Cubic Interpolation Profile Method For Transient Hydrodynamics of Solid Particles in Enclosure

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Abstract – The goal of this study is to determine the effect of transient vortex structure on solid particles and explain this behaviour in terms of particles’ trajectories. In the present study, an alternative numerical scheme was proposed to predict the fluid flow and coupled with a Lagrangian scheme on the prediction of solid phase. The dynamics of solid particle in a lid-driven cavity was investigated at a wide range of Reynolds numbers. The results of this study suggest that the particle trajectories are critically dependence on the magnitude of Reynolds numbers and the vortex behaviour in the cavity. Good comparisons with the experimental and previous studies demonstrate the multidisciplinary applications of the present scheme.

Keywords: Fluid-solid interaction, Cubic interpolation profile, Lid-driven cavity, Solid particle
I. Introduction

The phenomenon of multiphase flow can be seen not only in daily live situations but also in almost all engineering applications. The importance in understanding this problem results in many technical papers appear in recent years discussing its impacts on engineering. Among the researches pertinent to this problem, comparatively very few researchers devoted their study on the interaction between solid particles and fluid flow. Interestingly, this type of multiphase fluid flow plays an important role in the seeds drying technology, separation of grains, productions of milk powder, fluidized beds, coal combustion and many others.

It is believed that the main reason of lack of understanding on the fluid-solid interaction phenomenon is the complicated nature of the problem. The size of solid particles can be as big as grains seed or very tiny such as dust pollutant. Till present day, most researchers rely on computational rather than experimental approach to study the behavior of these particles in fluid flow. To the best of authors’ knowledge, only Tsorng et al. [1] reported details experimental results on the behavior of solid particles in lid-driven cavity flow from micro to macro size of particles. Other experimental works are Adrian [2], Han et al. [3], Matas et al. [4], Ushijima and Tanaka [5], Ide and Ghil [6], Hu [7], Liao [8], Ramkissoon and Rahaman [9], Mahmut and Kemal [10], etc. However, according to these papers, high accuracy of laser equipments together with high-speed digital image capture and data interpretation system is required to obtain reliable experimental data. Such high cost devices will not be affordable if not supported by research fund.

As an alternative approach, many researchers considered fully computational scheme in their investigations [11-14]. Kosinski et al. [15-16] provides extensive numerical results on the subject. From the behavior of one particle in a lid-driven cavity flow to thousands of particles in expansion horizontal pipe has been studied in their research works sheds new hope in understanding this problem. Kosinski et al. applied the combination of continuum Navier-Stokes equations to predict fluid flow and second Newton’s law for solid particle.

Definitely, a proper numerical model is required to predict the interaction between the fluid and solid particle. With a precise treatment, the trajectory of a solid particle in a complex fluid structure, which will be demonstrated in this paper, can be reproduced at certain level of accuracy. In this paper, a lid-driven cavity flow is used as a benchmark problem due to its simple geometry and complicated flow behaviours. It is usually very difficult to capture the flow phenomena near the singular points at the corners of the cavity. Therefore, the objective of this study is both to propose a numerical scheme that can be used to predict the interaction between the fluid and solid particle, as well as to analyze the flow structure in the lid-driven cavity.

II. Problem physics and the governing equations

The physical domain of the problem is represented by a cavity with top lid is constantly moved to the right direction at different constant velocity $U_{wall}$ to give the Reynolds number $(Re = U_{wall}H/u)$ range from 100 to 1000. The aspect ratio was set up as unity. In the present analysis, the computations are conducted on a two-dimensional plane. This two-dimensional approximation was undertaken based on a physical assumption that the behaviour of the lid driven vortex is relatively unaffected by the three dimensionality of the flow. In present study, the governing equation of the incompressible and two-dimensional formulation is considered. Therefore, the governing continuity and x- and y-momentum equations can be expressed as follow

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$  \hspace{1cm} (1)

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$  \hspace{1cm} (2)

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right)$$  \hspace{1cm} (3)

In this work, the pressure term in the Eq. (2) and (3) are eliminated and rewrite in terms of vorticity function as follow

$$\frac{\partial \omega}{\partial t} + u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y} = \nu \left( \frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2} \right)$$  \hspace{1cm} (4)

In terms of stream function, the equation defining the vorticity becomes

$$\omega = \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}$$  \hspace{1cm} (5)

Before considering any numerical solution to the above set of equations, it is convenient to rewrite the equations...
in terms of dimensionless variables. The following dimensionless variables will be used here

\[ \Psi = \frac{\psi}{u_x D}, \quad \Omega = \frac{\alpha D^2 \text{Pr}}{\nu} \]

\[ U = \frac{u}{u_x}, \quad V = \frac{v}{u_x} \]

\[ X = \frac{x}{D}, \quad Y = \frac{y}{D}, \quad T = \frac{t u_x}{D} \]

In terms of these variables, Eqs. (4) and (5) become

\[ \frac{\partial \Omega}{\partial T} + U \frac{\partial \Omega}{\partial X} + V \frac{\partial \Omega}{\partial Y} = \frac{1}{\text{Re}} \left( \frac{\partial^2 \Omega}{\partial X^2} + \frac{\partial^2 \Omega}{\partial Y^2} \right) \]

(7)

\[ \Omega = \left( \frac{\partial^2 \psi}{\partial X^2} + \frac{\partial^2 \psi}{\partial Y^2} \right) \]

(8)

where the dimensionless parameter Reynolds number, \( \text{Re} \) is defined as

\[ \text{Re} = \frac{u_x D}{\nu} \]

(9)

### III. Solution Approach

Cubic interpolation Profile method (CIP) was proposed and has been highly proven to be a universal solver for hyperbolic type of equations [17]. The CIP is known as a numerical method for solving the advection term with low numerical diffusion. This method constructs a solution inside the grid cell close enough to the real solution of the given equation [18].

To see this, we begin by recalling Eq. (7) and express in one-dimensional form as follow.

\[ \frac{\partial \Omega}{\partial T} + U \frac{\partial \Omega}{\partial X} = 0 \]

(10)

Note that we dropped the right hand side of the original equation and Eq. (10) reduces to a pure wave equation without source term. The theoretical solution of Eq. (10) is obtained by shifting a profile

\[ \Omega(X, T + \Delta T) = \Omega(X - U \Delta T, T) \]

(11)

Which represents a simple translation of profile with constant velocity \( U \). If we differentiate Eq. (10) with spatial variable \( X \), then we get

\[ \frac{\partial \Omega}{\partial T} + U \frac{\partial \Omega}{\partial X} = 0 \]

(12)

where \( \Omega_X = \partial \Omega/\partial X \). Eq. (12) coincides with Eq. (10) and represents the translation of \( \Omega_X \) with velocity \( U \). The novel idea behind this approach is, we trace the time evolution of both \( \Omega \) and \( \Omega_X \) using Eqs. (12) and (10) and the profile at each points after one step is specified according to Eq. (12). With this restriction, we can greatly reduce the numerical diffusion when we construct the profile [19-20].

In this method, the spatial quantities in the point interval are approximated with constrained polynomial using \( \Omega \) and \( \Omega_X \) at neighbouring points as follow

\[ F_i(X) = a_i \bar{X}^3 + b_i \bar{X}^2 + \Omega_X \bar{X} + \Omega_i \]

(13)

where \( \bar{X} = X - X_i \). The coefficients \( a \) and \( b \) are then determined so that the interpolation function and its first derivatives are continuous at both ends. As a result, we have

\[ a_i = \left( \frac{\Omega_{X,j} + \Omega_{X,j-1}}{\Delta X^2} \right) - \frac{2(\Omega_i - \Omega_{i+1})}{\Delta X^2} \]

(14)

\[ b_i = \left( \frac{2\Omega_{X,j} + \Omega_{X,j-1}}{\Delta X} \right) - \frac{3(\Omega_i - \Omega_{i-1})}{\Delta X^2} \]

(15)

where \( \Delta X = X_i - X_{i-1} \). Once \( F_i(X) \) is determined for all point intervals, the spatial derivatives are calculated as

\[ F_{X,i}(X) = (3a_i X_i + 2b_i)X_i + \Omega_{X,j} \]

(16)

After all, the advected profile is given by

\[ \Omega_{i+1} = F_i(X_i + \xi) = 3a_i \xi \]

(17)

where \( \xi = -U\Delta T \) and the superscript \( n \) indicates the time evolution.

In order to demonstrate the efficiency of the proposed approach, we firstly apply the method to predict the propagation of a square wave. Fig. 1 shows the plots of profile obtained from the present method, Lax-
Wendroff and first order upwind methods. As expected, the CIP scheme shows smaller diffusion and dispersion errors compared to the other solution methods. The average percentage of error produced by each method is then calculated and summarized in Tab. 1.

Figure 1 Numerical solution to advection equation

Table 1 Computed average error for every solution method

<table>
<thead>
<tr>
<th>Solution Method</th>
<th>First order upwind</th>
<th>Lax-Wendroff</th>
<th>Present method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average Error (%)</td>
<td>6.820</td>
<td>5.421</td>
<td>1.454</td>
</tr>
</tbody>
</table>

From Fig.1 and Tab.1, they can be seen that the proposed method gives the best accuracy compared to other well-known numerical solution to advection equation.

For two-dimensional solution, we begin by recalling Eq. (7) and it’s spatial derivatives, and split them into advection and nonadvection phases as follow:

Advection phase:

\[
\frac{\partial \Omega}{\partial t} = \left[ U \frac{\partial \Omega}{\partial X} + V \frac{\partial \Omega}{\partial Y} \right] \tag{18}
\]

\[
\frac{\partial \Omega_X}{\partial t} = \left[ U \frac{\partial \Omega_X}{\partial X} + V \frac{\partial \Omega_X}{\partial Y} \right] \tag{19}
\]

\[
\frac{\partial \Omega_Y}{\partial t} = \left[ U \frac{\partial \Omega_Y}{\partial X} + V \frac{\partial \Omega_Y}{\partial Y} \right] \tag{20}
\]

Nonadvection phase:

\[
\frac{\partial \Omega}{\partial t} = \frac{1}{Re} \left( \frac{\partial^2 \Omega}{\partial X^2} + \frac{\partial^2 \Omega}{\partial Y^2} \right) \tag{21}
\]

\[
\frac{\partial \Omega_X}{\partial t} = \frac{1}{Re} \left( \frac{\partial^3 \Omega}{\partial X^3} + \frac{\partial^3 \Omega}{\partial X^2 \partial Y} \right) - \frac{\partial U}{\partial X} \frac{\partial \Omega}{\partial X} - \frac{\partial U}{\partial X} \frac{\partial \Omega}{\partial X} \tag{22}
\]

\[
\frac{\partial \Omega_Y}{\partial t} = \frac{1}{Re} \left( \frac{\partial^3 \Omega}{\partial Y^3} + \frac{\partial^3 \Omega}{\partial X \partial Y^2} \right) - \frac{\partial U}{\partial X} \frac{\partial \Omega}{\partial X} - \frac{\partial U}{\partial X} \frac{\partial \Omega}{\partial X} \tag{23}
\]

where \( \Omega_X = \frac{\partial \Omega}{\partial X} \) and \( \Omega_Y = \frac{\partial \Omega}{\partial Y} \).

In the proposed method, the advection phase of the spatial quantities in the grid interval are approximated with constrained polynomial using the value the it’s spatial derivative at neighboring grid points as follow:

\[
F_{i,j}(X, Y) = \left[ a_1 \overline{X} + a_2 \overline{Y} + a_3 \right] \overline{X} + a_4 \overline{Y} + \Omega_X \overline{X}
+ \left[ a_5 \overline{Y} + a_6 \overline{X} + a_7 \right] \overline{Y} + \Omega_Y \overline{Y} \tag{24}
\]

where \( \overline{X} = X - X_{i,j} \) and \( \overline{Y} = Y - Y_{i,j} \). The coefficients of \( a_1, a_2, \ldots, a_7 \) are determined so that the interpolation function and its first derivatives are continuous at both ends. With this restriction, the numerical diffusion can
be greatly reduced when the interpolated profile is constructed. The spatial derivatives are then calculated as

$$F_{X,i,j}(X,Y) = (3a_1X + 2a_2Y + a_3)X + (a_4 + a_6Y) + \Omega_X$$

(25)

$$F_{Y,i,j}(X,Y) = (2a_2Y + a_3)X + (3a_2Y + 2a_6X + 2a_7)Y + \Omega_Y$$

(26)

In two-dimensional case, the advected profile is approximated as follow

$$\Omega_{i,j}^n = F_{i,j}(X + \eta, Y + \xi)$$

(27)

$$\Omega_{X,i,j}^n = F_{X,i,j}(X + \eta, Y + \xi)$$

(28)

$$\Omega_{Y,i,j}^n = F_{Y,i,j}(X + \eta, Y + \xi)$$

(29)

where \(\eta = -U \Delta T\) and \(\xi = -V \Delta T\). The newly calculated spatial quantities are then used to solve non-advection phase of Eqs. (21) to (23) and vorticity formulation of Eq. (8). In the present study, the explicit central finite different discretisation method is applied with second order accuracy in time and space. For example, the treatment for Eqs. (21) and (8) is

$$\Omega_{i,j}^{n+1} = \Omega_{i,j}^n + \frac{\Delta T}{Re} \left( \frac{\Omega_{i,j}^n - 2\Omega_{i,j}^{n+1} + \Omega_{i,j}^{n+1}}{(\Delta X)^2} \right)$$

(30)

$$\Omega_{X,i,j}^{n+1} = \Omega_{X,i,j}^n + \frac{\Delta T}{Re} \left( \frac{\Omega_{i,j}^n - 2\Omega_{X,i,j}^{n+1} + \Omega_{i,j}^{n+1}}{(\Delta Y)^2} \right)$$

$$\Psi_{i,j}^{n+1} = \frac{\Psi_{i+1,j}^{n+1} + \Psi_{i-1,j}^{n+1}}{(\Delta X)^2} + \frac{\Psi_{i,j+1}^{n+1} + \Psi_{i,j-1}^{n+1} + \Omega_{i,j}^{n+1}}{(\Delta Y)^2}$$

(31)

where superscript \(n\) represent the increment of time step and subscripts \(i\) and \(j\) represent the discretised \(x\) and \(y\) directions.

In summary, the evolution of the proposed scheme consists of three steps. The initial value of \(\Omega_{i,j}^n, \Omega_{X,i,j}^n\) and \(\Omega_{Y,i,j}^n\) are specified at each grid point. Then the system evolves in the following steps;

1. Since the pre-advected value of \(\Omega_{i,j}^n, \Omega_{X,i,j}^n\) and \(\Omega_{Y,i,j}^n\) are known on each grid, the constrained interpolation process can be completed according to Eqs. (27), (28) and (29).

2. After the interpolation, advection takes place, and \(\Omega_{i,j}^n, \Omega_{X,i,j}^n\) and \(\Omega_{Y,i,j}^n\) are obtained.

3. The values of \(\Omega_{i,j}^{n+1}, \Omega_{X,i,j}^{n+1}\) and \(\Omega_{Y,i,j}^{n+1}\) on the mesh grid are then computed from the newly advected values in step 2 by solving the nonadvective phase of the governing equation. Then the interpolation and the advection processes are repeated.

To predict the dynamics of solid particles in shear driven cavity flow, the equation of motion for solid particle must be expressed as

$$m_p \frac{dv_p}{dt} = f_p$$

(32)

where \(m_p\), \(v_p\) and \(f_p\) are the mass of particle, its velocity and drag force acting on particle due to surrounding fluid respectively. According to Kosinski et al. [15], the drag force can be written as follow

$$f_p = C_D A_p \rho \frac{|u - v_p|(|u - v_p|)}{2}$$

(33)

where \(A_p\) is the projected area of solid particle and \(C_D\) is the drag coefficient which is given as

$$C_D = \frac{24}{Re_p}$$

(34)

The particle’s Reynolds number in the above equation is calculated as follow

$$Re_p = \frac{d_p |u - v_p|}{v}$$

(35)

where \(d_p\) is the diameter of solid particle.
In the computational technique, the new value of particles’ velocity \( \mathbf{v}_p^{n+1} \) can be determined since the pre-calculated value of \( \mathbf{v}_p^n \) is known at previous time step as follow

\[
m_p \frac{\mathbf{v}_p^{n+1} - \mathbf{v}_p^n}{\Delta t} = \mathbf{f}_p
\]

(36)

Then the new position of solid particle can be determined as follow

\[
\mathbf{x}_p^{n+1} = \mathbf{v}_p^n \Delta t + \mathbf{x}_p^n
\]

(37)

IV. Results and Discussion

The code was first validated against other experimental results by comparing the trajectory of a particle with approximately the same density with the surrounding fluid so that the neutral buoyancy was obtained. For the simulation, the top lid is constantly moved so that the resultant Reynolds number is 470 as in Tsorng et al. [1].

In their report, Tsorng et al. discussed a three-dimensional measurement of a particle suspended in a fluid enclosed in a transparent cubic cavity. Before the experiments, the particle was plunged into the cavity so that it touched the lid and its initial location was approximately at the middle above of the lid. Fig. 2 indicates the comparison between numerical solution and experimental work as a trajectory of particle. As the simulation is done in dimensionless mode so the real times depending on velocity of fluid can be calculated.

At the first 20 seconds, both numerical and the experimental results match very well. Nevertheless, after this time, some differences appear that may be a result of the following:

1. The actual flow is 3D and these three-dimensional effects do not make it possible to simulate the real flow for a long period of time (where 2D modeling is assumed).
2. It is only possible to estimate the approximate initial location of the particle in the experiments.
3. There is some lubrication flow that occurs through the small gaps between the conveyor belt and the top of the cavity. This may slightly influence the flow pattern in the cavity.

We suppose that the first issue is of main importance, since Tsorng et al. [1] report a motion of the particle in the lateral direction after a few seconds after the beginning of the process. This cannot be simulated using 2D assumption.

A similar conclusion can be drawn while analyzing for instance reference [21], where studies of rotating filtration are reported. The authors investigate Taylor–Couette flow involving a rotation inner cylinder and a stationary outer cylinder. This configuration resembles our research involving, as it does, a rotational flow with particles. The main difference between this reference and our research is the three-dimensional flow leading to very interesting conclusions and results: the flow in the third direction is responsible for a special segregation of the particles.

In our next predictions, the top lid velocity is set at various values so that the resultant Reynolds number falls in between 100 to 1000. Fig. 3 shows the trajectory a solid particle suspended in a square cavity. They also demonstrate the transient behaviour of fluid indicated by the vortex structures in the cavity. As can be seen from the figures, at low Reynolds number (\( Re = 100 \)), the particle immediately spirals outwards the centre on the cavity. However, for the simulation at higher Reynolds number (\( Re = 1000 \)), the particle firstly makes few small spirals near the upper right of the cavity and then gradually spiral outwards the center of the cavity. This is due to the different transient
behaviour of vortex structure of fluid for these two values of Reynolds number. Further analysis on the transient vortex structure will be discussed again later.

![Figure 3a](image1) Particle’s trajectory for $Re = 100$.

![Figure 3b](image2) Particle’s trajectory for $Re = 1000$.

Next, the predictions were performed to predict the dynamics of particles in a lid-driven cavity at Reynolds number of 100, 400 and 1000. 2000 particles were randomly located in the cavity in the range of 0.25 to 0.75 in both $x$ and $y$ direction.

The snapshots of the transient hydrodynamics of particles are shown in Fig. 4. Surprisingly, the particles in the cavity with the lowest Reynolds in the present study started to move earlier than those in the higher values of Reynolds number. This can be explained by analysing the behaviour of the main vortex in the cavity for each Reynolds number. For $Re = 100$, the main vortex immediately moves to the centre of the cavity and drags the particles into it. However, for the higher Reynolds numbers, the main vortex initially moves to the right corner of the cavity before propagating to the center where the particles are located. Then, the rotating fluids drag the particles into motion and responsible for the drift of the particles. The vortex strength also influences the dynamics behaviour of the particles. At low Reynolds number ($Re = 100$), a weak vortex is formed and gradual gradient of flow velocity from the vortex center to the moving lid. This leads the particles move in bigger group along the flow streamline compared to the condition at high Reynolds numbers. For the all cases, due to the high inertia force acts on the moving particles, they are centrifuged outward and eventually all the particles propagating along the outer side of the vortex in the cavity.

For the simulation at high Reynolds number ($Re = 400$ and 1000), a small vortex appears near the vertical right wall and bottom right corner of the cavity. As the main vortex gradually increases, the wall vortex propagates to the lower part of the cavity and eventually joins with the lower corner vortex. This can be clearly seen at Reynolds number 1000. Gatski et al. [22] and Goodrich and Soh [23] predicted the same phenomena using the conventional finite different solution to the Navier-Stokes equation but failed to reproduce the right wall vortex in their investigations. Recently, Quartapelle [24] predicted the transient flow in a square cavity at $Re = 1000$ and showed that the solution is unstable and the vortex near the moving lid exhibits a large oscillatory behavior. This instability phenomenon is not encountered in the present investigation.
V. Conclusions

Numerical computations of solid particle in a lid-driven cavity flow were performed using the coupled cubic interpolation scheme for Navier-Stokes equation and Newton’s second law (Eulerian-Lagrangian scheme). Results of the present computations show that, almost all the physical detail of this transient flow at wide range of Reynolds numbers are reproduced by the current scheme. The computed particle’s trajectories clearly indicate the influence of vortex structure on the dynamics of particle in the cavity. These demonstrate the capability and the multidisciplinary applications of the present numerical scheme. Future efforts need to extend the current formulation for investigation at various types of solid fluid flow related to real engineering problems.

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