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## TWO ALGORITHMS FOR SOLVING COUPLED PARTICLE DYNAMICS AND FLOW FIELD EQUATIONS IN TWO-PHASE FLOWS

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#### ABSTRACT

Two methods for solving coupled particle dynamics and flow field equations simultaneously by considering fluidparticle interactions to simulate two-phase flow are presented and compared. In many conditions, such as magnetic micro mixers and shooting high velocity particles in fluid, the fluidparticle interactions can not be neglected. In these cases it is necessary to consider fluid-particle interactions and solve the related coupled equations simultaneously. To solve these equations, suitable algorithms should be used to improve convergence speed and solution accuracy. In this paper two algorithms for solving coupled incompressible Navier-Stokes and particle dynamics equations are proposed and their efficiencies are compared by using them in a computer program. The main criterion that is used for comparison is the time they need to converge for a specific accuracy. In the first algorithm the particle dynamics and flow field equations are solved simultaneously but separately. In the second algorithm in each iteration for solving flow field equations, the particle dynamics equation is also solved. Results for some test cases are presented and compared. According to the results the second algorithm is faster than the first one especially when there is a strong coupling between phases.

#### NOMENCLATURE

d	[ <i>m</i> ]	Particle diameter
m	[kg]	Particle mass
$\vec{V}$	[m/s]	Fluid's velocity vector
$\vec{V}_p$	[m/s]	Particle's velocity vector
$\vec{V}_{rel}$	[m/s]	Particle's velocity relative to the fluid velocity
t	[s]	Time
р	$[N/m^2]$	Pressure
F	[N]	Force
f	[N]	Force
$C_{M}$	[-]	Added mass coefficient

Re	[-]	Reynolds number
$F_{d}$	[N]	Drag force
$F_{g}$	[N]	Gravity force
$F_L$	[N]	Lift force
$F_s$	[N]	Fluid stress gradients force
$F_h$	[N]	Basset history force
Fw	[N]	Wall interaction force
$C_D$	[-]	Drag coefficient
$A_P$	$[m^2]$	Cross section area of the particle
х	[ <i>m</i> ]	Cartesian axis direction
у	[m]	Cartesian axis direction
$R^2$	[-]	Coefficient of determination
r	[ <i>m</i> ]	Position
	[1/s]	Velocity gradient $(\partial V / \partial y)$
	[1/s]	Particle angular velocity

 $\Omega_p [m^3]$ Particle volume

- W [-] Ratio of particle density to fluid density
- μ [kg/ms] Fluid dynamic viscosity
- $[kg/m^3]$ Density ρ

Subscripts

р	Particle
rel	Relative
f	Fluid
0	Initial

#### **INTRODUCTION**

Nowadays two-phase flows are common in industries. Chemical industries, MEMS, aerospace systems, combustion technology and biological applications are a few examples [1,2]. Two-phase flow simulation by using CFD is a powerful tool for reducing costs and doing optimization in industry. Two-phase flow that is considered in this paper is related to motion of solid particles in continuum fluid surrounding. Approaches of the dispersed-phase (solid particles, droplets, or bubbles) are commonly classified by their treatment as Eulerian vs. Lagrangian [1]. In the Eulerian approach it is assumed that the particles properties such as velocity, temperature and concentration can be described as a continuum. In the Lagrangian approach particles positions are carefully traced and the properties are extracted by using them. Both have pros and cones. For example Eulerian simulation gives a good physical insight but needs large computer resources and Lagrangian particle tracking is economical, feasible and flexible but it has some limitations on accuracy and resolution [3]. Two methods are presented in the Lagrangian approach: first is "point-volume" representation and second is "resolved-volume" representation [1].

In Figure 1 these two methods are presented. There is another classification in two-phase flow modeling: One-way coupling and two-way coupling. When the fluid flow affects the particles dynamics but particles have no effect on the fluid flow, the condition is one-way coupling. If particles can change the fluid flow, two-way coupling is occurred. To model the two-way coupling there are two general algorithms in the literature [4-8]. In fact these general algorithms talk about the sequences and steps that should be done between fluid flow and dispersed phase simulations. In this paper two algorithms for pointvolume two-way coupling Lagrangian particle tracking are presented and their efficiency are compared by using them in a code that is written for this purpose. Tests are done in a micro channel by using micro spheres. The emphasis is very much on the time they need to converge to a specific error. At the end the better algorithm is introduced.



Figure 1: Comparison of point-volume and resolved-volume particle representations [1].

### A REVIEW OF TWO GENERAL ALGORITHMS FOR SOLVING TWO-WAY COUPLING TWO-PHASE FLOW

Several kinds of forces act on solid particles accelerating in liquid flow. If we consider drag force as the dominant force in a two-way coupling two-phase flow in point-volume two-phase flow model, as it is usual in literature [1], then the two-way coupling problem could be split into three major problems (in an incompressible isothermal fluid surrounding):

- 1. Flow field calculation
- 2. Calculating drag force
- 3. Calculating particle velocity

By considering these three steps, regardless of the CFD method that is used for velocity and pressure field calculations and the method used for drag calculation, two general algorithms could be made:

*I.* **Algorithm1**: At each time step: continue the following steps until all the variables converge, i.e. velocity field, pressure field and particle velocity (Figure 2):

- *i)* Calculating velocity and pressure field until they converge.
- *ii)* Calculating drag force exerted on the particle.
- *iii)* Calculating particle velocity

The drag force that is exerted on the particle is in fact the force exerted on the fluid elements but in the opposite direction. Therefore this force is used in velocity and pressure field calculation.



Figure 2: Algorithm 1

II. Algorithm2: In each iteration to solve flow field equations to reach the convergence criteria, particles dynamics equations are also solved (Figure 3).

The first algorithm is called "explicit coupling between two phases" and the second is called "implicit coupling between two phases" [7].

The time they consume to converge is a highly competitive factor that shows their efficiency. Therefore this factor will be used for comparing these two algorithms in this paper.



Figure 3: Algorithm 2

#### THEORY AND ASSUMPTIONS

The model that is used in this paper is called "point-volume" which is a branch of two-phase flow simulation models. This method belongs to an approach that models drag forces and lift forces instead of calculating them by using fine mesh around the object. For using this method there is a necessary condition: particle's dimensions should be smaller than the cell's dimensions. In this approach angular velocity could also be modelled. At limit, when the particle's volume fraction of dispersed phase is very small, particles are treated as "points". It is a very usual method that is used by many researchers such as [4, 11]. In this situation particle's volume is assumed to be zero, therefore there is no angular velocity and the only equation that should be solved is the linear momentum equation.

The fluid is assumed to be Newtonian incompressible isothermal liquid. The behavior of fluid is governed by incompressible continuity and Navier-Stokes equations:

$$\nabla \cdot \vec{V} = 0 \tag{1}$$

$$\rho_f \left( \frac{\partial V}{\partial t} + (\vec{V} \cdot \nabla) \vec{V} \right) = -\nabla P + \mu \nabla^2 \vec{V} + \vec{f}(\vec{r}, t)$$
(2)

According to the point-volume model,  $\vec{f}$  in equation (2) is the force that is exerted by the particle on the fluid element at point  $\vec{r}$  and at time t.

In a general form, dynamics equation of a moving particle in fluid is [1]:

$$\rho_p \Omega_p (l + C_M / \psi) \frac{dV_p}{dt} = \sum F_k \tag{3}$$

$$\sum F_{k} = F_{d} + F_{g} + F_{l} + F_{s} + F_{h} + F_{w}$$
(4)

Usually  $\vec{F}_d$  and  $\vec{F}_g$  are dominant forces [1]. In the case that is discussed in this paper  $\vec{F}_g$  is  $8.1 \times 10^{-3}$  pN, and  $\vec{F}_d$  is in the

order of 1 pN, therefore, gravitational force can be neglected. Particle's density in our case is in the order of fluid density and the particle experience a high acceleration; therefore, it is reasonable to consider the added mass effect. Magnus lift force is a function of particle's angular velocity. Because we have used "point-volume" method, this force does not exist in our case. According to [12], when  $D_p \zeta \operatorname{Re}_p / (V - V_p) \ge 1.0$ , the magnitude order of Saffman lift is the same as Stokes drag.  $\zeta = \partial V / \partial y$ , y is the perpendicular direction relative to the main stream flow. The flow velocity between two parallel plate, based on our assumptions, is [4]:  $V_x(y) = 3/2V_0(1-4y^2/w^2)$ . By doing some calculation it can be deduced that the maximum value of  $D_p \zeta \operatorname{Re}_p / (V - V_p)$  could be about  $8 \times 10^{-5}$ . Therefore this force can surely be omitted. No collision is done in this case, therefore,  $F_w = 0$ .

It would be useful to notice an important point. Our study is in fact a comparison between two ways for solving coupled equations. Here we have incompressible fluid flow equations and particle dynamics equation which are coupled due to high velocity of the particle and as a result: high momentum coupling between phases. Therefore if some forces in this study were neglected, it would not disadvantage the result.

*Therefore the equation of motion becomes:* 

$$\rho_p \Omega_p (l + C_M / \psi) \frac{dV_p}{dt} = \vec{F}_d \tag{5}$$

 $\vec{F}_d$  is calculated from the below equation [2]:

$$\vec{F}_{d} = \frac{1}{2} \rho_{f} C_{D} A_{p} (\vec{V} - \vec{V}_{p}) / \vec{V} - \vec{V}_{p} /$$
(6)

where  $C_D$  depends on the Reynolds number that is considered in the code. In a general case, equations (1), (2) and (3) should be solved simultaneously. Therefore, it is a coupled problem.

The cases simulated in this paper are in micro scales. Because of micro channel's small dimensions and very slow fluid velocity, Reynolds number is below 1. Additionally, due to very small dimension of micro sphere and its low mass, it is not necessary to model turbulence. It is clear from the results that when the micro sphere is shot into the fluid, it does not disturb the streamlines seriously, therefore this assumption is correct.

#### NUMERICAL SCHEME AND THE CODE ABILITIES

A computer code for taking numerical tests is developed to calculate flow field. Particle's dynamics equation is integrated by using "improved Euler method" that is equivalent to "second order Runge-Kutta" [9]. Gauss-Seidel algorithm is used to solve linear system of equations.

This code can calculate flow field and dynamics of desired number of particles by considering momentum exchange between them and the flow field. The code is capable of using both algorithm1 and algorithm2 to solve two-way coupling in an unsteady mode. Grid generation subroutine is also included in the code that can make structured grid.

The geometry that is considered for the numerical tests is a two dimensional channel. No-slip boundary conditions are applied on the channel walls. Constant velocity inlet is the inlet boundary and at the channel outlet, zero pressure is applied.

#### Code validation

To validate the code, the analytical solution of particle dynamics equation is used. It is assumed that a micro sphere with a high-velocity is injected into the middle of a micro channel. Because the velocity of fluid is very low (about 0.00 Im/s), it is assumed that the particle is injected in a stationary surrounding. The drag force exerted on the micro sphere is as follows [2]:

$$Re_{p} = \rho_{f} (\vec{V_{p}} - \vec{V}) d / \mu$$
(7)  
if :  $l < Re_{p} < 800$   
 $\vec{F_{d}} = 3\pi\mu d \vec{V_{rel}} (l + 0.15 (Re_{p})^{0.687})$ (8)

The dynamics equation of the particle which should be solved is:

$$\rho_p \Omega_p (1 + C_M / \psi) \frac{dV_p}{dt} = \vec{F}_d \tag{9}$$

Suppose that the micro sphere is injected with velocity equal to 50m/s. Micro sphere properties are:

 $m = 8.27 \times 10^{-16} kg$   $d = 10^{-6} m$   $\Omega_p = 5.236^{-19} m^3$ Fluid properties are:

$$\mu = 10^{-3} kg/ms$$
$$\rho_f = 1000 kg/m^3$$

$$C_{M} = 0.5$$

*By integrating equation (8) and applying initial conditions, following equation is achieved:* 

$$e^{-(3\pi\mu l/(m+\Omega_p\rho_f C_M))t} = \frac{1}{9.17934} \frac{V_p^{2.4340}}{(0.15V_p^{1.687} + V_p)^{1.4556}} (10)$$

In Figure 4 analytical and numerical results are plotted. Numerical results are coincident and are in good agreement with the analytical result. Injection is done in x and y-directions using either algorithm.

The disturbed and the undisturbed streamlines are shown in Figure 5 and 6 respectively. In the disturbed case, the particle is injected in the y-direction. It is clear that the particle momentum has affected the flow field and two-way coupling is done

Position and velocity of injection are as follows:  

$$x(0) = 0.0001m, y(0) = 0.000072m$$
  
 $\overline{V_p}(0) = 50m/s$ 



Figure 4: Particle injection test



Figure 5: Undisturbed flow field



Figure 6: Disturbed flow field

#### TESTS AND RESULTS

To compare implicit with explicit coupling methods, some numerical experiments are performed. In these experiments a particle which is  $10^{-6}$  m in diameter, is injected into a micro channel, which is 0.0008m in length and 0.00015m in height. The particle is shot along channel's length with various velocities, from 10m/s to 150m/s. The momentum of the particle affects the flow field and disturbs it. In addition, because of drag force exerted on the particle, it decelerates and its velocity decreases. Time that each algorithm needs to reach 1.5m/s for particle velocity is the factor of efficiency. This experiment is performed for both algorithms for errors $10^{-6}$ ,  $10^{-7}$  and  $10^{-8}$ . In this paper error refers to the error in mass balance for solving flow field equations and also shows the error of calculating particle's velocity. Both of these errors are set to be equal in calculations.

Inlet velocity of the micro channel is  $10^{-3}$  m/s and fluid properties are the same as in the validation part.  $\Delta x$  and  $\Delta y$ 

in the grid in physical domain are  $8 \times 10^{-6}$  m and  $7.5 \times 10^{-6}$  m respectively. Number of grid points along the x-axis the y-axis is 100 and 20 respectively. By a simple calculation it can be shown that the cross section area of the particle is only 1.3% of a computational cell, therefore, the point-volume assumption is correct.

In Figure 7, results with error equal to  $10^{-6}$  are plotted.



**Figure 7:** Result for error equal to  $10^{-6}$ 

It can be observed in Figure 7 that at low velocities (in this figure until 20m/s) both algorithms need equivalent time. But by increasing the injection velocity, algorithm 2 becomes faster. Curve fitting can be done for the results to achieve a better insight. A curve fitting has been done on both curves and results are in Figure 8. A power function and a logarithmic function are fitted on the data of algorithm 1 and algorithm 2 respectively. The results are shown in Figure 8.

It is clear that at low velocities the times needed to reach the specified velocity for both algorithms are almost the same. However by increasing the shooting velocity, the difference becomes larger. According to this curve, algorithm 2 is faster than algorithm 1. A curve fitting has been done on both curves and results are in Figure 10. A power function is fitted on the data of algorithm 1 and a logarithmic curve fitting is performed on the data of algorithm 2.



*Figure 8:* Curve fitting on results with error equal to  $10^{-6}$ 

In Figure 9, results with error equal to  $10^{-7}$  are plotted.



**Figure 9:** Result for error equal to  $10^{-7}$ 



*Figure 10:* Curve fitting on results with error equal to  $10^{-7}$ 

In Figure 11, results with error equal to  $10^{-8}$  are plotted. Similar to the results with error equal to  $10^{-7}$ , at low velocities the results for both algorithms are close, but by increasing the injection velocity, the difference becomes larger. Again algorithm 2 is faster than algorithm 1.

*Curve fitting is also done for these data. It is presented in Figure 12. Types of functions are the same as the previous case and they only differ on constants.* 

Figure 13 shows the ratio of run-times in case 3(error equal to  $10^{-8}$ ) to run-times in case 2(error equal to  $10^{-7}$ ), for each

algorithm. It is noticeable that in this factor, similar to the runtime factor, algorithm 2 is the faster one.







*Figure 12:* Curve fitting on results with error equal to  $10^{-8}$ 



Figure 13: Relative increment in run-times

#### CONCLUSION

According to the obtained results, it can be understood that the implicit coupling algorithm is faster than the explicit one, especially in high velocity cases. In the other hand, the implicit method is more suitable when the coupling is very strong. Additionally, if a better accuracy is needed (it means a lower error), relative increment in computational time for implicit method is less than the explicit method. Velocity of injection could be a sign of coupling between two phases; because in higher velocity the momentum exchange is higher and two-way coupling is noticeable, because at limit when the particle's velocity is equal to the fluid velocity there is no coupling between phases and by increasing the particle's velocity coupling becomes more serious. Therefore it is reasonable to assume that the time consumption in an algorithm is proportional to:

A "Power function" of two-way coupling for algorithm 1.

A "Logarithmic function" of two-way coupling for algorithm 2.

As a general conclusion : in two-way coupling two-phase flow, if there is a strong coupling, implicit method should be used; and if coupling is negligible, there is not a significant difference between explicit and implicit algorithms. In other words if there is a high momentum exchange in a multiphase flow (regardless of the source of the coupling: high volume fraction of the dispersed phase or high velocity of the particles) algorithm 2 can reduces the cost of calculations.

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