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MOVING PARTICLE SEMI-IMPLICIT METHOD: FULLY LAGRANGIAN ANALYSIS OF INCOMPRESSIBLE FLOWS

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Abstract. *Moving Particle Semi-implicit (MPS) method is based on fully Lagrangian description. Particle interaction models are prepared for differential operators, such as gradient, divergence and Laplacien. Governing equations are transformed to interactions among moving particles. Grids are not necessary. Large deformation of interfaces can be analyzed without grid tangling. Numerical diffusion does not arise because the convection terms are not discretized. Collapse of a water column is calculated by MPS method. Fragmentation and coalescence of water is successfully analyzed. MPS method is applied to wave breaking on slopes. Two modes of wave breaking are in good agreement with experimental data. A gridless convection scheme named Meshless Advection using Flow-directional Local-grid (MAFL) is developed for arbitrary Lagrangian-Eulerian (ALE) description in combining MPS method. The combined method, MPS-MAFL, enables us to analyze wider range of thermal-hydraulic problems: for example, those involving inflow and outflow boundaries where Eulerian treatment is better. Local concentration of the computing points is easier in MPS-MAFL method. Bubble growth and departure in a nucleate boiling cycle is calculated and the heat transfer agrees well with that of an experiment.*

1. INTRODUCTION

Moving Particle Semi-implicit (MPS) method is based on fully Lagrangian description. Particle interaction models are prepared for differential operators, such as gradient, divergence and Laplacian. Governing equations are transformed to interactions among moving particles. Grids are not necessary. Incompressible flows are solved by using a semi-implicit algorithm; the incompressibility is implicitly satisfied by solving Poisson equation of pressure, while the other terms are explicitly calculated. Large deformation of interfaces is clearly analyzed by fully Lagrangian treatment. Grid tangling does not arise. In addition, MPS method is free from numerical diffusion because the convection terms are not discretized.

A pure particle method, where grids are not used at all, was first developed as Particle-and-Force (PAF) method[1]. Smoothed Particle Hydrodynamics (SPH) was developed by Lucy for astronomy[2]. In SPH a kernel function is used for smoothing discretized values at particles' positions. Derivatives are obtained by differentiating the smoothed distribution. Compressible flows are solved with a fully explicit algorithm. Spatial resolution is automatically controlled by clustering or dispersing of the particles, so that it is fitted to astrophysical problems involving large difference of gas density[3,4]. Moving Particle Semi-implicit (MPS) method was proposed to simulate incompressible viscous flows using a semi-implicit algorithm[5,6]. In MPS derivatives in the governing equations are transformed to interactions among the neighboring particles. A semi-implicit algorithm was also employed in SPH for incompressible flow analysis[7].

A gridless method was proposed by Batina[8]. A value at an arbitrary position was interpolated based on the least-square method. Only grid points, which are fixed in space, are necessary for this interpolation. Connectivity information among the grid points is not necessary, which means "gridless". Tanaka improved the accuracy of the gridless method by using Cubic-Interpolated Pseudoparticle (CIP) scheme[9]. Tanak also pointed out that the combination of a particle method and a gridless method leads to arbitrary Lagrangian-Eulerian description which possesses wider applicability to fluid dynamics problems. Yoon et al. developed a new gridless method, named Meshless Advenction using Flow-directional Local-grid (MAFL), and proposed a particle-gridless hybrid method by combining MAFL and MPS[10]. This hybrid method enables us to move the computing points, which have the same meaning with the particles, to anywhere in each time step as the ALE description.

MPS method was applied to collapse of a water column, and good agreement with an experiment was obtained even if splashing of the fluid occurred on a vertical wall[6]. Since no grids were used in the calculation, separation and coalescence of fluids as well as large deformation of free surfaces can be solved. Wave breaking on slopes was calculated by MPS[11] method. Two modes of wave breaking, spilling and plunging breakers, appeared in the calculation results. The critical condition between the two modes agreed with experiments. MPS method has been applied to thermal hydraulic problems for the nuclear safety; melt

fragmentation processes in vapor explosions[12], molten-core concrete interactions[13] and sodium leakage and combustion accidents[14]. Phase change processes are modeled as particle dynamics; boiling is represented by generation of new vapor particles and solidification is simulated by stopping the motion of the particles. Flow regimes of gas-liquid two phase flows were calculated by a two-particle model in MPS method[15]. Bubble growth and departure on a horizontal heated wall in subcooled nucleate boiling was calculated by MPS-MAFL method[16]. The calculated heat transfer agreed well with experimental data. Sloshing in an elastic tank was calculated where thin structures were also modeled by particle interactions[17]. A particle model of thick elastic structures was recently developed from the particle interaction models in MPS method[18,19].

In the present paper, the fundamental theory of MPS and MPS-MAFL methods are explained, and then three calculation examples are shown; collapse of a water column, wave breaking on slopes and bubble growth and departure in nucleate boiling.

2. MOVING PARTICLE SEMI-IMPLICIT METHOD

2.1 Governing equations

Mass, momentum and energy conservation equations for incompressible flows are solved:

$$\frac{d\rho}{dt} = 0 \tag{1}$$

$$\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho}\nabla P + \nu\nabla^2\mathbf{u} + \mathbf{f} \tag{2}$$

$$\frac{DT}{Dt} = \frac{k}{\rho Cp}\nabla^2 T + \frac{S}{\rho Cp} \tag{3}$$

The continuity equation is written with density for the particle modeling, while velocity divergence is usually employed in the finite volume method. The operator D/Dt denotes the Lagrangian derivative involving advection terms which are directly calculated by the moving particles.

2.2 Weight function

A weight function

$$w(r) = \begin{cases} \dfrac{r_e}{r} - 1 & 0 \le r < r_e \\ 0 & r_e \le r \end{cases} \tag{4}$$

is used for particle interaction models, where r is the distance between two particles and r_e is a parameter limiting the neighborhood (Fig.1). The weight function increases to infinity when the distance approaches zero. This characteristic shows good stability in the incompressibility calculation.

Summation of the weight function is called particle number density which is used as a normalization factor for averaging.

$$n_i = \sum_{j \neq i} w\left(\left|\mathbf{r}_j - \mathbf{r}_i\right|\right) \tag{5}$$

The particle number density is in proportion to the fluid density.

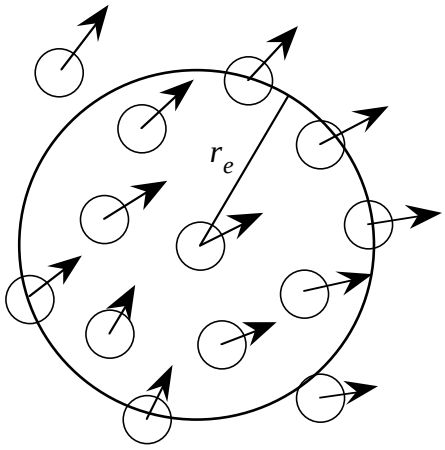

Figure 1. Particle interactions within weight function

2.3 Particle interaction models

If ϕ and $\mathbf{u}$ are arbitrary scalar and vector respectively, particle interaction models for differential operators are expressed as

$$\langle \nabla \phi \rangle_i = \frac{d}{n^0} \sum_{j \neq i} \left[\frac{\phi_j - \phi_i}{\left|\mathbf{r}_j - \mathbf{r}_i\right|^2} \left(\mathbf{r}_j - \mathbf{r}_i\right) w\left(\left|\mathbf{r}_j - \mathbf{r}_i\right|\right) \right] \tag{6}$$

$$\langle \nabla \cdot \mathbf{u} \rangle_i = \frac{d}{n^0} \sum_{j \neq i} \left[\frac{\left(\mathbf{u}_j - \mathbf{u}_i\right) \cdot \left(\mathbf{r}_j - \mathbf{r}_i\right)}{\left|\mathbf{r}_j - \mathbf{r}_i\right|^2} w\left(\left|\mathbf{r}_j - \mathbf{r}_i\right|\right) \right] \tag{7}$$

$$\left\langle \nabla^2 \phi \right\rangle_i = \frac{2d}{\lambda n^0} \sum_{j \neq i} \left[\left(\phi_j - \phi_i\right) w\left(\left|\mathbf{r}_j - \mathbf{r}_i\right|\right) \right] \quad , \tag{8}$$

where d is the number of space dimensions, n^0 is a particle number density fixed for incompressibility and λ is

$$\lambda = \frac{\sum_{j \neq i} \left|\mathbf{r}_j - \mathbf{r}_i\right|^2 w\left(\left|\mathbf{r}_j - \mathbf{r}_i\right|\right)}{\sum_{j \neq i} w\left(\left|\mathbf{r}_j - \mathbf{r}_i\right|\right)} \cong \frac{\int_V w(r) r^2 dv}{\int_V w(r) dv} \quad . \tag{9}$$

The gradient model is obtained as the average of gradient vectors which are determined between particle i and its neighboring particles j (Fig.2). The Laplacian model is derived from

the physical concept of diffusion. Part of a quantity at particle i is distributed to neighboring particles j (Fig.3). Parameter λ is introduced to keep the same variance increase as that of the analytical solution.

The parameter r_e of the weight function is $2.1l_0$ and $4.0l_0$ in the gradient and the Laplacian models respectively, where l_0 is the spacing between adjacent particles. These values were optimized from the viewpoint of accuracy[6].

Substituting the above particle interaction models into the differential operators in the governing equations, we obtain a kinematics of particles simulating fluid flows.

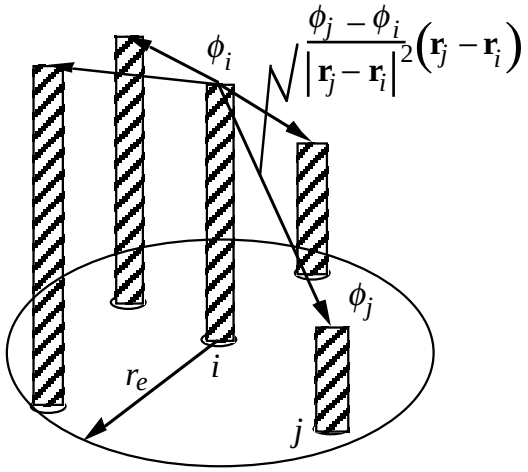

Figure 2. Gradient model

2.4 Semi-implicit algorithm

A semi-implicit algorithm was developed for incompressible flow analysis in MPS method. The continuity equation requires that the fluid density is constant. This is equivalent to the particle number density being constant; this constant value is denoted by n^0. The continuity equation and the pressure gradient term in the momentum conservation equation are implicitly calculated and the other terms are explicitly calculated by two steps (Fig.4).

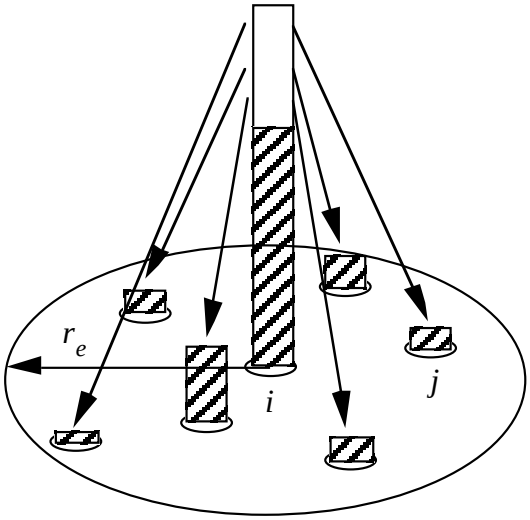

Figure 3. Laplacian model

In the first step, all terms in the momentum conservation equations except for the pressure gradient term are explicitly calculated and temporal velocities and positions of the particles are obtained. At this moment, the temporal particle number density n^* is not n^0. In the second step, Poisson equation of pressure

$$\nabla^2 P^{n+1} = -\frac{\rho}{\Delta t^2}\frac{n^* - n^0}{n^0} \tag{10}$$

is solved. The source term is the deviation of the temporal particle number density from the constant. Applying the present Laplacian model to the left hand side of Eq.(10), we obtain a symmetric matrix equation which can be solved by, for example, incomplete Cholesky

decomposition conjugate gradient (ICCG) method. The pressure gradient term is calculated and the velocities and the positions of the particles are modified.

2.5 Boundary condition

(1) fixed wall

Fixed walls are represented by three arrays of wall particles which are fixed in space. This

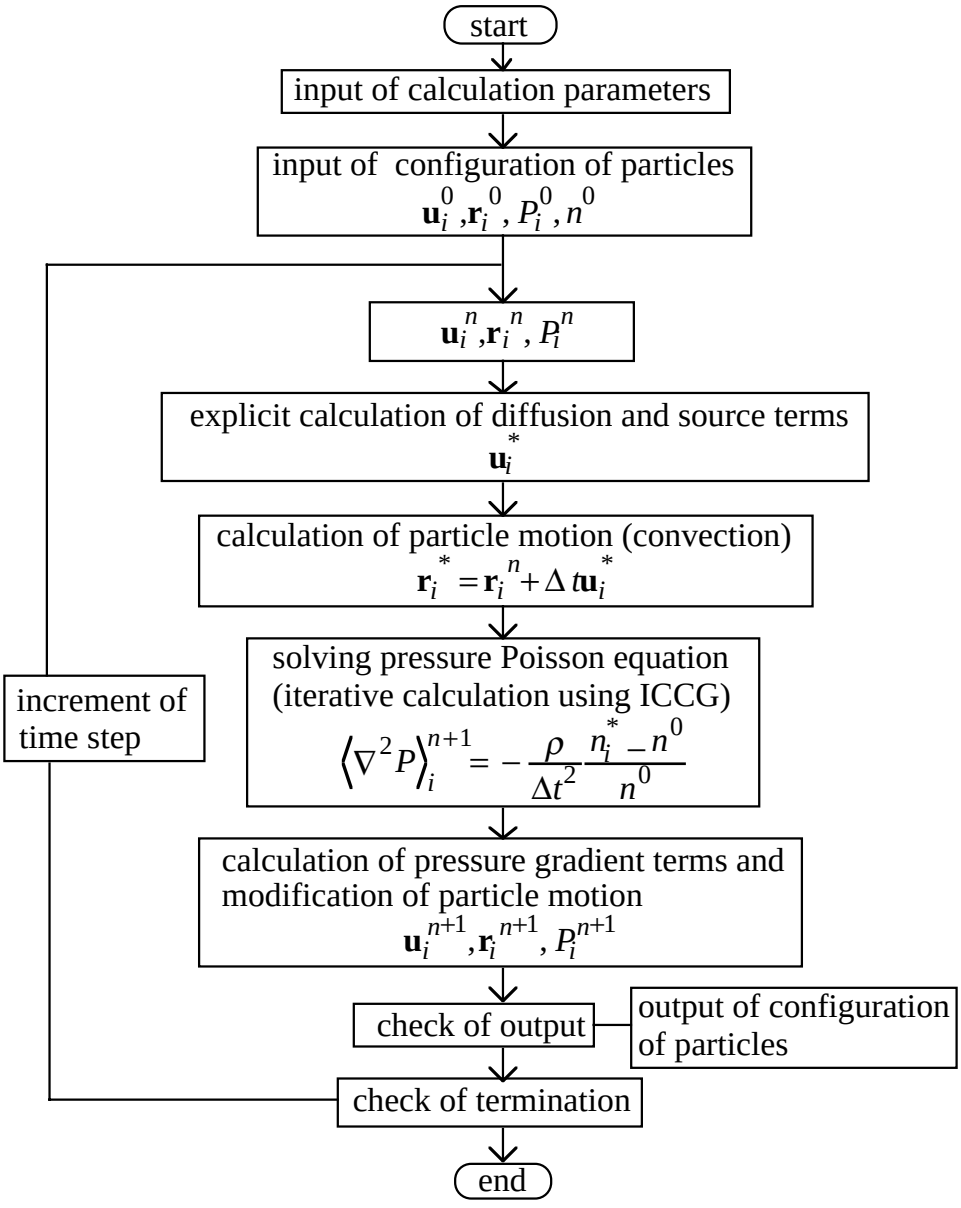

Figure 4. Semi-implicit algorithm in MPS method

is because enough particles should be located within the weight function. The most inner array, which contacts with the fluid particles, is included in the pressure calculation. When a fluid particle approaches the wall, the particle number density increases and repulsive force works between the fluid particle and the most inner wall particles. Negative velocities of the corresponding fluid particles are given to the wall particles as the non-slip conditions.

(2) free surface

Free surfaces are naturally tracked by fully Lagrangian motion of the particles. Since no fluid particles exist outside, the particle number density decreases on the free surfaces. Thus, the particles that satisfy the following condition are considered as on the free surface.

$$n_i^* < \beta n^0 \tag{11}$$

where β is a parameter below 1.0 (0.97 in this study). P=0 is applied to these particles in the pressure calculation.

It is not necessary to draw contours of the free surfaces in this scheme. Separation and coalescence of the fluid can be analyzed by this simple formulation.

3. MESHLESS ADVECTION USING FLOW-DIRECTIONAL LOCAL-GRID

Although MPS method has potential to analyze complex motion of interfaces, it has disadvantages for wider application to fluid dynamics problems. One is that fully Lagrangian description is not preferable in steady-state problems and those involving inflow and outflow boundaries. In MPS method inflow and outflow are calculated as generation and removal of particles. Another is that local enhancement of spatial resolution is difficult. Small particles, which are placed for high resolution, will move to somewhere as the calculation proceeds.

Meshless Advection using Flow-directional Local-grid (MAFL) scheme was developed for a gridless calculation of the convection terms. A one-dimensional grid line is generated at each particle in the direction of its velocity vector (Fig.5). Temporal grid points are located on the grid line. The values at the temporal grid points are interpolated from those of the neighboring particles. Finally, a one-dimensional difference scheme, for example the upwind scheme, QUICK, etc., is applied to the local grid. The accuracy can be controlled by selecting the difference scheme. MAFL scheme is easily extended to three-dimensional calculations because the local grid is one-dimensional.

Combining MPS and MAFL methods, we have an ALE method, called MPS-MAFL, in keeping the gridless framework. The concept is illustrated in Fig.6. The computing points are moved as fully Lagrangian description using MPS method, and then they are relocated arbitrarily with the calculation of convection using MAFL method. Fully Eulerian description is realized by relocating to the previous positions. In MPS-MAFL method the disadvantages

of fully Lagrangian description are overcome. Besides, MPS-MAFL method allowed us to change the number of the computing points arbitrarily during the calculation.

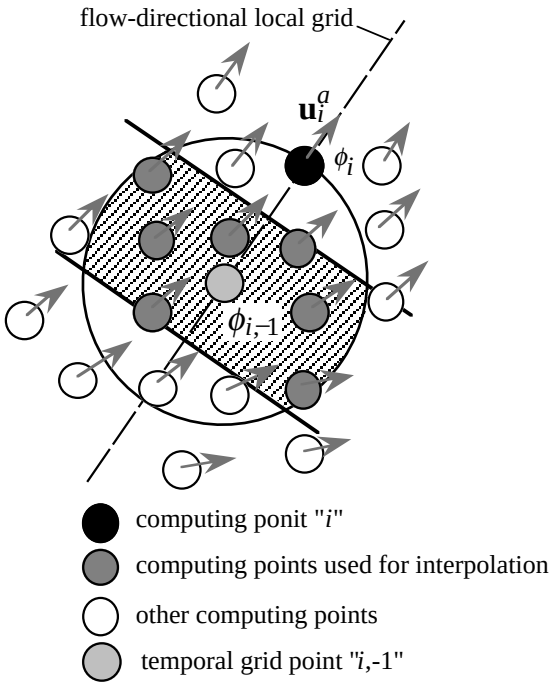

Figure 5. MAFL scheme for convection

4. CALCULATION EXAMPLES

4.1 Collapse of a water column

Collapse of a water column has been widely used for verification of free surface flow analysis codes. We carried out a calculation using MPS method[6]. An experiment was also carried out. The calculation and experimental results are shown in Figs.7 and 8, respectively. Water collapses (0.2sec), splashes on the right vertical wall (0.4sec), falls down (0.6) and splashes to the left (0.8sec). The calculated water behavior is similar to that of the experiment.

Figure 9 shows the leading edge position during the initial collapse of water. The calculated position agrees well with a reference calculation using Volume of Fluid (VOF) method[20], but it moves faster than our experiment and a reference experiment[21]. This may be attributed to the friction with the bottom wall. We can see that the shape of the leading edge is a little rounded in the experiment. This may decrease the spreading speed of water.

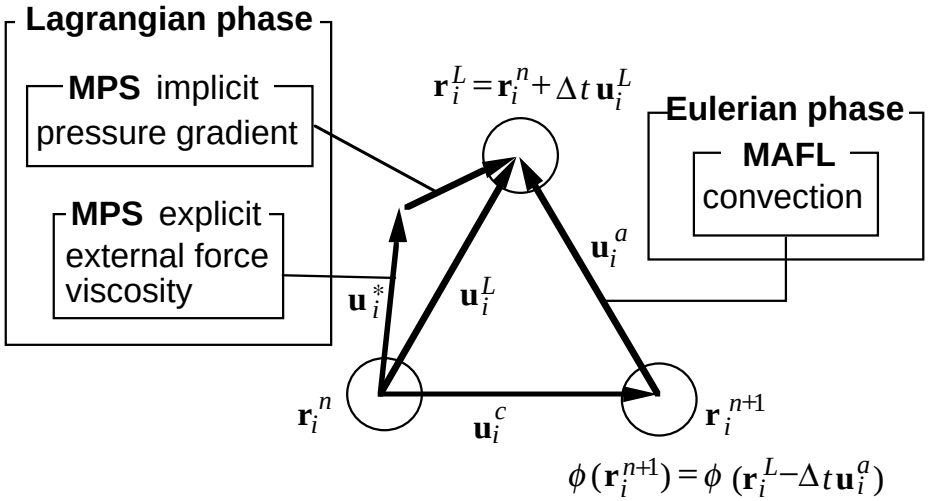

Figure 6. Arbitrary Lagrangian-Eulerian calculation in MPS-MAFL method

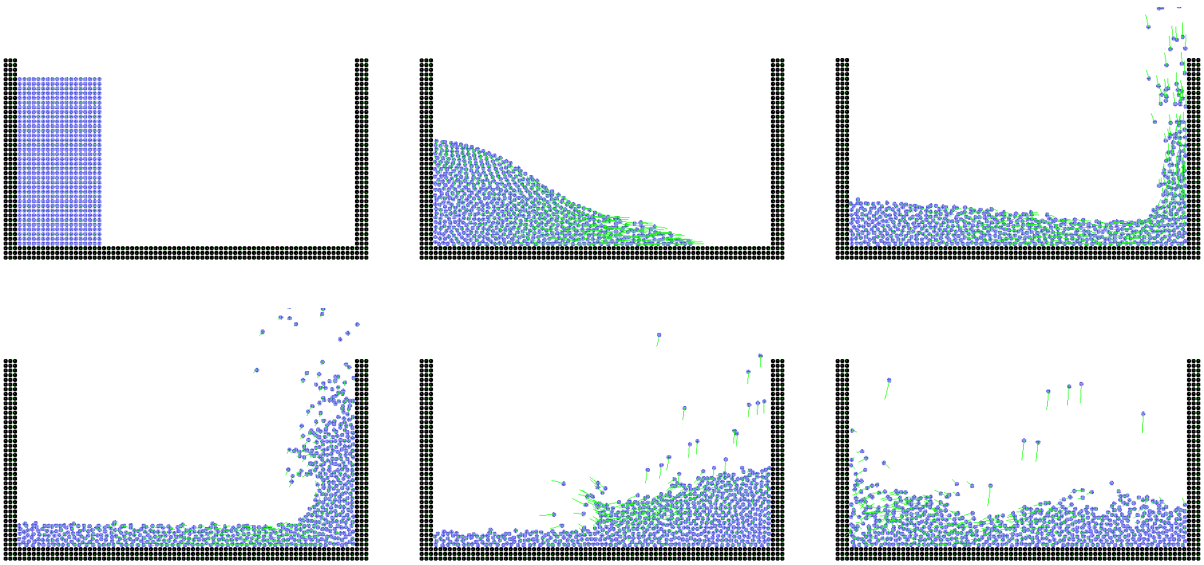

Figure 7. Calculation result of collapse of a water column: time interval=0.2sec

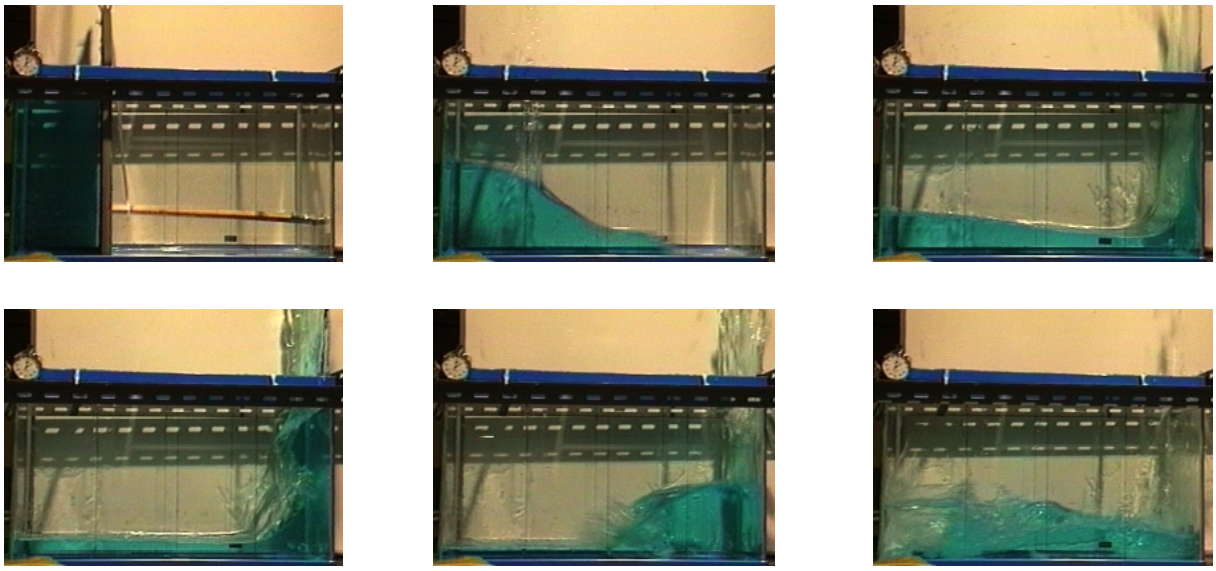

Figure 8. Experimental result of collapse of a water column: time interval=0.2sec

4.2 Wave breaking on slopes

Wave breaking occurs when waves propogate on slopes. Figure 10 shows the calculation geometry. A vertical wall is oscillated to generate waves. The motion of the wall is non-linear and the amplitude is vertically changed to follow finite amplitude waves. This complex motion is easily realized using particles.

It is known that wave breaking can be classified to several modes. Figure 11 shows the result of a plunging breaker; the wave front is forced to be steep and turns over. The calculation was carried out by varying the wave frequency and the slope tangent. The angular moment of the wave front was evaluated from the calculation results. When this was above a certain value, the breaking mode was considered as plunging; otherwise it was considered as spilling. Figure 12 shows the wave breaking modes obtained in this calculation. Plunging breakers were likely to occur when the wave frequency was smaller or

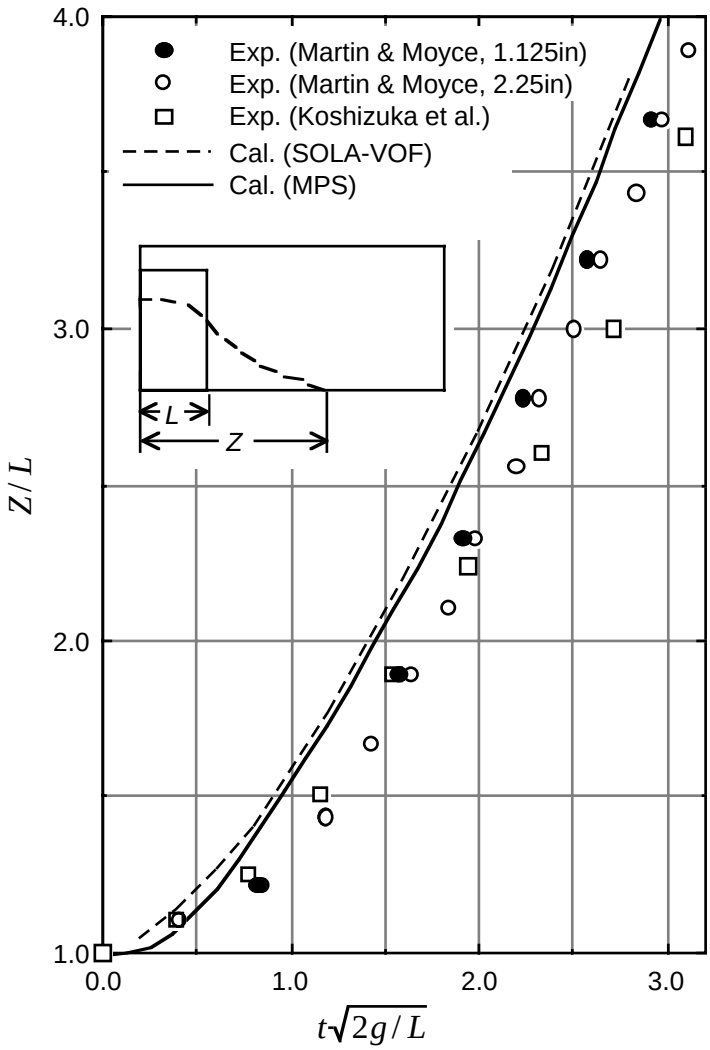

Figure 9. Leading edge position

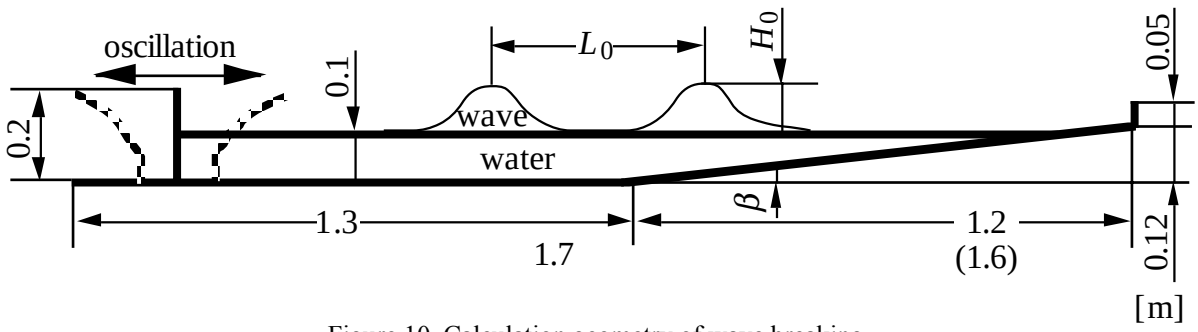

Figure 10. Calculation geometry of wave breaking

the slope was steeper. The results were compared with past experimental studies[22,23]. The boundary between the two modes agreed with the references within the range of data scattering.

4.3 Bubble growth and departure in nucleate boiling cycle

In nucleate boiling, bubbles periodically grow and depart from the heated wall. This cycle was calculated by MPS-MAFL method. Since this method is based on arbitrary Lagrangian-

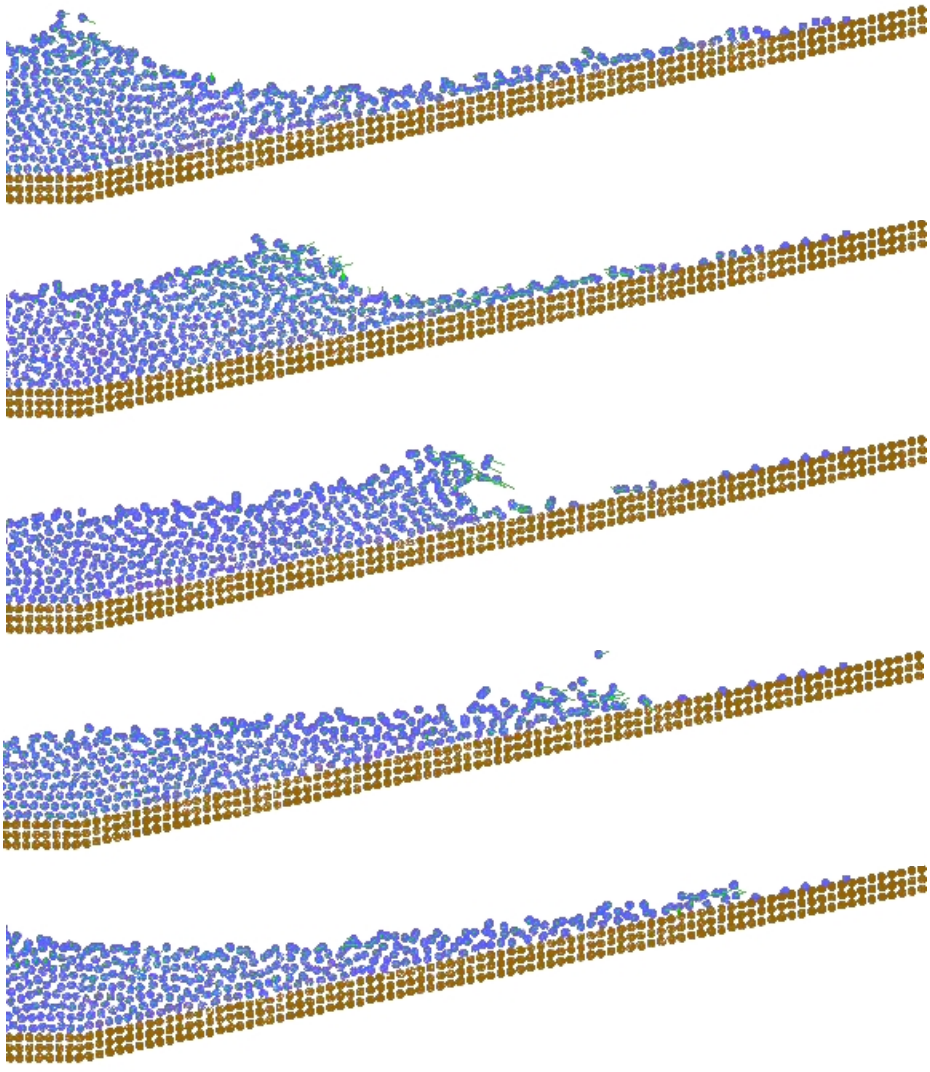

Figure 11. Plunging breaker on a slope

Eulerian, the computing points were locally concentrated in thin temperature boundary layers. There had been no successful numerical simulation to analyze the whole cycle of the bubble growth and departure in the past studies.

The calculation conditions were the same as those of an experiment carried out by Han and Griffith[24,25]. The bulk water temperature was 96°C at atmospheric pressure. The wall temperature was kept constant. In the calculation the temperature

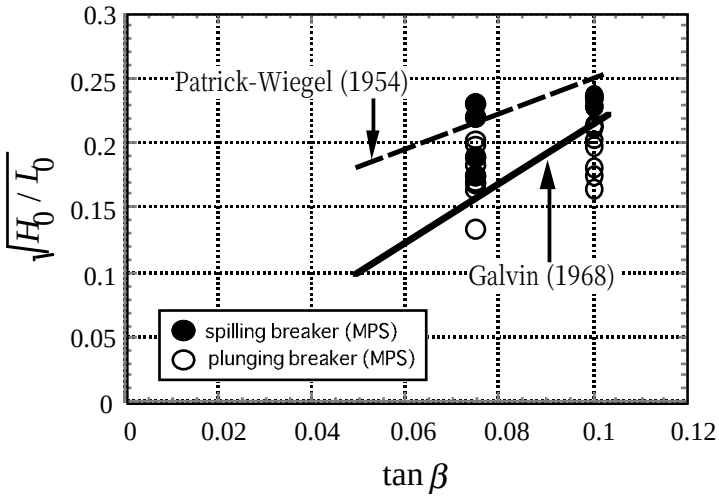

Figure 12. Modes of wave breaking

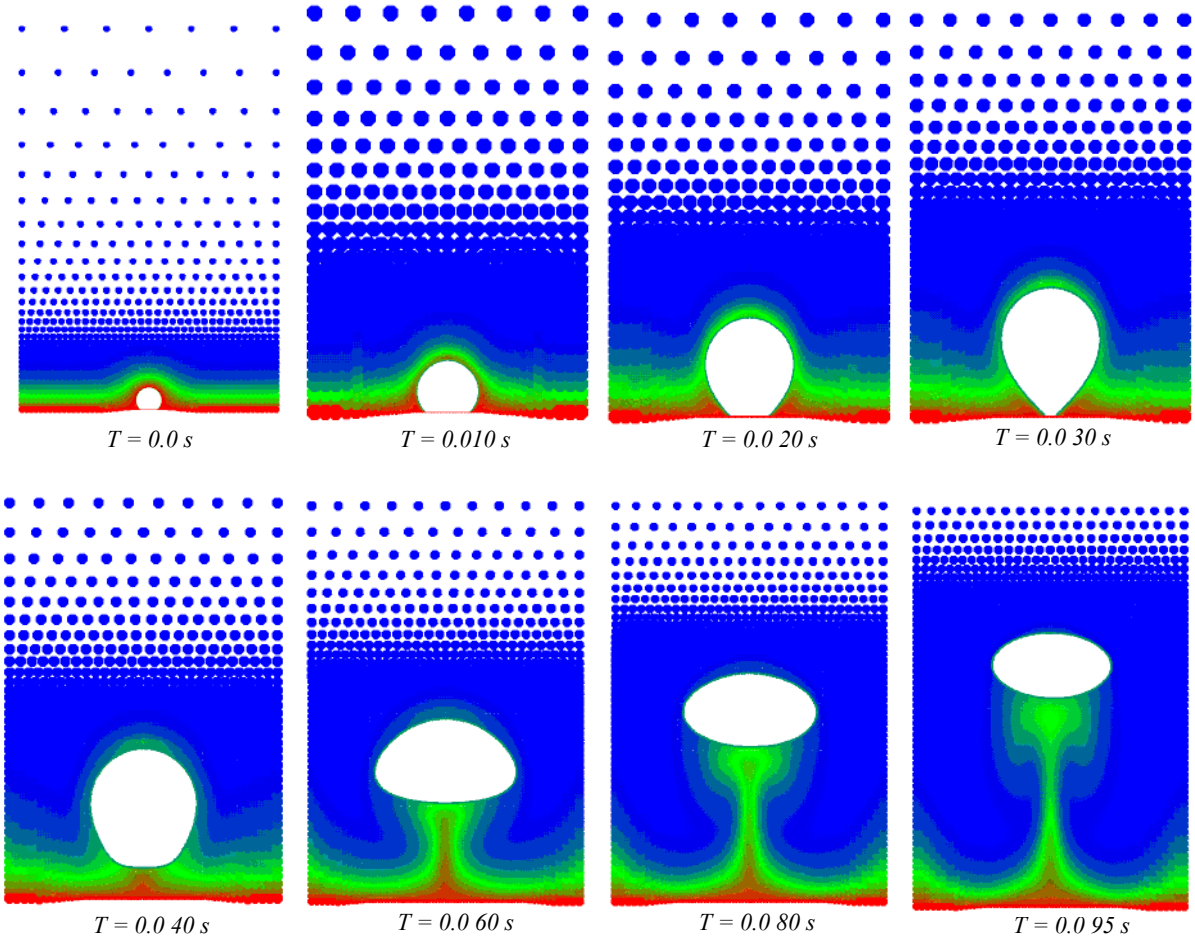

Figure 13. Bubble growth and departure in nucleate boiling

boundary layer on the wall was developed as pure conduction calculation during the waiting period, and then a small circular bubble of radius 0.3mm was placed as the initial condition. The contact angle was kept constant as 45°.

Figure 13 shows the calculation result when the wall temperature was kept at 110°C. The initial small bubble rapidly grows and departs from the wall by buoyancy force. Hot water in the boundary layer is lifted up behind the rising bubble.

Bubble growth speed was compared with the experimental data as shown in Fig.14. In the experiment bubble generation cycles were not strictly the same. Three cases were provided in the paper. We can see good agreement between the calculation and the three cases of the experiment. Compared with one-dimensional spherical bubble growth in a uniform temperature field of water, the bubble growth speed was decelerated when the bubble was expanded. This was due to condensation which was effective when the bubble was larger than the temperature boundary layer and contacted with the bulk subcooled water.

The heat transfer was evaluated by considering three mechanisms: latent heat, conduction and convection. The calculation result was transferred from x-y to r-z coordinates. We used the number of bubbles which were detected in the experiment. The evaluated total heat transfer is compared with experimental data in Fig.15. The heat transfer increases with the temperature difference between the bulk water and the heated wall. The calculation agrees well with the experiment.

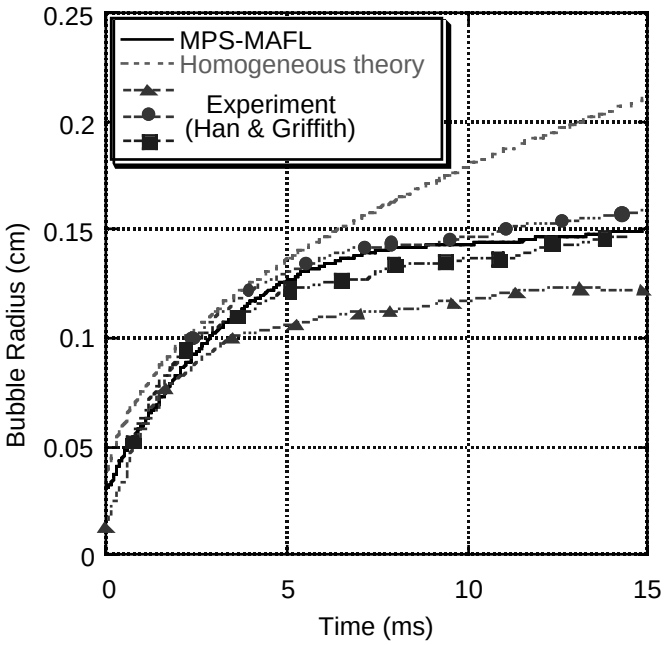

Figure 14. Bubble radius

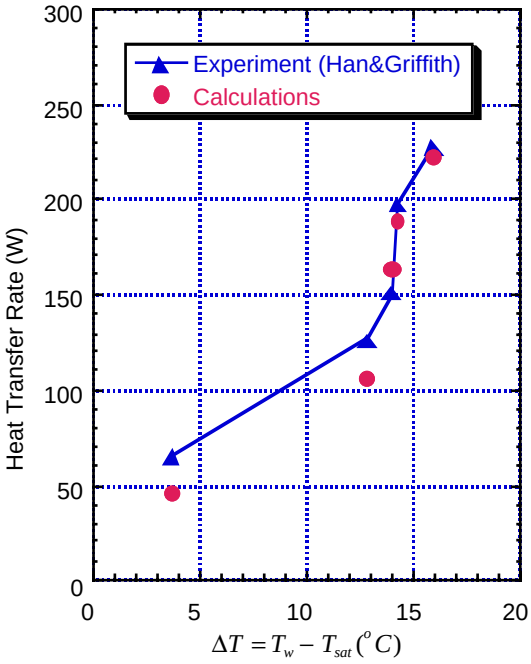

Figure 15. Total heat transfer rate

5. CONCLUSIONS

Gridless methods, MPS for pure Lagrangian and MPS-MAFL for arbitrary Lagrangian-Eulerian, were developed to analyze complex fluid dynamics with large deformation of interfaces. Since the grids are not necessary at all, large motion of boundaries can be tracked without the troubles of grid tangling. Numerical diffusion does not arise because of fully Lagrangian description. The concept of MPS method is that differential operators in the governing equations are transformed to equivalent particle interactions. Incompressibility is solved by a semi-implicit algorithm using Poisson equation of pressure. Free surfaces are simply identified by decrease in particle number density. MAFL scheme provides a gridless calculation of convection terms. A one-dimensional flow-directional local grid is temporarily generated at each computing point. MPS-MAFL is the combination of MAFL and MPS. Local concentration of the computing points is easy in MPS-MAFL method.

Two calculation examples of MPS method are shown. In collapse of a water column, fluid separation and coalescence are successfully calculated. In wave breaking, two modes of spilling and plunging breakers are simulated. Bubble growth and departure processes in nucleate boiling are calculated using MPS-MAFL method. The bubble growth speed and the heat transfer agree well with experimental data.

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