Journal of Computational Physics 229 (2010) 4279–4290

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Stabilization and smoothing of pressure in MPS method by Quasi-Compressibility

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ARTICLE INFO

Article history:
Received 8 April 2009
Received in revised form 2 October 2009
Accepted 11 February 2010
Available online 24 February 2010

Keywords:
Particle method
MPS
Smoothing of pressure
Incompressible fluid
Stabilization
Quasi-Compressibility

ABSTRACT

In this paper, a method to stabilize simulations and suppress the pressure oscillation in Moving Particle Semi-implicit method for an incompressible fluid is presented. To make the pressure smooth in terms of both of space and time, a new representation of the incompressible condition is proposed. The incompressible condition consists of two parts: the Divergence-Free condition and the Particle Number Density condition. The Divergence-Free condition has the effect of making the pressure smooth in terms of both space and time. The Particle Number Density condition is necessary to keep the fluid volume constant. In this work, the Quasi-Compressibility is also introduced for stabilization. A dam break is simulated more stably and the space distribution and the time variation of pressure are evaluated more smoothly than the traditional method. Moreover, surface particles are detected more accurately. Nevertheless the proposed method is computationally cheaper. Some simulations such as a Fluid–Structure Interaction are supposed to be more accurate using this method.

1. Introduction

MPS (Moving Particle Semi-implicit) method [1,2] was developed to simulate incompressible fluids using a particle method. Any kind of meshes are not needed in particle methods and such mesh-free methods are suitable for simulations of large deformations and multi-physics phenomena. Until now not only fluids but also rigid bodies [3], elastic bodies [4] and FSI (Fluid–Structure Interaction) [5] have been simulated. Accurate simulations of FSI are needed in CAE (Computer Aided Engineering) and MPS method is expected to be applied to it. In MPS method, however, there is a big problem that the space distribution and the time variation of pressure oscillate drastically. To simulate FSI using MPS method, the numerical oscillation of pressure is likely to cause unreal behaviors of structures. It is very important to suppress the pressure oscillation for more accurate FSI simulations.

There have been some researches to suppress the pressure oscillation in MPS method. It is common to resolve Poisson's equations two times [6,7]. First, the pressure to move particles is computed as with traditional methods. This pressure oscillates in terms of both space and time. Secondly, the pressure for validation is evaluated to make the divergence of the velocity field zero. This pressure for validation is not relative to particle motions. Such approaches, however, are computationally expensive and pressure for validation does not have physical meanings. Kondo and Koshizuka [8] have proposed a method to consider the error in the incompressible condition that the divergence of the velocity field should be zero and correct the source term.

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0021-9991/$ - see front matter
doi:10.1016/j.jcp.2010.02.011

There have been also some researches to stabilize MPS method. Ataie-Ashtiani and Farhadi [9] attempted several weight functions and chose the best one to stabilize simulations. However, only the number of free surface particles is discussed and the accuracy is not validated at all. Changing a weight function cannot be the critical solutions to stabilize simulations or make them more accurate even if some improvements can be achieved.

In this paper, we propose an approach to stabilize simulations and also make the pressure smoother in terms of both space and time. We introduce the Quasi-Compressibility to make simulations more stable and correct the source term to make the fluid volume constant at the same time to obtain smooth pressure. Lee et al. [10] has compared the explicit weakly-compressible method and the implicit incompressible one in SPH (Smoothed Particle Hydrodynamics) and concluded the incompressible one is more efficient and accurate. Our Quasi-Compressibility is not the same with this weakly-compressibility. Ours is just for numerical stability. We demonstrate that our method is superior to the traditional one in terms of not only accuracy but also computational costs by comparing them.

2. Traditional MPS method

The traditional MPS method is shown below. The governing equations are the continuum equation and the Navier–Stokes equation. These equations for incompressible fluids are represented as

$$\nabla \cdot \boldsymbol{v} = 0 \tag{1}$$

and

$$\frac{D\boldsymbol{v}}{Dt} = -\frac{1}{\rho}\nabla P + \nu\nabla^2 \boldsymbol{v} + \boldsymbol{g} \tag{2}$$

where $\boldsymbol{v}$ is a velocity vector, t is time, ρ is the constant density, P is pressure, ν is dynamic viscosity and $\boldsymbol{g}$ is gravity acceleration. Particle interactions are evaluated using a weight function such as

$$w(r,R) = \begin{cases} \frac{R}{r} - 1 & (r \leqslant R) \\ 0 & (r > R) \end{cases} \tag{3}$$

where r is distance between particles and R is the effect radius. We use $R = 2.1L$ for the effect radius in this paper, where L is the diameter of particles. The sum of the weight function is so-called the particle number density and is defined as

$$n_i = \sum_{j \neq i} w_{ij} \tag{4}$$

where w_{ij} is the weight function between particle i and j as

$$w_{ij} = w(r_{ij}, R) \tag{5}$$

where r_{ij} is distance between particle i and j. The particle number density in an incompressible state is called the particle number density criterion n^0.

In this paper, a relative vector between particle i and j is represented as

$$\boldsymbol{\Phi}_{ij} = \boldsymbol{\Phi}_j - \boldsymbol{\Phi}_i \tag{6}$$

The differential operators of gradient, Laplacian and divergence are formulated as

$$\langle \nabla\phi \rangle_i = \frac{d}{n^0}\sum_{j \neq i}\left[\frac{\phi_j - \phi_i}{r_{ij}^2}\boldsymbol{x}_{ij} w_{ij}\right] \tag{7}$$

$$\langle \nabla^2\phi \rangle_i = \frac{2d}{n^0\lambda_i}\sum_{j \neq i}[(\phi_j - \phi_i) w_{ij}] \tag{8}$$

$$\langle \nabla \cdot \boldsymbol{\Phi} \rangle_i = \frac{d}{n^0}\sum_{j \neq i}\left[\frac{\boldsymbol{\Phi}_{ij} \cdot \boldsymbol{x}_{ij}}{r_{ij}^2} w_{ij}\right] \tag{9}$$

where ϕ is an arbitrary scalar, Φ is an arbitrary vector, d is the number of dimensions, $\boldsymbol{x}$ is the coordinate of a particle and λ is a coefficient in Laplacian model which is defined as

$$\lambda_i = \frac{\sum_{j \neq i}\left(w_{ij} r_{ij}^2\right)}{\sum_{j \neq i} w_{ij}} \tag{10}$$

Note that these differentiated operator models are not consistent when the particle arrangement is not uniform, and this problem might be one of reasons for the pressure oscillation although this problem is not considered in this paper.

The algorithm of MPS method is similar to SMAC (Simplified Marker and Cell) as depicted in Fig. 1(a). First, all terms except the pressure term are computed explicitly and subsequently the pressure term is resolved implicitly to make the fluid incompressible. This methodology is commonly used in a variety of simulations of incompressible fluids.

Two kinds of incompressible conditions have been already suggested. Traditionally used one is that the particle number density should be constant, that is,

$$n_i = n^0 \tag{11}$$

Using this condition the following Poisson's equation is derived and pressure is evaluated by solving this equation.

$$\nabla^2 P = \frac{\rho}{\Delta t^2}\frac{n^0 - n^*}{n^0} \tag{12}$$

where n^* is temporary particle number density after computation of explicit terms and Δt is simulation time step. This condition is called the PND (Particle Number Density) condition in this paper.

The other condition is that the divergence of the velocity field should be zero. The theoretical incompressible condition is shown in Eq. (1) originally and the following Poisson's equation is derived from this.

$$\nabla^2 P = \frac{\rho}{\Delta t}\nabla \cdot \boldsymbol{v}^* \tag{13}$$

where $\boldsymbol{v}^*$ is temporary velocity before resolving the pressure term. This equation can be discretized directly in MPS method and has been used in MPS–MAFL (Meshless Advection using Flow-directional Local-grid) method [11–13] in which the particle distribution is not uniform. This condition is called the Divergence-Free condition in this paper.

The boundary condition to evaluate pressure is that the pressure values of free surface particles are zero. Surface particles are detected by

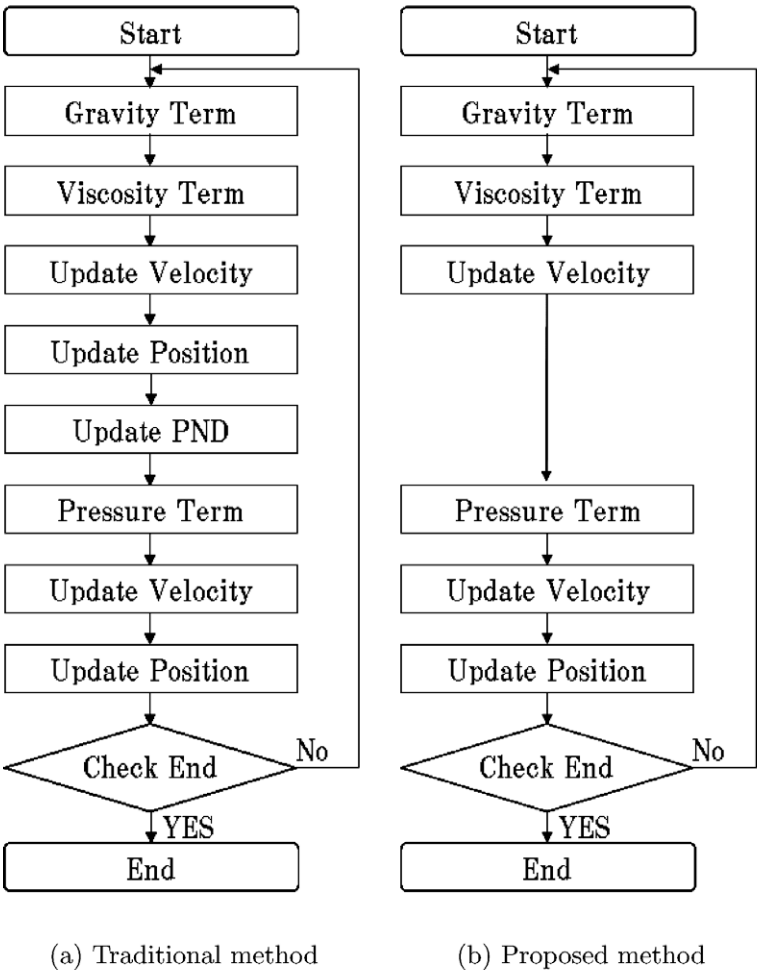


Fig. 1. Flow charts.

$$n_i < \beta n^0 \tag{14}$$

where β is a coefficient for surface detection and the value 0.97 has been adopted ordinarily.

To apply the divergence model of MPS method to the pressure gradient term, velocity variation in the pressure term is represented as

$$\Delta \boldsymbol{v} = -\frac{\Delta t}{\rho}\frac{d}{n^0}\sum_{j\neq i}\left[\frac{P_j - P_i}{r_{ij}^2}\boldsymbol{x}_{ij}w_{ij}\right] \tag{15}$$

however, in MPS method the following equation is used instead for stabilization.

$$\Delta \boldsymbol{v} = -\frac{\Delta t}{\rho}\frac{d}{n^0}\sum_{j\neq i}\left[\frac{P_j - \hat{P}_i}{r_{ij}^2}\boldsymbol{x}_{ij}w_{ij}\right] \tag{16}$$

where $\hat{P}_i$ is minimum pressure in neighboring particles of particle *i*. Using this equation, all particle interaction forces become repulsive ones and the simulation comes to be more stable.

Although MPS method is for simulating incompressible fluids, a simple way to consider Restricted Compressibility is suggested [14]. The Poisson's equation of pressure is represented as

$$\nabla^2 P^{k+1} = \frac{\rho}{\Delta t^2}\left(\frac{n^0 - n^*}{n^0} + \alpha P_i^{k+1}\right) \tag{17}$$

where α is compressibility ratio. Considering compressibility like this, the simulation comes to be more stable because the diagonal elements of the coefficient matrix are bigger. This compressibility is called the Restricted Compressibility in this paper.

3. Proposed method

3.1. Incompressible condition

Two incompressible conditions have been proposed in MPS method: the PND condition and the Divergence-Free condition. In the PND condition, pressure is implicitly solved to relax particle number density of each particle to a constant. However, particle number density is non-linear with respect to coordinates and does not accord with the particle number density criterion even though the pressure term is solved implicitly. Moreover, solving Eq. (12) directly causes instability. Traditionally the right-hand side of Eq. (12) is commonly lessened for stabilization. In this condition, the incompressible condition is made using the difference between the present particle number density and the particle number density criterion, and hence the error does not accumulate even if the source term is lessened. In other words changing the source term does not always break the incompressible condition while the incompressible condition is not filled completely. A little compressibility is allowed as with the penalty method in this condition. There are also some problems in the PND condition. One is that the pressure oscillates drastically in terms of both space and time. In particular when simulation time step is small particles behave unnaturally.

On the other hand, the Divergence-Free condition has some advantages one of which is that comparatively smoother pressure can be obtained. This is because even though particles arrange ununiformly the divergence of the velocity field can be obtained plausibly and the source term is relatively smooth. This condition is commonly adopted in MPS–MAFL in which particle arrangement is not uniform. Another advantage is that temporary coordinates and particle number density are not necessary and hence the computational cost is cheaper. One problem is that the error might accumulate and therefore the volume of a fluid is likely to increase or decrease after simulating many time steps. This is because the present state is assumed as incompressible.

The proposed method has both advantages of the PND condition that the error is not stored and of the Divergence-Free condition that the smoother pressure is obtained. The source term is divided into two parts as with the approach by Kondo and Koshizuka [8].

$$\nabla^2 P = \frac{\rho}{\Delta t^2}\frac{n^k - n^*}{n^0} + \frac{\rho}{\Delta t^2}\frac{n^0 - n^k}{n^0} \tag{18}$$

The first term of the right-hand side represents the difference of the particle number density from that at the time step *k*. The second term represents the difference of the particle number density at the time step *k* from the particle number density criterion. The former is supposed to be similar to the Divergence-Free condition. The source term can be rewritten as

$$\nabla^2 P = \frac{\rho}{\Delta t}\nabla\cdot\boldsymbol{v}^* + \frac{\rho}{\Delta t^2}\frac{n^0 - n^k}{n^0} \tag{19}$$

Solving this equation leads not only smoother pressure distribution to be obtained but also the fluid volume to be kept constant. However, the source term is too big that the simulation diverges. To prevent the numerical divergence, the second term of the source term should be smaller as

$$\nabla^2 P = \frac{\rho}{\Delta t}\nabla\cdot\boldsymbol{v}^* + \gamma\frac{\rho}{\Delta t^2}\frac{n^0 - n^k}{n^0} \tag{20}$$

where γ is a relaxation coefficient which is about 1.0e−3 and it should be chosen so that the fluid volume does not increase nor decrease. The larger γ is, the harder the pressure oscillates. In this algorithm temporary coordinates and particle number density are not needed as with the Divergence-Free condition. The flow chart of the proposed method is depicted in Fig. 1(b).

3.2. Quasi-Compressibility

As mentioned above, introducing the Restricted Compressibility makes the diagonal elements of the coefficient matrix bigger and stabilizes computations. Such compressibility is useful for numerical stabilization, not for the accurate simulation of compressible fluids. This Restricted Compressibility is, however, not scalable for length. In a large scale of length, the diagonal elements of the coefficient matrix are relatively bigger. Therefore, the effect of compressibility is stronger and simulations are more stable. Conversely in a small scale of length, simulations are less stable. In the PND condition, a little compressibility does not influence the fluid behavior because the error does not accumulate. On the other hand, the fluid volume decreases in the Divergence-Free condition. Especially in a large scale of length, the effect of compressibility is too strong that the fluid volume decreases greatly.

In the proposed method, the diagonal element of the coefficient matrix is enlarged to keep the stability at the same time to exclude the scalability. The Poisson's equation of pressure is rewritten as

$$\frac{2d}{n^0\lambda_i}\sum_{j\neq i}[(P_j - cP_i)w_{ij}] = \frac{\rho_i}{\Delta t}[\nabla\cdot\boldsymbol{v}^*]_i + \gamma\frac{\rho_i}{\Delta t^2}\frac{n^0 - n_i^k}{n^0} \tag{21}$$

where c is a multiplication coefficient and should be chosen appropriately. To make c bigger, calculations is more stable, however, the effect of compressibility is stronger and the fluid motion might be unnatural.

3.3. Surface detection

Conventionally surface particles have been detected using Eq. (14). In the PND condition, the difference between the present particle number density n_i and the criterion n^0 has a direct influence on the pressure values. If particles exist whose particle number density is much different from the criterion, the fluid motion becomes unstable and the simulation might diverge. This surface detection prevents this unstable and unnatural motion well. However, not only surface particles but also inside particles are detected as surfaces and this is one of causes of the pressure oscillation.

In the proposed method, the number of neighbor particles N_i is used for surface detection as

$$N_i < \beta' N^0 \tag{22}$$

where N^0 is the number of neighbor particles in the incompressible state. The number of neighbor particles N_i is defined as

$$N_i = \sum_{j\neq i} w_{ij}^s \tag{23}$$

where w^s is a weight function for surface detection and is formulated as

$$w_{ij}^s = \begin{cases} 1 & (r_{ij} \leqslant R) \\ 0 & (r_{ij} > R) \end{cases} \tag{24}$$

3.4. Pressure gradient

Conventionally the pressure gradient has been computed by Eq. (16). The momentum is not conserved in this equation. To overcome this problem, Eq. (16) is improved as

$$\Delta\boldsymbol{v} = -\frac{\Delta t}{\rho}\frac{d}{n^0}\sum_{j\neq i}\left[\frac{P_j + P_i}{r_{ij}^2}\boldsymbol{x}_{ij}w_{ij}\right] \tag{25}$$

Assuming that particles are arranged uniformly around particle i,

$$\sum_{j\neq i}\left[\frac{\boldsymbol{x}_{ij}w_{ij}}{r_{ij}^2}\right] = 0 \tag{26}$$

is approved and Eq. (25) is almost the same with Eq. (16). A similar equation has been applied in SPH. Note that Eq. (26) is not strictly approved when particles are arranged randomly and $\Delta\boldsymbol{v}$ in Eq. (25) can be nonzero even if the pressure field is constant.

4. Results and discussions

4.1. Effect of Restricted Compressibility

At first results of dam break simulations by a traditional method in two dimensions are shown. The simulation condition is illustrated in Fig. 2. The wall is a square whose side is 100*L* where *L* is a diameter of particles. In the initial state, the height of the fluid is 80*L* and the width is 40*L*. The gravity acceleration is 9.8 m/s^2 and viscosity is not considered. Some cases of three different length-scales were simulated. The diameter of particles is 1.0e−4, 1.0e−2 and 1.0e−0 m, respectively. The time steps were chosen to satisfy the CFL (Courant–Friedrichs–Lewy) condition and Δt = 1.0e−5, 1.0e−4, 1.0e−3 s were used in each length-scale. In each length-scale, two cases with and without the Restricted Compressibility represented by Eq. (17) were simulated.

In the PND condition, the Restricted Compressibility in small length-scale simulation had little influence on the fluid behavior. The pressure distribution in small length-scale is shown in Fig. 3. In the traditional MPS method, simulations are unstable if minus pressure is considered and hence it is taken to be zero pressure. There are many particles which were detected as surface or whose pressure was minus in Fig. 3 and the pressure distribution is not smooth. Nonetheless the fluid motion was quantitatively natural. This reason is supposed as below. The fluid is compressed and the pressure is induced to be high. The repulsive force acts between particles by high pressure and the decrease of the fluid volume is prevented. However, the fluid expands by the inertia force and the pressure of many particles becomes minus. This cycle of high and minus

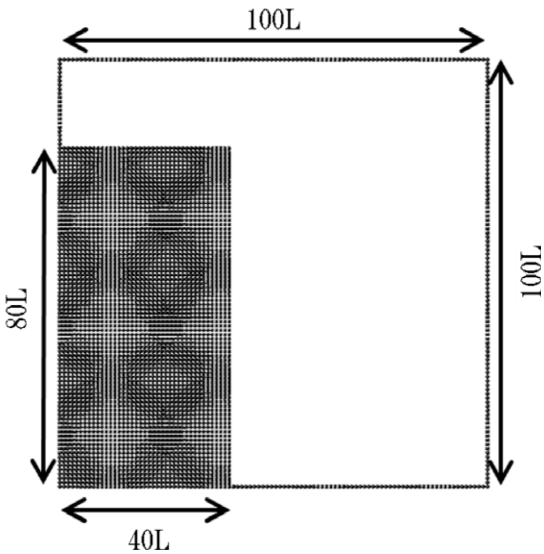


Fig. 2. Simulation condition of dam break.

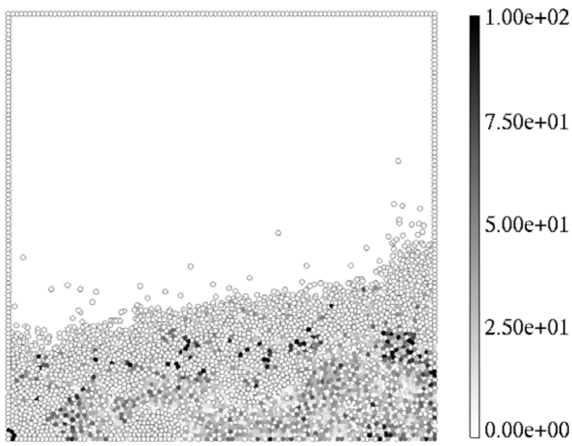


Fig. 3. Pressure distribution of small length-scale dam break.

pressure continues. After all, the fluid motion is observed naturally even though the pressure is not evaluated correctly. The smooth pressure distribution cannot be obtained in the PND condition, that is, a mathematically strict incompressible condition without any compressibility.

On the other hand, the Restricted Compressibility played an important role in large length-scale simulation. No inside particles were detected as surfaces and the pressure distribution was smoother as shown in Fig. 4. The fluid motion was natural as well.

In the Divergence-Free condition, in the absence of the Restricted Compressibility the fluid could be simulated in any length-scales even though the simulations were unstable. In these simulations if the results could be obtained, the fluid volume was almost constant. The pressure was smooth in terms of space while it oscillated hard in terms of time. In the presence of the Restricted Compressibility the fluid volume decreased apparently while the computation was very stable. Especially in large length-scale, the effect of the compressibility is too strong that the fluid did not behave as like a fluid. To consider the compressibility in the Divergence-Free condition, some methods to keep the volume constant are needed.

4.2. Volume conservation and pressure distribution

The Quasi-Compressibility is developed to stabilize simulations and smooth pressure in terms of both space and time in any length-scales. Also the incompressible condition is improved as Eq. (20) to keep the fluid volume constant. Two coefficients, a multiplication coefficient of the diagonal elements c and a relaxation coefficient of the source term γ should be adjusted appropriately. The multiplication coefficient c does not have a physical meaning. It is just an adjust parameter to realize the stability and the smoothing of pressure. The value 1.05 is applied in this work. By this operation, a little compressibility is introduced and thus the fluid volume is induced to decrease. A relaxation coefficient γ is adjusted to make the fluid volume constant with keeping stability.

To optimize the relaxation coefficient, dam break simulations were carried out until the surface was stationary. The conservation of the fluid volume was validated by the height of the surface. The diameter of particles was 1.0e−2 m. Six cases were simulated in which the relaxation coefficient γ was 1.0e−4, 3.16e−4, 1.0e−3, 3.16e−3, 1.0e−2 and 3.16e−2, respectively. The height of the surface is illustrated in Fig. 5. The difference between the height of each simulation and the theoretical value is shown in Table 1 and Fig. 6. In the simulations of γ = 3.16e−2 and upwards, the effect of the PND condition was too strong that particles on the surface moved hard. The height was a little higher than the theoretical value. Enlargement of γ caused unnatural motion. On the other hand, in the simulations of γ = 1.0e−3 or less, the fluid volume decreased and the error of the height was larger. The simulation of γ = 1.0e−2 and 3.16e−3 produced almost the same results. In these cases, the pressure distribution was very smooth as shown in Fig. 7. The simulation was more stable and the motion of surface particles was natural. The proposed Quasi-Compressibility does not depend on length-scale. This parameter, however, is likely to depend on time-scale and should be adjusted in each case. This approach is regarded as one kind of penalty methods. In the simulations where there are many particles in the vertical direction, the fluid volume is likely to decrease.

4.3. Time variation of pressure

In the proposed method, the pressure oscillation can be suppressed in terms of time as well as space. To confirm that, dam break simulations illustrated in Fig. 2 were carried out by both the PND condition and the proposed one. The diameter of particles is 1.0e−2 m and the simulation time is 3.0 s. The pressure was measured in every time step at the lower right corner in Fig. 2. The pressure distributions in terms of time in both the traditional and the proposed method are shown in Fig. 8. The

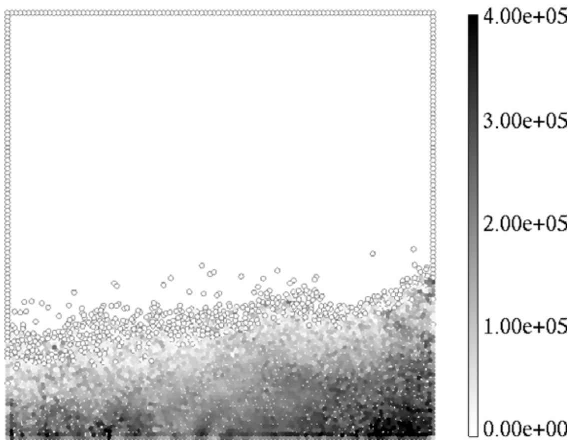


Fig. 4. Pressure distribution of large length-scale dam break.

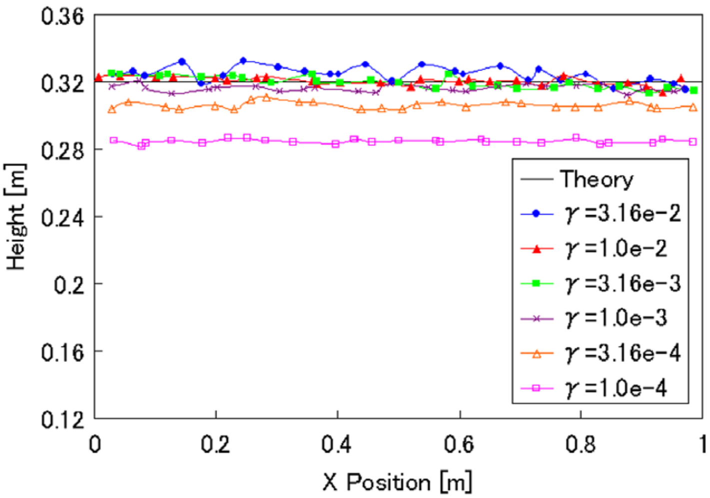


Fig. 5. Heights of fluid surface against γ.

Table 1
Error of height.

γ	Error (%)
3.16e−2	1.30
1.0e−2	0.09
3.16e−3	0.10
1.0e−3	1.22
3.16e−4	4.39
1.0e−4	11.13

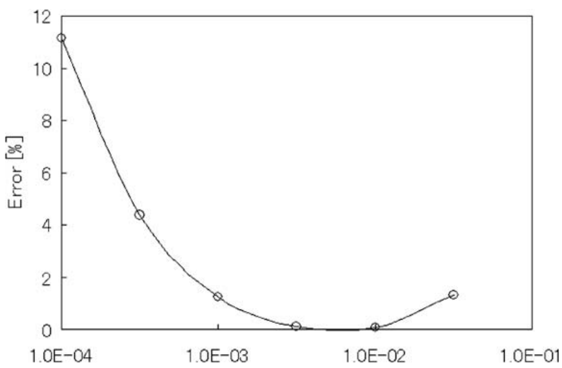


Fig. 6. Error of height.

pressure was measured by linear weighted average in the effect radius. The space pressure oscillation is removed to some extent. It is clear that the pressure is much smoother than the traditional method.

4.4. Effect of pressure gradient scheme

In the proposed method, Eq. (25) is applied in the pressure gradient while Eq. (16) has been used in the traditional MPS method. Two cases of the dam break with different pressure gradient schemes were simulated. The diameter of particles is 1.0e−2 m and the simulation time is 2.0 s. The pressure is measured in every time step in the same manner as described above. The results are depicted in Fig. 9. While the pressure oscillated in the traditional method, the pressure was much smoother in the proposed method. Particle motions were stabilized by conserving the momentum, and in the consequence of that, the pressure was evaluated smoother.

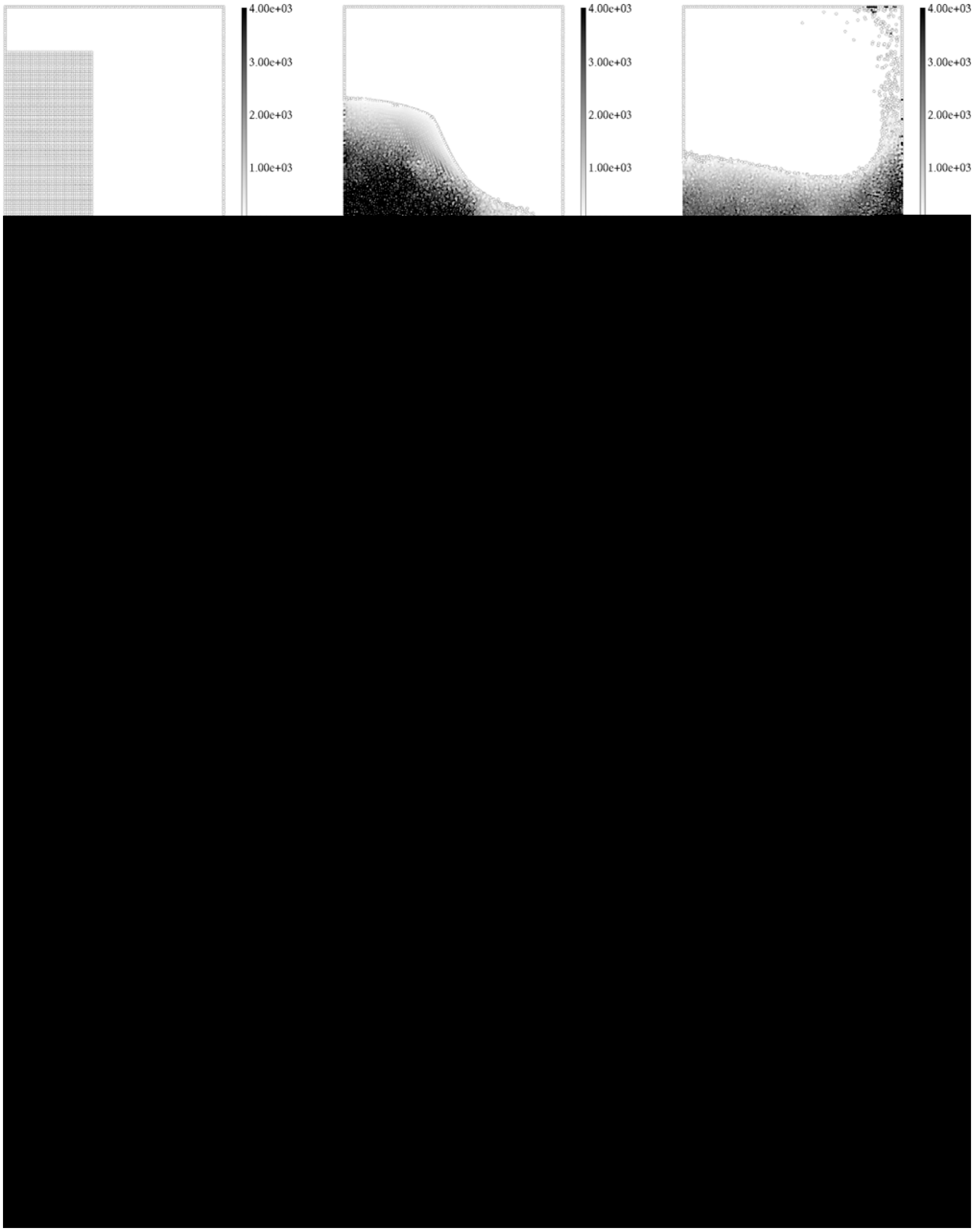


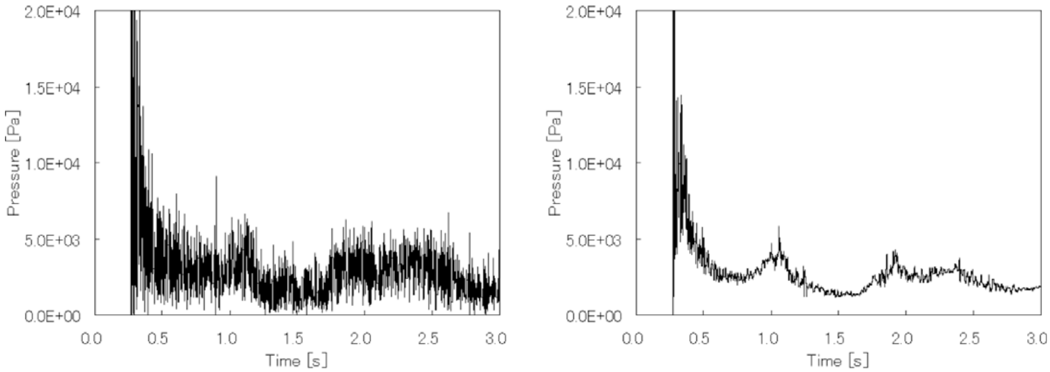
Fig. 7. Pressure distributions of proposed method.

4.5. Computational time

In the proposed method, the temporary coordinates and particle number density are not needed and hence the computational cost is expected to be cheaper. Three cases of dam break simulations were conducted where the total number of particles were 4436, 15236 and 56036, respectively. The computational times by the traditional and proposed method are shown in Table 2. The computational load is reduced down in any cases.

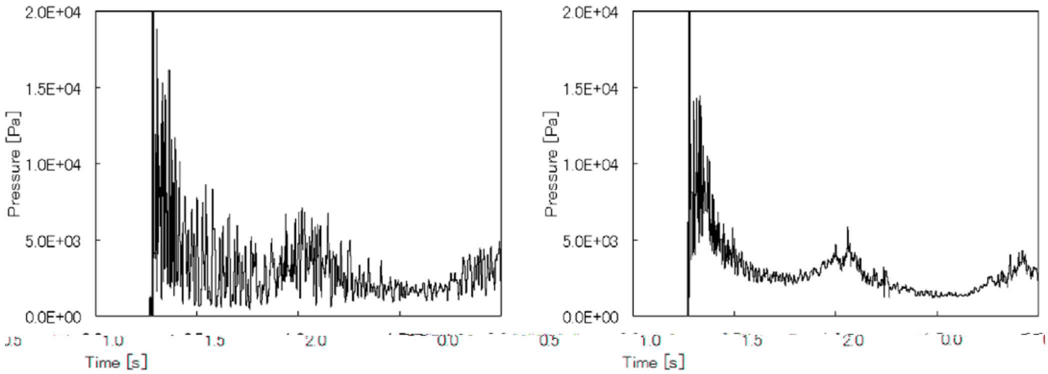
4.6. Accuracy of surface detection

In the traditional method, Eq. (14) has been used to detect surface particles. This is for preventing the instability in the case that the particle number density is far different from the criterion. Applying this detection method, some inside particles are detected as the surface and its pressure is regarded as zero. This is one of reasons of pressure oscillation. The result of the traditional method is illustrated in Fig. 10(a). The dark particles represent surface particles. The simulation was not con-



(a) Traditional method (b) Proposed method

Fig. 8. Comparison of pressure profile between traditional and proposed method.



[raditional method (b) Proposed method (a) T

Fig. 9. Pressure profiles by two kinds of pressure gradient.

Table 2
Calculation time per timestep.

Number of particles	Traditional method (s)	Proposed method (s)
4436	0.022630	0.015224
15,236	0.102967	0.075713
56,036	0.411720	0.290015

verged using the proposed surface detection method in the traditional incompressible condition. The proposed incompressible condition is based on the Divergence-Free condition and the proposed surface detection method can be applied to it. Consequently the surface detection came to be more accurate as depicted in Fig. 10(b). Although it is not considered in this research, the surface tension calculation needs accurate surface detection. This surface detection is useful in such a simulation.

4.7. Hydrostatic pressure

Four simulations to confirm the accuracy of the pressure calculation were conducted. The simulation condition is illustrated in Fig. 11. The diameter was $L = 1.0\text{e}{-2}$ m and the height of the fluid was $20L$, $40L$, $60L$ and $80L$, respectively. The coefficient $\gamma = 1.0\text{e}{-3}$ was chosen. The hydrostatic pressures at the bottom of the vessel and the theoretical values are shown in Fig. 12. In the cases of shallow ones, for example the height is $20L$ or $40L$, the simulation results are in good agreement with the theoretical values. However, if the pool is deeper, the difference between the simulation and theory is larger. When the number of particles in the vertical direction is larger, the effect of the Quasi-Compressibility is bigger and that is supposed to be one reason of the error of the hydrostatic pressure. The relaxation coefficient γ should be adjusted in each simulation.

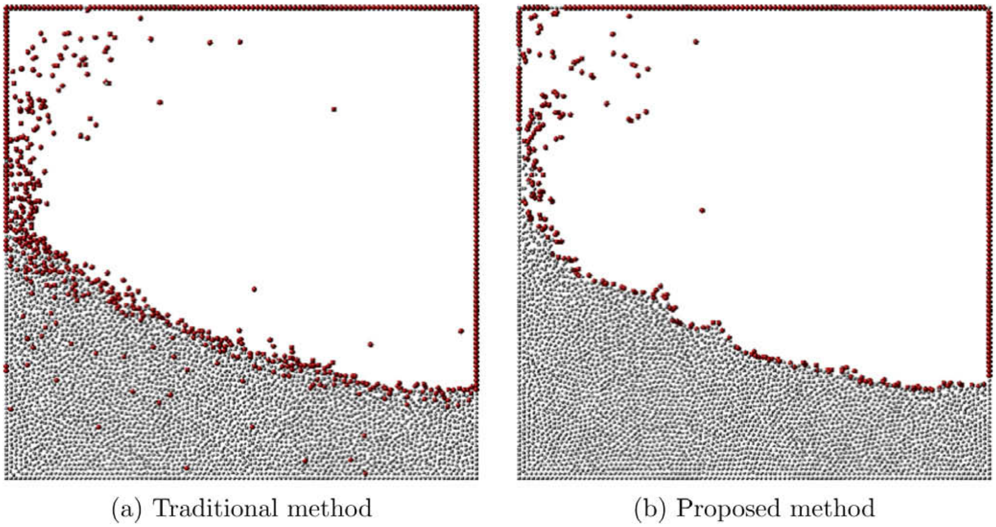


Fig. 10. Surface particles.

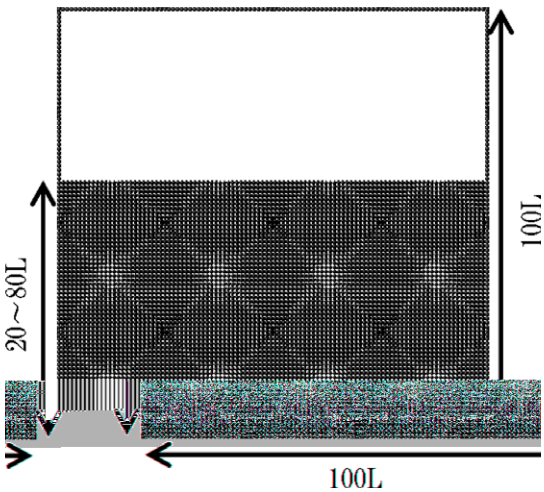


Fig. 11. Simulation condition of hydrostatic problem.

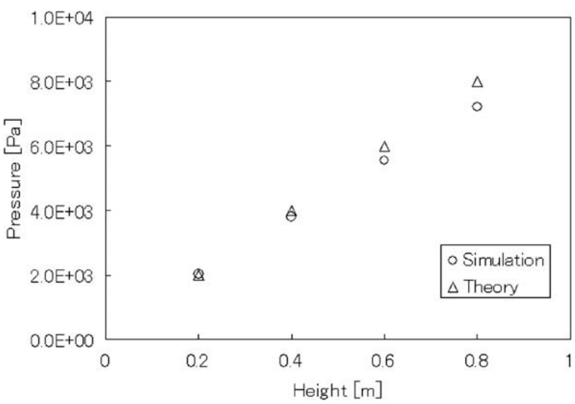


Fig. 12. Simulation results and theoretical values of hydrostatic pressure.

5. Conclusions

In this research, the MPS method was improved to be more stable and to suppress the pressure oscillation by coupling two incompressible conditions and introducing the Quasi-Compressibility. The pressure came to be much smoother than the traditional method in terms of both space and time. The computational cost was cheaper because the temporary coordinates and particle number density before the pressure term were not needed. Using this proposed method in which smooth pressure distribution can be obtained, the accurate fluid-solid interaction can be simulated. The Quasi-Compressibility in this method does not depend on length-scale. However, some compressibility is allowed as well as a penalty method and some parameters should be adjusted in each case. This is one of future works.

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