discretization order. So, an attendant question is how to choose the optimal grid density and discretization order in the practical high-order simulation, in order to meet the accuracy requirements, at the same time has the shortest solution time. For high-order simulation, the mesh-independent test is no longer available, and the generally used methods to determine the optimal mesh and the optimal discretization order are heuristic methods. To the best of our knowledge, there are no relative theory for Mesh–order independent study in high-order CFD simulation.

This paper starts from a practical point of view and launches a series of studies which focus on the configuration of grid spacing and discretization order in high-order CFD simulation. Specifically, the contributions of this article can be summarized as follows:

- A general theory for grid spacing and discretization order selection for high-order CFD simulation, Mesh–Order Independence, is proposed.
- An algorithm of searching the optimal Mesh–order independent pair is designed, and the key technologies are analyzed in detail.
- The verification and validation of the proposed theory are performed in practical high-order FEM simulation.

In addition, there are two points that need to be emphasized. First, the concept of Mesh–Order Independence proposed in this paper can be regarded as a generalized abstraction of the conventional mesh independence in low-order simulation, because when the discretization order is fixed, the Mesh–Order Independence is actually degenerate into the mesh independence; the second is that although the simulation cases in this paper are based on high-order FEM method, the theory and method proposed also have profound guiding significance for other high-order methods.

The rest of this paper is organized as follows: Section II provides a brief introduction to background knowledge and related work to this article. Section III presents the theory of Mesh–Order Independence. Section IV gives a practical algorithm to find the optimal Mesh–order independent pair, and details the required key technologies. Section V is the experiment, followed by the conclusions and the future work.

II. BACKGROUNDS AND RELATED WORK

A. NUMERICAL ERROR

The essence of CFD simulation is solving the linear systems of equations, which is obtained by the discretization of the partial differential equations (PDEs) that describe the physical problems. The solution of the original continuous partial differential equation is called the analytical solution, or the exact solution, while the solution of the linear system of equations is the numerical solution. Generally, the numerical solution is not equal to the analytical solution, but only close to the analytical solution. This is mainly because the numerical simulation will inevitably introduce errors. According to the different sources, the numerical errors of the simulation can be divided into three parts [10]: the discretization error caused by the approximation of the PDE, the iterative

convergence error due to the iteration is not sufficient, and the round-off error caused by approximate representation of numbers. In general, discretization error accounts for more than 90% of all errors. Therefore, the error discussed in the subsequent part of this article refers to discretization error unless otherwise stated. For a practical simulation, the error is defined as:

$$e = |u^* - u_h^p| \quad (1)$$

where u_h^p is the numerical solution to the discrete equations on a mesh with a representative cell length of h , and u^* is the exact solution to the differential equations.

$$\|e\|_{L_2(K)} = \left(\int_K |u^* - u_h|^2 dx \right)^{1/2} \quad (2)$$

$$\|e\|_{H^1(K)} = \left(\int_K |u^* - u_h|^2 dx + \int_K |\nabla(u^* - u_h)|^2 dx \right)^{1/2} \quad (3)$$

Eq. 1 is a typical definition of error, which describes the local error of a variable. However, unknown variables are usually vectors or tensors in simulations, and the global error is more concerned. Eq. 2 and 3 are two of the most widely used models describing the global error, L_2 norm and H^1 norm, where K represents the smallest discrete element. Here in this paper, unless otherwise stated, the global error refers to the global L_2 error.

B. MESH INDEPENDENCE

For a stable and fixed-order numerical scheme, the simulation accuracy will gradually increase as the mesh density increases. It is well known that the numerical error is the most commonly used quantitative indicators to describe the simulation accuracy in CFD. If E is the numerical error, h is the grid spacing, then we have the following relation for a first order scheme [11]:

$$E \propto k * h \quad (4)$$

where k is a coefficient independent of h , but may change in space or time. In other words, E and h are in a proportional relationship. Similarly, if T represents the overhead of the simulation process, then it will increase as the decrease of h , so T and h are inversely proportional. Here, the overhead T can be all kinds of the resource consumption, such as the execution time and the memory consumption of the simulation. The factor g is a coefficient independent of h .

Because of the existence of simulation overheads, we can not increase the accuracy of the simulation by reducing the grid spacing infinitely. The mesh independent study is critical to balance the accuracy and performance in practical simulations, and it is also an essential process to conduct verification and validation of the simulation [12], [13]. The purpose of mesh independent study is to find the optimal mesh with the largest grid spacing to meet the accuracy requirements. In general, the first step is to solve the same problem using three different meshes: coarse, medium and fine. Then the simulation error is calculated. If the simulation

error on coarse mesh can meet the accuracy requirements of the problem, then, according to Eq. 4, the simulation on medium mesh and fine mesh will certainly be able to meet the accuracy requirements. At this time, in order to make the simulation overhead lowest, obviously the coarse mesh is the optimal. At present, the vast majority of mesh independent test process is performed in a heuristic approach [14], that is, the researchers select three different meshes mainly based on their experience, and then determine the optimal one.

C. ADAPTIVE REFINEMENT

The trade-off between performance and accuracy has been one of the most concerned problems in CFD simulations. In order to improve the accuracy of the simulation with lowest cost, researchers have proposed a variety of mesh adjustment methods [15], including h-adaptive, p-adaptive, hp-adaptive and so on. In the case of h-adaptive refinement, the main process is as follows: First, a complete simulation is performed on a relatively coarse initial mesh and the errors of all cells are estimated. Then, cells with relatively large errors will be marked. Finally, the marked cells are refined, and the previous processes are repeated until error of all the cells meet the accuracy requirements. The refinement process of p-adaptive and hp-adaptive refinement are similar to h-adaptive refinement, except that p-adaptive refinement is achieved by increasing the discretization order on the cells with large error, while hp-adaptive refinement is achieved by changing either the grid spacing or the discretization order.

No matter what kind of adaptive refinement methods, the basic idea is to refine the local mesh or increase the local discretization order iteratively to improve the local accuracy, and thus improve the global accuracy. With adaptive refinement, the problem of low local accuracy due to the existence of singularities can be solved satisfactorily. However, the current adaptive research focuses almost on the various optimization based on the heuristic algorithm, which lacks uniform theoretical guidance. To solve this problem, this paper is going to study the theory of hp adjustment for CFD simulation from the perspective of global refinement. It should be noted that the choice of global hp adjustment rather than local adjustment is mainly because:

- 1) Local adjustment is related to lots of factors, which leading to a complex modeling. Global adjustment can be treated as a theoretical basis for local adjustment.
- 2) Solutions of certain smooth problems converge monotonically as the grid is global refined, thus has a practical significance.

III. MESH–ORDER INDEPENDENCE

A. MESH–ORDER PAIR

The accuracy and performance of CFD simulation are affected by many factors, such as physical model, discretization scheme, linear solution method and so on. A myriad of researchers have discussed the impact of the different models and solution methods on the simulation results in detail. We will focus on the discretization order and grid spacing in

this paper, and try to analyze the impact of these two factors on the performance and accuracy of CFD simulation from the perspective of quantification model. First of all, for the sake of convenience, we define the concept of a Mesh–order pair in simulation as follows.

Definition. For CFD simulations with all parameters fixed except grid spacing and discretization order, the **Mesh–order pair** represents a simulation configuration with the grid spacing h and the discretization order p , denoted as $\text{pair}(h, p)$.

It should be noted that the grid spacing h is not consistent with all cells when the mesh is nonuniform in practical CFD simulations. Therefore, the grid spacing here is conventionally defined as the maximum value of the distance between two adjacent cells. When the mesh is refined or coarsened, all the cells have to be adjusted simultaneously. For example, if the grid spacing is halved, then the size of all cells are halved simultaneously. In this way, the grid spacing after the refinement and coarsening can be expressed as $h/2$. In addition, for models with multiple unknowns, the discretization scheme may be different for different field variables, such as velocity, pressure and temperature. Here, we only consider the case with one variable’s order change at a time.

B. MESH–ORDER INDEPENDENT PAIR

It is known that as the grid spacing decreases, or the discretization order increases, the numerical solution will gradually approach the exact solution, so the error will gradually decrease and the accuracy will be improved. At the same time, with the decrease of grid spacing and the increase of discretization order, the cost of simulation will increase gradually. Therefore, it is necessary to compromise between accuracy and performance. In practical engineering applications and scientific computing, a threshold is usually specified for the error. When the simulation error is less than or equal to this threshold, the accuracy requirement for the simulation is considered to be satisfied. For example, it is generally believed that the error is less than 10^{-2} to meet the engineering accuracy, and for the high accuracy of 10^{-6} arises in some scientific applications [16]. When the error satisfies a certain accuracy requirement, it is generally noneconomic to further reduce the error by further reducing the grid spacing, or by increasing the discretization order. On the one hand, the degree of error reduction is very low; on the other hand, the resulting overhead will increase dramatically. In order to describe the special simulation state when the error is less than or equal to the specified threshold, we propose the concept of “Mesh–Order Independence”, which is defined as follows:

Definition. Let e be the error of a CFD simulation with a configuration of $\text{pair}(h, p)$, that is, the grid spacing is h and the discretization order is p , then for a prescribed threshold ε , if

$$e \leq \varepsilon$$

is satisfied, then the $\text{pair}(h, p)$ is called **Mesh–order independent pair**, denoted as $\Lambda(h, p)$.

The benefit of using this error description is straightforward, but the problem is that the magnitude of the numerical solution directly determines the quality and reliability of the description. Let us consider the case where the error threshold is fixed to 10^{-2} . When the exact solution of the original continuous equation is large, such as 100, in order to achieve the required accuracy, the numerical solution should be in the range of [99.99, 100.01]. However, if the exact solution is equivalent to the error threshold, 0.01 for example, the numerical solution should be in the range of [0,0.02] in order to satisfy the accuracy requirement. Although the absolute errors in these two cases are the same, the relative errors are very different. If we use formula

$$e' = \frac{e}{x^*} = \frac{|u^* - u_h^p|}{|u^*|} \quad (5)$$

to calculate the relative error, then the relative error for the two cases described above is calculated to be 10^{-4} and 1, respectively. Obviously, the simulation accuracy of the former case is higher than the latter. In the practical simulation, an effective method to improve the simulation accuracy of the latter case is to reduce the error threshold. Another common method is to describe the accuracy of the simulation with the relative error rather than the absolute error. Inspired by this idea, we use the relative error to redefine the concept of Mesh-Order Independence in the previous section as follows:

Definition. Let e' be the relative error of a CFD simulation with a configuration of pair (h, p) , that is, the grid spacing is h and the discretization order is p , then for a prescribed threshold ε , if

$$e' \leq \varepsilon$$

is satisfied, then the Mesh-order pair (h, p) relative Mesh-Order Independence, denoted as $\hat{\Lambda}(h, p)$.

The following properties can be derived from the concept of Mesh-order independent pair:

- **Infinity** For a specified threshold ε , there may be infinite Mesh-order independent pairs, all the combinations of h and p that makes the simulation error under ε is a Mesh-order independent pair.
- **Transitivity** If the threshold $\varepsilon_1 < \varepsilon_2$, then all the Mesh-order independent pair under the threshold ε_1 are also the Mesh-order independent pair under the threshold ε_2 .

C. OPTIMAL MESH-ORDER INDEPENDENT PAIR

In the previous section we propose a definition of Mesh-order independent pair, and simply analyze its properties. It is not difficult to know that there are a large number of Mesh-order independent pairs that satisfy a certain accuracy requirement. However, in the practical simulation, if the performance is taken into account, then the Mesh-order independent pair with the lowest cost is the most concerned among all Mesh-order pairs that meet the accuracy requirements. How to find this optimal Mesh-order independent pair is worthy of further study.

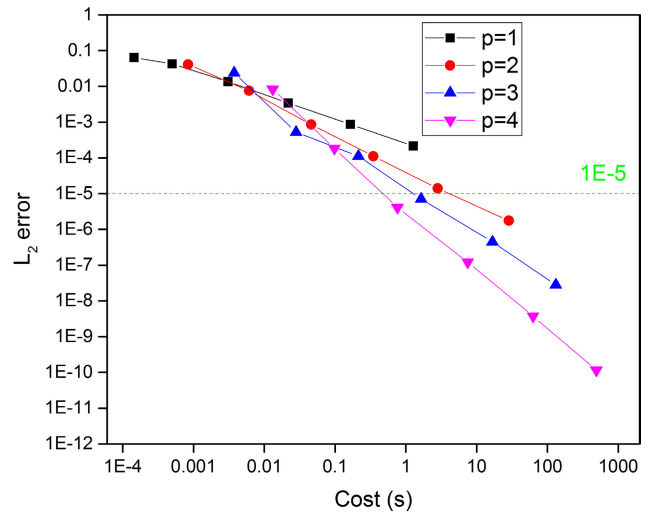


FIGURE 1. The relationship between cost and error for a high-order FEM simulation of helmholtz problem.

Fig. 1 shows the results of a practical CFD simulation process, where the abscissa represents the cost of the simulation and the ordinate indicates the accuracy of the simulation. Specifically, the total time required for a complete simulation is used to represent the overhead of the simulation, and the accuracy of the simulation is described using L_2 errors. The color of the curve in the figure represents the discretization order, and the points on each curve represent the Mesh-order pair with different grid spacing. There are six points on each curves, and the grid spacing from left to right are $h_i (i = 1, 2, \dots, 6)$ respectively. The grid spacing of the first point on all curves is the same, and the grid spacing of the right side is half of the left side, that is, the grid density is doubled. In order to find a Mesh-order pair that satisfies a certain accuracy requirement, such as $\varepsilon = 10^{-5}$, it is only need to make a straight line $y = 10^{-5}$ in the direction parallel to the x-axis, and then all the points below the straight line meet the required accuracy. At this point, all the Mesh-order independent pairs make up a set:

$$A = \{\Lambda(h_6, p_2), \Lambda(h_4, p_3), \Lambda(h_5, p_3), \Lambda(h_6, p_3), \Lambda(h_3, p_4), \Lambda(h_4, p_4), \Lambda(h_5, p_4), \Lambda(h_6, p_4)\}$$

In all of these pairs, the one which meets a certain performance requirements is often the focus of user's attention. Here, if we use the most commonly used performance indicator, the execution time, as a evaluation index, then the optimal pair would be $\Lambda(h_3, p_4)$ according to Fig. 1. Thus, when considering both the accuracy and performance of the simulation, we can define the optimal Mesh-order independent pair as follows:

Definition: Among all the Mesh-order independent pairs respect to a prescribed error threshold ε , the one which has the minimal cost is the **optimal Mesh-order independent pair**, denoted as $\hat{\Lambda}(h, p)$.

It should be noted that the cost in the definition of the optimal Mesh–order independent pair can be either the execution time, the storage consumption, or some other performance metrics. Here in the rest part of this paper, the optimal Mesh–order independent pair are all evaluated with execution time unless otherwise stated.

IV. FIND THE $\hat{\lambda}(H, P)$ IN FEM SIMULATION

In Section III, we present a series of concepts respect to Mesh–order pair. One of the most significant aspects of these theories is that they can be used to guide practical CFD simulations. For instance, it is quite recommend for the user to start the simulation with the specific grid spacing and discretization order indicated by the optimal Mesh–order independent pair, so that the performance of the simulation is optimal, as well as the accuracy requirement is met. Next, we will take FEM simulation as an example, and first give a general flow for the search of optimal Mesh–order independent pair, then analyze and discuss the key technologies involved in the process.

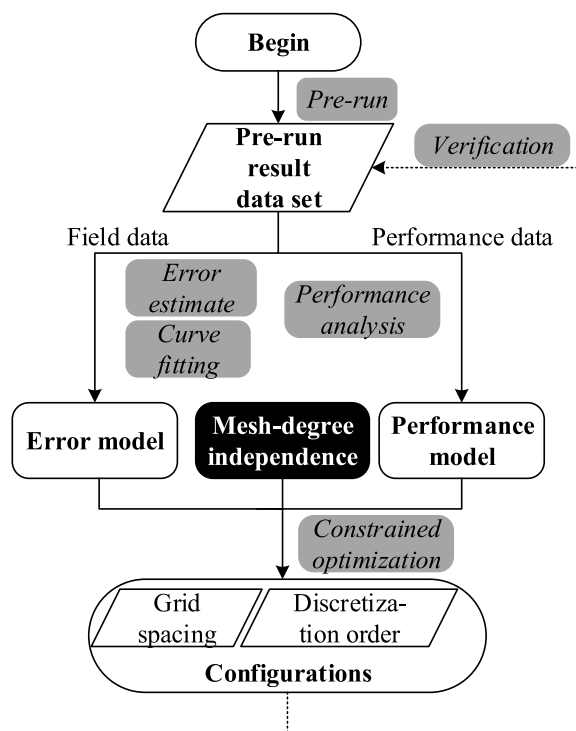


FIGURE 2. The simulation parameter optimization based on mesh–order independence.

A. OVERALL PROCESS

Fig. 2 shows the flow chart using Mesh–order independent theory to guide the parameter configuration in FEM simulation. First, a series of pre-runs are conducted. A pre-run is to run the case a few iterations with tentative grid spacing h_i and discretization order p_i , and the results of the user concerned variables u_1, u_2, \dots, u_n will be sampled. Here, u_i

may be either the field data such as pressure, a component of velocity, or the performance data such as storage costs, execution time. In general, the grid spacing for pre-run should be as large as possible while the discretization order should be as low as possible to reduce the execution time. The number of pre-runs is related to the problem to be solved, generally at least two pre-runs are required for simple problems and three for complex problems. The results of the pre-runs are usually stored in a data set $D_i(h_i, p_i, u_1, u_2, \dots, u_n)$, where $i = 1, 2, \dots, n$. Next, based on the field data obtained by pre-runs, the simulation error is estimated, and the accuracy model is further established. The error estimation is still a hot topic in the field of CFD, and the specific method used in this paper will be described in detail later. In addition to the accuracy model, it is also necessary to establish a performance model based on the performance data obtained from the pre-runs. Then, based on the combination of established accuracy model, performance model and the Mesh–order independent theory, the optimal grid and order configuration problem can be converted into a single-objective optimization problem. Finally, the optimal configurations to meet the accuracy requirement can be solved with the help of mathematical tools, for example Matlab.

B. ERROR ESTIMATION

It can be seen from the Eq. 1 that the error is determined by both the simulation solution and the exact solution, thus the way to estimate the error is closely related to whether the exact solution is known or not. When the exact solution is known, the L_2 error can be calculated simply according to Eq. 2. However, getting the analytical solutions of PDEs is not always a simple matter. In fact, for most of the equations derived from real physical process, it is difficult to calculate the exact solutions. Therefore, other way is necessary. For these problems, the most common way of estimating error is to use the standard Richardson Extrapolation (RE) method [17], [18] and some improved algorithms based on this method, such as the generic RE method [19], the mixed RE method, and the Grid Convergence Index (GCI) method [20]. Appendix VI gives a detailed procedure of how to use the standard RE method to obtain an exact solution.

C. CURVE FITTING

Curve fitting is widely used in scientific and engineering computing to deal with discrete data due to its usability and practicability [21], [22]. The essence of curve fitting is to use a continuous function to approximate a series of discrete data, which may be either experimental results or simulation results. The most commonly used curve fitting function is a polynomial function, and nonlinear fitting functions includes exponential function, power function and logarithmic function. When applying curve fitting to practical problems, the fitting function is usually determined with experience, otherwise heuristic methods are considered. Regardless of which fitting function is used, the undetermined coefficients need to be evaluated. Generally, the method of linear least

squares (LLS) is widely used to determine the parameters in the fitting function. Appendix VI gives an example of the parameter evaluation in linear fitting.

Nevertheless, the undetermined coefficient can not be obtained simply by solving the equation as Eq. 17 for nonlinear fitting, thus it is usually necessary to transform the model from nonlinear to linear using mathematical methods. For example, the logarithmic function can be used to convert the nonlinear exponential function model and the power function model into a linear function, and then a problem like Eq. 15 can be obtained using the linear least squares method. If the nonlinear function can not be transformed into a linear function, the numerical optimization algorithms [23] such as gradient descent method, Levenberg-Marquardt (LM) algorithm [24], [25], and Gaussian Newton algorithm can also be considered.

D. CONSTRAINED OPTIMIZATION

The essence of finding the optimal Mesh–order independent pair in FEM simulation is an optimization problem. Here, the constraints mainly include two aspects, one is the accuracy constraints, that is, Mesh–order independent theory, the other is the resource constraints of the platform, such as the memory limitation. The only goal of the optimization is to optimize the performance of the simulation, so this is a typical single-objective optimization problem that can be expressed as

$$\begin{cases} \min & y = f(h, p) \\ \text{s.t.} & g_1(h, p) \leq 0 \\ & g_2(h, p) \leq 0 \\ & h \in D_1, \quad p \in D_2 \end{cases} \quad (6)$$

where h and p are decision variables that correspond to the grid spacing and discretization order, f is the objective function, g_1 and g_2 are the two inequality constraints that correspond to the accuracy constraints and resource constraints, respectively. $D_1 = \{h \in R | 0 < h < 1\}$ and $D_2 = \{p \in N^+ | 0 < p\}$ are the searching space of the two decision variables.

Since there are two decision variables in Eq. 6, the most intuitive way to solve the global optimal solution of the constraint optimization problem is to use the traversal method. Specifically, a decision variable such as the discretization order is firstly fixed, then the searching space of the other decision variable is traversed to find a temporary optimal solution that satisfies the constraints. Then, the new local optimal solution is obtained by traversing the searching space of the fixed decision variable in the previous step, that is, the discretization order. Finally, the new local optimal solution is the global optimal solution. The specific algorithm description is shown in Algorithm 1.

It should be noted that, since this paper focuses on the Mesh–order independent theory and its application in practical scientific and engineering computations, Algorithm 1 only gives a general and intuitive solution to such

Algorithm 1 The Traversing Algorithm to Search the Optimal Mesh–Order Independent Pair

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1: Initial  $f_{optimal}$ 
2: for all  $p$  such that  $p \in D_2$  do
3:   for all  $h$  such that  $h \in D_1$  do
4:     Calculate the error and cost of the Mesh–order pair
        $(h, p): e_{temp}, f_{temp}$ 
5:     if  $(e_{temp} \leq \varepsilon) \ \& \ (f_{optimal} > f_{local})$  then
6:        $f_{optimal} = f_{local}$ 
7:     end if
8:   end for
9: end for
10: return the  $\hat{\Lambda}(h, p)$  respect to  $f_{optimal}$ 

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a multi-variable optimization problem, and may not be the velocity optimal. In fact, the optimization problem has always been one of the hotspots in the field of science and engineering. Researchers have proposed a number of optimization methods for practical problems, including the genetic algorithm, ant colony algorithm, particle swarm algorithm and so on. In recent years, with the rapid development of artificial intelligence technology, researchers have tried to use machine learning and deep learning techniques to solve the problem of constrained optimization. Taking into account the subject of this study, as well as the limitations of space, this article does not discuss these algorithms in-depth.

V. EXPERIMENT

A. METHODOLOGY

To demonstrate the significance of the Mesh–Order Independence theory in the practical CFD simulation, two benchmark cases are carried out in this section: the Helmholtz problem in a square domain and the Laplace problem in an L-shaped domain. Both of the problems have been widely studied, such as [26]–[29].

First, the Helmholtz problem in a square region $[-1, 1]^2$ is solved under different mesh density and discretization order, and the accuracy and performance of the solution are record and quantified. Here, the accuracy is described by L_2 error, while performance mainly refers to the execution time. In this test, the Lagrange element is used. The discretization order starts from $p = 1$ and increases gradually. The maximum discretization order is $p = 6$. Similarly, the initial mesh is a structured mesh with a size of 4×4 , and the grid spacing is 0.5. Then global refinement is used to uniformly refine the mesh, and the maximum mesh size is 1024×1024 . Fig. 3 shows the mesh under different grid spacing, which are sparse, medium and fine. It should be noted that, due to the memory limitation of the test platform, for $p = 5$ and $p = 6$, the maximum mesh size is 256×256 . Since the geometric shape is structured and simple, it is a typical case

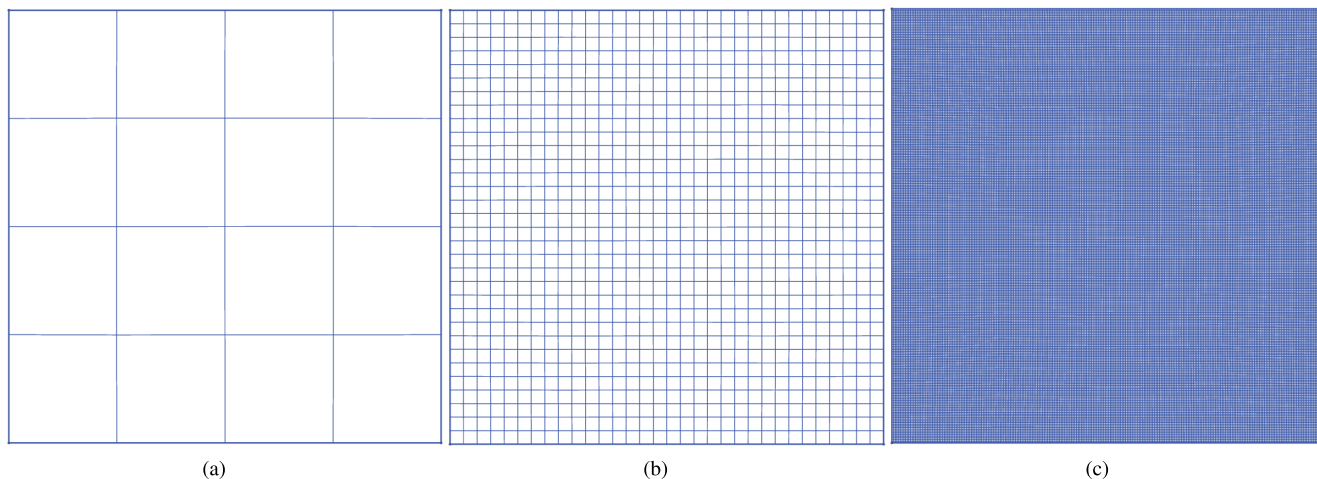


FIGURE 3. The meshes for the helmholtz problem. Left: The coarse mesh with 4×4 cells. Center: The medium mesh consists of 32×32 elements. Right: The fine mesh with 256×256 cells.

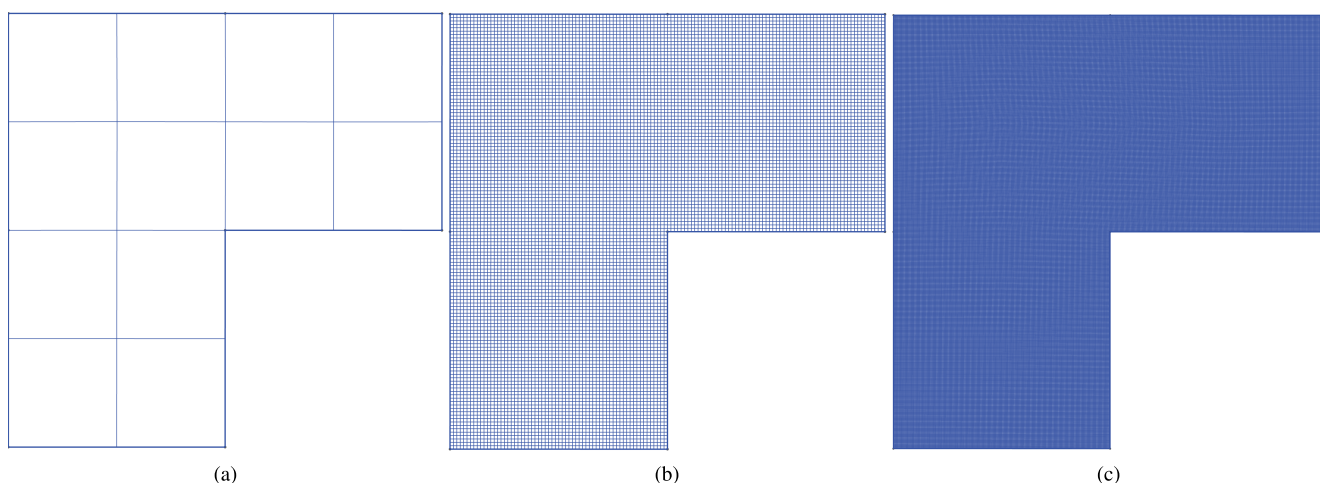


FIGURE 4. The L-shaped domain meshes used in simulations. The coarse mesh on the left consists of 21 vertices and 12 elements. The medium mesh on the center consists of 833 vertices and 768 elements. The fine mesh on the right consists of 197633 vertices and 196608 elements.

with smooth solution, and the exponential model can be used to establish the accuracy model. The performance model of the simulation will be established based on the degree of freedom (dofs). Finally, based on the established model and the theory of mesh degree independence, we will focus on the determination of the optimal Mesh–order independent pair and the prediction of the shortest simulation time under the prescribe accuracy.

Then, a singular solution to the Laplace problem in an L-shaped domain is considered as another model problem, see Fig. 4. For this case, the minimum and maximum size of the mesh are 12 and 196608, respectively, and the discretization order is also increasing from $p = 1$ to $p = 6$. Since the case is a singular problem, a linear function is used to model its simulation accuracy.

B. PLATFORM AND TEST CASES

1) SOFTWARE AND HARDWARE

Deal.II is an open source FEM software which offers support for a variety of finite elements, such as Lagrange elements

of any order, Nedelec and Raviart-Thomas elements of any order. For its portability, reliability, efficiency and usability, deal.II is widely used in many academic and commercial projects.

Deal.II version 8.4.1 is compiled with GCC-4.9.1 on a HPC cluster. Each of the computing nodes contains 12 Intel Xeon 2.1 GHz E5-2620 CPU cores and a total memory of 16GB.

2) TEST CASES

The Helmholtz equation is an elliptic partial differential equation describing electromagnetic waves, which has a wide range of applications in the fields of electromagnetic radiation, acoustics and seismology. For the sake of convenience, the equation that we are going to solve here is the Helmholtz equation “with the nice sign”:

$$-\Delta u + u = f$$

The boundary conditions are summarized as

$$\begin{cases} \Gamma_1 : u = g_1 \\ \Gamma_2 : n \cdot \nabla u = g_2 \end{cases}$$

where $\Gamma_1 = \{x = 1\} \cup \{y = 1\}$ and $\Gamma_2 = \{x = -1\} \cup \{y = -1\}$. To get the numerical solution of the above equation, the method of manufactured solutions is used. By choosing

$$\begin{cases} \bar{u}(x) = \sum_{i=1}^3 \exp\left(-\frac{|x-x_i|^2}{\sigma^2}\right) \\ f = -\Delta\bar{u} + \bar{u} \\ g_1 = \bar{u}|_{\Gamma_1} \\ g_2 = n \cdot \nabla\bar{u}|_{\Gamma_2} \end{cases}$$

where $\sigma = \frac{1}{8}$, $x_1 = (-\frac{1}{2}, \frac{1}{2})$, $x_2 = (-\frac{1}{2}, -\frac{1}{2})$ and $x_3 = (\frac{1}{2}, -\frac{1}{2})$, a numerical solution with $u = \bar{u}$ is obtained.

The singular Laplace problem in an L-shaped domain is widely used in the study of the mesh refinement. Here in this paper, the test case is similar to the problem in references [28]–[30] and the benchmark case on NIST (National Institute of Standards and Technology) AMR benchmarks site.¹ The equation and boundary conditions are summarized as

$$-\Delta u = 0$$

and

$$\begin{cases} \Gamma_1 : u = 0 \\ \Gamma_2 : n \cdot \nabla u = g \end{cases}$$

where the two edges meeting at the origin are denoted by Γ_1 and the other edges belong to the boundary Γ_2 . The exact solution to this problem is

$$\bar{u} = r^{2/3} \sin(2\theta/3)$$

where $r = \sqrt{x^2 + y^2}$, $\theta = \tan^{-1}(y/x)$.

C. THE RESULTS OF HELMHOLTZ PROBLEM

1) MODELLING

According to the type of finite element, the performance model based on the degree of freedom is:

$$Dofs = \left(\frac{p}{h} + 1\right)^2$$

As is described in Section V-A, the accuracy model can be built with the exponential function using nonlinear fitting. Here, the model is $e = a \times h^{p+1} + b$, while a and b are undetermined coefficients. It should be noted that since the value of e is small in magnitude, we first take the logarithm of the two sides of the model according to the method described in Section IV-C, and obtain a new equivalent model, and then use the fitting technique to obtain the undetermined coefficient. The other case is similar and will not be repeated.

It is clearly that the quality of the model depends on the number of pre-runs. Thus, three independent models are tested with the results of different pre-runs. Specifically, with the pre-runs of the following Mesh–order pairs:

$$A = \{pair(0.125, 1), pair(0.0625, 1), pair(0.125, 2), pair(0.0625, 2)\}$$

¹<http://math.nist.gov/amr-benchmark/index.html>

model A is built as:

$$\|e\|_A = 2^{1.654 \times \log_2 h \times p - 1.068 \times \log_2 h + 4.442 \times p - 6.651}$$

With the pre-runs of the following Mesh–order pairs:

$$B = A + \{pair(0.03125, 1), pair(0.03125, 2)\}$$

model B is built as:

$$\|e\|_B = 2^{1.596 \times \log_2 h \times p - 0.4748 \times \log_2 h + 4.25 \times p - 4.673}$$

Finally, model C:

$$\|e\|_C = 2^{1.406 \times \log_2 h \times p + 0.0273 \times \log_2 h + 3.552 \times p - 2.832}$$

is built with the pre-runs of the following Mesh–order pairs:

$$C = B + \{pair(0.015625, 1), pair(0.015625, 2)\}$$

2) PRACTICAL TEST RESULTS

To investigate the practical performance of different Mesh–order pairs, the results of practical test are shown in Fig. 5. Specifically, Fig. 5a shows the change of the actual accuracy of the simulation. It can be seen that the simulation error decreases exponentially with the discretization order increases, so it is reasonable to establish the error model with the exponential function. In the modeling of performance, the degree of freedom directly determines the size of the linear system of equations obtained by discrete partial equations, thus it is used as the evaluation index. The change of the error with the degree of freedoms is shown in Fig. 5b. In fact, the use of degrees of freedom to evaluate performance is a simplification because the efficiency of the solution of the linear systems is related not only to the size of the coefficient matrix, but also to some other factors such as the element distribution of the coefficient matrix, the condition number and so on. Thus, as can be seen in Fig. 5c, the relationship between simulation time and the degrees of freedom is not completely linear. Finally, In Fig. 5d we show the relationship between the actual simulation accuracy (i.e. L_2 error) and performance (i.e. execution time). It can be seen that for high accuracy requirements, a high discretization order is usually the optimal, while for low accuracy requirements, there is no such conclusion. This is consistent with the conclusions from Mitchell [16] and others.

According to the above test results, the optimal Mesh–order independent pair respect to prescribed accuracy can be easily obtained, as is shown in Table 1.

3) VERIFICATION

Based on the above-mentioned accuracy models and performance model, the optimal Mesh–order independent pairs under different accuracy requirements are predicted using the constrained optimization algorithm described in section IV-D. Table 2 shows the prediction results with model A. When compared with Table 1, it can be found that the prediction consistent with the tested results except accuracy requirement are 1.00E-1, 1.00E-3 and 1.00E-4. That is to say, the prediction accuracy is about 66.7% with 4 pre-runs.

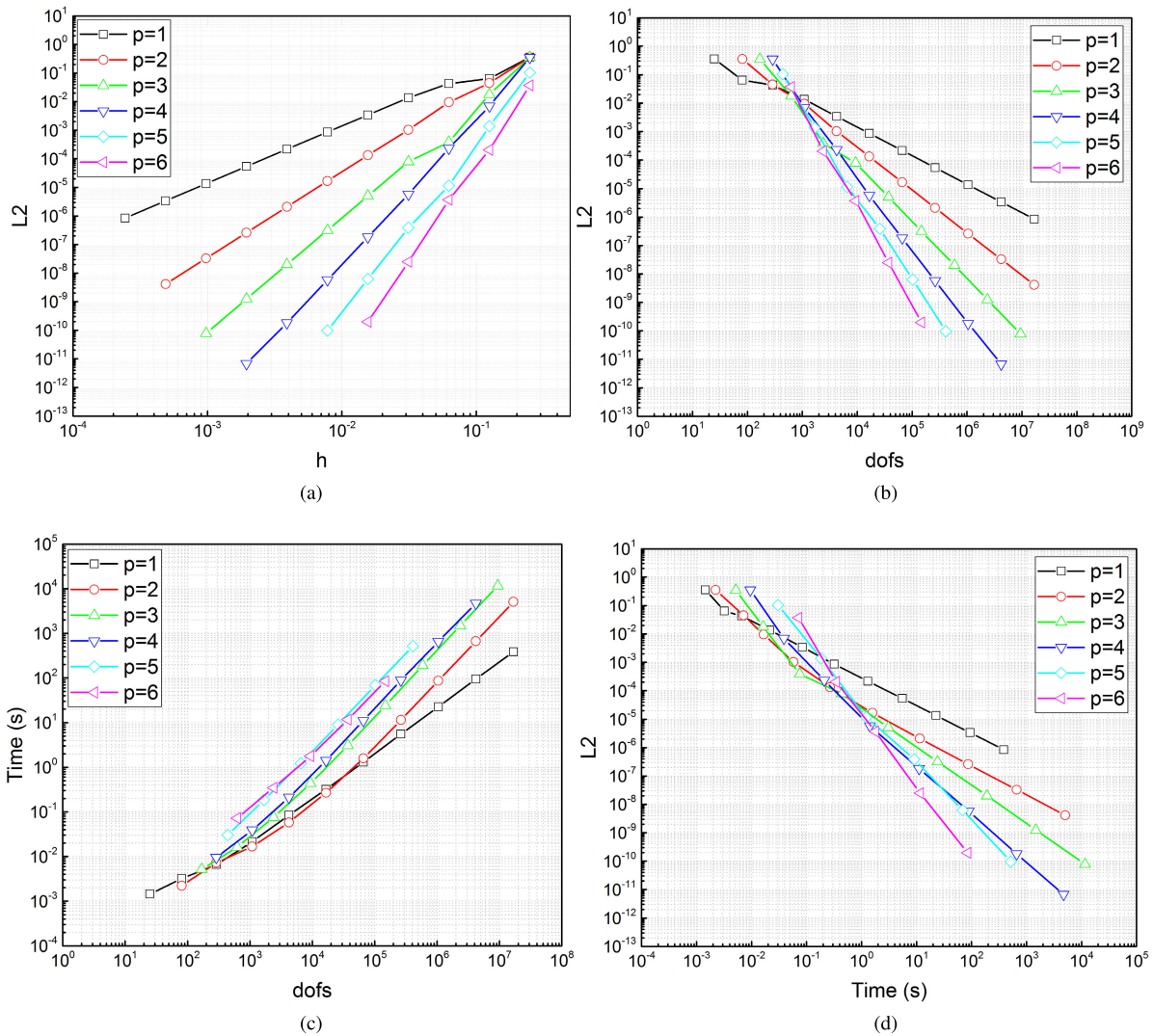


FIGURE 5. The solution results of the helmholtz problem. The different colors in all the figures represent the discretization order. Figure (a) is the log-log graph of the simulation accuracy versus grid size. Figure (b) is the log-log graph of the accuracy versus dofs. Figure (c) is the log-log graph of the simulation time versus dofs. Figure (d) is the log-log graph of the simulation accuracy versus execution time.

TABLE 1. The tested optimal mesh-order independent pairs for helmholtz problem.

| Accuracy | h | p | error | time |
|----------|----------|---|----------|--------|
| 1.00E-01 | 0.125 | 1 | 6.40E-02 | 0.0032 |
| 1.00E-02 | 0.0625 | 2 | 9.46E-03 | 0.0166 |
| 1.00E-03 | 0.0625 | 3 | 3.87E-04 | 0.0754 |
| 1.00E-04 | 0.03125 | 3 | 7.93E-05 | 0.438 |
| 1.00E-05 | 0.03125 | 4 | 5.76E-06 | 1.42 |
| 1.00E-06 | 0.03125 | 5 | 3.89E-07 | 9.1 |
| 1.00E-07 | 0.03125 | 6 | 2.47E-08 | 11.7 |
| 1.00E-08 | 0.015625 | 5 | 6.19E-09 | 69.1 |
| 1.00E-09 | 0.015625 | 6 | 1.96E-10 | 84.8 |

TABLE 2. The predicted optimal mesh-order independent pairs for helmholtz problem with model A.

| Accuracy | h | p | error | time |
|-----------------|---------------|----------|-----------------|----------------|
| 1.00E-01 | 0.25 | 1 | 3.57E-01 | 0.00245 |
| 1.00E-02 | 0.0625 | 2 | 9.46E-03 | 0.0166 |
| 1.00E-03 | 0.0625 | 4 | 2.32E-04 | 0.211 |
| 1.00E-04 | 0.0625 | 6 | 3.70E-06 | 1.78 |
| 1.00E-05 | 0.03125 | 4 | 5.76E-06 | 1.42 |
| 1.00E-06 | 0.03125 | 5 | 3.89E-07 | 9.1 |
| 1.00E-07 | 0.03125 | 6 | 2.47E-08 | 11.7 |
| 1.00E-08 | 0.015625 | 5 | 6.19E-09 | 69.1 |
| 1.00E-09 | 0.015625 | 6 | 1.96E-10 | 84.8 |

The prediction results with model B is shown in Table 3, and it is seen that the prediction accuracy increased to 77.8%. Further increase the number of pre-runs for nonlinear fitting,

we get model C, whose prediction result is the same as model B. Therefore, a prediction with 6 pre-runs is enough to get a prediction accuracy of 77.8% for this case.

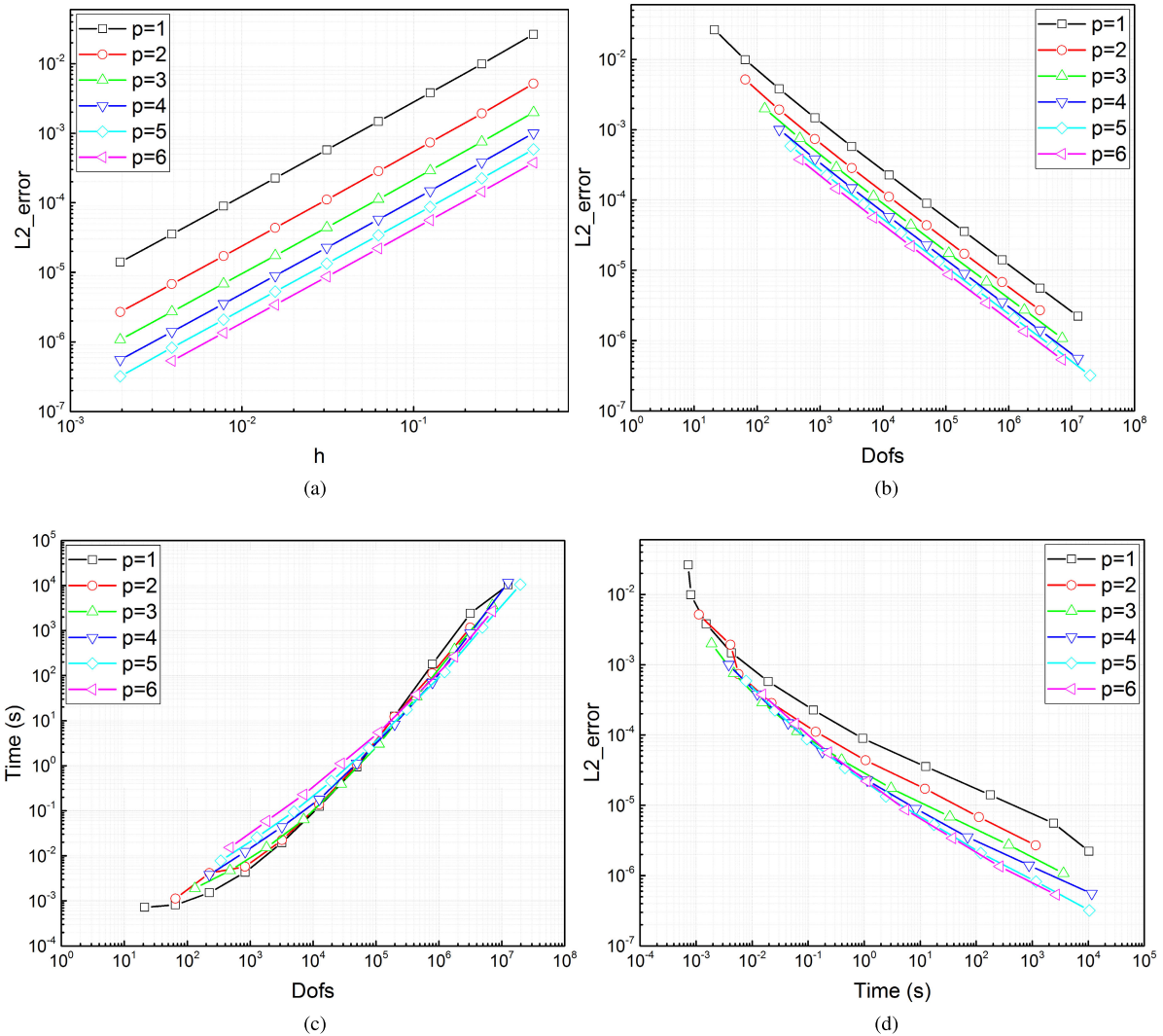


FIGURE 6. The solution results of the laplace problem. The different colors in all the figures represent the discretization order. Figure (a) is the log-log graph of the simulation accuracy versus grid size. Figure (b) is the log-log graph of the accuracy versus dofs. Figure (c) is the log-log graph of the simulation time versus dofs. Figure (d) is the log-log graph of the simulation accuracy versus execution time.

TABLE 3. The predicted optimal mesh-order independent pairs for helmholtz problem with model B and C.

| Accuracy | h | p | error | time |
|-----------------|---------------|----------|-----------------|--------------|
| 1.00E-01 | 0.125 | 1 | 6.40E-02 | 0.0032 |
| 1.00E-02 | 0.0625 | 2 | 9.46E-03 | 0.0166 |
| 1.00E-03 | 0.0625 | 4 | 2.32E-04 | 0.211 |
| 1.00E-04 | 0.0625 | 5 | 1.15E-05 | 1.23 |
| 1.00E-05 | 0.03125 | 4 | 5.76E-06 | 1.42 |
| 1.00E-06 | 0.03125 | 5 | 3.89E-07 | 9.1 |
| 1.00E-07 | 0.03125 | 6 | 2.47E-08 | 11.7 |
| 1.00E-08 | 0.015625 | 5 | 6.19E-09 | 69.1 |
| 1.00E-09 | 0.015625 | 6 | 1.96E-10 | 84.8 |

Since this article focuses on the application of the Mesh-Order Independence theory in practical simulation, all the modeling process has been simplified. First of all, the

accuracy model is simplified as an exponential function, which may need a more elaborate description. Then, all the models are established using curve fitting based on the results of the pre-runs, and there is a certain degree of fitting error. Last but not least, the use of degrees of freedom to approximate the simulation performance also has some error. Therefore, to study how to improve the prediction accuracy may be an open and interesting question in a subsequent project, and it will not be detailed here for the reason of the length of this paper.

D. THE RESULTS OF LAPLACE PROBLEM

1) MODELLING

This is a typical singular case, whose accuracy model is not suitable to establish with exponential function, so we use polynomial function instead. Two accuracy models:

$$\|e\|_A = 2^{(1.401 \times \log_2(h) - 2.185 \times p^{1.058} - 1.662)}$$

and

$$\|e\|_B = 2^{(1.413 \times \log_2(h) - 151.7 \times p^{0.02213} + 147.3)}$$

are established using the non-linear fitting method as in the previous case with the following Mesh–order pairs:

$$A = \{pair(0.5, 1), pair(0.25, 1), pair(0.5, 2), pair(0.25, 2)\}$$

and

$$B = \{pair(0.5, 1), pair(0.25, 1), pair(0.5, 2), pair(0.25, 2), pair(0.5, 3), pair(0.25, 3)\}$$

Similar to the Helmholtz problem, the performance model is still established based on degrees of freedom. According to the type of finite element and mesh refinement method, the performance model is:

$$Dofs = 3 \times \left(\frac{p}{h}\right)^2 + 4 \times \frac{p}{h} + 1$$

2) TEST AND PREDICTION RESULTS

The tested results of this case are shown in Fig. 6, and according to the tested results, the optimal Mesh–order independent pairs for this problem are shown in Table 4.

TABLE 4. The tested optimal mesh–order independent pairs for laplace problem.

| Accuracy | h | p | error | time |
|----------|----------|---|----------|----------|
| 1.00E-01 | 0.5 | 1 | 2.63E-02 | 0.000725 |
| 1.00E-02 | 0.5 | 2 | 5.15E-03 | 0.001121 |
| 1.00E-03 | 0.5 | 5 | 5.88E-04 | 0.007795 |
| 1.00E-04 | 0.125 | 5 | 8.72E-05 | 0.095401 |
| 1.00E-05 | 0.03125 | 6 | 8.65E-06 | 5.48201 |
| 1.00E-06 | 0.003906 | 5 | 8.25E-07 | 1169.12 |

TABLE 5. The predicted optimal mesh–order independent pairs for laplace problem with model A.

| Accuracy | h | p | error | time |
|-----------------|------------|----------|-----------------|-----------------|
| 1.00E-01 | 0.5 | 1 | 2.63E-02 | 0.000725 |
| 1.00E-02 | 0.5 | 2 | 5.15E-03 | 0.001121 |
| 1.00E-03 | 0.5 | 3 | 1.99E-03 | 0.001887 |
| 1.00E-04 | 0.5 | 4 | 1.01E-03 | 0.003823 |
| 1.00E-05 | 0.5 | 5 | 5.88E-04 | 0.007795 |
| 1.00E-06 | 0.5 | 5 | 5.88E-04 | 0.007795 |

As is similar to the previous test case, the optimal Mesh–order independent pair for this Laplace problem can be predicted by solving the optimization problem which is defined by the accuracy model and the performance model. As is shown in Table 5, the prediction accuracy with model A is poor, and only the first two prediction are correct. However, when the model is established with 6 pre-runs, the prediction

result is consistent with the actual results very well. Since this result is exactly the same as Table 4, it is not shown here.

According to the prediction results, when the accuracy requirements are high, such as less than 10^{-4} , the high order simulation shows a better performance than the lower ones, which is consistent with the results in the Helmholtz problem.

VI. CONCLUSIONS

A Mesh–order independent theory was proposed for high-order CFD simulation. It is designed to deal with the trade-offs between the simulation performance and accuracy, specifically by adjusting two critical impact factors, the grid spacing h and discretization order p . In order to demonstrate the specific procedure of choosing h and p based on this theory, a detailed flow chart is given with high-order finite element simulation as an example, and the key technologies involved are described in detail.

With the theoretical modeling and experimental verification of the solution of the benchmark cases, it is found that the Mesh–order independent theory proposed in this paper has a guiding significance on the configuration of the key parameters h and p in the practical simulation, especially in the case of high accuracy requirements, for example, the scientific computing accuracy requirements. In addition, although the proposed theory is applied only to high-order FEM simulations, it is universal and independent of the particular discrete method, and it is possible to be extended to other high-order methods.

The current study focuses mainly on the concept of Mesh–Order Independence, thus only the simple benchmark cases are discussed. Future work should consider the application of the proposed theory to some more complex and practical cases. For example, the modeling and application to the solution of Navier–Stokes equations on unstructured grid should be investigated. Other possible research directions include the extension of the theory to parallel CFD simulation.

APPENDIX A

The standard RE method is a method proposed by Richardson in the early 1900s to obtain a fourth order precision solution from the second order precision interpolation. The essence of this method is to treat the exact solution of the problem to be solved as an unknown variable, and then an equation system is obtained according to the numerical simulation results under two different sets of grids, and then the equations are solved to get the exact solution of the original problem. Let f^* be the exact solution of the original PDE, f is the second-order numerical solution of the original problem under the grid spacing h , then the following relationship holds:

$$f^* = f + ah^2 + O(h^2) \tag{7}$$

When the grid spacing is h_1 and h_2 , the numerical solutions f_1 and f_2 are substituted into Eq. 7:

$$\begin{cases} f^* = f_1 + ah_1^2 + O(h_1^3) \\ f^* = f_2 + ah_2^2 + O(h_2^3) \end{cases} \tag{8}$$

Ignore the high order terms (HOT) in Eq. 8, then solve the system of linear equations in two unknowns:

$$\begin{cases} a = (f_2 - f_1)/3h_1^2 \\ f^* = f_1 + (f_2 - f_1)/3 \end{cases} \quad (9)$$

Consider a more general case, such as the discrete accuracy p is unknown, then the Eq. 7 becomes:

$$f^* = f + a_p h^p + O(h^{p+1}) \quad (10)$$

where a new variable p is added. Since there are three unknowns, at least three equations need to be solved together, and then the simulation results of three sets of grid, h_1 , h_2 and h_3 , are needed. Taking into account the convenience of calculation and simulation, usually h_1 , h_2 and h_3 are choose to meet $h_1/h_2 = h_2/h_3 = r$, then:

$$\begin{cases} f^* = f_1 + a_p h_1^p + O(h_1^{p+1}) \\ f^* = f_2 + a_p h_2^p + O(h_2^{p+1}) \\ f^* = f_3 + a_p h_3^p + O(h_3^{p+1}) \end{cases} \quad (11)$$

Ignore the HOT in the system of Eq. 11, then we get

$$\begin{cases} p = \frac{\ln((f_3 - f_2)/(f_2 - f_1))}{\ln(r)} \\ a_p = \frac{f_2 - f_1}{r^p - 1} \\ f^* = f_1 + \frac{f_2 - f_1}{r^p - 1} \end{cases} \quad (12)$$

The Eq. 12 is the exact solution of the original equation obtained using the general RE method. It should be noted that the accuracy p obtained here is the observed degree of the numerical method. Thus, this method is also used to evaluate the true accuracy of discretization methods.

APPENDIX B

Taking the linear fitting function as an example, let the discrete data set be $\{x_i, y_i\}_{i=1}^n$, substituting the abscissa x_i of the discrete points into the model, the result is \hat{y}_i , and $\hat{y}_i = ax_i + b$ where $i = 1, 2, \dots, n$. The error between the estimated value \hat{y}_i and the actual value y_i is:

$$\Delta y_i = y_i - \hat{y}_i \quad (13)$$

The objective function S is defined as the sum of squares of errors between n actual and estimated values:

$$S = \sum_{i=1}^n \Delta y_i^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \sum_{i=1}^n (ax_i + b - y_i)^2 \quad (14)$$

Then, the fitting process is to find the appropriate coefficient a and b makes the objective function S minimum, that is,

$$a, b = \arg \min_{a^*, b^*} \sum_{i=1}^n (a^* x_i + b^* - y_i)^2 \quad (15)$$

According to the extremum theory, a and b that make S reach the minimum should satisfy the following relation:

$$\begin{cases} \frac{\partial S}{\partial a} = 2 \sum_{i=1}^n x_i (ax_i + b - y_i) = 0 \\ \frac{\partial S}{\partial b} = 2 \sum_{i=1}^n (ax_i + b - y_i) = 0 \end{cases} \quad (16)$$

Eq. 16 can be expressed in matrix form:

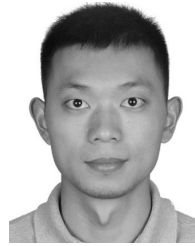
$$\underbrace{\begin{bmatrix} \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & n \end{bmatrix}}_A \cdot \underbrace{\begin{bmatrix} a \\ b \end{bmatrix}}_X = \underbrace{\begin{bmatrix} \sum_{i=1}^n x_i y_i \\ \sum_{i=1}^n y_i \end{bmatrix}}_B \quad (17)$$

When the matrix A is column full, we have a LLS solution for Eq. 17 as $X = A^{-1}B$.

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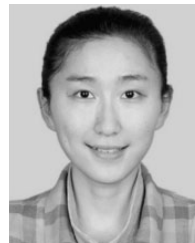


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