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Multiquadric Finite Difference (MQ-FD) Method and its Application

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Abstract. The conventional finite difference (FD) schemes are based on the low order polynomial approximation in a local region. This paper shows that when the polynomial approximation is replaced by the multiquadric (MQ) function approximation in the same region, a new FD method, which is termed as MQ-FD method in this work, can be developed. The paper gives analytical formulas of the MQ-FD method and carries out a performance study for its derivative approximation and solution of Poisson equation and the incompressible Navier-Stokes equations. In addition, the effect of the shape parameter c in MQ on the formulas of the MQ-FD method is analyzed. Derivative approximation in one-dimensional space and Poisson equation in two-dimensional space are taken as model problems to study the accuracy of the MQ-FD method. Furthermore, a lid-driven flow problem in a square cavity is simulated by the MQ-FD method. The obtained results indicate that this method may solve the engineering problem very accurately with a proper choice of the shape parameter c.

AMS subject classifications: 41A10, 41A30, 65N05

Key words: MQ–FD method, shape parameter, central FD method.

1 Introduction

Finite difference (FD) schemes are the most popular approaches used in engineering. In its most general form, the FD method is based on approximating some derivative of a function u at a given point by using a linear combination of the values of u at some surrounding points. Basically, the generation of the finite difference schemes is based on the polynomial approximation. Apart from polynomials, there are a lot of

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other approximate functions such as radial basis functions (RBFs) that can be used to generate finite difference schemes. RBFs are a primary tool for interpolating multidimensional scattered data. Due to their "mesh-free" nature, in the past decade, RBFs have received an increasing attention for derivative approximation and solution of partial differential equations (see, e.g., [1–8]). However, most of these methods are actually based on the function approximation by a global collocation approach. The global collocation approach generally results in a large, ill-conditioned linear system. Furthermore, function approximation approach is very complicated for solving nonlinear problems. These may be the reasons why the method has not so far been extensively applied to solve practical problems.

To resolve these problems and make RBF methods more feasible in solving PDEs, a local method named "local radial basis function-based differential quadrature method" has recently been proposed by Shu et al. [9]. This method adopted the idea of direct approximation of derivative through the differential quadrature (DQ) method, thus can be consistently well applied to linear and nonlinear problems. The DQ method was first proposed by Bellman et al. [10, 11] and its essence is that the derivatives of unknown function can be approximated in terms of the function values at a set of points, either uniformly or non-uniformly distributed. Suppose that a function $f(x)$ is sufficiently smooth, then its mth order derivative with respect to x at a point x_i can be approximated by DQ as

$$\frac{\partial^m f}{\partial x^m}\bigg|_{x_i} = \sum_{j=1}^{N} w_{i,j}^{(m)} f(x_j), \tag{1.1}$$

where x_j are the discrete points in the domain, $f(x_j)$ and $w_{i,j}^{(m)}$ are the function values at these points and the related weighting coefficients. This definition is actually similar to that of the finite difference method, so we can consider the DQ method as a "special" finite difference method. The key to the DQ method is to determine the weighting coefficients in derivative discretization of various orders. In the local RBF-DQ method, based on the analysis of a linear vector space and function approximation, RBFs are taken as the test functions in the DQ approximation to compute the weighting coefficients. Therefore, this method bears both the advantages of RBF approximation, e.g., mesh-free nature, and the advantages of DQ discretization, such as, easy implementation for both linear and nonlinear problems.

In implementing the local RBF-DQ method to solve fluid flow problems, we only need to substitute a set of RBF base functions into Eq. (1.1) and numerically solve the resultant linear equations to obtain the weighting coefficients. Although the procedure is quite simple, we cannot get its analytical formulas for derivative approximation. As a result, it is difficult to theoretically analyze this scheme, such as the influence of shape parameter. In addition, it is very difficult to compare this meshless method with the conventional numerical methods, such as finite difference scheme. In this paper, we apply the idea of local RBF-DQ method to the stencil of the central difference scheme to derive the new MQ-FD method, which has analytical form so that it can be compared with the conventional central difference scheme. In the paper, we mainly focus on the derivation of the RBF-FD method and its performance study for derivative approximation and solution of partial differential equations.

Currently, there are a number of RBFs, such as MQs, thin-plate splines, Gaussians and inverse MQs. Among them, MQ, which was first presented by Hardy [12], is the most popular one. Franke [13] carried out a comprehensive study on various RBFs, and found that MQ generally performs better for the interpolation of 2D scatter data. Compared with other RBFs, MQ RBFs are more accurate and converge faster at an exponential rate. Therefore, in our work, we will concentrate on MQ RBFs. Despite the excellent performance of MQ, however, it contains a shape parameter c, which strongly influences the accuracy of MQ approximation and must be determined by the user. A lot of work has been done on the choice of optimal shape parameters and some of them can be found in [13–15]. In this paper, we also study the effect of the shape parameter on the formulas of the MQ-FD method, especially when c goes to infinity. Furthermore, we numerically study the effect of the shape parameter on the accuracy of the MQ-FD method for derivative approximation in one-dimensional (1-D) space and solution of partial differential equations in two-dimensional (2-D) space.

This paper is structured as follows. In Section 2, we derive the MQ-FD method both in 1-D space and 2-D space. In addition, the effect of the shape parameter c on the formulas of the MQ-FD method is systematically studied. In Section 3, we numerically study the performance of the MQ-FD method for derivative approximation and solution of partial differential equations. A fluid flow problem is simulated by the MQ-FD method in Section 4 to demonstrate its capability for solving the incompressible fluid flow problems accurately. Some concluding remarks are given in Section 5.

2 Description of MQ-FD methods and comparison with central FD schemes

In this section, the derivation of the MQ-FD methods both in 1-D space and 2-D space is presented in detail. The basic idea to derive MQ-FD method is the same as that in local MQ-DQ method [9]. A global nodal index is used to identify points in the domain. For any reference point i, there is a supporting region, as shown in Fig. 1 (for 1-D space) and Fig. 2 (for 2-D space). A local nodal index is used to identify the supporting points for the reference point.

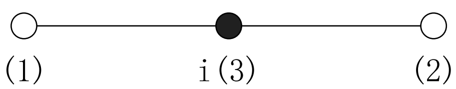


Figure 1: A supporting region for point i in 1-D space.

2.1 MQ-FD method in 1-D space

If a function $f(x)$ is assumed to be sufficiently smooth, its first and second order derivatives with respect to x at a point x_i can be approximated by the MQ-FD method as

$$f_x^{(1)}(x_i) = \sum_{k=1}^{3} w_{i,k}^{(1)} f(x_{i,k}), \tag{2.1}$$

$$f_x^{(2)}(x_i) = \sum_{k=1}^{3} w_{i,k}^{(2)} f(x_{i,k}), \tag{2.2}$$

where $w_{i,k}^{(1)}$ and $w_{i,k}^{(2)}$ are the related weighting coefficients, which need to be determined. $x_{i,k}$ represents the position of the kth supporting point for reference point i.

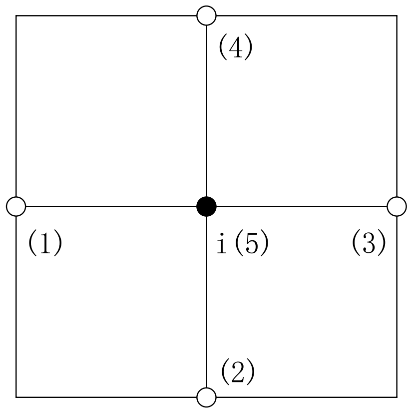


Figure 2: A supporting region for point i in 2-D space.

As shown in Fig. 1, in the supporting region for reference point i, function $f(x)$ can be locally approximated by MQ RBFs as

$$f(x) = \sum_{j=1}^{2} \lambda_j g_j(x) + \lambda_3, \tag{2.3}$$

where

$$g_j(x) = \sqrt{(x-x_j)^2 + c^2} - \sqrt{(x-x_3)^2 + c^2}, \qquad c > 0, \tag{2.4}$$

c is the shape parameter given by the user.

From the property of a linear vector space, if all the base functions, $g_j(x)$ $(j=1,2)$ and $g_3(x)=1$, satisfy the linear relationship (2.1) or (2.2), so does any function represented by Eq. (2.3). Thus when the weighting coefficients of DQ approximation are determined by all the base functions, they can be used to discretize the derivatives in a PDE, whose solution can actually be represented by Eq. (2.3).

Substituting the three base functions into Eqs. (2.1) and (2.2), we can get a set of linear equations, which can be expressed in the matrix form as

$$[D] = [G][W], \tag{2.5}$$

where

$$[D] = \begin{bmatrix} 0 & 0 \\ C & E \\ -C & E \end{bmatrix}, \quad [G] = \begin{bmatrix} 1 & 1 & 1 \\ A & B & -A \\ B & A & -A \end{bmatrix}, \quad [W] = \begin{bmatrix} w_{i,1}^{(1)} & w_{i,1}^{(2)} \\ w_{i,2}^{(1)} & w_{i,2}^{(2)} \\ w_{i,3}^{(1)} & w_{i,3}^{(2)} \end{bmatrix},$$

$$A = c - \sqrt{\Delta^2 + c^2}, \quad B = \sqrt{4\Delta^2 + c^2} - \sqrt{\Delta^2 + c^2},$$

$$C = \frac{\Delta}{\sqrt{\Delta^2 + c^2}}, \qquad E = \frac{c^2}{(\sqrt{\Delta^2 + c^2})^3} - \frac{1}{c},$$

where Δ is the mesh spacing. Based on Cramer's rule, the elements of matrix $[W]$ can be obtained. First of all, we will illustrate the procedure of obtaining the weighting coefficients for the first order derivative. Determinants of matrices can be expressed as

$$|G| = \begin{vmatrix} 1 & 1 & 1 \\ A & B & -A \\ B & A & -A \end{vmatrix} = -2AB + 3A^2 - B^2 = (3A+B)(A-B),$$

$$|G_{11}| = \begin{vmatrix} 0 & 1 & 1 \\ C & B & -A \\ -C & A & -A \end{vmatrix} = 3AC + BC = (3A+B)C,$$

$$|G_{21}| = \begin{vmatrix} 1 & 0 & 1 \\ A & C & -A \\ B & -C & -A \end{vmatrix} = -3AC - BC = -(3A+B)C,$$

$$|G_{31}| = \begin{vmatrix} 1 & 1 & 0 \\ A & B & C \\ B & A & -C \end{vmatrix} = 0.$$

Thus, the weighting coefficients are

$$w_{i,1}^{(1)} = \frac{|G_{11}|}{|G|} = \frac{(3A+B)C}{(3A+B)(A-B)} = \frac{C}{A-B},$$

$$w_{i,2}^{(1)} = \frac{|G_{21}|}{|G|} = \frac{-(3A+B)C}{(3A+B)(A-B)} = \frac{-C}{A-B},$$

$$w_{i,3}^{(1)} = \frac{|G_{31}|}{|G|} = \frac{0}{(3A+B)(A-B)} = 0.$$

With the above weighting coefficients, the first order derivative can be expressed as

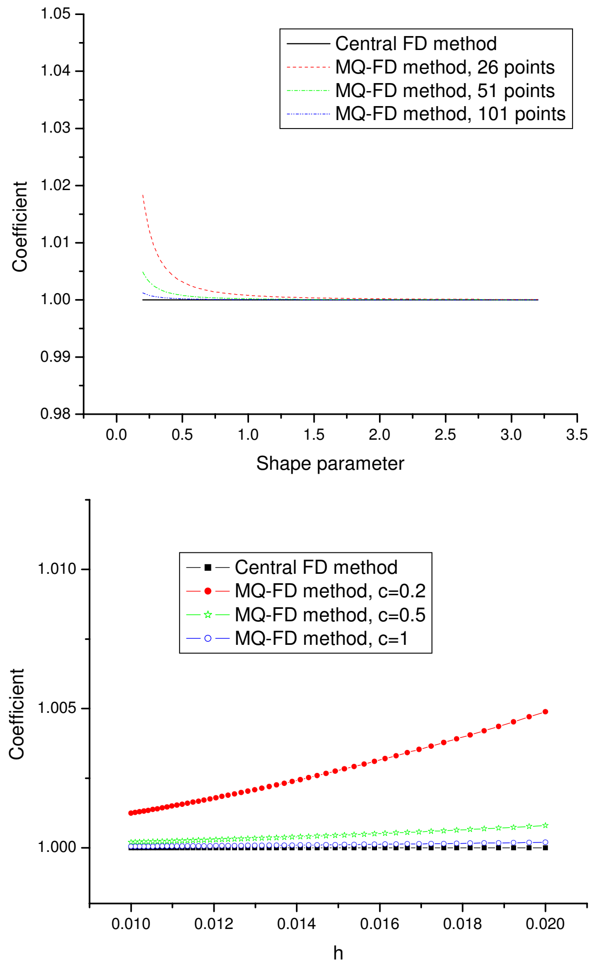


Figure 3: Effect of shape parameter c and mesh spacing h on the coefficient of formula for first order derivatives. (a) Coefficient variation with regard to shape parameter c. (b) Coefficient variation with regard to mesh spacing h.

$$
\begin{aligned}
f_x^{(1)}(x_i) &= \frac{C}{A-B}\Big(f(x_{i,1}) - f(x_{i,2})\Big) \\
&= \frac{\Delta}{(\sqrt{4\Delta^2+c^2}-c)\sqrt{\Delta^2+c^2}}\Big(f(x_{i,2}) - f(x_{i,1})\Big).
\end{aligned} \tag{2.6}
$$

Compared with the formula of the central FD scheme for the first order derivative, i.e.,

$$
f_x^{(1)}(x_i) = \frac{1}{2\Delta}\Big(f(x_{i,2}) - f(x_{i,1})\Big),
$$

the formula of the MQ-FD method is dependent on the value of the shape parameter c. In the following, we will discuss the effect of the shape parameter on the formula of the MQ-FD method.

1. When c goes to infinity, according to the Binomial Theorem, we have

$$\begin{aligned}
&\lim_{c\to\infty}\sqrt{\Delta^2+c^2}\\
=&\lim_{c\to\infty}c\big(1+\frac{\Delta^2}{c^2}\big)^{\frac{1}{2}}=\lim_{c\to\infty}c\big(1+\frac{1}{2}\frac{\Delta^2}{c^2}-\frac{1}{8}\frac{\Delta^4}{c^4}+\cdots\big)=\lim_{c\to\infty}(c+\cdots),\\
&\lim_{c\to\infty}(\sqrt{4\Delta^2+c^2}-c)\\
=&\lim_{c\to\infty}[c(1+\frac{1}{2}\frac{4\Delta^2}{c^2}-\frac{1}{8}\frac{16\Delta^4}{c^4}+\cdots)-c]=\lim_{c\to\infty}(\frac{2\Delta^2}{c}+\cdots),
\end{aligned}$$

and

$$\begin{aligned}
&\lim_{c\to\infty}\frac{\Delta}{(\sqrt{4\Delta^2+c^2}-c)\sqrt{\Delta^2+c^2}}\\
=&\frac{\Delta}{\lim_{c\to\infty}(\sqrt{4\Delta^2+c^2}-c)\lim_{c\to\infty}\sqrt{\Delta^2+c^2}}\\
=&\frac{\Delta}{\lim_{c\to\infty}(\frac{2\Delta^2}{c}+\cdots)\lim_{c\to\infty}(c+\cdots)}=\frac{1}{2\Delta}.
\end{aligned}$$

Thus, when c goes to infinity, we can get

$$f_x^{(1)}(x_i)=\frac{1}{2\Delta}\Big(f(x_{i,2})-f(x_{i,1})\Big),$$

which is the same as the formula of the central FD scheme. This observation shows that the "classical" polynomial-based FD scheme can be reproduced by the MQ-FD method in the limit of $c\to\infty$.

2. When $0<c<\infty$, we numerically compare the formula of the MQ-FD method with that of the central FD scheme. Dividing the formula of the MQ-FD method by that of the central FD scheme, we can get a coefficient of

$$\frac{2\Delta^2}{(\sqrt{4\Delta^2+c^2}-c)\sqrt{\Delta^2+c^2}}.$$

Fig. 3(a) plots the curves of the coefficient according to the shape parameter c with Δ to be 0.04 (26 points), 0.02 (51 points) and 0.01 (101 points), respectively. From this figure, we can see that the coefficient is always larger than 1 and when c goes to infinity, the coefficient approaches 1, which is consistent with the above observation. Another point to be emphasized here is that if the shape parameter c is fixed, with decreasing Δ, the coefficient gets closer to 1. This phenomenon can also be seen from Fig. 3(b), in which the curves of coefficient with regard to Δ are displayed for the shape parameter c of 0.2, 0.5 and 1, respectively.

The procedure for the weighting coefficients of the second order derivative is the same. Determinants of matrices are

$$|G_{12}| = \begin{vmatrix} 0 & 1 & 1 \\ E & B & -A \\ E & A & -A \end{vmatrix} = AE - BE = (A-B)E,$$

$$|G_{22}| = \begin{vmatrix} 1 & 0 & 1 \\ A & E & -A \\ B & E & -A \end{vmatrix} = AE - BE = (A-B)E,$$

$$|G_{32}| = \begin{vmatrix} 1 & 1 & 0 \\ A & B & E \\ B & A & E \end{vmatrix} = 2BE - 2AE = -2(A-B)E.$$

Thus, the weighting coefficients can be obtained as

$$w_{i,1}^{(2)} = \frac{|G_{12}|}{|G|} = \frac{(A-B)E}{(3A+B)(A-B)} = \frac{E}{3A+B},$$
$$w_{i,2}^{(2)} = \frac{|G_{22}|}{|G|} = \frac{(A-B)E}{(3A+B)(A-B)} = \frac{E}{3A+B},$$
$$w_{i,3}^{(2)} = \frac{|G_{32}|}{|G|} = \frac{-2(A-B)E}{(3A+B)(A-B)} = -2\frac{E}{3A+B}.$$

With these weighting coefficients, the second order derivative can be expressed as

$$\begin{aligned} f_x^{(2)}(x_i) &= \frac{E}{3A+B}\Big(f(x_{i,1}) + f(x_{i,2}) - 2f(x_{i,3})\Big) \\ &= \frac{\frac{c^2}{(\sqrt{\Delta^2+c^2})^3} - \frac{1}{c}}{3c - 4\sqrt{\Delta^2+c^2} + \sqrt{4\Delta^2+c^2}}\Big(f(x_{i,1}) + f(x_{i,2}) - 2f(x_{i,3})\Big). \end{aligned} \tag{2.7}$$

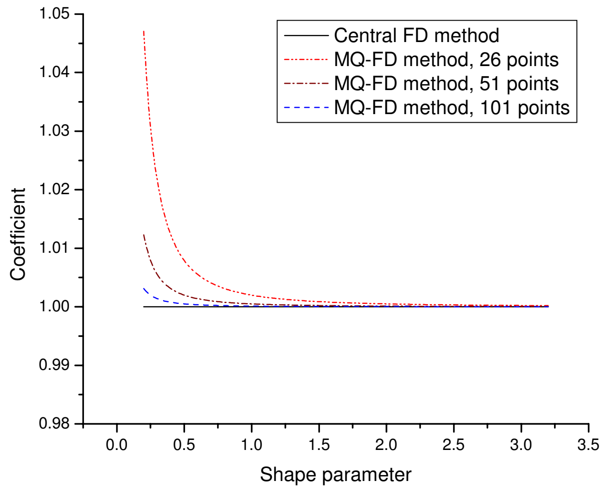
Similar to the procedure for the first order derivative, we study the effect of the shape parameter c on the formula of MQ-FD method for the second order derivative.

1. When c goes to infinity,

$$\begin{aligned} &\lim_{c\to\infty}\Big(\frac{c^2}{\sqrt{\Delta^2+c^2}^3} - \frac{1}{c}\Big) = \lim_{c\to\infty}\frac{c^3 - \sqrt{\Delta^2+c^2}^3}{c\sqrt{\Delta^2+c^2}^3} \\ =& \lim_{c\to\infty}\frac{c^3 - c^3\big(1 + \frac{3}{2}\frac{\Delta^2}{c^2} + \frac{3}{8}\frac{\Delta^4}{c^4} + \cdots\big)}{c^4\big(1 + \frac{3}{2}\frac{\Delta^2}{c^2} + \frac{3}{8}\frac{\Delta^4}{c^4} + \cdots\big)} = \lim_{c\to\infty}\Big(-\frac{3}{2}\frac{\Delta^2}{c^3} + \cdots\Big), \end{aligned}$$

and

$$\begin{aligned} &\lim_{c\to\infty}\Big(3c - 4\sqrt{\Delta^2+c^2} + \sqrt{4\Delta^2+c^2}\Big) \\ =& \lim_{c\to\infty}\Big[3c - 4c\big(1 + \frac{1}{2}\frac{\Delta^2}{c^2} - \frac{1}{8}\frac{\Delta^4}{c^4} + \cdots\big) + c\big(1 + \frac{1}{2}\frac{4\Delta^2}{c^2} - \frac{1}{8}\frac{16\Delta^4}{c^4} + \cdots\big)\Big] \\ =& \lim_{c\to\infty}\Big(-\frac{3}{2}\frac{\Delta^4}{c^3} + \cdots\Big). \end{aligned}$$



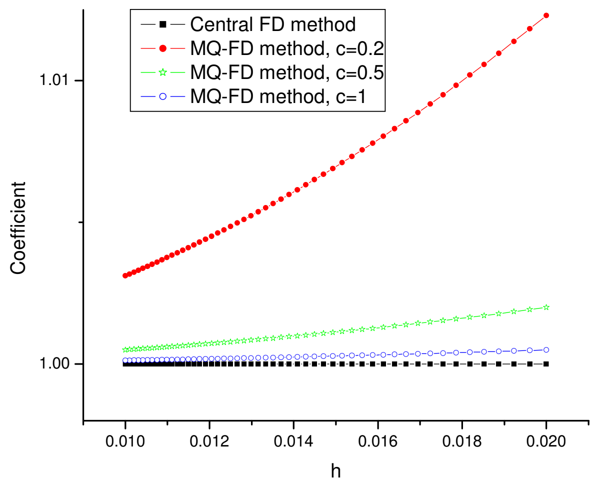


Figure 4: Effect of shape parameter c and mesh spacing h on the coefficient of formula for second order derivatives. (a) Coefficient variation with regard to shape parameter c. (b) Coefficient variation with regard to mesh spacing h.

Thus, when c goes to infinity, we have

$$f_x^{(2)}(x_i) = \frac{1}{\Delta^2}\Big(f(x_{i,1}) + f(x_{i,2}) - 2f(x_{i,3})\Big).$$

This formula is also the same as that by the central difference scheme, which confirms the above observation.

2. When $0<c<\infty$, we also numerically compare the formula of the MQ-FD method with that of the central FD scheme. The corresponding coefficient for the second order derivative is

$$\frac{\frac{c^2}{(\sqrt{\Delta^2+c^2})^3} - \frac{1}{c}}{3c - 4\sqrt{\Delta^2+c^2} + \sqrt{4\Delta^2+c^2}}\Delta^2.$$

Fig. 4(a) plots the curves of the coefficient according to the shape parameter c with Δ to be 0.04 (26 points), 0.02 (51 points) and 0.01 (101 points), respectively. Fig. 4(b) presents the curves of coefficient with regard to Δ with the shape parameter c to be 0.2, 0.5 and 1, respectively. From these two figures, we can see that, similar to those for the first order derivatives, with Δ fixed, the larger the c, the closer the coefficient approaches 1 and with c fixed, the smaller the Δ, the closer the coefficient approaches 1.

2.2 MQ-FD method in 2-D space

If a function $f(x,y)$ is assumed to be sufficiently smooth, its second order derivatives with respect to x and with respect to y, at a point (x_i, y_i) can be approximated by the MQ-FD method as

$$f_x^{(2)}(x_i, y_i) = \sum_{k=1}^{5} w_{i,k}^{(2)} f(x_{i,k}, y_{i,k}), \tag{2.8}$$

$$f_y^{(2)}(x_i, y_i) = \sum_{k=1}^{5} \bar{w}_{i,k}^{(2)} f(x_{i,k}, y_{i,k}), \tag{2.9}$$

where $w_{i,k}^{(2)}$ and $\bar{w}_{i,k}^{(2)}$ are the related weighting coefficients in the x and y directions, which need to be determined. $(x_{i,k}, y_{i,k})$ represents the position of the kth supporting point for reference point i.

As shown in Fig. 2, in the supporting region for reference point i, function $f(x,y)$ can be locally approximated by MQ RBFs as

$$f(x,y) = \sum_{j=1}^{4} \lambda_j g_j(x,y) + \lambda_5, \tag{2.10}$$

where

$$g_j(x,y) = \sqrt{(x-x_j)^2 + (y-y_j)^2 + c^2} - \sqrt{(x-x_5)^2 + (y-y_5)^2 + c^2}. \tag{2.11}$$

Substituting the five base functions, $g_j(x,y)$ $(j=1,\cdots,4)$ and $g_5(x,y)=1$, into Eqs. (2.8) and (2.9), we can obtain a set of linear equations, which can be expressed in the matrix form as

$$[D] = [G][W], \tag{2.12}$$

where

$$[D] = \begin{bmatrix} 0 & 0 \\ X & Y \\ Y & X \\ X & Y \\ Y & X \end{bmatrix}, \quad [G] = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ A & B & C & B & -A \\ B & A & B & C & -A \\ C & B & A & B & -A \\ B & C & B & A & -A \end{bmatrix}, \quad [W] = \begin{bmatrix} w_{i,1}^{(2)} & \bar{w}_{i,1}^{(2)} \\ w_{i,2}^{(2)} & \bar{w}_{i,2}^{(2)} \\ w_{i,3}^{(2)} & \bar{w}_{i,3}^{(2)} \\ w_{i,4}^{(2)} & \bar{w}_{i,4}^{(2)} \\ w_{i,5}^{(2)} & \bar{w}_{i,5}^{(2)} \end{bmatrix},$$

where

$$A = c - \sqrt{\Delta^2 + c^2}, \qquad B = \sqrt{2\Delta^2 + c^2} - \sqrt{\Delta^2 + c^2},$$

$$C = \sqrt{4\Delta^2 + c^2} - \sqrt{\Delta^2 + c^2}, \quad X = \frac{c^2}{(\sqrt{\Delta^2 + c^2})^3} - \frac{1}{c}, \quad Y = \frac{1}{\sqrt{\Delta^2 + c^2}} - \frac{1}{c}.$$

The procedure for coefficients in 2-D space is similar to that in 1-D space. Compared with the 3×3 dimensional matrix in 1-D space, G in 2-D space is a 5×5 dimensional matrix. Thus we cannot compute the determinants of matrices directly. Instead, the software Maple is used to compute the determinants. Determinants of matrices are:

$$\begin{aligned}
|G| &= (C-A)^2(5A + C + 2B)(A + C - 2B), \\
|G_{11}| &= (C-A)^2(XC + 3XA - 2YA - 2BY), \\
|G_{21}| &= (C-A)^2(YC + 3YA - 2XA - 2XB), \\
|G_{31}| &= (C-A)^2(XC + 3XA - 2YA - 2BY), \\
|G_{41}| &= (C-A)^2(YC + 3YA - 2XA - 2XB), \\
|G_{51}| &= -2(C-A)^2(A + C - 2B)(X + Y).
\end{aligned}$$

Thus, the weighting coefficients can be obtained as

$$\begin{aligned}
w_{i,1}^{(2)} &= \frac{|G_{11}|}{|G|} = \frac{XC + 3XA - 2YA - 2BY}{(5A + C + 2B)(A + C - 2B)}, \\
w_{i,2}^{(2)} &= \frac{|G_{21}|}{|G|} = \frac{YC + 3YA - 2XA - 2XB}{(5A + C + 2B)(A + C - 2B)}, \\
w_{i,3}^{(2)} &= \frac{|G_{31}|}{|G|} = \frac{XC + 3XA - 2YA - 2BY}{(5A + C + 2B)(A + C - 2B)}, \\
w_{i,4}^{(2)} &= \frac{|G_{41}|}{|G|} = \frac{YC + 3YA - 2XA - 2XB}{(5A + C + 2B)(A + C - 2B)}, \\
w_{i,5}^{(2)} &= \frac{|G_{51}|}{|G|} = -2\frac{(X + Y)}{5A + C + 2B}.
\end{aligned}$$

When c goes to infinity, based on the binomial theorem, we have:

$$\begin{aligned}
\lim_{c\to\infty} \sqrt{\Delta^2 + c^2} &= \lim_{c\to\infty} \Big(c + \frac{1}{2}\frac{\Delta^2}{c} - \frac{1}{8}\frac{\Delta^4}{c^3} + \cdots \Big), \\
\lim_{c\to\infty} \sqrt{2\Delta^2 + c^2} &= \lim_{c\to\infty} \Big(c + \frac{\Delta^2}{c} - \frac{1}{2}\frac{\Delta^4}{c^3} + \cdots \Big), \\
\lim_{c\to\infty} \sqrt{4\Delta^2 + c^2} &= \lim_{c\to\infty} \Big(c + 2\frac{\Delta^2}{c} - 2\frac{\Delta^4}{c^3} + \cdots \Big), \\
\lim_{c\to\infty} (\Delta^2 + c^2)^{-\frac{3}{2}} &= \lim_{c\to\infty} \Big(\frac{1}{c^3} - \frac{3}{2}\frac{\Delta^2}{c^5} + \frac{15}{8}\frac{\Delta^4}{c^7} + \cdots \Big), \\
\lim_{c\to\infty} (\Delta^2 + c^2)^{-\frac{1}{2}} &= \lim_{c\to\infty} \Big(\frac{1}{c} - \frac{1}{2}\frac{\Delta^2}{c^3} + \frac{3}{8}\frac{\Delta^4}{c^5} + \cdots \Big).
\end{aligned}$$

Thus, we can get:

$$
\begin{aligned}
&X+Y=\lim_{c\to\infty}\Big(-2\frac{\Delta^2}{c^3}+\cdots\Big),\\
&5A+C+2B=\lim_{c\to\infty}\Big(-2\frac{\Delta^4}{c^3}+\cdots\Big),\\
&A+C-2B=\lim_{c\to\infty}\Big(-\frac{\Delta^4}{c^3}+\cdots\Big),\\
&XC+3XA-2YA-2BY=X(C+3A)-2Y(A+B)=\lim_{c\to\infty}\Big(2\frac{\Delta^6}{c^6}+\cdots\Big),\\
&YC+3YA-2XA-2XB=Y(C+3A)-2X(A+B)=0.
\end{aligned}
$$

Finally, the coefficients can be obtained as:

$$
\begin{aligned}
&w_{i,1}^{(2)}=w_{i,3}^{(2)}=\frac{\lim\limits_{c\to\infty}\Big(2\frac{\Delta^6}{c^6}+\cdots\Big)}{\lim\limits_{c\to\infty}\Big(-2\frac{\Delta^4}{c^3}+\cdots\Big)\lim\limits_{c\to\infty}\Big(-\frac{\Delta^4}{c^3}+\cdots\Big)}=\frac{1}{\Delta^2},\\
&w_{i,2}^{(2)}=w_{i,4}^{(2)}=0,\qquad w_{i,5}^{(2)}=-2\frac{\lim\limits_{c\to\infty}\Big(-2\frac{\Delta^2}{c^3}+\cdots\Big)}{\lim\limits_{c\to\infty}\Big(-2\frac{\Delta^4}{c^3}+\cdots\Big)}=\frac{-2}{\Delta^2}.
\end{aligned}
$$

Thus, when c goes to infinity, we have:

$$
\begin{aligned}
f_x^{(2)}(x_i,y_i)&=\sum_{k=1}^{5}w_{i,k}^{(2)}f(x_{i,k},y_{i,k})\\
&=\frac{1}{\Delta^2}\Big(f(x_{i,1},y_{i,1})+f(x_{i,3},y_{i,3})-2f(x_{i,5},y_{i,5})\Big).
\end{aligned}\tag{2.13}
$$

Based on the symmetric property, we have

$$
f_y^{(2)}(x_i,y_i)=\frac{1}{\Delta^2}\Big(f(x_{i,2},y_{i,2})+f(x_{i,4},y_{i,4})-2f(x_{i,5},y_{i,5})\Big),\tag{2.14}
$$

when c goes to infinity. These formulas are the same as those by the central difference scheme, which is consistent with the above observation.

3 Performance study of MQ-FD methods for derivative approximation and solution of Poisson equations

In this section, we study the performance of the MQ-FD methods for derivative approximation and solution of Poisson equations. Derivatives in 1-D space and Poisson equations in 2-D space are taken as model problems and results are compared with those obtained by the central FD scheme.

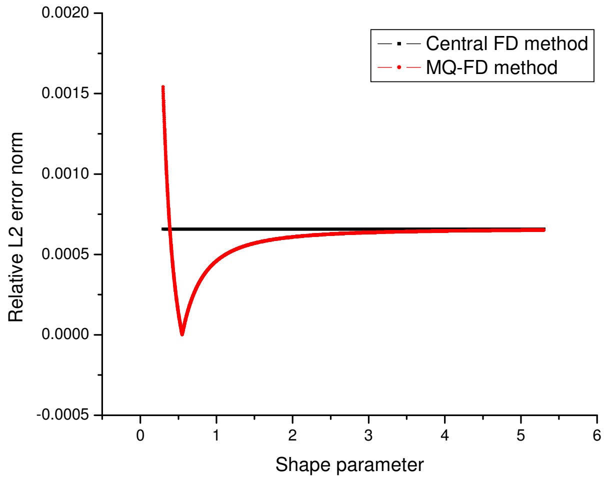
3.1 Derivative approximation of the MQ-FD method in 1-D space

In this part, the first and second order derivatives of two functions,

$$f = \sin(\pi x) \quad \text{and} \quad f = x^4,$$

are approximated by both the MQ-FD method and the central FD scheme. Accuracy obtained by the MQ-FD method with different shape parameters is shown in Figs. 5 and 6, in which, accuracy by the central FD scheme is also displayed for comparison. The grid is chosen to be 51×51 and the function values on the grid points are taken as known.

Fig. 5 indicates that, as compared with the central FD scheme, the MQ-FD method may approximate the derivatives of the function f=$\sin(\pi x)$ more accurately or less



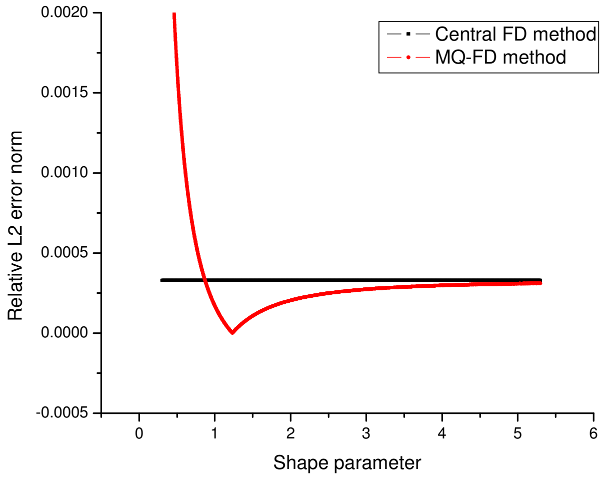


Figure 5: Derivative approximation of $\sin(\pi x)$ by the central FD method and the MQ-FD method. (a) First order derivative. (b) Second order derivative.

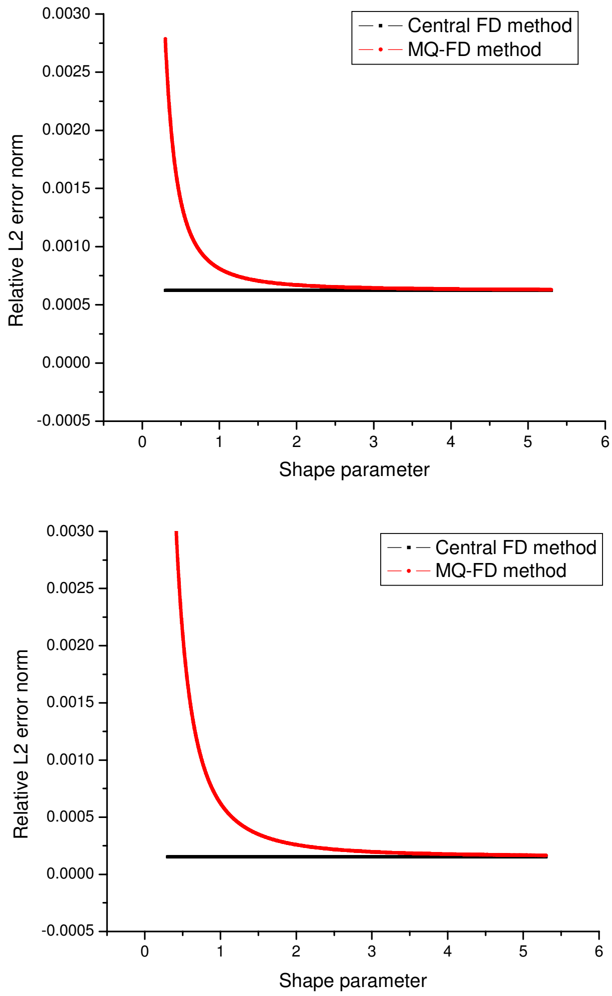


Figure 6: Derivative approximation of x^4 by the central FD method and the MQ-FD method. (a) First order derivative. (b) Second order derivative.

accurately according to the choice of shape parameter c. When the value of c is very small, the accuracy of derivative approximation by the MQ-FD method is very low. With increase of the c value, there exists a range of c with which the MQ-FD method approximates the derivatives more accurately than the central FD scheme does. When the value of the shape parameter c goes to infinity, the accuracy achieved by the MQ-FD method approaches that by the central FD scheme. Comparatively, the accuracy of derivative approximation of the function $f=x^4$ achieved by the MQ-FD method is always lower than that by the central FD scheme whatever c is, as shown in Fig. 6. However, when c goes to infinity, the accuracy by the MQ-FD method also goes to that by the central FD scheme. This is in good agreement with what we have derived in the last section that when c goes to infinity, the MQ-FD method can be reduced to the central FD scheme.

3.2 Application for solution of Poisson equations in 2-D space

In this part, we study the performance of the MQ-FD method for solution of Poisson equation in 2-D space. Poisson equation is taken as a model problem, which can be written as:

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}=f(x,y), \quad \text{in } \Omega=\{(x,y)|0\leqslant x,y\leqslant 1\}, \tag{3.1a}$$

$$T=g, \quad \text{on } \partial\Omega, \tag{3.1b}$$

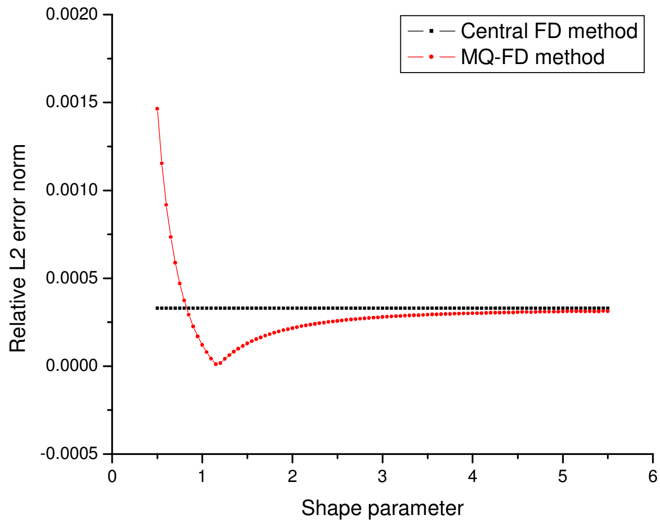
where f and g are determined in such a manner that the exact solution T of the Poisson equation is the given one.

To study the performance of the MQ-FD method in simulating two classical types of flow problems: periodic boundary value problems and general boundary value problems, we take

$$T=\sin(\pi x)\sin(\pi y) \quad \text{and} \quad T=x^4+y^4,$$

as two typical solution functions. Here, T=$\sin(\pi x)\sin(\pi y)$ can represent the solution of the periodic boundary value problems and T=x^4+y^4 can stand for the solution of the general boundary value problems. First, we will observe the effect of the shape parameter c on the MQ-FD result. Accuracy obtained by the MQ-FD method with different shape parameters is shown in Fig. 7, in which, accuracy by the central FD scheme is also displayed for comparison. The grid is chosen to be 51×51. Comparing Figs. 5, 6 and 7, we can see that the effect of the shape parameter on the performance of the MQ-FD method for the solution of Poisson equations in 2-D space is very similar to that on its performance for derivative approximation in 1-D space.

Then we illustrate the convergence rate of the MQ-FD method as the grid is refined. To study the convergence rate of the method, we choose ten different values of the shape parameter c, ranging from 0.02 to 10, and solve the Poisson equation with grid of 21×21, 41×41, 61×61, 81×81 and 101×101. Convergence rate of the MQ-FD method with different shape parameters and that of the central FD scheme are shown in Fig. 8. From this figure, we can see that the slope of the convergence rate of the MQ-FD method with certain shape parameter c, say from 0.1 to 5, is parallel to that of the central FD scheme. However, when the shape parameter is very small (0.02 and 0.05) or very large (8 and 10), the symbols representing the accuracy of solution are not in a line. This is reasonable. It is well known that when c is very small, the MQ-FD method can not solve the Poisson equation accurately and when c is very large, the condition number of matrix G in Eq. (2.12) becomes very large. That is, matrix G becomes highly ill-conditioned, leading to a large numerical error of MQ-FD method. Another point to be emphasized here is that for T=$\sin(\pi x)\sin(\pi y)$, with the increase of the shape parameter c, the accuracy of the MQ-FD method can be improved to be higher than that of the central FD scheme. However, with further increase of the shape parameter c, the accuracy of the MQ-FD method will be decreased due to ill-condition of the MQ-FD matrices. For T=x^4+y^4, with the increase of the shape parameter c, the



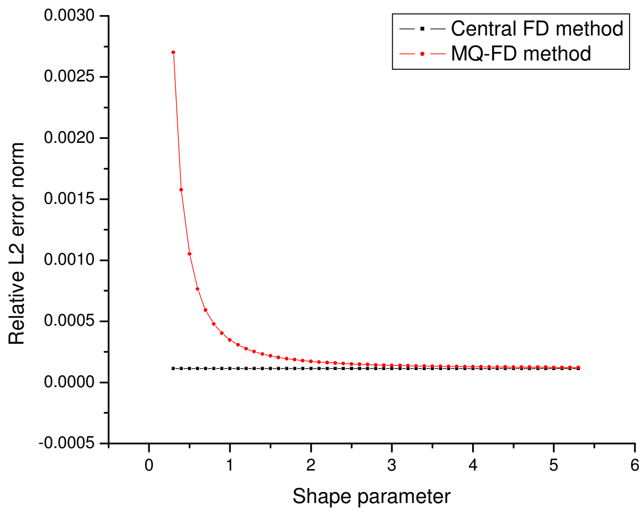


Figure 7: Comparison of accuracy between the MQ-FD method and the central FD method for solution of Poisson equations. (a) $\sin(\pi x)\sin(\pi y)$. (b) x^4+y^4.

accuracy of the MQ-FD method can be improved to approach that of the central FD scheme. These results are consistent with those in Fig. 7.

4 Simulation of lid-driven flow in a square cavity

In the last section, we have carried out the performance study of the MQ-FD methods for derivative approximation and solution of Poisson equations. Now, we will illustrate the ability of the MQ-FD method for solving fluid flow problems accurately. In this study, a steady incompressible lid-driven flow in a square cavity is taken as a model problem, as shown schematically in Fig. 9. The governing equations are the two dimensional steady incompressible Navier-Stokes equations in the vorticity-stream function form, which can be written as

$$u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y} = \frac{1}{Re}\Big(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2}\Big), \tag{4.1}$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = \omega, \tag{4.2}$$

where Re is the Reynolds number, ω is the vorticity, ψ is the stream function, u, v denote the components of velocity in the x and y directions, which can be calculated

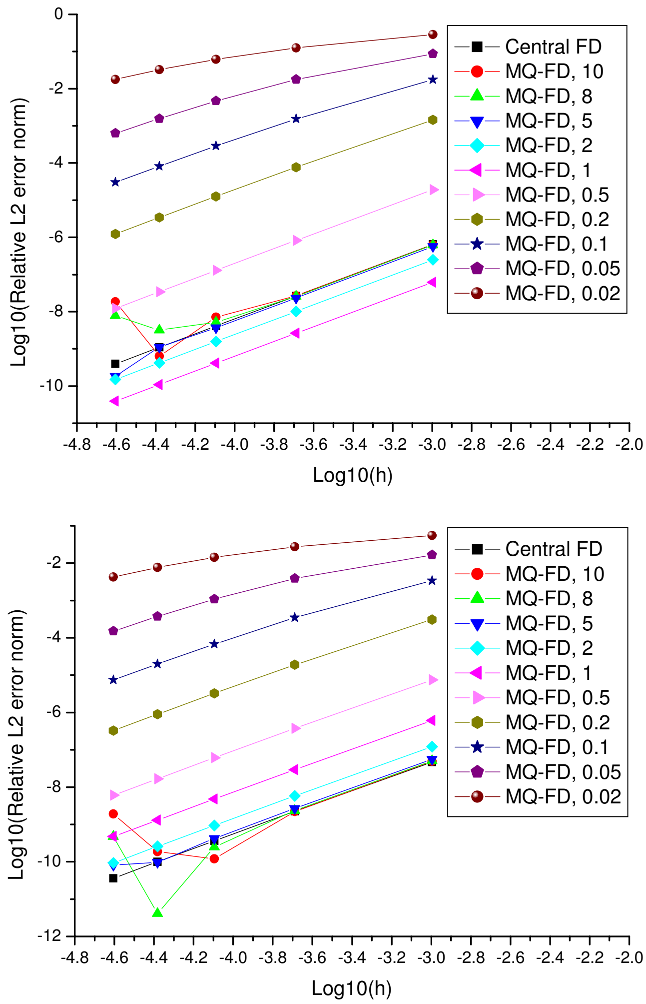


Figure 8: Convergence rate of the MQ-FD methods with different shape parameters for solution of Poisson equation. (a) $T = \sin(\pi x)\sin(\pi y)$. (b) $T = x^4 + y^4$.

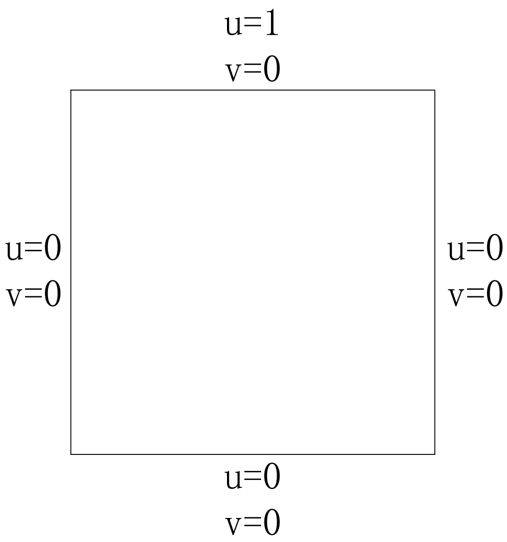


Figure 9: Configuration of a lid-driven flow in a square cavity.

from the stream function

$$u = \frac{\partial \psi}{\partial y}, \quad v = -\frac{\partial \psi}{\partial x}. \tag{4.3}$$

For this model problem, Re is chosen to be 1000 and 5000, respectively.

In this study, the governing Eqs. (4.1)-(4.3) are discretized by the MQ-FD method. The discretization form of the governing equations at a general node i can be written as:

$$u_i \sum_{k=1}^{5} w_{i,k}^{(1)} \omega_i^k + v_i \sum_{k=1}^{5} \bar{w}_{i,k}^{(1)} \omega_i^k = \frac{1}{Re}\Big(\sum_{k=1}^{5} w_{i,k}^{(2)} \omega_i^k + \sum_{k=1}^{5} \bar{w}_{i,k}^{(2)} \omega_i^k \Big), \tag{4.4}$$

$$\sum_{k=1}^{5} w_{i,k}^{(2)} \psi_i^k + \sum_{k=1}^{5} \bar{w}_{i,k}^{(2)} \psi_i^k = \omega_i, \tag{4.5}$$

$$u_i = \sum_{k=1}^{5} \bar{w}_{i,k}^{(1)} \psi_i^k, \qquad v_i = -\sum_{k=1}^{5} w_{i,k}^{(1)} \psi_i^k. \tag{4.6}$$

The boundary conditions of this problem can be written as:

$$\begin{aligned}
&u = 0, \quad v = 0, \quad \psi = 0, \quad \text{at } x = 0, 1, \quad 0 \le y < 1, \\
&u = 0, \quad v = 0, \quad \psi = 0, \quad \text{at } y = 0, \quad\;\; 0 \le x \le 1, \\
&u = 1, \quad v = 0, \quad \psi = 0, \quad \text{at } y = 1, \quad\;\; 0 \le x \le 1.
\end{aligned}$$

The boundary condition for ω can be derived from Eq. (4.2), i.e.,

$$\omega|_{wall} = \frac{\partial^2 \psi}{\partial x^2}\Big|_{wall} + \frac{\partial^2 \psi}{\partial y^2}\Big|_{wall}. \tag{4.7}$$

The general solution procedure of the MQ-FD method for the above governing equations is shown below:

1. Set up the node distribution (uniform Cartesian grid points) in the domain.
2. Determine the supporting points for each reference point.
3. Calculate the weighting coefficients for the related derivatives in the governing equations. Actually it is only necessary to compute the coefficients once and apply them all over the discretization.
4. Discretize the governing equations with the computed weighting coefficients.
5. Solve the resultant algebraic equations.

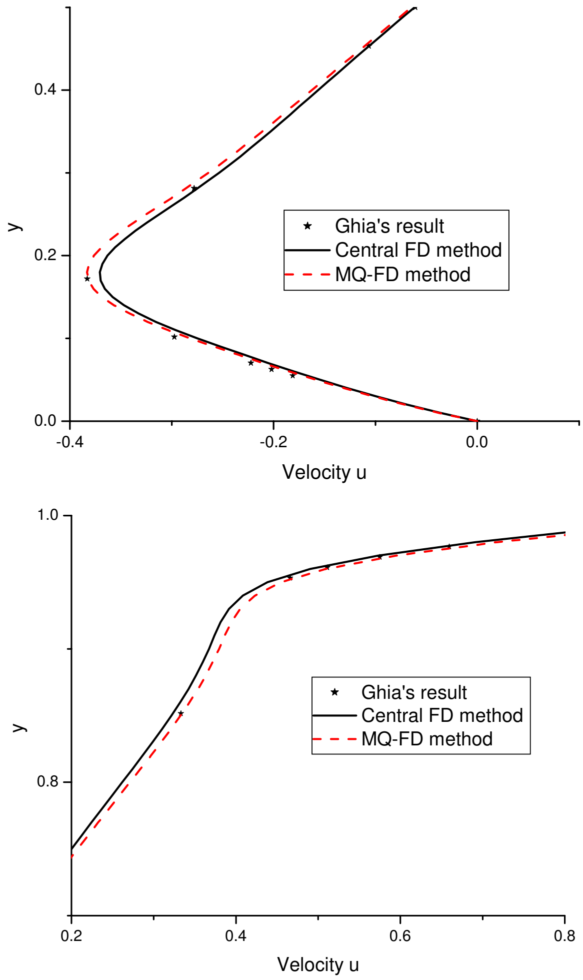


Figure 10: Local u-velocity profile along vertical centerline $Re = 1000$. (a) Enlarged view around $y = 0.2$. (b) Enlarged view around $y = 0.9$.

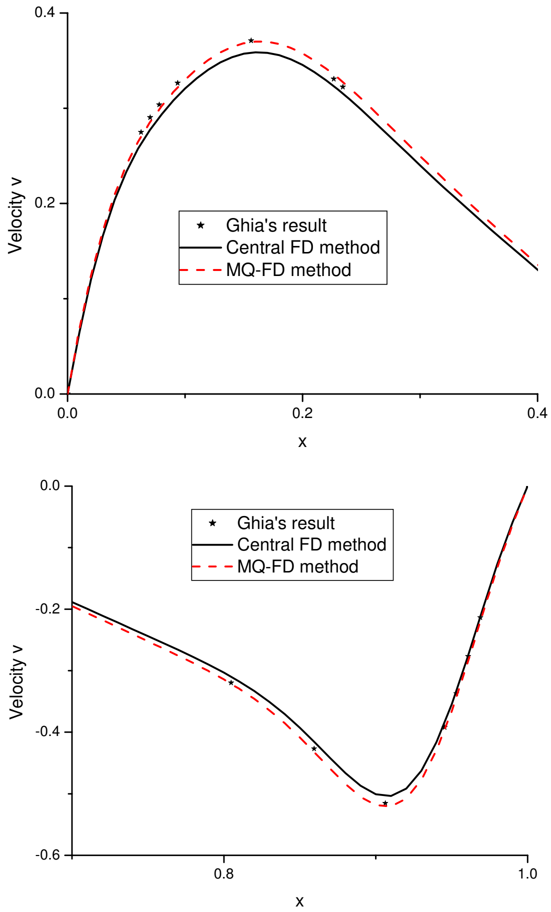
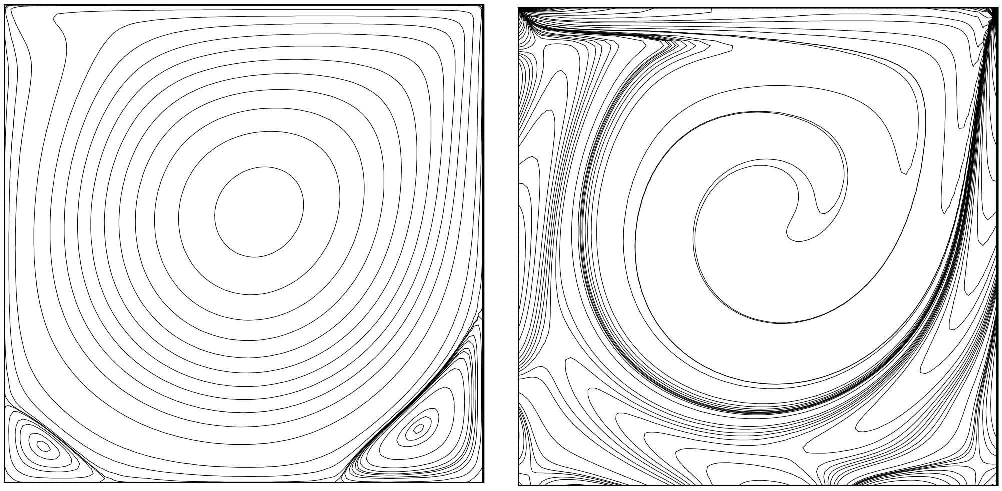


Figure 11: Local v-velocity profile along horizontal centerline at $Re = 1000$. (a) Enlarged view around $x = 0.2$. (b) Enlarged view around $x = 0.9$.

Firstly, the problem is solved by the MQ-FD method with a Cartesian mesh of 101×101 for Re=1000. The shape parameter c is chosen to be 0.03 in this case. After discretizing the governing equations on all the interior points by the MQ-FD method, we get a set of linear algebraic equations. To solve the resultant equations, the successive over-relaxation (SOR) method is used. The computed velocity component u at the vertical centerline of x=0.5 and v at the horizontal centerline of y=0.5 are plotted in Figs. 10 and 11. Since there is no analytical solution for this problem, the result of Ghia et al. [16] is adopted as the benchmark data to validate the present results. The numerical results by the central FD scheme with the same grid are also plotted in the figure for comparison. In order to see the accuracy difference of these two methods clearly, only the enlarged view of the velocity component u around y=0.2 & 0.9 and v around x=0.2 & 0.9 is presented, where the biggest differences occur. From these figures, we can see that although both methods solve the problem very accurately, the numerical results of the MQ-FD method agree better with the benchmark solution. This means

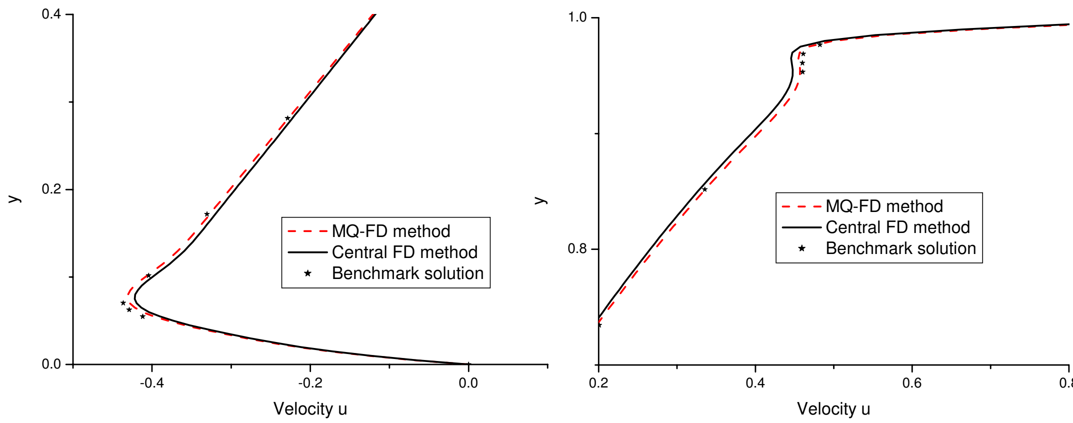


(a) Streamlines (b) Vorticity contour

Figure 12: Contours of lid-driven cavity flow at $Re = 1000$.

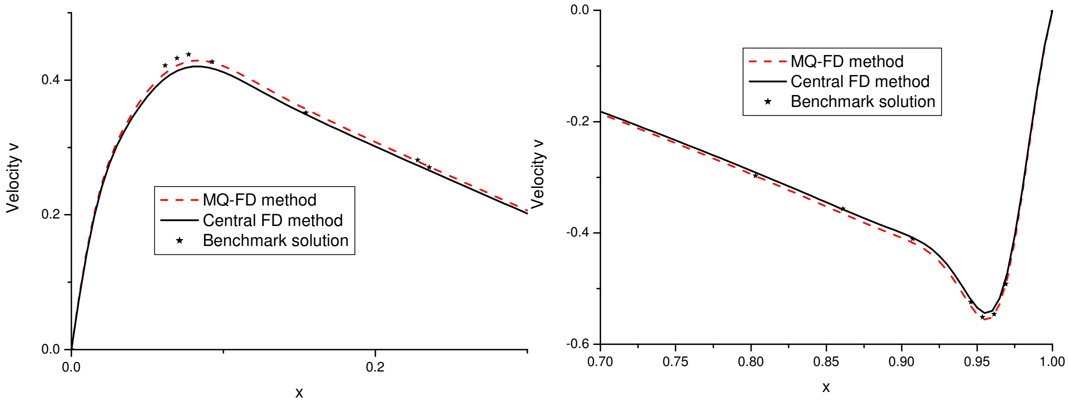
that if a proper shape parameter c is chosen, the MQ-FD method may simulate this fluid flow problem more accurately than the central FD scheme with the same Cartesian mesh. The streamlines and vorticity contours of this case by the MQ-FD method on the uniform mesh of 101×101 are shown in Fig. 12. They also agree well with those in the work of Ghia et al. [16].

For Re=5000, the Cartesian mesh is chosen to be 201×201 and the shape parameter is taken as 0.02. It is well known that as compared with the case of Re=1000, the flow with Re=5000 is much more difficult to be simulated. The computed velocity



(a) Enlarged view around $y = 0.2$ (b) Enlarged view around $y = 0.9$

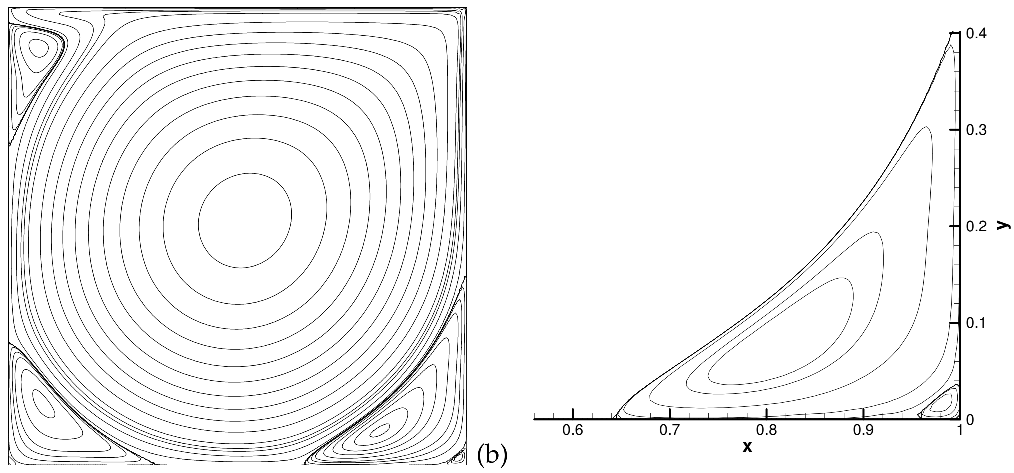
Figure 13: Local u-velocity profile along vertical centerline at $Re = 5000$.



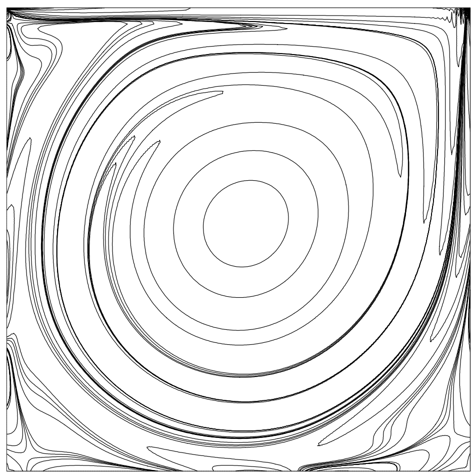
(a) Enlarged view around $x = 0.2$ (b) Enlarged view around $x = 0.9$

Figure 14: Local v-velocity profile along horizontal centerline at $Re = 5000$.

(a)



(b)



(c)

Figure 15: Contours of lid-driven cavity flow at $Re = 5000$. (a) Streamlines. (b) Enlarged view of the left bottom corner. (c) Vorticity contour.

component u at the vertical centerline of x=0.5 and v at the horizontal centerline of y=0.5 are plotted in Figs. 13 and 14, together with the results of Ghia et al. [16] and those by the central FD scheme. From these figures, we can also observe that the results by the MQ-FD method agree better with the benchmark solution as compared with those of the central FD scheme. Fig. 15 shows the streamlines and vorticity contours of this case. To display the secondary vortices clearly, an enlarged view of the left bottom corner is also included. These results, including the configuration and positions of the vortices, are in good agreement with those of Ghia et al. [16]. This implies that the MQ-FD method can simulate incompressible fluid flows with high Reynolds numbers accurately.

5 Conclusions

In this paper, the MQ-FD method was derived and its performance for derivative approximation and solution of Poisson equation and incompressible Navier-Stokes equations was investigated. In addition, the effect of the shape parameter c on the formulas and accuracy of the MQ-FD method was analyzed. It was found that when c goes to infinity, the MQ-FD formulas of derivative approximation are the same as those given by the central FD scheme. With regard to the accuracy of the MQ-FD methods, it was found that if the shape parameter c is properly chosen, the MQ-FD method may solve periodic boundary value problems more accurately than the central FD scheme does. For general boundary value problems, however, the accuracy by the MQ-FD method may not be as accurate as that by the central FD scheme. When the value of c is not very small, the accuracy by these two methods is very close. The lid-driven flow in a square cavity is simulated by the MQ-FD method. Results showed that with a proper shape parameter c, the MQ-FD method can simulate this flow problem very accurately, as compared with the central FD scheme.

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