Fundamental Study of Smoothed Particle Hydrodynamics -Treatment of Two-Phase Flow - *

Haruki OBARA **, Jhun SUEMURA ** and Mariko HONDA **

**University of TOYAMA

3190 Gofuku, Toyama City, 930-8555 Japan

E-mail: Obarah@eng.u-toyama.ac.jp

Abstract

The smoothed particle hydrodynamics (SPH) method developed by Monaghan and Liversky, et al. is beset with the problem of numerical disorder at the interface of a two-phase flow such as that of gas and liquid. In this paper, new formulas for the SPH method, termed relaxation equations, suitable for treating the two-phase flow of nonviscous fluid are proposed. The relaxation equations are developed on the basis of the mass and momentum conservation equations. By using these equations, it is possible to suppress numerical disorder around the interface of two fluids.

Key words: SPH, Particle Method, Numerical Disorder, Two Phase Flow

1. Introduction

The smoothed particle hydrodynamics (SPH) method developed by Monaghan⁽¹⁾ and Liversky⁽²⁾ et al., which is a Lagrangian particle method, treats a continuum as an aggregation of particles and is gridless. The SPH method does not require connectivity between particles, surface definition and the physical value of the free surface. Therefore, it is suitable for treating the splashing of water, the fracture fragmentation of materials and other problems that are not easy to treat by FEM and FDM. In addition, it has potential for treating different materials without having to define the contact surface. The SPH method was first used in solving astrophysics problems. Since the early 1990s, the application of the SPH method has been extended to the modeling of solid and fluid mechanics.

In spite of the above merits, the SPH method is beset with some problems that need to be solved. One of these problems is numerical disorder at the interface of different materials. The particle method has potential to simulate the interaction problem of two materials without having to define the interface between them. It eases the difficulties in the simulation of the complex interaction between different materials. However, when we use traditional SPH formulas for the interaction of two different materials such as gas and liquid, an unexpected large numerical disorder appears around the interface. This makes it difficult to continue the simulation. The disorder is caused by the differences in density and compressibility between the two materials. If this problem is prevented, the SPH method will have a high potential for application in a wide range of fields. Our aim is to develop a new particle method that can treat gas, liquid and solid simultaneously. In this paper we propose new formulas for suppressing numerical disorder around the interface of different materials.

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2. SPH Method

The SPH method is based on the kernel approximation of the function f . The discrete formulas for evaluating f and $\partial f / \partial x$ at the position X_i are,

$$\langle f(X_i) \rangle = \sum_{j=1}^N f_j \frac{m_j}{\rho_j} W(X_i - X_j, h), \quad (1)$$

$$\langle \frac{\partial f(X)}{\partial x} \rangle_i = \sum_{j=1}^N f_j \frac{m_j}{\rho_j} \frac{\partial W(X - X_j, h)}{\partial x} \quad (2)$$

Here, $\langle f(X_i) \rangle$ and $\langle \partial f / \partial x \rangle_i$ are smoothed values of f and $\partial f / \partial x$ at the position X_i , respectively. W is a kernel function and has an integrated value of 1 in infinite space. Usually, the Gauss function or B Spline function is used for the kernel function. j is the particle number and N is the total number of particles in the influence domain around particle i . m_j and ρ_j are the mass and density of particle j in the domain, respectively. h is the smoothing length and is usually defined as

$$h = \eta \left(\frac{m}{\rho} \right)^{\frac{1}{3}}. \quad (3)$$

Usually, $\eta=1$. For the conservative equation of mass, Liberskey et al.⁽²⁾ used Equation (4), and Takaoka et al.⁽³⁾ used Equation (5).

$$\frac{d\rho_i}{dt} = -\rho_i \sum_j \frac{m_j}{\rho_j} \left\{ [u_j - u_i] \frac{\partial W}{\partial x} + [v_j - v_i] \frac{\partial W}{\partial y} + [w_j - w_i] \frac{\partial W}{\partial z} \right\} \quad (4)$$

$$\frac{d\rho_i}{dt} = -\sum_j m_j \left\{ [u_j - u_i] \frac{\partial W}{\partial x} + [v_j - v_i] \frac{\partial W}{\partial y} + [w_j - w_i] \frac{\partial W}{\partial z} \right\} \quad (5)$$

Here, u , v and w are the velocities in the x -, y - and z -axis of the particle, respectively. We use h_j for h and a derivative of W along the x -axis at the position i for $\partial W / \partial x$, where W is located at the position j . These values of h and $\partial W / \partial x$ will be discussed in our next report.

Using Eq.(2), we obtain the following discrete momentum equation for the x -axis, for a nonviscous fluid.

$$\frac{du_i}{dt} = -\frac{1}{\rho_i} \sum_j \frac{m_j}{\rho_j} p_j \frac{\partial W}{\partial x} \quad (6)$$

We call this a primitive equation. However, this equation does not conserve the momentum of particles i and j . Usually, Equation (7) by Monaghan⁽¹⁾ is used.

$$\frac{du_i}{dt} = -\sum_j m_j \left(\frac{p_j}{\rho_j^2} + \frac{p_i}{\rho_i^2} \right) \frac{\partial W}{\partial x} \quad (7)$$

Here, p is the pressure of the particle.

3. Problem of Two-Phase Flow

3.1 Models for Evaluating Error around Interface of Two-Phase Flow

The SPH method has potential for treating different materials simultaneously without defining the interface of two materials. For example, SPH was applied to the analysis of the behavior of a hypervelocity impact of an aluminum sphere on a thin wall of different materials⁽⁴⁾, or the detonation of an explosive surrounded by water⁽⁵⁾. However, when the densities or other parameters of two materials are markedly different, the acceleration and pressure around the interface of the two materials have numerical disorder, and the analysis

is discontinued. We call this the two-phase flow problem.

To study the two-phase flow problem, we need a model for estimating the error around the interface. Here, we propose the following quasi-steady two-phase flow model. For simplicity, we treat a one-dimensional flow. The conservative equation of mass is transformed to the following pressure equation:

$$\frac{dp}{dt} = -\rho C^2 \frac{\partial u}{\partial x}, \quad C^2 = \frac{dp}{d\rho}. \quad (8)$$

C is the sound velocity of a fluid. The one-dimensional momentum equation is

$$\frac{du_i}{dt} = -\frac{1}{\rho} \frac{\partial p}{\partial x}. \quad (9)$$

Here, we assume a situation in which gas and liquid flow without separation. In this situation, the pressure p at the interface of two fluids is the same across the interface, thus, the dp/dt values of the two fluids should be equal. This requires the following relationship between the velocity gradient of two fluids based on Eq. (8):

$$-\rho_{\text{gas}} C_{\text{gas}}^2 \frac{\partial u}{\partial x} \Big|_{\text{gas}} = -\rho_{\text{liquid}} C_{\text{liquid}}^2 \frac{\partial u}{\partial x} \Big|_{\text{liquid}}. \quad (10)$$

This equation indicates that the velocity gradient of each fluid is inversely proportional to ρC^2 . Similarly, the velocity u and du/dt of two fluids are continuous across the interface. Thus, we obtain the following equation on the basis of Eq. (9):

$$-\frac{1}{\rho_{\text{gas}}} \frac{\partial p}{\partial x} \Big|_{\text{gas}} = -\frac{1}{\rho_{\text{liquid}}} \frac{\partial p}{\partial x} \Big|_{\text{liquid}}. \quad (11)$$

This means that the pressure gradient of the two fluids across the interface is proportional to the density of the fluid. Therefore, when the distributions of velocity and pressure around the interface of two fluids are supplied on the basis of Eqs. (10) and (11), the du/dt and dp/dt values of the two fluids should be even. The difference between the analytical and theoretical values indicates the error of analysis.

3.2 Errors of Traditional Equations

Errors of traditional equations from Eqs. (4) to (7) are analyzed using the quasi-steady two-phase flow model of air and water. Particles are located uniformly in a 3-dimensional infinite space. Figures 1 and 2 show the velocity and pressure distributions, respectively. h is 1 m, and the density of air and water are 1.29 kg/m^3 and 1000 kg/m^3 , respectively. The sound velocities C in air and water are 330 m/sec and 1400 m/sec , respectively. The

Fig. 1 Velocity distribution model

Fig.2 Pressure distribution model

interface position is $x=5.5$ m.

Figure 3 shows the distribution of dp/dt obtained using Eqs. (4) and (5) around the interface of two fluids in Fig. 1. The Gauss function is used for the kernel function. The radius of the influence domain is $3h$. The expected dp/dt is -14193 Pa/s, but the calculated results differ from the expected value by 3~4 orders of magnitude.

Figure 4 shows the distribution of du/dt obtained using Eqs. (6) and (7) around the interface of two fluids in Fig. 2. The expected du/dt is 10 m/s², but the calculated results differ from the expected value by 2~7 orders of magnitude.

Fig.3 dp/dt distribution around the interface

Fig.4 du/dt distribution around the interface

4. Relaxation Equations

4.1 Symmetrical Momentum Equation

In order to solve the problem of two-phase flow, we first derive a new discrete momentum equation instead of Eq. (7). We study the conservation of momentum of particles i and j . From Eq. (6), the force acting on particle i by particle j is

$$m_i \frac{du_i}{dt} = -\frac{m_i m_j}{\rho_i \rho_j} p_j \frac{\partial W_j}{\partial x_i}, \quad (12),$$

and the force acting on particle j by particle i is

$$m_j \frac{du_j}{dt} = -\frac{m_i m_j}{\rho_i \rho_j} p_i \frac{\partial W_i}{\partial x_j}. \quad (13).$$

The summation of Eq. (12) and (13) is not 0. Therefore, Eq. (6) does not conserve the momentum of particles. On the other hand, Eq. (7) derived by Monaghan conserves the momentum of particles i and j under the condition of $h_i = h_j$. However, we use another equation. We add the momentum increase of particle j caused by the reaction of particle i to Eq. (12), because the force acting on particle j acts on particle i as a reaction force. It yields

$$\frac{du_i}{dt} = -\frac{1}{\rho_i} \sum_j \frac{m_j}{\rho_j} \left\{ p_j \frac{\partial W_j}{\partial x_i} - p_i \frac{\partial W_i}{\partial x_j} \right\}, \quad (14)$$

which is truly symmetrical and conserves the momentum, even under the condition of $h_i \neq h_j$. Eq. (14) leads to Eq. (15) under the condition of $h_i = h_j$, which corresponds to the relationship of $\partial W_j / \partial x_i = -\partial W_i / \partial x_j$.

$$\frac{du_i}{dt} = -\frac{1}{\rho_i} \sum_j \frac{m_j}{\rho_j} (p_i + p_j) \frac{\partial W_j}{\partial x_i} \quad (15)$$

Eq. (15) coincides with the 3rd momentum formula described by Monaghan⁽¹⁾. Eq. (14) has an additional term of p_i compared with Eq. (6). This term vanishes with the summation over an infinite space. Therefore, Eq. (14) is consistent with the primitive momentum Eq. (6). We call Eq. (14) or (15) the symmetrical momentum equation.

4.2 Relaxation Equations

4.2.1 Relaxation equation for pressure

We use the following 1-dimensional discrete formula derived from Eq. (8) for pressure.

$$\frac{dp_i}{dt} = -\left\langle \rho C^2 \frac{\partial u}{\partial x} \right\rangle_i = -\left\langle \rho C^2 \frac{\partial (u - u_i)}{\partial x} \right\rangle_i = -\sum_j \frac{m_j}{\rho_j} \rho_j C_j^2 (u_j - u_i) \frac{\partial W}{\partial x} \quad (16)$$

For example, we assume that particle i is air and particle j is water, and that there is an interface at the position x between particles i and j . Based on the quasi-steady two-phase flow model, the ρC^2 of water is large and the gradient of velocity is very small. On the other hand, the ρC^2 of air is small and the gradient of velocity is large. However, the $u_j - u_i$ used in Eq. (16) contains not only the velocity difference in water but also the velocity difference in air. Thus, the product of $\rho_j C_j^2$ and $u_j - u_i$ yields an excessive value. This is the reason for the numerical disorder. To overcome this problem, we replace Eq. (16) with Eq. (17), by dividing $\rho_j C_j^2 (u_j - u_i)$ into two terms.

$$\frac{dp_i}{dt} = -\sum_j \frac{m_j}{\rho_j} \left[\rho_j C_j^2 (u_j - u_x) + \rho_i C_i^2 (u_x - u_i) \right] \frac{\partial W}{\partial x} \quad (17)$$

The first term in brackets in Eq. (7) is the influence of particle j (water), and the second term is the influence of particle i (air). When $\rho_j C_j^2$ is large but $(u_j - u_x)$ is small, and $\rho_i C_i^2$ is small but $(u_x - u_i)$ is large, their summation does not have an excessive value. However, u_x ,

which is the velocity at the interface position x , is unknown. To overcome this difficulty, we assume that the first and second terms in the brackets are the same; thus,

$$\rho_i C_i^2 [u_x - u_i] = \rho_j C_j^2 [u_j - u_x]. \quad (18)$$

We transform Eq. (17) using the u_x derived from Eq. (18) and extend it for a three-dimensional space, resulting in the following equation for pressure:

$$\frac{dp_i}{dt} = -\sum_j \frac{m_j}{\rho_j} \frac{2\rho_i C_i^2 \rho_j C_j^2}{\rho_i C_i^2 + \rho_j C_j^2} \left\{ [u_j - u_i] \frac{\partial W}{\partial x} + [v_j - v_i] \frac{\partial W}{\partial y} + [w_j - w_i] \frac{\partial W}{\partial z} \right\}. \quad (19)$$

4.2.2 Relaxation equation for acceleration

We transform Eq. (14) and obtain

$$\frac{du_i}{dt} = -\sum_j \frac{m_j}{\rho_j} \left\{ \frac{p_i}{\rho_i} \left(\frac{\partial W_j}{\partial x_i} - \frac{\partial W_i}{\partial x_j} \right) + \frac{p_j - p_i}{\rho_i} \frac{\partial W_j}{\partial x_i} \right\}. \quad (20)$$

Again, we assume the interface at the position x between particles i and j , and by dividing $(p_j - p_i)/\rho_i$ of Eq. (20) into two terms, we obtain

$$\frac{du_i}{dt} = -\sum_j \frac{m_j}{\rho_j} \left\{ \frac{p_i}{\rho_i} \left(\frac{\partial W_j}{\partial x_i} - \frac{\partial W_i}{\partial x_j} \right) + \left(\frac{p_x - p_i}{\rho_i} + \frac{p_j - p_x}{\rho_j} \right) \frac{\partial W_j}{\partial x_i} \right\}. \quad (21)$$

p_x is unknown; however, by assuming that

$$\frac{p_x - p_i}{\rho_i} = \frac{p_j - p_x}{\rho_j}, \quad (22)$$

by deriving p_x from Eq. (22), and by substituting it in Eq. (21), we obtain the following equation for momentum:

$$\frac{du_i}{dt} = -\sum_j \frac{m_j}{\rho_j} \left\{ \frac{p_i}{\rho_i} \left(\frac{\partial W_j}{\partial x_i} - \frac{\partial W_i}{\partial x_j} \right) + 2 \frac{p_j - p_i}{\rho_i + \rho_j} \frac{\partial W_j}{\partial x_i} \right\}. \quad (23)$$

This equation conserves momentum under the condition $h_i = h_j$, but not under the condition $h_i \neq h_j$. This problem will be discussed in our next report.

Figures 5 and 6 show the dp/dt and du/dt calculated using Eqs. (19) and (23) around the interface of air and water, using the pressure and velocity distributions of Figs. 1 and 2. The errors of dp/dt and du/dt in the figures are markedly reduced or relaxed compared with those in Figs. 3 and 4. The maximum error is 10 % or less. When the interface is placed on particles i or j , the error increases up to 20%. Eqs. (19) and (23) are not ideal formulas, but they can markedly reduce or relax the errors around the interface and enables the continuation of the simulation. We call them relaxation equations (Rex. eqs).

Fig.5 dp/dt distribution around interface of two-phase flow in case of Rex. eq.

Fig.6 du/dt distribution around interface of two-phase flow in case of Rex. eq.

5. Simulation of Two-phase Flow

Figure 7 shows the particle distribution of the analyzed model to test the relaxation equations. The particles are located uniformly on a three-dimensional regular lattice having a distance of 0.01 m in the x , y and z directions. The outer three-layer particles except those in the $+x$ -direction are on a rigid wall. The $+x$ direction is free. We boldly assume the wall particles to be iron to confirm the efficiency of the relaxation equations. The wall surrounds air and water particles. The left-side particles from Nos. 4 to 8 in the x direction are air particles having a pressure of 1.013×10^5 Pa. The residual right-side particles are water particles having pressure of 0 Pa. The air expands adiabatically. In this model, shock waves are transmitted in the $+x$ direction. Note that the quasi-steady flow condition is not satisfied in the initial pressure distribution. Simulations are performed explicitly. The average pressure and velocity in the x -plane are used for the wall particles. Artificial viscosity is not used. Calculation using traditional SPH equations is difficult even if Δt is set at $0.1h/C$. Figure 8 shows the pressure distribution in the $y=0.07$ m plane at each time using relaxation equations. Δt was set at $0.5h/C$. The shock wave front is not sharp. This may be caused by numerical diffusion. The pressure distribution of air is flat, but there is pressure oscillation at the shock wave front. The oscillation in the x -axis may be caused by the difference in physical value between air and water. The oscillation in the z -axis may be caused by the difference in density between fluids and the iron wall. Note that the relaxation equations are constructed for the quasi-steady two-phase flow, having pressure and velocity distributions respectively as shown in Figs. 1 and 2; however, these equations may also be used for shock wave analysis, which does not satisfy the condition of a quasi-steady two-phase flow.

Fig.7 Three dimensional analyzed model

Fig.8 Analyzed pressure distribution by relaxation equations for model of Fig.7
(plane: $y=0.07\text{[m]}$, rigid wall: $x=0\sim0.02\text{[m]}$, air : $x=0.03\sim0.07\text{[m]}$, water : $x=0.08\text{[m]}\sim$)

6. Conclusions

To decrease the numerical disorder in the SPH method around the interface of a two-phase flow, relaxation equations for the pressure and acceleration of a nonviscous flow are constructed on the basis of a quasi-steady two-phase flow model. The efficiency of these equations is confirmed to be effective for a three-dimensional air-water two-phase flow having shock front.

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