Density-Independent Smoothed Particle Hydrodynamics for a Non-Ideal Equation of State

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Abstract

The smoothed particle hydrodynamics (SPH) method is a useful numerical tool to study a variety of astrophysical and planetological problems. However, it turned out that the standard SPH algorithm has problems in dealing with hydrodynamical instabilities. This problem is due to the assumption that the local density distribution is differentiable. In order to solve this problem, a new SPH formulation, which does not require the differentiability of the density, was proposed. This new SPH method improved the treatment of hydrodynamical instabilities. This method, however, is applicable only to the equation of state (EOS) of an ideal gas. In this paper, we describe how to extend the new SPH method to non-ideal EOS. We present the results of various standard numerical tests for non-ideal EOS. Our new method works well for non-ideal EOS. We conclude that our new SPH can handle hydrodynamical instabilities for an arbitrary EOS, and that it is an attractive alternative to the standard SPH.

Key words: hydrodynamics — methods: numerical

1. Introduction

In the field of astrophysics and planetary science, fluid dynamical processes play important roles on virtually all length and mass scales from galaxies to planets. The smoothed particle hydrodynamics (SPH) method (Lucy 1977; Gingold & Monaghan 1977) is one of the most popular simulation methods to solve the motion of a fluid in astrophysical problems (for reviews, see Monaghan 1992; Rosswog 2009; Springel 2010). In the SPH method, fluid elements are represented by hypothetical particles (so-called SPH particles). Thus, the dynamical equations are written in the Lagrangian form of hydrodynamical equations. Compared to grid-base methods, the SPH method is suitable to problems in which inhomogeneities, such as large empty regions and small dense core, develop. Furthermore, it is easy to incorporate various physical effects to the SPH scheme, such as self-gravity, radiative cooling and chemical reactions. Because of these advantages, various astrophysical problems, such as star-formation, planetesimal collisions and galaxy formation, have been studied using the SPH method.

Recently, however, it has been pointed out that the standard SPH method has difficulties in dealing with hydrodynamical instabilities, such as the Kelvin-Helmholtz instability (KHI) or the Rayleigh-Taylor instability (RTI) (e.g., Okamoto et al. 2003; Agertz et al. 2007; Valcke et al. 2010; McNally et al. 2012). Agertz et al. (2007) has concluded that this difficulty is due to the requirement of the standard SPH, that the density must be continuous and differentiable. This requirement is not satisfied at contact discontinuities. As a result, at contact discontinuities, the pressure of the low-density side is overestimated, and that of the high-density side is underestimated. Thus, pressure is also overestimated at the low-density side of the contact discontinuity, and a “unphysical” repulsive force appears. This unphysical repulsive force causes a surface tension effect that suppresses the growth of hydrodynamical instabilities.

To resolve this issue, modifications of the standard SPH method have been proposed. Price (2008) introduced an artificial thermal conductivity term in the SPH equation to smooth the thermal energy at the contact discontinuity (Price 2008; Valdarnini 2012). Cha et al. (2010) and Murante et al. (2011) showed that the Godunov SPH, originally developed by Inutsuka (2002), can describe hydrodynamical instabilities. However, the Godunov scheme is difficult to extend to non-ideal equation of state (EOS), though methods exist (e.g., Colell & Glaz 1985). Read et al. (2010) showed that KHI takes place with the equation of motion of Ritchie and Thomas (2001), and with a kernel function that has a larger number of neighbours. Heß and Springel (2010) replaces the density estimate in the standard SPH by a new density estimate with Voronoi tesselation. Abel (2011) used the relative pressure instead of the absolute value of the pressure in the equation of motion. However, this approach does not satisfy the conservation of momentum. García-Senz et al. (2012) present a new formulation that is based on a tensor approach.

Saitoh and Makino (2013) have proposed a new formulation of SPH. They pointed out that the problematic requirement of the differentiability of the density arises from the formula used to estimate the volume element associated with a particle in the standard SPH. The volume element used in the standard SPH is \( \Delta V_i = m_i / \rho_i \), where \( \Delta V_i \), \( m_i \), and \( \rho_i \) are the volume element, the mass and the density of a particle \( i \), respectively. Thus, by using an estimate of the volume element that is independent of the mass and density, we can avoid the necessity for the differentiability of the density. In particular,
Saitoh and Makino (2013) used $U_i/q_i$ as the volume element, where $U_i$ is the internal energy and $q_i$ is the energy spatial density. As a result, their formulation does not require differentiability of the density. In the case of the EOS of ideal gas, the pressure is proportional to the energy spatial density. Thus, the requirement of the differentiability of the energy spatial density corresponds to the requirement of the differentiability of the pressure. Their formulation does not introduce any physically non-existent term, and does not break any conservation property. They showed that their new SPH can handle hydrodynamical instabilities well.

However, their new formulation can be applied only to ideal gas. In many astrophysical problems, the EOS is non-ideal. In this paper, we present an extension of their new SPH to non-ideal EOS. As is shown in Saitoh and Makino (2013), we can choose an arbitrary basis for the volume element. Thus, using a different choice of the estimate of the volume element, we can extend the new SPH to non-ideal EOS, without losing any advantages of Saitoh and Makino (2013)'s formulation.

This paper is organized as follows. In section 2, we present a brief overview of the formulation of Saitoh and Makino (2013). Then, in section 3, our new formulation is described. In section 4, the results of various test calculations with our new SPH are shown. Finally, in section 5, we summarize this paper.

2. Overview of the Density Independent SPH

Let us consider the following set of equations that describes the motion of fluid:

\[
\begin{align*}
\frac{dp}{dt} &= -\rho \nabla \cdot \mathbf{v}, \\
\frac{dv}{dt} &= -\frac{1}{\rho} \nabla p, \\
\frac{du}{dt} &= -\frac{p}{\rho} \nabla \cdot \mathbf{v},
\end{align*}
\]

(1)

(2)

(3)

Here, $\rho$, $\mathbf{v}$, $\mathbf{p}$, $u$, and $t$ are the density, velocity, pressure, specific internal energy and time, respectively. The pressure $\rho$ is given by EOS, $p = p(\rho, u)$.

In the SPH method, a fluid is expressed by a number of SPH particles. Physical quantities at a point are approximated by the summation of the contributions of these particles. First, we approximate a function $f(x)$ by convolution with a kernel function, $W(x, h)$:

\[ f(x) = \int f(x') W(x - x'; h) dV'. \]

(4)

where $x$ is the position vector, $W$ is the kernel function and $h$ is the smoothing length. The kernel function must be differentiable for $|x|$ and have following two properties:

\[ \int W(x - x'; h) dV' = 1, \]

\[ \lim_{h \to 0} W(x - x'; h) = \delta(x - x'). \]

(5)

(6)

We can use an arbitrary kernel function, as long as the above conditions are satisfied. Throughout this paper, we use the cubic spline function proposed by Monaghan and Lattanzio (1985):

\[
W(x; h) = \frac{\sigma}{h^D} \times \begin{cases} 
\frac{1}{4} (4 - 6s^2 + 3s^3) & (0 \leq s < 1), \\
\frac{1}{4} (2 - s)^2 & (1 \leq s < 2), \\
0 & (2 \leq s).
\end{cases}
\]

(7)

where $s = |x|/h$, $D$ is number of dimensions and $\sigma$ is the normalization constant that takes values of $2/3$, $10/7\pi$, $1/\pi$ in one-, two- and three-dimensional cases, respectively. Note that the use of this cubic spline kernel, for the derivative sometimes causes clustering of the SPH particles. In order to avoid this clustering of the SPH particles, we adopt a gradient of the kernel, which has a triangular shape, as done by Thomas and Couchman (1992):

\[
\nabla W(x; h) = -\frac{\sigma x}{h^{D+1}|x|} \times \begin{cases} 
1 & (0 \leq s < 2/3), \\
\frac{3}{4} s(4 - 3s) & (2/3 \leq s < 1), \\
\frac{3}{4} (2 - s)^2 & (1 \leq s < 2), \\
0 & (2 \leq s).
\end{cases}
\]

(8)

The essential solution is to adopt the kernels that do not show the pairing instability (Read et al. 2010; Dehnen & Aly 2012).

In order to evaluate the value of the physical quantities at the positions of particles, we need to discretize equation (4). By approximating the integral by summation over the particles, we obtain the following equation:

\[
\{f(x)\} = \sum_j f_j W(x - x_j; h) \Delta V_j,
\]

(9)

where the subscript $j$ denotes particle index and $f_j$ is the value of $f(x)$ of particle $j$. In the formulation of Saitoh and Makino (2013), the volume element $\Delta V_j$ is replaced by $U_j/q_j$, where $U_j = m_j u_j$ is the internal energy and $q_j = \rho_j u_j$ is the energy spatial density of the $j$-th particle. Thus, $f_i$ can be written as

\[
f_i = \sum_j f_j \frac{U_j}{q_j} W(x_{ij}; h).
\]

(10)

where $x_{ij} = x_i - x_j$. By substituting $q$ into $f$, we obtain

\[
q_i = \sum_j U_j W(x_{ij}; h).
\]

(11)

From equations (10), the derivative of $f_i$ is given by

\[
\nabla f_i = \sum_j f_j \frac{U_j}{q_j} \nabla W(x_{ij}; h).
\]

(12)

Now, we first derive the equation of energy, and then the equation of motion.

In order to derive the equation of energy, we need an expression of $\nabla \cdot \mathbf{v}$. We use the following relation:

\[
\nabla (q \mathbf{v}) = \mathbf{v} \cdot \nabla q + q \nabla \cdot \mathbf{v}.
\]

(13)

Note that in the case of an ideal gas, the pressure is proportional to $q$. Thus, around the contact discontinuity, $q$ is differentiable. By applying equation (12) to equation (13), we obtain

\[
q_i \nabla \cdot \mathbf{v}_i = -\sum_j U_j w_{ij} \cdot \nabla W(x_{ij}; h).
\]

(14)
where \( \mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j \). Here, the density, \( \rho_i \), is

\[
\rho_i = \frac{m_i q_i}{U_i}.
\]

By applying equations (14) and (15) to equation (3), we can write the equation of energy as

\[
\frac{dU_i}{dt} = \sum_j \frac{U_i p_i}{q_i^2} U_j \mathbf{v}_{ij} \cdot \nabla W(r_{ij};h).
\]

(16)

Now we define the change in the internal energy of the \( i \)-th particle due to the interaction with the \( j \)-th particle as \( dU_{ij}/dt \). From equation (16), we obtain

\[
\frac{dU_{ij}}{dt} = U_i U_j p_i q_j \mathbf{v}_{ij} \cdot \nabla W(x_{ij};h).
\]

(17)

From the equation of energy, we derive the equation of motion. The change of the internal energy is the same as that of the kinetic energy with an opposite sign,

\[
\frac{dU_i}{dt} + \frac{dU_{ij}}{dt} = -\frac{d}{dt}(K_i + K_j).
\]

(18)

where \( K_i \) and \( K_j \) are the kinetic energy of the \( i \)-th and \( j \)-th particle, respectively. Here, we consider the change of \( K_i \) due to the interaction with the \( j \)-th particle only. From equation (17), the left hand side of equation (18) can be written as

\[
\frac{dU_{ij}}{dt} + \frac{dU_{ji}}{dt} = U_i U_j \left( \frac{p_i}{q_i^2} + \frac{p_j}{q_j^2} \right) \mathbf{v}_{ij} \cdot \nabla W(x_{ij};h).
\]

(19)

Here, \( K_i + K_j \) is

\[
K_i + K_j = \frac{1}{2} m_i v_i^2 + \frac{1}{2} m_j v_j^2
\]

\[
= \frac{1}{2} \left( m_i + m_j \right) \left( \frac{m_i v_i + m_j v_j}{m_i + m_j} \right)^2 + \frac{1}{2} \frac{m_i m_j}{m_i + m_j} v_{ij}^2.
\]

(20)

Thus, the change of the kinetic energy can be written as

\[
\frac{d}{dt}(K_i + K_j) = \frac{1}{2} \frac{m_i m_j}{m_i + m_j} \frac{d}{dt} \left( \frac{m_i v_i + m_j v_j}{m_i + m_j} \right)^2 + \frac{m_i m_j}{m_i + m_j} \mathbf{v}_{ij} \cdot \frac{d\mathbf{v}_{ij}}{dt}.
\]

(21)

Since the total momentum of two particles is conserved, we have

\[
\frac{d}{dt}(m_i \mathbf{v}_i + m_j \mathbf{v}_j) = 0.
\]

(22)

Thus, the first term of the right-hand side of equation (21) is zero. By substituting equations (19) and (21) into equation (18), we obtain

\[
\frac{m_i m_j}{m_i + m_j} \frac{d\mathbf{v}_{ij}}{dt} = U_i U_j \left( \frac{p_i}{q_i^2} + \frac{p_j}{q_j^2} \right) \nabla W(x_{ij};h).
\]

(23)

By using equation (22), we can eliminate \( \mathbf{v}_j \) in equation (23), and we finally obtain

\[
\frac{m_i d\mathbf{v}_i}{dt} = -\sum_j U_i U_j \left( \frac{p_i}{q_i^2} + \frac{p_j}{q_j^2} \right) \nabla W(x_{ij};h).
\]

(24)

Note that for the case of a variable kernel size, \( \nabla W(x_{ij};h) \) must take a symmetrical form in the smoothing length to satisfy the conservation of energy and momentum. This condition is achieved by replacing \( \nabla W(x_{ij};h) \) with \( \nabla W(x_{ij};h_i) + \nabla W(x_{ij};h_j)/2 \) or \( \nabla W[x_{ij};(h_i + h_j)/2] \). Throughout this paper, we adopt the former form.

Hopkins (2013) and Saitoh and Makino (2013) derived the equation of motion from a Lagrangian. The advantage of this derivation is that it includes the variation of \( h \) naturally. This term, so-called the "\( \nabla h \)" term, is important in simulations in which extremely strong shocks are present [see subsection 3.5 in Saitoh and Makino (2013)].

3. Extension to Non-Ideal EOS of DISPH

In the previous section, we summarized the formulation of Saitoh and Makino (2013). As stated above, the formulation of Saitoh and Makino (2013) has one assumption: that the pressure is proportional to the energy spatial density. In this section, we extend their new SPH to an arbitrary EOS. In order to construct a new SPH formulation, we introduce the following quantity:

\[
Y_i = \frac{p_i}{\rho_i} \Delta V_i.
\]

(25)

In our formulation, we use the following new volume element:

\[
\Delta V_i = \frac{Y_i}{\rho_i}.
\]

(26)

By substituting equation (26) into equation (9), we obtain the following two equations:

\[
f_i = \sum_j f_j \frac{Y_j}{\rho_j} W(x_{ij};h),
\]

(27)

\[
\nabla f_i = \sum_j f_j \frac{Y_j}{\rho_j} \nabla W(x_{ij};h).
\]

(28)

By substituting \( p \) into \( f \) in equation (27), we obtain the smoothed pressure \( p \),

\[
p_i = \sum_j Y_j W(x_{ij};h).
\]

(29)

We first derive the equation of energy, and then we derive the equation of motion, following the derivation of Saitoh and Makino (2013).

3.1. Equation of Energy

In order to derive the equation of energy, we need an expression of \( \nabla \cdot \mathbf{v} \) in our new SPH. Here, we use

\[
p \nabla \cdot \mathbf{v} = \nabla \cdot (p \mathbf{v}) - \mathbf{v} \cdot \nabla p.
\]

(30)

which can be obtained by replacing \( q \) in equation (13) by \( p \). Thus, the expression of \( \nabla \cdot \mathbf{v} \) is

\[
\nabla \cdot \mathbf{v}_i = -\frac{1}{\rho_i} \sum_j Y_j v_{ij} \cdot \nabla W(x_{ij};h).
\]

(31)

In our new SPH, the density \( \rho_i \) can be expressed as

\[
\rho_i = \frac{m_i p_i}{Y_i}.
\]

(32)
By applying equations (31) and (32) to equation (3), the equation of energy can be written as

$$\frac{dU_i}{dt} = \sum_j Y_i Y_j \frac{p_i}{p_j} v_{ij} \cdot \nabla W(x_{ij}; h).$$  \hspace{1cm} (33)

Hence, the equation corresponding to equation (17) is

$$\frac{dU_{ij}}{dt} = Y_i Y_j \frac{p_i}{p_j} v_{ij} \cdot \nabla W(x_{ij}; h).$$  \hspace{1cm} (34)

### 3.2. Equation of Motion

From the equation of energy, we derive the equation of motion. By using equation (34) instead of equation (17), we obtain the analogue of equation (23):

$$- \frac{m_i m_j}{m_i + m_j} \frac{d}{dt} \frac{dY_{ij}}{dt} = Y_i Y_j \left( \frac{1}{p_i} + \frac{1}{p_j} \right) \nabla W(x_{ij}; h).$$  \hspace{1cm} (35)

Thus, the equation of motion becomes

$$m_i \frac{d^2 v_i}{dt^2} = - \sum_j Y_i Y_j \left( \frac{1}{p_i} + \frac{1}{p_j} \right) \nabla W(x_{ij}; h).$$  \hspace{1cm} (36)

### 3.3. The Equation for $Y$

In the previous section, we derived the equation of energy and the equation of motion. These equations determine the evolution of a fluid. However, in order to actually perform the numerical integration, we need to determine new values of the pressure, by solving an implicit equation, equation (29), for a given position, $x_i$, and a specific internal energy, $u_i$. We solve equation (29) by iteration. Here, we summarize the actual procedure.

**Step 1**: We calculate the density using equation (32).

**Step 2**: From the EOS, density and internal energy, we obtain the non-smoothed pressure $\tilde{p} = p(\rho, u)$.

**Step 3**: We update $\tilde{Y}$ from the equation, $\tilde{Y} = m \tilde{p} / \rho$.

**Step 4**: We calculate $p$ by using equation (29). If necessary, we go back to Step 1.

Unless otherwise noted, only one cycle of the above iteration is applied.

We calculate the initial guess of $\tilde{Y}$ by integrating the time derivative of $Y$. It is given by

$$\frac{dY}{dt} = p \frac{dV}{dt} + \Delta V \frac{dp}{dt} = p \Delta V \left( \frac{1}{\Delta V} \frac{d\Delta V}{dt} + \frac{1}{p} \frac{dp}{dt} \right) = Y \left( \frac{1}{\Delta V} \frac{d\Delta V}{dt} + \frac{\Delta V}{p} \frac{1}{\Delta V} \frac{dp}{dt} \right) = Y \frac{1}{\Delta V} \frac{d\Delta V}{dt} \left( 1 + \frac{\Delta V}{p} \frac{dp}{d\Delta V} \right).$$  \hspace{1cm} (37)

From the continuity equation, equation (1), and $\Delta V = m / \rho$, we obtain

$$\frac{1}{\Delta V} \frac{d\Delta V}{dt} = \nabla \cdot \mathbf{v},$$  \hspace{1cm} (38)

$$\frac{\Delta V}{\frac{p}{\rho}} \frac{dp}{d\Delta V} = - \frac{\rho}{p} \frac{dp}{d\rho}.$$  \hspace{1cm} (39)

By substituting equations (38) and (39) into equation (37), we obtain

$$\frac{dY_i}{dt} = (\gamma_i - 1) \sum_j Y_i Y_j \frac{p_i}{p_j} v_{ij} \cdot \nabla W(x_{ij}; h).$$  \hspace{1cm} (40)

where

$$\gamma_i := \frac{p_i}{\rho_i} \frac{dp}{d\rho}_i.$$  \hspace{1cm} (41)

When equation (29) is satisfied, we should have $p_i = p(\rho_i, u_i)$. If we express this as an equation for a specific internal energy, $u_i$, we have $u(p_i, \rho_i) = u_i$, where $u(p_i, \rho_i)$ comes from the EOS. Therefore, the quantity

$$\Delta u_i = \left| u(p_i, \rho_i) - u_i \right|.$$  \hspace{1cm} (42)

3.4. Smoothing Length

The smoothing length is the effective length of the kernel function. In general, individual and time-varying smoothing lengths are used. In this paper, we use the following equation to determine $h_i$:

$$h_i = \eta \left( \frac{m_i}{\rho_i} \right)^{1/D} = \eta \left( \frac{Y_i}{\rho_i} \right)^{1/D}.$$  \hspace{1cm} (43)

Unless otherwise specified, we set the parameter to $\eta = 1.2$.

3.5. A Conservative Formulation of Our New SPH Using the Action Principle

As stated above, we derived the equation of motion and equation of energy of our new SPH from the fundamental equations of fluid. However, as Springel and Hernquist (2002) did, the equations for the SPH method can be also derived from the Lagrangian. Recently, Hopkins (2013) derived the equation of motion for Saioto and Makino (2013)’s new SPH from the Lagrangian. In this section, we derive the equation of motion for our new SPH from the Lagrangian, and show the corresponding expression of $\nabla h$ term for our new SPH.

Here, we consider the Euler–Lagrangian equation,

$$\frac{d}{dt} \frac{\partial L}{\partial Q_i} - \frac{\partial L}{\partial Q_i} = \sum_j \lambda_{ij} \frac{\partial \phi_j}{\partial Q_i},$$  \hspace{1cm} (45)

where $L$, $\lambda_{ij}$, and $\phi_i$ are the Lagrangian, Lagrange multipliers and appropriate constraints, respectively. According to Hopkins (2013), we use the following constraint equation:

$$\phi_i = \frac{4\pi}{3} (Hh_i)^3 \frac{1}{\Delta V_i} - N_{\text{SPH}} = 0,$$  \hspace{1cm} (46)

where $H$ is the kernel-support radius. This constraint equation gives a condition that there are an approximately constant number of particles in the kernel for three dimensions, if the mass of each SPH particle is equal. The Lagrangian can be written as...
where \( \mathbf{Q} = (x_1, \ldots, x_N, h_1, \ldots, h_N) \). By substituting equations (46) and (47) into equation (45), we obtain \( 2N \) equations.

Let us consider the second half of the above \( 2N \) equations. By substituting \( h_i \) into \( \mathbf{Q_i} \), the right-hand side of the Euler–Lagrangian equation becomes

\[
\sum_j \lambda_j \frac{\partial \mathbf{p}_j}{\partial h_i} = \lambda_i \frac{\partial}{\partial h_i} \left[ \frac{4\pi H^3 h_j^2}{3} \frac{1}{\Delta V_j} - N_{\text{SPH}} \right] \frac{\partial}{\partial h_i} \left( 1 - \frac{h_i}{3} \frac{\partial \Delta V_i}{\partial h_i} \right). 
\]

(48)

The left-hand side becomes

\[
\frac{d}{dt} \frac{\partial L}{\partial \mathbf{p}_j} = \frac{\partial}{\partial h_i} \frac{\partial L}{\partial \mathbf{h}_i} = -p_i \frac{\partial \Delta V_i}{\partial h_i}. 
\]

(49)

Note that here we used the following relation from the first law of thermodynamics,

\[
\frac{\partial U_i}{\partial \mathbf{Q}_i} = -p_i \frac{\partial \Delta V_i}{\partial \mathbf{Q}_i}. 
\]

(50)

From equations (48) and (49), we obtain the Lagrangian multipliers as

\[
\lambda_i = \frac{p_i \Delta V_i \frac{\partial \Delta V_i}{\partial h_i}}{4\pi H^3 h_j^2 \frac{\partial}{\partial h_i} \left( 1 - \frac{h_i}{3} \frac{\partial \Delta V_i}{\partial h_i} \right)}. 
\]

(51)

By substituting the positions of SPH particles into \( \mathbf{Q}_i \), in equations (45) and (51), we obtain the equation of motion,

\[
m_i \frac{d \mathbf{v}_i}{dt} = \sum_j \left( p_j - \frac{4}{3} \pi H^3 h_j^2 \lambda_j \frac{1}{\Delta V_j^2} \right) \nabla(\Delta V_j). 
\]

(52)

Here, we recall that in our new SPH, the volume element, \( \Delta V_i \), is estimated as \( Y_i/p_i \). Thus, we obtain following equations:

\[
\frac{\partial \Delta V_i}{\partial h_i} = \frac{Y_i}{p_i^2} \frac{\partial p_i}{\partial h_i}, 
\]

\[
\nabla(\Delta V_j) = \frac{Y_j}{p_j} \nabla p_j = -\frac{Y_j}{p_j} \left[ Y_j \nabla W(x_{ij}; h_i) + \delta_{ij} \sum_k Y_k \nabla W(x_{ik}; h_i) \right]. 
\]

(53)

(54)

(55)

where \( \delta_{ij} \) is Kronecker’s delta. By substituting equation (53) into equation (51), we obtain \( \lambda_i \):

\[
\lambda_i = \frac{Y_i^2}{4\pi H^3 h_j^2} \frac{\partial p_i}{\partial h_i} \left( 1 + \frac{h_i}{3} \frac{\partial p_i}{\partial h_i} \right)^{-1}. 
\]

(56)

By substituting equations (54) and (55) into equation (52), we obtain the equation of motion as

\[
m_i \frac{d \mathbf{v}_i}{dt} = -\sum_j Y_j \left[ \frac{f_{i,\text{grad}}^{\text{grad}}}{p_i} \nabla W(x_{ij}; h_i) + \frac{f_{i,\text{grad}}^{\text{grad}}}{p_j} \nabla W(x_{ij}; h_i) \right], 
\]

(57)

where

\[
f_{i,\text{grad}}^{\text{grad}} = \left( 1 + \frac{h_i}{3} \frac{\partial p_i}{\partial h_i} \right)^{-1}. 
\]

In order to calculate the time evolution of the specific internal energy explicitly, we need the equation of energy. We derive the equation of energy with the \( \nabla h \) term as follows. From the first law of thermodynamics, we obtain

\[
\frac{d U_i}{dt} = -p_i \frac{d \Delta V_i}{dt}. 
\]

(58)

Here,

\[
\frac{d \Delta V_i}{dt} = \frac{d}{dt} \left( \frac{Y_i}{p_i} \right) = -\frac{Y_i}{p_i} \frac{d p_i}{dt} = -\frac{Y_i}{p_i} \frac{d}{dt} \sum_j Y_j W(x_{ij}; h_i) = -\frac{Y_i}{p_i} \sum_j Y_j \left[ \frac{\partial W(x_{ij}; h_i)}{\partial h_i} + \frac{d h_i}{dt} \frac{\partial W(x_{ij}; h_i)}{\partial h_i} \right]. 
\]

(59)

From equations (46), we obtain the following equation:

\[
\frac{d h_i}{dt} = \frac{h_i}{3} \frac{d \Delta V_i}{dt}. 
\]

(60)

By substituting equation (60) into equation (59),

\[
\frac{d \Delta V_i}{dt} = -\frac{Y_i}{p_i} \sum_j Y_j \left[ \frac{\partial W(x_{ij}; h_i)}{\partial h_i} + \frac{h_i}{3} \frac{d}{dt} \frac{\partial W(x_{ij}; h_i)}{\partial h_i} \right] = -\frac{Y_i}{p_i} \sum_j Y_j \frac{\partial W(x_{ij}; h_i)}{\partial h_i} \frac{d \Delta V_j}{dt}. 
\]

(61)

From the above equation we obtain

\[
\frac{d \Delta V_i}{dt} = -f_{i,\text{grad}}^{\text{grad}} \sum_j Y_j \frac{\partial W(x_{ij}; h_i)}{\partial h_i}. 
\]

(62)

By substituting equation (62) into equation (58), we obtain the equation of energy, as follows:

\[
\frac{d U_i}{dt} = \sum_j Y_j \frac{f_{i,\text{grad}}^{\text{grad}}}{p_i} \nabla W(x_{ij}; h_i). 
\]

(63)

With the equation of energy, we can obtain the analogue to equation (40), as follows:

\[
\frac{d Y_i}{dt} = (y_i - 1) \sum_j Y_j f_{i,\text{grad}}^{\text{grad}} \frac{\partial W(x_{ij}; h_i)}{\partial h_i}. 
\]

(64)

Note that here we discuss only the three-dimensional case. However, by using an appropriate constraint, we can easily derive the expression of \( f_{i,\text{grad}}^{\text{grad}} \) in the one- or two-dimensional case, as follows:

\[
f_{i,\text{grad}}^{\text{grad}} = \left( 1 + \frac{h_i}{D} \frac{\partial p_i}{\partial h_i} \right)^{-1}. 
\]

(65)
3.6. Artificial Viscosity

We need to introduce artificial viscosity to handle shocks. There are several different forms of artificial viscosity (e.g., Lattanzio et al. 1985; Monaghan 1997). In this paper we adopt the following form of the artificial viscosity proposed by Monaghan (1997). It is expressed as

$$\Pi_{ij} = -\frac{\alpha_{AV} v_{ij}^{\text{sig}} w_{ij}}{\rho_i},$$

(66)

where

$$v_{ij}^{\text{sig}} = c_i + c_j - 3 w_{ij},$$

(67)

$$w_{ij} = \begin{cases} \frac{v_{ij} \cdot x_{ij}}{|x_{ij}|} & \text{if } x_{ij} \cdot v_{ij} < 0, \\ 0 & \text{otherwise}, \end{cases}$$

(68)

$$\rho_{ij} = \frac{1}{2}(\rho_i + \rho_j).$$

(69)

Note that the use of equation (32) for calculating the artificial viscosity sometimes leads to an unstable behavior under strong shocks. It seems to be safer to use the smoothed density,

$$\rho_i = \sum_j m_j W(x_{ij}; h_i).$$

(70)

In order to suppress the shear viscosity, we apply the Balsara switch (Balsara 1995). It is given by

$$F_i = \frac{\left| \nabla \cdot v_i \right|}{\left| \nabla \cdot v_i \right| + \left| \nabla \times v_i \right| + \varepsilon_b c_i / h_i},$$

(71)

where $\varepsilon_b$ is a small value introduced to prevent numerical overflow. In this paper we set $\varepsilon_b = 0.0001$. Here, the rotation of velocity is given by

$$\nabla \times v_i = - \sum_j \frac{V_j}{p_i} v_{ij} \times \nabla W(x_{ij}; h_i).$$

(72)

Consequently, the viscosity terms for the equation of motion and the equation of energy are given by

$$\left( m_i \frac{dv_i}{dt} \right)_{AV} = -m_i \sum_j m_j \frac{1}{2} (F_i + F_j) \Pi_{ij}$$

$$\times \frac{1}{2} \left[ \nabla W(x_{ij}; h_i) + \nabla W(x_{ij}; h_j) \right],$$

(73)

$$\left( \frac{dU_i}{dt} \right)_{AV} = \frac{m_i}{2} \sum_j m_j \frac{1}{2} (F_i + F_j) \Pi_{ij} v_{ij}$$

$$\times \frac{1}{2} \left[ \nabla W(x_{ij}; h_i) + \nabla W(x_{ij}; h_j) \right],$$

(74)

respectively.

One might imagine that the use of the smoothed density in the artificial viscosity would be inconsistent with the formulation of our new SPH. The artificial viscosity is, however, a mimic of the molecular dissipation, which is not included in the original set of equations for hydrodynamics. Thus, the choice of the form of the artificial viscosity is independent from the formulation of the SPH.

3.7. Timestep

The timesteps for integration are limited by the Courant condition for numerical stability. The timesteps of the $i$-th particle, $dt_i$, are given by

$$dt_i = C_{CFL} \frac{2h_i}{\max_j v_{ij}^{\text{sig}}},$$

(75)

where we set $C_{CFL} = 0.3$.

4. Numerical Tests

4.1. Shock Tube Tests

The shock tube test is one of the most common test problems. It is designed to test the ability of a numerical method to capture the shock. We place the initial discontinuity at the origin of the coordinates. We place equal-mass particles. The particle separation varies according to the density distribution. We use a shared timestep, and adopt $dt = \min_i dt_i$ as the time step of each step. Throughout this paper, we adopt $C_{CFL} = 0.3$.

Figure 3 shows the relative error of the specific internal energy for each particle, as defined in equation (43). At the contact discontinuity, $x \simeq 0.2$, large errors can be seen.
Fig. 1. Snapshots from the 1D shock tube test for the Tamman EOS with our new SPH at $t = 0.01$. The dots indicate SPH particles and the solid curves represent the exact solution.

Fig. 2. Same as figure 1, but with the standard SPH. At the contact discontinuity, a large pressure blip can be seen. This causes a suppression of fluid mixing.
However, for any particle, the absolute value of the error is less than 0.01%.

4.2. Hydrostatic Equilibrium Tests

This test clearly shows the ability of a scheme to handle the contact discontinuity. A similar test has been performed by Saitoh and Makino (2013) with the ideal gas EOS. In order to check the ability of our new SPH to the non-ideal EOS, we use the Tillotson EOS (see below), instead of the ideal gas EOS. We set a high-density region in a low-density ambient, at a pressure equilibrium. We use a 2D computational domain, $0 \leq x < 1$ and $0 \leq y < 1$. In both directions, the mirror boundary condition is imposed. The density is

$$\rho = \begin{cases} 4 & \text{for } 0.25 < x < 0.75 \text{ and } 0.25 < y < 0.75, \\ 1 & \text{otherwise.} \end{cases}$$

(78)

To express the above density distribution, we place equal-mass particles in a uniform grid. The number of particles in the dense square is 4225 and that in the ambient is 3007, respectively. The end time is $t = 8$. Since the system is in the hydrostatic equilibrium, particles should not move.

The Tillotson EOS (Tillotson 1962; Melosh 1989) is one of the most widely used EOS for giant impact simulations (e.g., Benz et al. 1986; Canup & Asphaug 2001; Genda et al. 2012). The Tillotson EOS contains 10 parameters, which we should choose to describe a given material. The Tillotson EOS takes three different functional forms, depending on the density, $\rho$, and the specific internal energy, $u$.

(A) condensed ($\rho > \rho_0$) or cold state ($u < u_{iv}$)

In this region, the Tillotson EOS is given by the following form:

$$p_{co} = a \rho u + \left[ \frac{b \rho u}{u_0 \eta^2} + 1 \right] A \mu + B \mu^2. \tag{79}$$

where $\eta = \rho/\rho_0$ and $\mu = \eta - 1$.

(B) expanded hot state ($\rho < \rho_0$ and $u > u_{cv}$)

In this region, the Tillotson EOS is given by the following form:

$$p_{ex} = a \rho u + \left[ \frac{b \rho u}{u_0 \eta^2} + 1 \right] A \mu \exp \left\{ -\alpha \left( 1 - \frac{1}{\eta} \right) \right\} \times \left[ \frac{\beta}{1 - \frac{1}{\eta}} \right]^2. \tag{80}$$

(C) intermediate region ($u_{iv} < u < u_{cv}$ and $\rho < \rho_0$)

In this region, a smooth transition between the above two states occurs. Thus, as Benz et al. (1986) did, we interpolated the pressure by using $p_{co}$ and $p_{ex}$:

$$p_{tr} = \frac{(u - u_{iv}) p_{ex} + (u_{cv} - u) p_{co}}{u_{cv} - u_{iv}}. \tag{81}$$

Here, $\rho_0$, $u_0$, $a$, $b$, $A$, $B$, $u_{cv}$, $u_{iv}$, $\alpha$, and $\beta$ are material parameters. In the present work, we used the values for granite: $\rho_0 = 2680 \text{ kg m}^{-3}$, $u_0 = 16 \text{ MJ kg}^{-1}$, $a = 0.5$, $b = 1.3$, $A = 18 \text{ GPa}$, $B = 18 \text{ GPa}$, $u_{cv} = 18 \text{ MJ kg}^{-1}$, $u_{iv} = 3.5 \text{ MJ kg}^{-1}$, $\alpha = 5$, and $\beta = 5$. We set the density unit, $\rho_0$, unit specific energy, $u_0$, and unit pressure, $\rho_0 u_0$.

Figure 4 shows the results of this test for the standard SPH and our new SPH. The difference between the two schemes is clear. With the standard SPH, although the pressures of each particle are initially equal, the high-density domain becomes a circle at $t = 8$. The reason why such an unphysical transform occurs is explained Saitoh and Makino (2013).

In contrast, with our new SPH, the high-density domain keeps its original shape, except for some local rearrangement near the boundary of two fluids. Our new SPH removes the unphysical surface tension completely, even for a non-ideal gas.

4.3. KHI tests

KHI is one of the most fundamental test problems for the ability of numerical methods to handle hydrodynamical instability. Initially, two layers in pressure equilibrium have different density, and move to opposite directions to each other.

We performed the KHI test for the Tillotson EOS. We used a 2D computational domain, $-0.5 < x < 0.5$ and $-0.25 < y < 0.25$. Periodic boundary conditions were imposed in the $x$-direction, and the mirror boundary condition was imposed in the $y$-direction. We set the density as follows:

$$\rho = \begin{cases} \rho_l & \text{for } y > 0, \\ \rho_h & \text{for } y \leq 0, \end{cases} \tag{82}$$

where $\rho_l$ and $\rho_h$ are the density of the low-density region and that of the high-density region, respectively. The shear velocity was set up in the $x$-direction. We set $v_{x,l} = 0.5$ for the high-density region and $v_{x,l} = -0.5$ for the low-density region, respectively. As a seed of the instability, a small perturbation was added to the particles around the initial contact discontinuity:

$$v_y = \Delta v_y \sin \left( \frac{2\pi x}{\lambda} \right) \text{ for } |y| < 0.025. \tag{83}$$

Here, $\Delta v_y$ and $\lambda$ are the amplitude and wavelength of the initial perturbation, respectively. We set $\Delta v_y = 0.025$ and $\lambda = 1/6$. 
Thus, six vortex rolls were expected to be developed in the computational domain. The growth time scale of the KHI is

\[ \tau_{\text{KH}} = \frac{\lambda (\rho_l + \rho_h)}{\sqrt{\rho_l \rho_h |v_{x,l} - v_{x,h}|}}. \]  

(84)

For our test case, \( \tau_{\text{KH}} \approx 0.35 \). In each region, we placed the equal-mass particles uniformly in a lattice. The particle separation in the low-density region was set to 1/512.

The equilibrium pressure was set to 3.5.

Figure 5 shows the density distributions at times \( t = 1.0 \tau_{\text{KH}} \) and \( 2.0 \tau_{\text{KH}} \). The upper row gives the results of our new SPH, and the lower row gives those of the standard SPH. There is an obvious difference between the two results, and our new SPH gives far better results compared to that of the standard SPH. With the standard SPH, perturbations grow until \( 1.0 \tau_{\text{KH}} \). However, the unphysical surface tension inhibits the growth of
the vortex rolls. The dense fluid is stretched. As a consequence, the standard SPH produces “blobs” of dense fluid (see figure 7 in Price 2008; figure 7 in Saitoh & Makino 2013). The mixing between the two layers is completely suppressed. On the other hand, our new SPH shows very good result. At \( t = 2.0 \, t_{KH} \), six vortex rolls are clearly visible.

Figure 6 shows the pressure distribution along the \( y \)-axis at \( t = 1.0 \, t_{KH} \). The left panel gives the result of the standard SPH, while the right panel gives that of our new SPH. With the standard SPH, there is a large pressure jump at the contact interface, \( y \approx 0 \). With our new SPH, on the other hand, the pressure jump is much smaller. Our new SPH eliminated the unphysical surface tension, even for a non-ideal gas. Thus, the growth of the KHI is not suppressed.

Figure 7 shows the distribution of the error of specific internal energy for each particle, as defined in equation (43). One iteration of the pressure summation loop is done. At the contact interface \( y \approx 0 \), particles have larger errors. However, even for the largest value, the error is about 1%. Figure 8 shows that the averaged of error of the specific internal energy, as defined in equation (42), decreases as the number of iterations of the pressure summation loop of our new SPH increases. For all cases, the averaged error of the specific internal energy is less than 0.1%, and the error becomes smaller by a factor of two after each iteration.

![Pressure distribution from the KHI test along the y-axis at \( t = 1.0 \, t_{KH} \). The left panel shows the result of the standard SPH, while the right panel shows that of our new SPH. Pressure is normalised to \( \rho_0 u_0 \).](image1)

![The distribution of the error of the specific internal energy of the KHI test along the y-axis at \( t = 1.0 \, t_{KH} \) with one iteration.](image2)

![The averaged error of the specific internal energy versus number of iterations for our new SPH.](image3)
5. Discussion and Summary

5.1. Treatment of Mixing

In a real fluid, mixing takes place due to physical dissipation, namely, the random motion of molecules. Thus, if we had an infinite number of particles, mixing would not take place at all, and we could resolve infinitely small vortices, as long as we do not include any physical diffusion term. For the test of KHI, however, our new SPH produces a somewhat noisy contact interface between two fluids. Therefore, one might think that other schemes, such as the AC term, are better than our new SPH. However, the noisy interface appears because we have a finite number of particles, and is at least partly due to the KHI, itself, at high-wavenumber, which is physically there. Thus, we argue that a noisy interface is not problematic.

It is worth noting that, in the case of a jump in the chemical composition, the standard AC term is insufficient, and it is necessary to introduce an artificial chemical diffusion term. Our scheme can handle any kind of discontinuity without any diffusion term. Of course, to express fluid mixing on the sub-resolution scale appropriately, we should introduce a turbulent diffusion term (Wadsley et al. 2008).

5.2. Summary

The SPH method is a powerful numerical tool for astrophysical and planetological problems. However, due to the requirement of the differentiability of density, the standard SPH has a problem in describing multi-phase flows and mixing. In this paper, we describe an alternative formulation of SPH in which the pressure is used as the basis of smoothing, instead of the density. In our formulation, we do not assume differentiability of the density, but assume that of the pressure. As a result, our new formulation shows great improvement in the treatment of contact discontinuity and hydrodynamical instabilities. Our new SPH can handle problems in which mixing takes place. Our new SPH is natural extension of that of Saitoh and Makino (2013). With our new SPH, the shock tube, the hydrostatic equilibrium test and the KHI test show good results for non-ideal gas. It is easy and straightforward to modify the existing SPH to our new method. In addition, our new SPH does not introduce any additional dissipation term, and does not break the conservation properties. The increase of the calculation cost is small.

Our new SPH can be easily incorporated with other improvements, for example inviscid SPH (Morris & Monaghan 1997; Cullen & Dehnen 2010) and a higher-order dissipation switch (Read & Hayfield 2012).

One important application of our new SPH is giant impact simulations, where the instabilities and mixing at the boundaries of different materials might play important roles. We are currently working to apply our new SPH to giant impact simulations. The results will be reported in a forthcoming paper. Of course, our new SPH can be applied to a variety other astrophysical and planetological problems.

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