An Improvement of Moving Particle Semi-implicit method for Navier-Stokes equation with Free Boundary

自由境界 Navier-Stokes 方程式を粒子法 MPS で数値解析するにあたっての一つの修正案

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1 Particle Methods(Implicit or Explicit)

1. Deformation of liquid with free surface

   Solve Navier-Stokes equation numerically
   based on Lagrangian material variables

2. Particle Methods **粒子法**

（a） Moving Particle Semi-implicit method (MPS)

・・・Semi-Implicit

（b） Smoothed Particle Hydrodynamics (SPH)

・・・Explicit

2 Implicit Method in Simulation

1. Thin and Flexible elastic bodies' deformation
   (cloth, butterflie's wing, flower's petal etc.)
   (a) Stiffness operator and Damping operator are non-linear
   (b) Linearize the evolution equation by Frechet derivatives
   (c) Solve Resolvent equation at each time

   " Implicit Method "

2. Yosida Approximation for Evolution Equations

   Mathematical Theory which verifies
   Implicit Method in Numerical Simulations

3 Elastic bodies' deformation

Elastic bodies' deformation is described
by this evolution equation

$$\frac{d}{dt}\begin{pmatrix} u(t) \\ v(t) \end{pmatrix} + \begin{pmatrix} -v(t) \\ K\left(u(t)\right) + L\left(v(t)\right) \end{pmatrix} = \begin{pmatrix} 0 \\ f(t) \end{pmatrix} \quad (1)$$

$u(t,x)$: displacement at each position x
$v(t,x)$: velocity at each position x
$f(t,x)$: external force at each position x

$K(\cdot)$: stiffness operator which is non-linear
$L(\cdot)$: damping operator which is non-linear

4 Discretize in small time interval Δt

The evolution equation is discretized into this
time difference equation by a small time interval Δt

$$\frac{1}{\Delta t}\begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix} + \begin{pmatrix} -v[n] - \Delta v \\ K\left(u[n] + \Delta u\right) + L\left(v[n] + \Delta v\right) \end{pmatrix}$$
$$= \begin{pmatrix} 0 \\ f[n+1] \end{pmatrix} \tag{2}$$

$n = 0, 1, 2, 3, \cdots$: discretized time
$u[n] = u(n\,\Delta t)$, $v[n] = v(n\,\Delta t)$, $f[n] = f(n\,\Delta t)$
$\Delta u = u[n+1] - u[n]$, $\Delta v = v[n+1] - v[n]$

5 Taylor expansions of spatial operators

Taylor expansion of stiffness $K(u)$ and damping $L(v)$ based on their Frechet derivatives $\partial K/\partial u$ and $\partial L/\partial v$

$$K\left(u[n] + \Delta u\right) = K\left(u[n]\right) + \frac{\partial K}{\partial u}[n]\,\Delta u \tag{3}$$

$$L\left(v[n] + \Delta v\right) = L\left(v[n]\right) + \frac{\partial L}{\partial v}[n]\,\Delta v \tag{4}$$

$$K[n] = K\left(u[n]\right) \quad , \quad L[n] = L\left(v[n]\right) \tag{5}$$

$$\frac{\partial K}{\partial u}[n] = \frac{\partial K}{\partial u}\left(u[n]\right) \quad , \quad \frac{\partial L}{\partial v}[n] = \frac{\partial L}{\partial v}\left(v[n]\right) \tag{6}$$

6 Solve Resolvent equation at each time

Resolvent equation whose unknowns are $(\Delta u, \Delta v)$

$$\left\{ \begin{pmatrix} I & O \\ O & I \end{pmatrix} + \Delta t \begin{pmatrix} O & -I \\ \frac{\partial K}{\partial u}[n] & \frac{\partial L}{\partial u}[n] \end{pmatrix} \right\} \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix}$$
$$= \Delta t \begin{pmatrix} v[n] \\ -K[n] - L[n] + f[n+1] \end{pmatrix} \tag{7}$$

Solve $(\Delta u, \Delta v)$ from the above Resolvent equation.

Next displacement $u[n+1]$ and Next velocity $v[n+1]$ is computed by

$$u[n+1] = u[n] + \Delta u \tag{8}$$
$$v[n+1] = v[n] + \Delta v \tag{9}$$

7 Deformation of liquid with free surface

1. Splashing water, Breaking waves and so on are computed by Moving Particle Semi-implicit method (which was proposed by Prof. S.KOSHIZUKA et al.)
   - (a) Time Evolution : Lagrangian material variable
   - (b) Spatial Derivative : Eulerian space variable

2. The original MPS must be modified mathematically
   - (a) It does not converge to Navier-Stokes equation
   - (b) Temporal Pressure → Real Pressure

8 Navier-Stokes equation (Eulerian)

$x = (x_1, x_2, \cdots, x_I)$: Eulerian space variable, $I = 2, 3, \cdots$

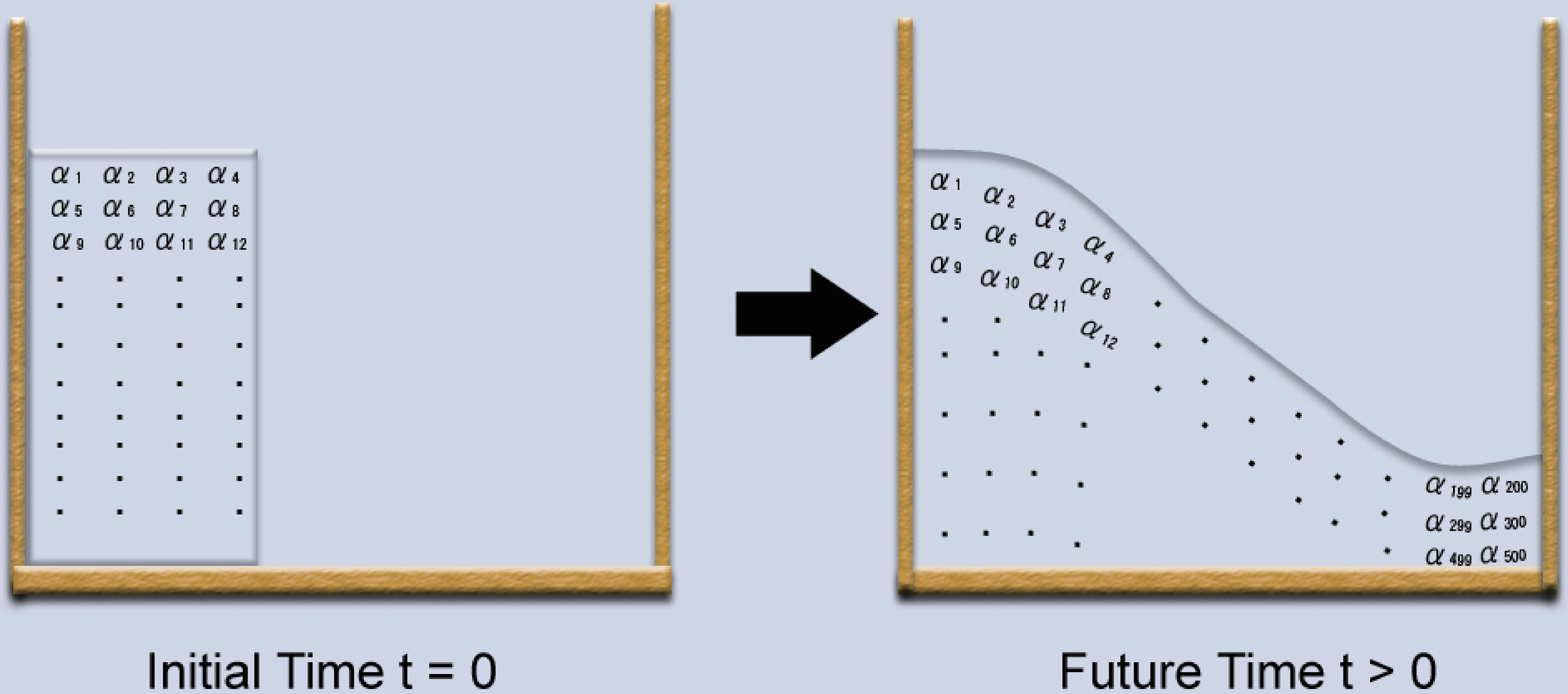
Navier-Stokes equation with free surface

$$\frac{D\ v(t,x)}{Dt} = \frac{\mu}{\rho(t,x)} \sum_{i=1}^{I} \frac{\partial^2 v(t,x)}{\partial x_i^2} - \frac{1}{\rho(t,x)} \frac{\partial p(t,x)}{\partial x} + g$$

$$\frac{Du(t,\alpha)}{Dt} = v\left(t, u(t,\alpha)\right) \tag{10}$$

The equation of continuity from mass conservation

$$0 = \frac{\partial \rho(t,x)}{\partial t} + \sum_{i=1}^{I} \frac{\partial}{\partial x_i} \left\{\rho(t,x) v_i(t,x)\right\} \tag{11}$$


Initial Time t = 0
Future Time t > 0

9 Lagrangian material variable

We analyze Navier-Stokes equation based on Lagrangian material variable.

Each liquid's particle is expressed by an initial position $\alpha = (\alpha_1,\ \alpha_2,\ \cdots, \alpha_I)^{\mathrm{T}}$ at initial time $t = 0$.

Let $u(t, \alpha) = (u_1(t, \alpha),\ u_2(t, \alpha),\ \cdots\ ,\ u_I(t, \alpha))^{\mathrm{T}}$ be a position of the particle $\alpha = (\alpha_1,\ \alpha_2,\ \cdots, \alpha_I)^{\mathrm{T}}$ at time $t \geq 0$.

Let $v(t, \alpha) = (v_1(t, \alpha),\ v_2(t, \alpha),\ \cdots\ ,\ v_I(t, \alpha))^{\mathrm{T}}$ be a velocity of the particle $\alpha = (\alpha_1,\ \alpha_2,\ \cdots, \alpha_I)^{\mathrm{T}}$ at time $t \geq 0$.

10 State variables around each particle

Let $u(t) = (u(t, \alpha)\ ;\ \alpha \in \Lambda)$
Let $v(t) = (v(t, \alpha)\ ;\ \alpha \in \Lambda)$
$u(t)$ expresses the liquid's shape at time $t \geq 0$.

- Let $\rho(t, \alpha)$ be mass density around the particle $\alpha = (\alpha_1,\ \alpha_2,\ \cdots, \alpha_I)^{\mathrm{T}}$ at time $t \geq 0$.
- Let $p(t, \alpha)$ be pressure around the particle $\alpha = (\alpha_1,\ \alpha_2,\ \cdots, \alpha_I)^{\mathrm{T}}$ at time $t \geq 0$.

Let $\rho(t) = (\rho(t, \alpha)\ ;\ \alpha \in \Lambda)$
Let $p(t) = (p(t, \alpha); \alpha \in \Lambda)$

11 Incompressibility Assumption

The mass density $\rho(t, \alpha)$ depends the volume expansion

$$\rho(t, \alpha) = \frac{\rho_0}{\det\left(\frac{\partial u(t,\alpha)}{\partial \alpha}\right)} \tag{12}$$

Assume that the flow is incompressible

$$1 = \det\left(\frac{\partial u(t, \alpha)}{\partial \alpha}\right) \tag{13}$$

Then, the mass density $\rho(t, \alpha)$ become a constant ρ_0

$$\rho(t, \alpha) = \rho_0 \tag{14}$$

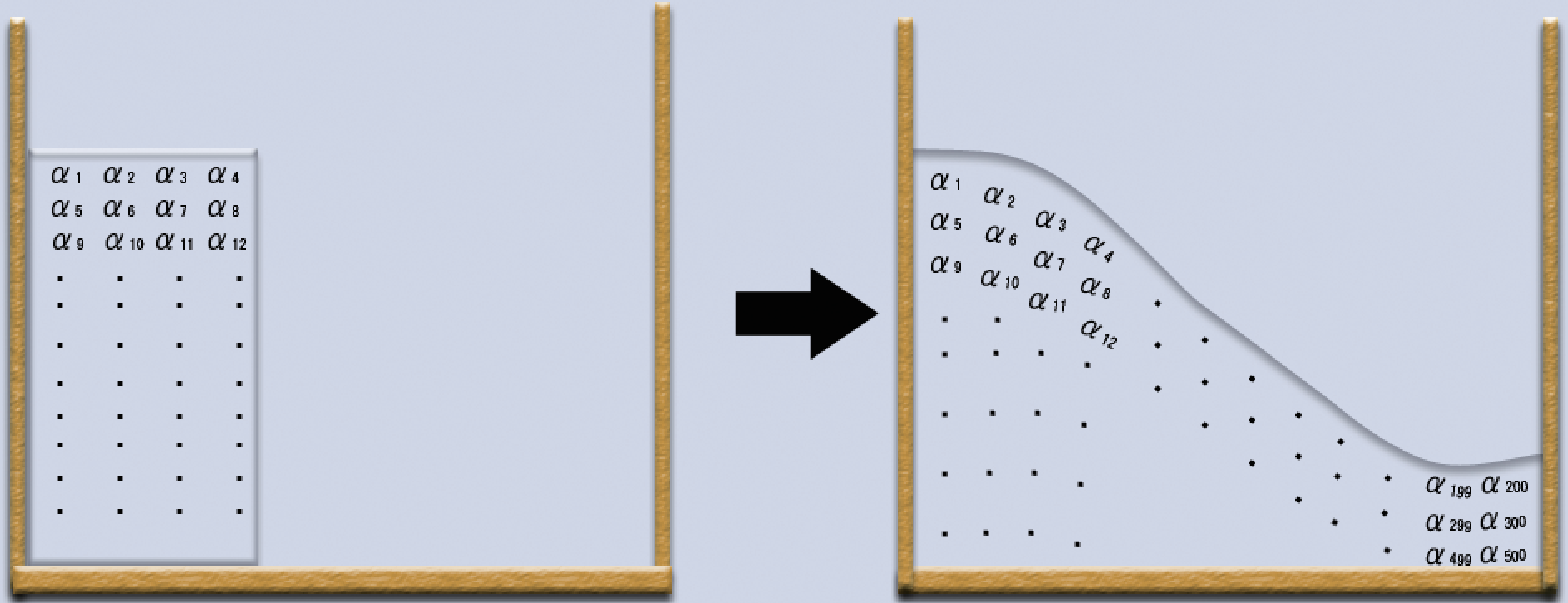
12 Lagrangian-Eulerian hybrid type Navier-Stokes equation

Based on Lagrangian material variable, we obtain

$$\frac{D\ v(t,\alpha)}{Dt} = \frac{\mu}{\rho_0} \sum_{i=1}^{I} \frac{\partial^2 v(t,\alpha)}{\partial u_i(t,\alpha)^2} - \frac{1}{\rho_0} \frac{\partial p(t,\alpha)}{\partial u(t,\alpha)} + g \quad (15)$$

$$\frac{Du(t,\alpha)}{Dt} = v(t,\alpha) \quad (16)$$

$$0 = \frac{D\rho(t,\alpha)}{Dt} + \rho(t,\alpha) \sum_{i=1}^{I} \frac{\partial v_i(t,\alpha)}{\partial u_i(t,\alpha)} \quad (17)$$



Initial Time t = 0

Future Time t > 0

13 Discretization by L particles

Lagrangian material variable is discretized by many particles $\alpha_{[l]} \quad (l = 1, 2, 3, \cdots, L = 5000)$.

Let $\alpha_{[l]}$ be a representative initial position $(l = 1, 2, \cdots, L)$ at initial time $t = 0$.

Position $u(t, \alpha) \quad (\alpha \in \Lambda)$ is discretized as $u(t, \alpha_{[l]}) \quad (l = 1, 2, \cdots, L)$.

Velocity $v(t, \alpha) \quad (\alpha \in \Lambda)$ is discretized as $v(t, \alpha_{[l]}) \quad (l = 1, 2, \cdots, L)$.

14 Discretization of Laplacian by MPS

$$
\sum_{i=1}^{I} \frac{\partial^2 \phi}{\partial U_i^2}(\alpha_{[l]}) = \tag{18}
$$

$$
2I \sum_{k \neq l} \frac{\left\{\phi(\alpha_{[k]}) - \phi(\alpha_{[l]})\right\}}{\lambda} \frac{w\left(\left|U(\alpha_{[k]}) - U(\alpha_{[l]})\right|\right)}{\rho_0}
$$

where

$$
\lambda = \frac{\sum_{k \neq l} \left|U(\alpha_{[k]}) - U(\alpha_{[l]})\right|^2 \; w\left(\left|U(\alpha_{[k]}) - U(\alpha_{[l]})\right|\right)}{\sum_{k \neq l} w\left(\left|U(\alpha_{[k]}) - U(\alpha_{[l]})\right|\right)}
$$

15 Discretization of gradient by MPS

$$
\begin{aligned}
&\frac{\partial \phi}{\partial U}(\alpha_{[l]}) \\
= &\frac{I}{\rho_0}\sum_{k\neq l}\frac{\phi(\alpha_{[k]})-\phi(\alpha_{[l]})}{\left|U(\alpha_{[k]})-U(\alpha_{[l]})\right|}\frac{U(\alpha_{[k]})-U(\alpha_{[l]})}{\left|U(\alpha_{[k]})-U(\alpha_{[l]})\right|} \\
&\frac{w\left(\left|U(\alpha_{[k]})-U(\alpha_{[l]})\right|\right)}{\rho_0}
\end{aligned}
\tag{19}
$$

Laplacian and gradient are discretized by mutual operations between particles.

16 Time Discretization (explicit)

$\tau = \Delta t$: sampling time

$t = n\tau \quad (\; n = 0, 1, 2, \cdots$: digital time)

Let $U[n](\alpha)$ be an approximate value for $u(n\tau, \alpha)$.

Let $V[n](\alpha)$ be an approximate value for $v(n\tau, \alpha)$.

$$\frac{V[n+1] - V[n]}{\tau} = \frac{\mu}{\rho_0} \sum_{i=1}^{I} \frac{\partial^2 V[n]}{\partial U_i[n]^2} - \frac{1}{\rho_0} \frac{\partial P}{\partial U} + g \quad (20)$$

$$\frac{U[n+1] - U[n]}{\tau} = V \quad (21)$$

$$\mathrm{Rho}[n] = \rho_0 \quad (22)$$

17 Temporal velocity V^* and Temporal position U^*

Temporal velocity V^* is computed only by viscosity term ignoring pressure term

$$\frac{V^* - V[n]}{\tau} = \frac{\mu}{\rho_0} \sum_{i=1}^{I} \frac{\partial^2 V[n]}{\partial U_i[n]^2} + g \tag{23}$$

Temporal position U^* is computed from Temporal velocity V^*

$$\frac{U^* - U[n]}{\tau} = V^* \tag{24}$$

18 Modifiers V' and U'

Recover effect of pressure P^* (unknown)
by modifiers V' and U'

$$V[n+1] = V^* + V' \qquad U[n+1] = U^* + U' \tag{25}$$

$$\frac{V'}{\tau} = \frac{-1}{\rho_0} \; \frac{\partial P^*}{\partial U^*} \tag{26}$$

$$\frac{U'}{\tau} = V' \tag{27}$$

$$\mathrm{Rho}^*(\alpha) = \frac{\rho_0}{\det\left(\frac{\partial U^*(\alpha)}{\partial \alpha}\right)} \tag{28}$$

19 N-S eq. modified by pressure P^*

By adding effects of modifiers V' and U'

$$\frac{V[n+1]-V[n]}{\tau} = \frac{\mu}{\rho_0}\sum_{i=1}^{I}\frac{\partial^2 V[n]}{\partial U_i[n]^2} - \frac{1}{\rho_0}\frac{\partial P^*}{\partial U^*} + g \tag{29}$$

$$\frac{U[n+1]-U[n]}{\tau} = V[n+1] \tag{30}$$

20 Find temporal pressure P^*

Considering modifier V' from effect of pressure P^*

$$(-1)\ \frac{\partial P^*}{\partial U^*} = \frac{\rho_0}{\tau}\ V' \tag{31}$$

By taking inner product with $\partial/\partial U^*$

$$(-\ \tau)\ \sum_{i=1}^{I} \frac{\partial^2 P^*}{\partial {U_i^*}^2} = \rho_0\ \sum_{i=1}^{I} \frac{\partial V_i'}{\partial U_i^*} \tag{32}$$

21 Find temporal pressure P^*

$$0 = \frac{D\rho}{Dt} + \rho_0 \sum_{i=1}^{I} \frac{\partial V_i[n+1]}{\partial U_i^*} \tag{33}$$

$$= \frac{D\rho}{Dt} + \rho_0 \sum_{i=1}^{I} \left(\frac{\partial V_i^*}{\partial U_i^*} + \frac{\partial V_i'}{\partial U_i^*} \right) \tag{34}$$

$$= \frac{\mathrm{Rho}[n+1] - \mathrm{Rho}^*}{\tau} + \frac{\mathrm{Rho}^* - \mathrm{Rho}[n]}{\tau} \tag{35}$$

$$+\rho_0 \sum_{i=1}^{I} \frac{\partial V_i^*}{\partial U_i^*} + \rho_0 \sum_{i=1}^{I} \frac{\partial V_i'}{\partial U_i^*}$$

22 Find temporal pressure P^*

Discretization of the equation of continuity

$$\frac{\mathrm{Rho}^* - \mathrm{Rho}[n]}{\tau} + \sum_{i=1}^{I} \frac{\partial V_i^*}{\partial U_i^*} = 0 \tag{36}$$

Here, since $\mathrm{Rho}[n+1] = \rho_0$ (incompressible assumption)

$$0 = \frac{\rho_0 - \mathrm{Rho}^*}{\tau} + \rho_0 \sum_{i=1}^{I} \frac{\partial V_i'}{\partial U_i^*} \tag{37}$$

23 Find temporal pressure P^*

Thus, we obtain

$$\rho_0 \sum_{i=1}^{I} \frac{\partial V_i'}{\partial U_i^*} = (-1) \, \frac{\rho_0 - \mathrm{Rho}^*}{\tau} \tag{38}$$

By substituting the above equation
into the following equation (32)

$$(-\,\tau) \sum_{i=1}^{I} \frac{\partial^2 P^*}{\partial {U_i^*}^2} = \rho_0 \sum_{i=1}^{I} \frac{\partial V_i'}{\partial U_i^*} \tag{39}$$

we have

24 Poisson equation determines P^*

$$(-\ \tau)\ \ \sum_{i=1}^{I} \frac{\partial^2 P^*}{\partial {U_i^*}^2} = (-1)\ \frac{\rho_0 - \mathrm{Rho}^*}{\tau} \tag{40}$$

Thus, we obtain Poisson type equation

$$\sum_{i=1}^{I} \frac{\partial^2 P^*}{\partial {U_i^*}^2} = \frac{\rho_0 - \mathrm{Rho}^*}{\tau^2} \tag{41}$$

By solving this PDE with B.C. from liquid's shape U^* , we find temporal pressure P^* .

25 Find next pressure $P[n+1]$

Time Difference N-S eq. with temporal pressure P^*

$$\frac{V[n+1]-V[n]}{\tau} = \frac{\mu}{\rho_0}\sum_{i=1}^{I}\frac{\partial^2 V[n]}{\partial U_i[n]^2} - \frac{1}{\rho_0}\frac{\partial P^*}{\partial U^*} + g \quad (42)$$

Compute next pressure $P[n+1]$ which sutisfies the following modified time difference N-S eq.

$$\frac{V[n+1]-V[n]}{\tau} = \frac{\mu}{\rho_0}\sum_{i=1}^{I}\frac{\partial^2 V[n]}{\partial U_i[n]^2} - \frac{1}{\rho_0}\frac{\partial P[n+1]}{\partial U[n+1]} + g$$

based on next velocity $V[n+1]$ and position $U[n+1]$.

26 Modified N-S eq. with next V and U

The approximate solutions V , U , P
from the time difference modified N-S eq.

$$\frac{V[n+1]-V[n]}{\tau} = \frac{\mu}{\rho_0}\sum_{i=1}^{I}\frac{\partial^2 V[n]}{\partial U_i[n]^2} - \frac{1}{\rho_0}\frac{\partial P[n+1]}{\partial U[n+1]} + g$$

with next velocity $V[n+1]$ and next position $U[n+1]$
may converge to the rigorous solutions v , u , p
of Lagrangian-Eulerian hybrid type N-S eq.

$$\frac{D\,v(t,\alpha)}{Dt} = \frac{\mu}{\rho_0}\sum_{i=1}^{I}\frac{\partial^2 v(t,\alpha)}{\partial u_i(t,\alpha)^2} - \frac{1}{\rho_0}\frac{\partial p(t,\alpha)}{\partial u(t,\alpha)} + g \quad (43)$$

27 Smoothed Particle Hydrodynamics

Discretize Navier-Stokes equation

$$\frac{D\ v(t,x)}{Dt} = \frac{\mu}{\rho(t,x)} \sum_{i=1}^{I} \frac{\partial^2 v(t,x)}{\partial x_i^2} - \frac{1}{\rho(t,x)} \frac{\partial p(t,x)}{\partial x} + g$$

and the state equation

$$p(t,\cdot) = F\left(\rho(t,\cdot)\right) \tag{44}$$

by kernel functions

1. Explicit Method
2. Incompressibility does not follows strictly

28 Conclusions

1. Deformation of liquid with free surface
   (Navier Stokes equation with Free Boundary)
2. Particle Method **粒子法**
   (a) MPS(Moving Particle Semi-implicit)· · ·Semi-implicit
   (b) SPH(Smoothed Particle Hydrodynamics)· · ·Explicit
3. Mathematical formulation of MPS
   Lagrangian-Eulerian hybrid type Navier-Stokes equation
4. Moving Particle Semi-implicit method were modified.
   (a) Temporal Pressure → Real Pressure
   (b) Approximate solution of modified MPS will converge to rigorous solution of L-E hybrid type N-S eq.

29 Appendix

自由境界 Navier-Stokes **方程式の数値解析において**
流体粒子 Lagrange **座標に基づく**
Lagrange-Euler **混合型** Navier-Stokes **方程式**

$$\frac{D\ v(t,\alpha)}{Dt} = \frac{\mu}{\rho_0} \sum_{i=1}^{I} \frac{\partial^2 v(t,\alpha)}{\partial u_i(t,\alpha)^2} - \frac{1}{\rho_0} \frac{\partial p(t,\alpha)}{\partial u(t,\alpha)} + g$$

へ
粒子法 Moving Particle Semi-implicit **が収束するよう、**
MPS **における 仮の圧力** P^* **を**
N-S **方程式に適合する 圧力** $P[n+1]$ **に**
計算し直す事を提案した。