

A NEW DERIVATION OF PRESSURE POISSON EQUATION IN MOVING PARTICLE SEMI-IMPLICIT METHOD

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Key words: Computational fluid dynamics, CFD, Particle method, Meshfree particle method, MPM, Moving particle simulation, MPS, Moving particle semi-implicit method,

Abstract. In order to simulate complex deformation of liquid with free surface, Koshizuka et al. proposed the Moving Particle Semi-implicit method (MPS). MPS is applied to make 3DCG animations about splashing waters, breaking waves, and so on. MPS computes the liquid's pressures by solving the Poisson equation with the feedback for mass density. This pressure Poisson equation is derived from the equation of continuity by assuming the flow's incompressibility. Although MPS computes the incompressible flows, compressibility is considered in the computing process. By considering this compressibility, the pressure Poisson equation is modified to the one with the feedback for the mass density and the divergence of the flow's velocity.

1 Introduction

In order to simulate complex deformation of liquid with free surface, Seiichi Koshizuka et al. proposed the Moving Particle Semi-implicit method (MPS) [1]. MPS is applied to make 3DCG animations about splashing waters, breaking waves, and so on. MPS simulates the incompressible flow of the liquid. MPS constructs the spatial differences by the particles at each time and discretize the Navier-Stokes equation spatially. In the time evolution scheme of MPS, pressures are computed as a solution of the Poisson type partial differential equation (the pressure Poisson equation).

Although the positions and the velocities of the liquid were computed suitably by MPS method, the computed pressures oscillate numerically. This is so-called the pressure oscillation problem of the MPS method [2] [3] [4],

In order to avoid this problem, i.e., in order to stabilize the pressures which is computed by MPS, Yoshimasa MINAMI improved the source term of the pressure Poisson equation heuris-

tically [3]. He modified the pressure Poisson equation to the one with the feedback by the mass density and the divergence of the flow's velocity. In this paper, the author explain the mathematical meaning of that improvement. He derives the pressure Poisson equation with the feedback by the mass density and the divergence of the flow's velocity.

Although MPS is proposed to compute incompressible flow [1], compressibility is considered in its computation process between the present time s and the next time $t = s + \Delta s$. In such compressible process, mass density varies as the time goes on. Considering the time varying mass density, the authors derived the pressure Poisson equation (59) with the feedback by the mass density and the divergence of the flow's velocity mathematically. This derivation guarantees the heuristic computation proposed by [3] theoretically.

In traditional hydrodynamics, the boundary condition of that Poisson type partial differential equation must be non-homogeneous. By the mathematical theory of partial differential equations, a non-homogeneous boundary condition of a partial differential equation is transformed to a source term of the partial differential equation. Thus we can compute the solution of the Poisson type partial differential equation based on a homogeneous boundary condition [5] [6].

2 Lagrangian material coordinate based on Fluid's particles

We simulate the deformation of liquid based on the Lagrangian material coordinate. Let Dim be the dimension of the space. Thus

$$\text{Dim} = 2, 3 \quad (1)$$

If a fluid particle whose position is $x = (x_1, x_2, \dots, x_{\text{Dim}}) \in \mathbb{R}^{\text{Dim}}$ at time $s > 0$ reaches to the position $z = (z_1, z_2, \dots, z_{\text{Dim}}) \in \mathbb{R}^{\text{Dim}}$ at time $t > s$ by the flow, then we write

$$z = u(t/s, x). \quad (2)$$

Let

$$v(t, z/s, x) = v(t/s, x) = v(t, z) \quad (3)$$

be the velocity of this particle whose position is x at time s and which reaches to the position z at time t by the flow.

Let

$$a(t, z/s, x) = a(t/s, x) = a(t, z) \quad (4)$$

be the acceleration of this particle whose position is x at time s and which reaches to the position z at time t by the flow.

Here

$$\text{the position } u = (u_1, u_2, \dots, u_{\text{Dim}}) \in \mathbb{R}^{\text{Dim}} \quad (5)$$

$$\text{the velocity } v = (v_1, v_2, \dots, v_{\text{Dim}}) \in \mathbb{R}^{\text{Dim}} \quad (6)$$

$$\text{the acceleration } a = (a_1, a_2, \dots, a_{\text{Dim}}) \in \mathbb{R}^{\text{Dim}} \quad (7)$$

Let

$$\rho(t, z/s, x) = \rho(t/s, x) = \rho(t, z) \quad (8)$$

be the mass density around this particle whose position is x at time s and which reaches to the position z at time t by the flow.

Let

$$p(t, z/s, x) = p(t/s, x) = p(t, z) \quad (9)$$

be the pressure around this particle whose position is x at time s and which reaches to the position z at time t by the flow.

Let $\Omega(s) \subset \mathbb{R}^{\text{Dim}}$ be the shape of the liquid at time $s > 0$. Of course $x \in \Omega(s)$. The liquid's shape $\Omega(s)$ changes to the shape $\Omega(t) \subset \mathbb{R}^{\text{Dim}}$ at time $t > s$. Of course $z \in \Omega(t)$.

$\Omega(0)$ means the initial shape of the liquid at initial time 0. The particle's position $\xi = (\xi_1, \xi_2, \dots, \xi_{\text{Dim}}) \in \Omega(0)$ at initial time 0 represents the fluid particle, id est, each particle's position z at time t can be expressed by

$$z = u(t/0, \xi) \quad (10)$$

for some particle's position $\xi \in \Omega(0)$ at initial time 0. For the initial position ξ of the particle at initial time 0,

$$u(0/0, \xi) = \xi \quad (11)$$

follows.

The mass density $\rho(t, z/s, x)$ depends the volume expansion as

$$\rho(t, z/s, x) = \rho_0 \left\{ \det \left(\frac{\partial u(t/s, x)}{\partial x} \right) \right\}^{-1} = \rho_0 \left\{ \det \left(\frac{\partial z}{\partial x} \right) \right\}^{-1} \quad (12)$$

where ρ_0 is the initial mass density at initial time 0.

3 The Navier-Stokes equation (Lagrangian type)

We simulate the liquid's deformation dynamics based on the Navier-Stokes equation

$$z = u(t/s, x) \quad (13)$$

$$\frac{D u(t/s, x)}{Dt} = v(t/s, x) \quad (14)$$

$$a(t/s, x) = \frac{D v(t/s, x)}{Dt} = \frac{\mu}{\rho(t/s, x)} \sum_{i=1}^{\text{Dim}} \frac{\partial^2 v(t, z/s, x)}{\partial z_i^2} - \frac{1}{\rho(t/s, x)} \frac{\partial p(t/s, x)}{\partial z} + g \quad (15)$$

and the continuity equation

$$0 = \frac{D \rho(t, z/s, x)}{Dt} + \rho(t, z/s, x) \sum_{i=1}^{\text{Dim}} \frac{\partial v_i(t, z/s, x)}{\partial z_i} \quad (16)$$

by the mass conservation. Here $g = (0, \dots, 0, -9.81[\text{m/s}^2])$ denotes the gravity acceleration.

Since the velocity v , the position u , and the mass density ρ are expressed by Lagrangian coordinate (s, x) , D/Dt denotes the Lagrangian time derivative. By letting

$$t = s + \Delta s \quad (17)$$

we can think that

$$\left[\frac{D u(t/s, x)}{Dt} \right]_{t=s} = \lim_{\Delta s \rightarrow 0} \frac{z - x}{\Delta s} \quad (18)$$

$$a(s, x/s, x) = \left[\frac{D v(t, z/s, x)}{Dt} \right]_{t=s} = \lim_{\Delta s \rightarrow 0} \frac{v(t, z/s, x) - v(s, x/s, x)}{\Delta s} \quad (19)$$

$$= \lim_{\Delta s \rightarrow 0} \frac{v(t, z) - v(s, x)}{\Delta s} \quad (20)$$

and

$$\left[\frac{D \rho(t, z/s, x)}{Dt} \right]_{t=s} = \lim_{\Delta s \rightarrow 0} \frac{\rho(t, z/s, x) - \rho(s, x/s, x)}{\Delta s} \quad (21)$$

$$= \lim_{\Delta s \rightarrow 0} \frac{\rho(t, z) - \rho(s, x)}{\Delta s} \quad (22)$$

Although the Lagrangian coordinate (s, x) is not used in [1], this paper describes equations based on (s, x) for mathematical clarity.

The boundary conditions for the position u and the velocity v are defined by

$$v(t/0, \xi) = 0 \quad (23)$$

$$u(t/0, \xi) = \xi \quad (24)$$

$$\rho(t/0, \xi) = \rho_0 \quad (25)$$

for

$$\xi \in \partial\Omega(0) \text{ and } \xi \text{ belongs to the solid wall.} \quad (26)$$

The particle ξ in the solid wall is regarded as fluid particles ξ whose velocities are zero ($v(t/0, \xi) = 0$) and whose positions do not change ($u(t/0, \xi) = \xi$) as the time t goes on.

The boundary conditions for the pressure p at the solid wall is defined by

$$\frac{\partial p}{\partial \sigma}(t/0, \xi) = 0 \quad (27)$$

for

$$\xi \in \partial\Omega(0) \text{ and } \xi \text{ belongs to the solid wall} \quad (28)$$

where $\sigma(\xi)$ is an inner normal vector of the wall at the solid particle $\xi \in \Xi_{\text{solid}}$. The effect of the gravity is expressed by the source term of the pressure Poisson partial differential equation, as we see in the section 5.4.

The boundary conditions for the pressure p at the free surface (the liquid which comes in contact with the atmosphere) is defined by

$$p(t/0, \xi) = 0 \quad (29)$$

for

$$\xi \in \partial\Omega(0) \text{ and } \xi \text{ belongs to the free surface.} \quad (30)$$

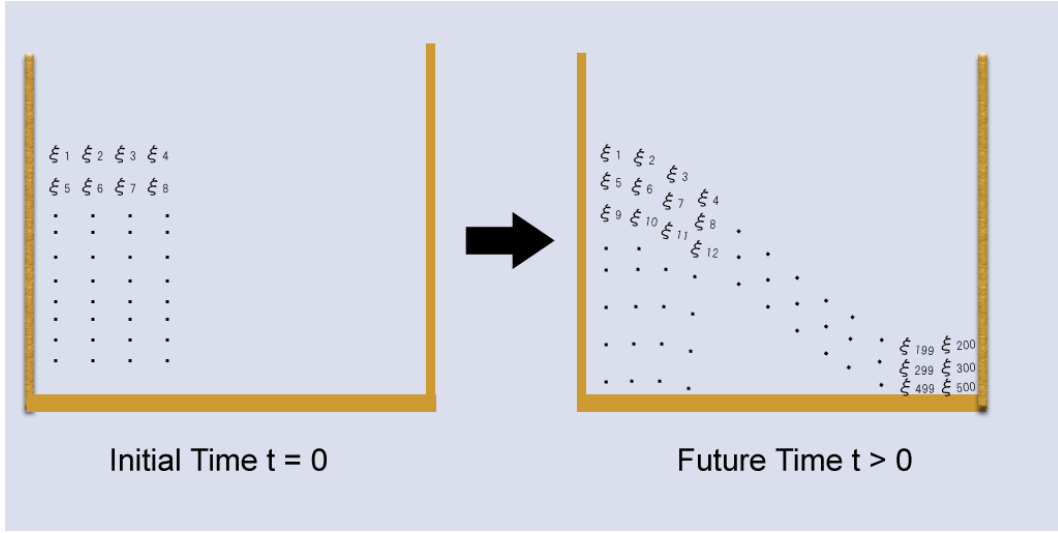


Figure 1: Spatial discretization by many particles.

4 Spatial discretization by Moving Particles

For $l = 1, 2, \dots, L$, let $\xi_{[l]}$ be a representative initial position in the initial shape $\Omega(0)$ of the liquid at initial time 0. Lagrangian material variables are discretized by many particles $\xi_{[l]}$ ($l = 1, 2, 3, \dots, L = 10000$). The position $u(t/0, \xi)$ ($\xi \in \Omega(0)$) is discretized as $u(t/0, \xi_{[l]})$ ($l = 1, 2, \dots, L$). The velocity $v(t/0, \xi)$ ($\xi \in \Omega(0)$) is discretized as $v(t/0, \xi_{[l]})$ ($l = 1, 2, \dots, L$). The Navier-Stokes equations (15), (14) and the the equation (16) of continuity are discretized spatially by the Moving Particle Semi-implicit method (MPS) [1].

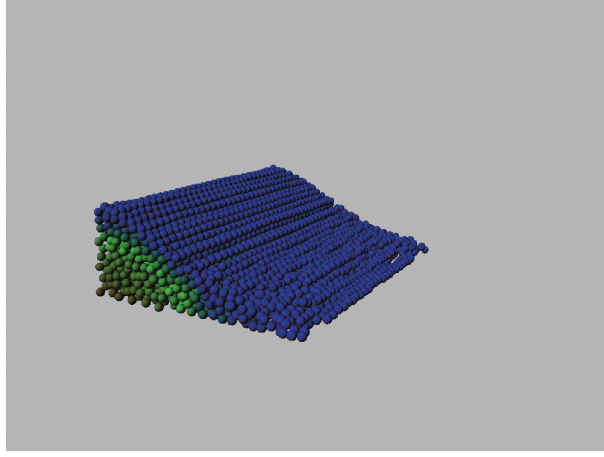


Figure 2: A numerical simulation by many fluid particles.

5 Time evolution scheme of the Moving Particle Semi-implicit method

If we observe the liquid's flow based on the macroscopic view point, it is regarded to be incompressible. Then we assume that

$$1 = \det\left(\frac{\partial u(t/s, x)}{\partial x}\right) = \det\left(\frac{\partial z}{\partial x}\right) \quad (31)$$

and the mass density $\rho(t/s, x)$ become a constant ρ_0

$$\rho(t/s, x) = \rho_0 \quad (32)$$

for times $t > s \geq 0$.

5.1 Time discretization to compute position $z = u(s + \Delta s)$ and velocity $v(s + \Delta s, z)$

By letting the equation (17), we obtain the approximating equation

$$\frac{z - x}{\Delta s} = v(s/s, x) = v(s, x) \quad (33)$$

based on the equation (18) and the approximating equation

$$\frac{v(s + \Delta s, z) - v(s, x)}{\Delta s} = \frac{\mu}{\rho(s, x)} \sum_{i=1}^{\text{Dim}} \frac{\partial^2 v(s, x)}{\partial x_i^2} - \frac{1}{\rho(s + \Delta s, z)} \frac{\partial p(s + \Delta s, z)}{\partial z} + g \quad (34)$$

based on the equations (20) and (15). The time discretization of the discrete time Navier-Stokes equation (34) is explicit for the valocity v and implicit for the pressure p .

5.2 The Poisson equation which computes the pressure $p(s + \Delta s, z)$ at next time $t = s + \Delta s$

In the original MPS proposed by Koshizuka et al. [1], the pressure at next time is computed by the Poisson type partial differential equation (pressure Poisson equation). We derive this pressure Poisson partial differential equation by considering the intermediate compressible procedure between the present time s and the next time $t = s + \Delta s$.

The temporal velocity $v_{(\text{tmp})}(s + \Delta s, y/s, x) = v_{(\text{tmp})}(s + \Delta s, y)$ at next time $t = s + \Delta s$ is computed only by the viscosity term and the gravity term, ignoring the pressure term as

$$\frac{v_{(\text{tmp})}(s + \Delta s, y) - v(s, x)}{\Delta s} = \frac{\mu}{\rho(s, x)} \sum_{j=1}^{\text{Dim}} \frac{\partial^2 v(s, x)}{\partial x_j^2} + g \quad (35)$$

Here the temporal position $y = u_{(\text{tmp})}(t/s, x)$ at next time $t = s + \Delta s$ is computed from the temporal velocity $v_{(\text{tmp})}(s + \Delta s, z)$ as

$$\frac{y - x}{\Delta s} = \frac{u_{(\text{tmp})}(t/s, x) - x}{\Delta s} = v_{(\text{tmp})}(s + \Delta s, y) \quad (36)$$

By considering the difference between the discrete time Navier-Stokes equation (34) and the equation (35), in order to recover the effect of pressure $p(s + \Delta s, z)$ (unknown) to the equation (35), we consider the modifiers v' , y' and the temporal mass density $\rho_{(\text{tmp})}(s + \Delta s, y)$ as

$$v(t, z) = v_{(\text{tmp})}(s + \Delta s, y) + v' \quad (37)$$

$$z = y + y' \quad (38)$$

where

$$\frac{v'}{\Delta s} = \frac{-1}{\rho(s + \Delta s, z)} \frac{\partial p(s + \Delta s, z)}{\partial z} \quad (39)$$

$$\frac{y'}{\Delta t} = v' \quad (40)$$

$$\rho_{(\text{tmp})}(s + \Delta s, y) = \rho_0 \left\{ \det \left(\frac{\partial u_{(\text{tmp})}(s + \Delta s/s, x)}{\partial x} \right) \right\}^{-1} = \rho_0 \left\{ \det \left(\frac{\partial y}{\partial x} \right) \right\}^{-1} \quad (41)$$

By adding the equation (35) and the equation (39), we obtain the discrete time Navier-Stokes equation (34) for velocity. By adding the equation (36) and the equation (40), we obtain the discrete time Navier-Stokes equation (33) for position.

By the equation (39), we have

$$(-\Delta s) \frac{\partial p(s + \Delta s, z)}{\partial z_j} = \rho(s + \Delta s, z) v'_j \quad (42)$$

for $j = 1, 2, \dots, \text{Dim}$. Assuming the flow's incompressibility leads to

$$(-\Delta s) \frac{\partial p(s + \Delta s, z)}{\partial z_j} = \rho_0 v'_j \quad (43)$$

By differentiating both sides of the above equation with respect to z_j , we have

$$(-\Delta s) \frac{\partial^2 p(s + \Delta s, z)}{\partial z_j^2} = \rho_0 \frac{\partial v'_j}{\partial z_j} \quad (44)$$

By adding both sides of the above equation with $j = 1, 2, \dots, \text{Dim}$, we obtain

$$(-\Delta s) \sum_{j=1}^{\text{Dim}} \frac{\partial^2 p(s + \Delta s, z)}{\partial z_j^2} = \rho_0 \sum_{j=1}^{\text{Dim}} \frac{\partial v'_j}{\partial z_j} \quad (45)$$

By considering the mass conservation from (s, x) to $(s + \Delta s, z)$, the discrete time equation of continuity becomes

$$0 = \frac{D\rho}{Dt} + \rho \sum_{j=1}^{\text{Dim}} \frac{\partial v_j}{\partial z_j} = \frac{\rho(s + \Delta s, z) - \rho(s, x)}{\Delta s} + \rho(s + \Delta s, z) \sum_{j=1}^{\text{Dim}} \frac{\partial v_j(s + \Delta s, z)}{\partial z_j} \quad (46)$$

$$= \frac{\rho(s + \Delta s, z) - \rho_{(\text{tmp})}(s + \Delta s, y)}{\Delta s} + \frac{\rho_{(\text{tmp})}(s + \Delta s, y) - \rho(s, x)}{\Delta s} \quad (47)$$

$$+ \rho(s + \Delta s, z) \sum_{j=1}^{\text{Dim}} \frac{\partial v_{(\text{tmp})j}(s + \Delta s, y)}{\partial z_j} + \rho(s + \Delta s, z) \sum_{j=1}^{\text{Dim}} \frac{\partial v'_j}{\partial z_j}$$

By considering the mass conservation from (s, x) to $(s + \Delta s, y)$, the discrete time equation of continuity becomes

$$0 = \frac{\rho_{(\text{tmp})}(s + \Delta s, y) - \rho(s, x)}{\Delta s} + \rho_{(\text{tmp})}(s + \Delta s, y) \sum_{j=1}^{\text{Dim}} \frac{\partial v_{(\text{tmp})j}(s + \Delta s, y)}{\partial y_j} \quad (48)$$

By taking the difference between the equation (47) and (48), we obtain

$$0 = \frac{\rho(s + \Delta s, z) - \rho_{(\text{tmp})}(s + \Delta s, y)}{\Delta s} \quad (49)$$

$$+ \rho(s + \Delta s, z) \sum_{j=1}^{\text{Dim}} \frac{\partial v_{(\text{tmp})j}(s + \Delta s, y)}{\partial z_j} - \rho_{(\text{tmp})}(s + \Delta s, y) \sum_{j=1}^{\text{Dim}} \frac{\partial v_{(\text{tmp})j}(s + \Delta s, y)}{\partial y_j}$$

$$+ \rho(s + \Delta s, z) \sum_{j=1}^{\text{Dim}} \frac{\partial v'_j}{\partial z_j}$$

For the 2nd term of the right hand side of the above equation

$$\frac{\partial v_{(\text{tmp})j}(s + \Delta s, y)}{\partial z_j} = \sum_{k=1}^{\text{Dim}} \frac{\partial v_{(\text{tmp})j}(s + \Delta s, y)}{\partial y_k} \frac{\partial y_k}{\partial z_j} = \sum_{k=1}^{\text{Dim}} \frac{\partial v_{(\text{tmp})j}(s + \Delta s, y)}{\partial y_k} \delta_{kj} = \frac{\partial v_{(\text{tmp})j}(s + \Delta s, y)}{\partial y_j} \quad (50)$$

since

$$\frac{\partial z_j}{\partial y_k} = \frac{\partial y_j}{\partial y_k} + \frac{\partial y'_j}{\partial y_k} \simeq \delta_{jk} \quad (51)$$

$$\frac{\partial}{\partial z} \simeq \frac{\partial}{\partial y} \quad (52)$$

Thus, the equation (49) leads to

$$0 = \frac{\rho(s + \Delta s, z) - \rho_{(\text{tmp})}(s + \Delta s, y)}{\Delta s} \quad (53)$$

$$+ \left[\rho(s + \Delta s, z) - \rho_{(\text{tmp})}(s + \Delta s, y) \right] \sum_{j=1}^{\text{Dim}} \frac{\partial v_{(\text{tmp})_j}(s + \Delta s, y)}{\partial y_j}$$

$$+ \rho(s + \Delta s, z) \sum_{j=1}^{\text{Dim}} \frac{\partial v'_j}{\partial z_j} \quad (54)$$

By considering the flow's incompressibility, we obtain

$$0 = \frac{\rho_0 - \rho_{(\text{tmp})}(s + \Delta s, y)}{\Delta s} + \left[\rho_0 - \rho_{(\text{tmp})}(s + \Delta s, y) \right] \sum_{j=1}^{\text{Dim}} \frac{\partial v_{(\text{tmp})_j}(s + \Delta s, y)}{\partial y_j} + \rho_0 \sum_{j=1}^{\text{Dim}} \frac{\partial v'_j}{\partial z_j} \quad (55)$$

Substituting this equation (55) to the equation (45), we obtain

$$(-\Delta s) \sum_{j=1}^{\text{Dim}} \frac{\partial^2 p(s + \Delta s, z)}{\partial z_j^2} = \rho_0 \sum_{j=1}^{\text{Dim}} \frac{\partial v'_j}{\partial z_j} = \quad (56)$$

$$(-1) \frac{\rho_0 - \rho_{(\text{tmp})}(s + \Delta s, y)}{\Delta s} + (-1) \left[\rho_0 - \rho_{(\text{tmp})}(s + \Delta s, y) \right] \sum_{j=1}^{\text{Dim}} \frac{\partial v_{(\text{tmp})_j}(s + \Delta s, y)}{\partial y_j} \quad (57)$$

This leads to the following Poisson type partial differential equation

$$\sum_{j=1}^{\text{Dim}} \frac{\partial^2 p(s + \Delta s, z)}{\partial z_j^2} = \frac{\rho_0 - \rho_{(\text{tmp})}(s + \Delta s, y)}{\Delta s^2} + \frac{\rho_0 - \rho_{(\text{tmp})}(s + \Delta s, y)}{\Delta s} \sum_{j=1}^{\text{Dim}} \frac{\partial v_{(\text{tmp})_j}(s + \Delta s, y)}{\partial y_j} \quad (58)$$

Since the next position z is unknown unfortunately, we cannot compute the pressure p from the above partial differential equation. By adopting the approximation (52) for spatial derivative, we obtain the solvable pressure Poisson partial differential equation

$$\sum_{j=1}^{\text{Dim}} \frac{\partial^2 p(s + \Delta s, z)}{\partial y_j^2} = \frac{\rho_0 - \rho_{(\text{tmp})}(s + \Delta s, y)}{\Delta s^2} + \frac{\rho_0 - \rho_{(\text{tmp})}(s + \Delta s, y)}{\Delta s} \sum_{j=1}^{\text{Dim}} \frac{\partial v_{(\text{tmp})_j}(s + \Delta s, y)}{\partial y_j} \quad (59)$$

By solving this pressure Poisson equation (59) with the boundary condition determined by the liquid's shape $\Omega(s + \Delta s)$, we can compute (estimate) the pressure $p(s + \Delta s, z)$ at next time $t = s + \Delta s$.

5.3 The boundary condition of the pressure Poisson equation

We will improve the description about the boundary condition of the pressure p as follows. Let $\sigma(\xi) = (\sigma_1(\xi), \sigma_2(\xi), \sigma_3(\xi))$ be an inner normal vector of the boundary solid wall at the position $\xi = (\xi_1, \xi_2, \xi_3)$. By considering the inner product between the both sides of the Navier-Stokes equation and the inner normal vector $\sigma(\xi)$, we obtain the non-homogeneous Neumann boundary condition

$$\frac{1}{\rho_0} \frac{\partial p}{\partial \sigma} = \sigma \cdot g \quad (60)$$

for pressure which is explained in traditional hydrodynamics.

For example, let

$$\Omega_{\text{liquid}} = \{r = (r_1, r_2, r_3) \in \mathbb{R}^3 ; r_3 > 0\} \quad (61)$$

$$\Omega_{\text{solid}} = \{r = (r_1, r_2, r_3) \in \mathbb{R}^3 ; r_3 < 0\} \quad (62)$$

be the domain of the liquid and the domain of the solid, respectively. The boundary $\partial\Omega_{\text{liquid}}$ of the liquid domain Ω_{liquid} becomes

$$\partial\Omega_{\text{liquid}} = \{r = (r_1, r_2, r_3) \in \mathbb{R}^3 ; r_3 = 0\}. \quad (63)$$

Considering the normal vector $\sigma = (0, 0, 1)$ of the boundary $\partial\Omega_{\text{liquid}}$, the boundary condition (60) becomes

$$\frac{1}{\rho_0} \frac{\partial p}{\partial u_3} = \begin{cases} g_z & \text{if } u \in \partial\Omega_{\text{liquid}} \\ 0 & \text{if } u \in \Omega_{\text{solid}} \end{cases} \quad (64)$$

Thus we obtain

$$\frac{1}{\rho_0} \frac{\partial^2 p}{\partial u_3^2} = \delta(u_3) \quad (65)$$

where $\delta(\cdot)$ is the Dirac's delta function.

In this way, the non-homogeneous boundary condition (60) of the pressure Poisson equation is transformed to the source term of the pressure Poisson equation.

6 Conclusion

We derived the time evolution scheme of the Moving Particle Semi-implicit method (MPS) by considering the compressible flow in the computation process and analyzed the boundary condition of the pressure Poisson equation(the Poisson type partial differential equation).

We modified the Poisson type partial differential equation which gives the pressure based on our previous research [6]. The Poisson type partial differential equation is modified to the one

with feedback for the mass density and the divergence of the flow's velocity. This modification guarantees the heuristic computation proposed by [3] theoretically.

Since the non-homogeneous boundary condition of the Poisson type partial differential equation is transformed to the feedback term(source term of the equation), we can compute the solution of the Poisson type partial differential equation based on the homogeneous boundary condition.

Acknowledgement :

The first author would like to express his thanks to Prof. Masato KIMURA (Kanazawa University) for his valuable advices about spatial derivatives at Nishijin Plaza in Kyushu University on February 19th 2013.

Also the first author would like to express his thanks to Master Tasuku TAMAI (The University of Tokyo, Koshizuka & Shibata Laboratory) for advicing him how to verify the approximation equation (52) numerically.

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