# A Moving Particle Method for Simulating Incompressible Flow

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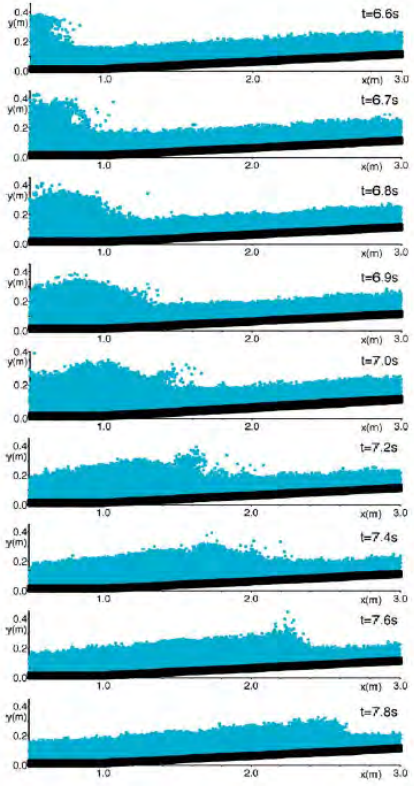
# Presentation Outline

- Origin of the conventional Moving Particle Semi-implicit (MPS) particle method.
- Limitations of MPS method.
- The proposed Moving Particle Pressure Mesh (MPPM) scheme.
- A new density interpolation scheme based on level-set function.
- Test cases: single- and multi-phase flow.
- Conclusion & on-going works

# The origin of MPS

- Moving Particle Semi-implicit (MPS) scheme → mesh-free Lagrangian method→ to simulate incompressible flow using a semi-implicit technique.
- Main Ref: Koshizuka, S., Nobe, A. and Oka, Y. (1998), "Numerical analysis of breaking waves using the moving particle semi-implicit method", *International Journal for Numerical Methods in Fluids*, Vol. 26, pp. 751-769.
- E.g. **Wave-breaking**

  (Gotoh and Sakai 2006):




**Multiphase flow** (Chen et al. 2011)

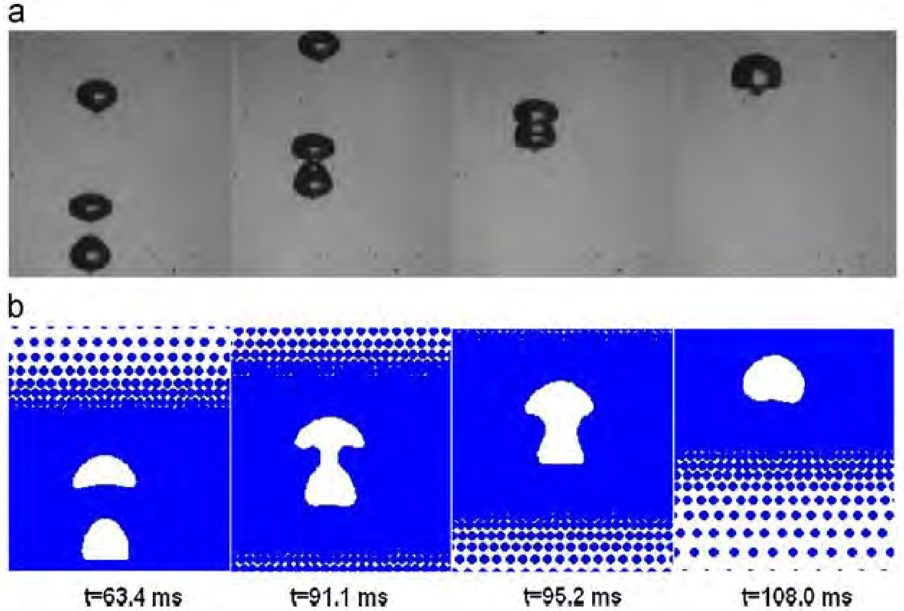



Fig. 6. Numerical results and experimental observations of in-line coalescence between two identical bubbles.

# The origin of MPS

- Similar to SPH, MPS uses particle interaction models to predict the differential operators:
  - $\nabla$ (p)
  - $\nabla^2$(u), $\nabla^2$(v), $\nabla^2$(w). No derivative of kernel function is involved in MPS.
  - E.g.:

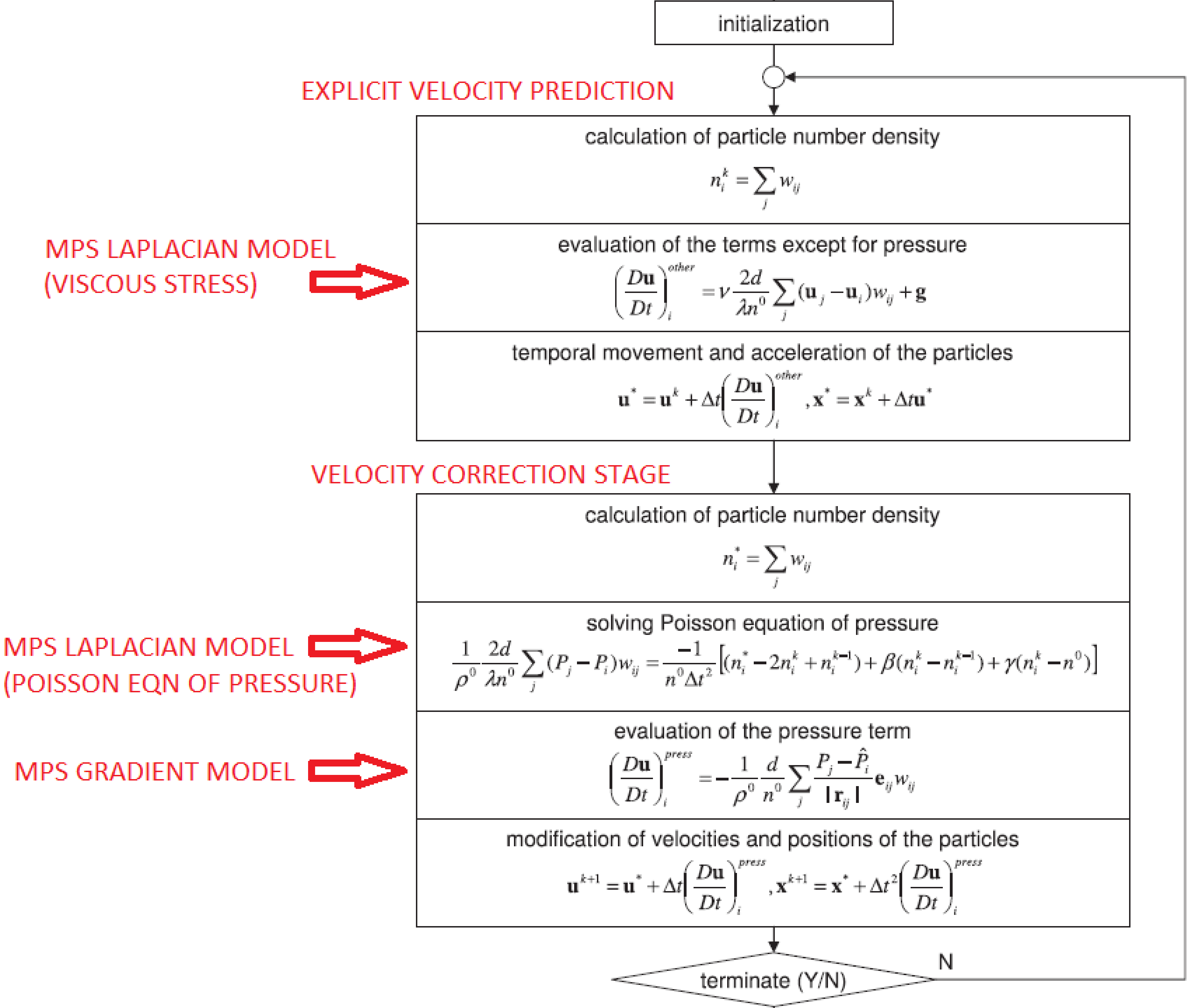
$$\left\langle \mu \nabla^2 (\vec{u}) \right\rangle_i^n = \frac{2d}{\sum_{j \neq i} w'_{ij}} \sum_{j \neq i} \mu_{ij} w'_{ij} \frac{(\vec{u}_j^n - \vec{u}_i^n)}{\left| \vec{r}_j^{\,n} - \vec{r}_i^{\,n} \right|^2}$$

$$w'_{ij} = \left| \vec{r}_j - \vec{r}_i \right|^N w\left( \left| \vec{r}_j - \vec{r}_i \right| \right)$$

# Basic MPS algorithm

Flow chart taken from

Kondo & Koshizuka (2011)



# Limitations of MPS 1: Source term of Pressure Poisson Equation

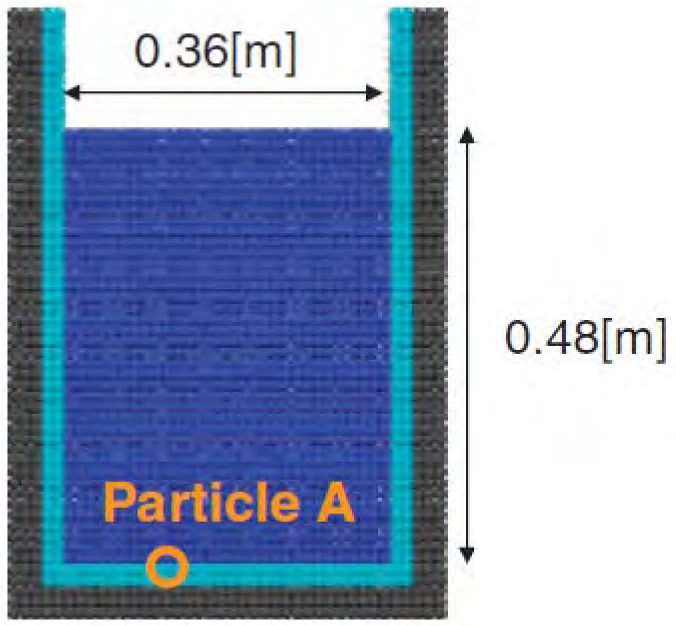
- In MPS, the initial particle density is represented by $n^0$, in which $n$ must be kept constant (incompressibility) when the solution progresses via solving the Poisson equation of pressure.

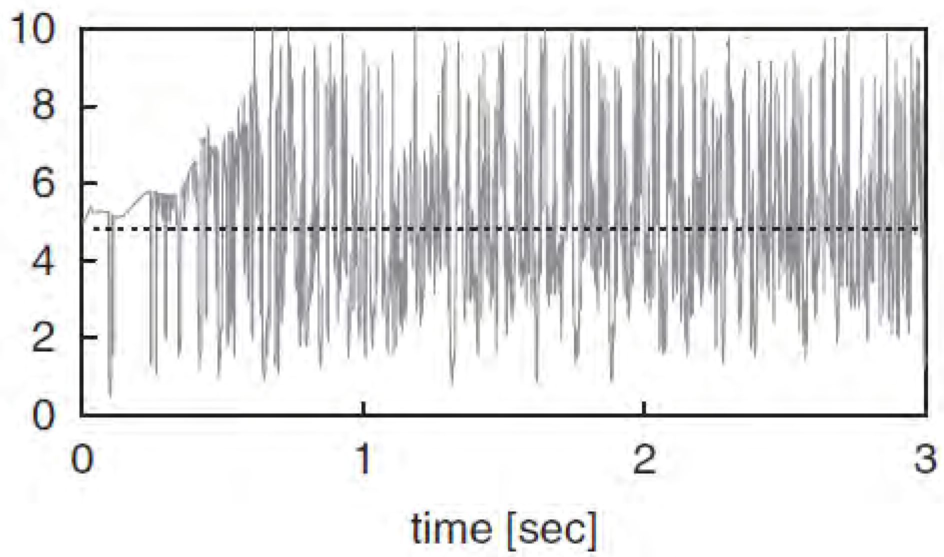
$$\langle \nabla^2 P^{n+1} \rangle_i = -\frac{\rho}{\Delta t^2} \frac{\langle n^* \rangle_i - n^0}{n^0}$$

- Problems:
  - The source term is wiggly across the flow field.
  - Spurious oscillations of pressure is commonly found although the volume of fluid particle can be preserved well $n^{n+1} \sim n^0$.

# Limitations of MPS 1: Source term of Pressure Poisson Equation

- Hydrostatic problem taken from Kondo and Koshizuka (2011)



# Limitations of MPS 1: Source term of Pressure Poisson Equation

- Proposals:
  - A hybrid source term is proposed by using the velocity divergence: (Tanaka and Masunaga 2010, Lee et al. 2011, Natsui et al. 2014)
  - The hybrid scheme is used to ensure the smoothness of pressure field while retaining the volume of each fluid particle.

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

  - However, parameter tuning of $\gamma$ must be performed.

# Limitations of MPS 2: Pressure gradient

- Tsuruta et al. (2013) claimed that the existing MPS schemes tend to over-predict the inter-particle attractive forces (causing clumping of particles)
- To solve this problem , an **artificial repulsive force** term is normally incorporated in the MPS pressure gradient model:
  - Minimum pressure model (widely used)

$$\langle \nabla p \rangle_i = \boxed{\frac{D_s}{n_0} \sum_{j \neq i} \frac{(p_j - p_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^2} (\boldsymbol{r}_j - \boldsymbol{r}_i) w(|\boldsymbol{r}_j - \boldsymbol{r}_i|)} + \boxed{\frac{D_s}{n_0} \sum_{j \neq i} \frac{(p_i - \hat{p}_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^2} (\boldsymbol{r}_j} \boxed{- \boldsymbol{r}_i) w(|\boldsymbol{r}_j - \boldsymbol{r}_i|)}$$

Actual MPS gradient model

# Limitations of MPS 2: Pressure gradient

- CMPS method (Khayyer and Gotoh 2008):

$$\langle \nabla p \rangle_i = \boxed{\frac{D_s}{n_0} \sum_{j \neq i} \frac{(p_j - p_i)}{|\mathbf{r}_j - \mathbf{r}_i|^2} (\mathbf{r}_j - \mathbf{r}_i) w(|\mathbf{r}_j - \mathbf{r}_i|)}$$

**Actual MPS gradient model**

$$\boxed{+ \frac{D_s}{n_0} \sum_{j \neq i} \frac{(p_i - \hat{p}_i) + (p_i - \hat{p}_j)}{|\mathbf{r}_j - \mathbf{r}_i|^2} (\mathbf{r}_j - \mathbf{r}_i) w(|\mathbf{r}_j - \mathbf{r}_i|)}$$

**Artificial repulsive force**

- It is important to note that artificial repulsive force term is not physical by nature.

# Limitations of MPS 3: Collision model

- At high Reynolds number (particularly free-surface flow), inter-penetration between particles occurs and it tends to de-stabilize the computation.
- In most of the MPS codes, a collision model (similar to X-SPH) is employed to modify the particle velocity (Shakibaeinia and Jin 2012; Natsui et al. 2014)

$$\boldsymbol{u}_i^* = \boldsymbol{u}_i - \frac{1}{\rho_{ij}} \sum_{j \in J} \left[ (1+\varepsilon) \frac{\rho_i \rho_j}{\rho_i + \rho_j} \boldsymbol{u}_{ij}^n \right]; \quad J = \{ j : r_{ij} < d_p \}$$

- Again, the velocity is subjected to tuning of parameter $\varepsilon$ and $d_p$.

# A proposal of particle method for incompressible flow

- A particle method should be free of rigorous tuning parameter.
- The pressure field should be smooth.
- The pressure gradient force should be in its original form and *involve no artificial treatments*.

# A proposal: Moving Particle Pressure Mesh (MPPM) method

- Firstly proposed by Hwang (2011).
- His ideas:
  - The moving particle strategy (Lagrangian particles) in MPS should be retained -- > numerical issues due to convective discretization.
  - Dissociation of PRESSURE variable from moving particles → treated as Eulerian variable instead.
    - Coz. no explicit evolution equation for PRESSURE for incompressible moving particles.
    - The mesh used for neighbouring-searching can be equally deployed for storing pressure.
  - Moving particles are merely acting as interpolating points to realize the related operators in the Poisson equation.

# MPPM approach

- Step 1: Evolution of moving particles to obtain the intermediate particle velocities

$$\vec{\boldsymbol{u}}_p^* = \vec{\boldsymbol{u}}_p^n + \Delta t\, \nu \nabla^2 \vec{\boldsymbol{u}}_p^n$$

$$\vec{\boldsymbol{r}}_p^* = \vec{\boldsymbol{r}}_p^n + \Delta t\, \vec{\boldsymbol{u}}_p^*$$

# MPPM approach

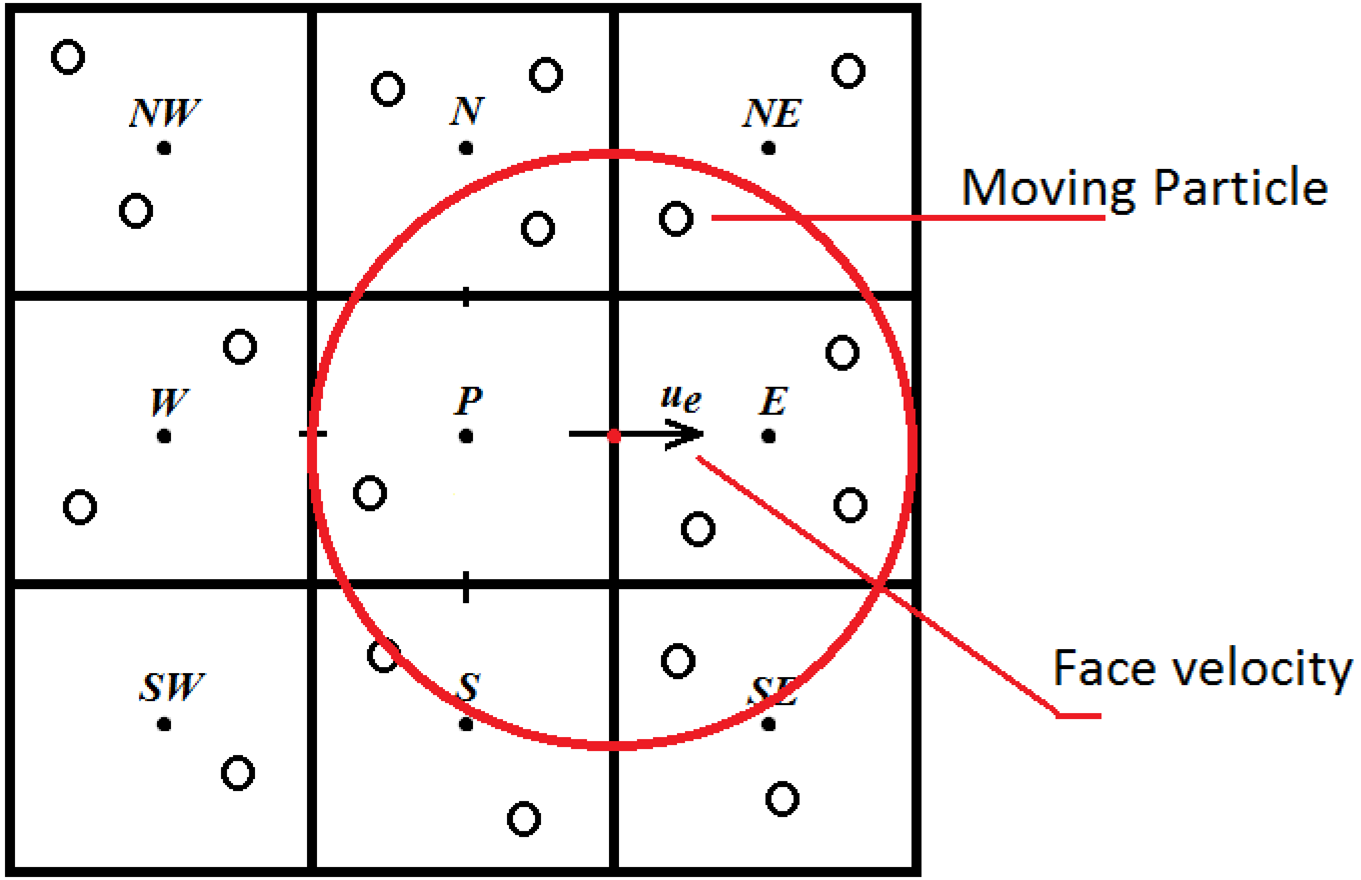
- Step 2: Form the Poisson equation of pressure on Eulerian pressure mesh

$$\boxed{2\left(\frac{\Delta x}{\Delta y}+\frac{\Delta y}{\Delta x}\right)} p_P^{n+1} = \boxed{\frac{\Delta y}{\Delta x}} p_E^{n+1} + \boxed{\frac{\Delta y}{\Delta x}} p_N^{n+1} + \boxed{\frac{\Delta x}{\Delta y}} p_W^{n+1} + \boxed{\frac{\Delta x}{\Delta y}} p_S^{n+1} - \frac{\rho}{\Delta t}\left[\left(u_e^* - u_w^*\right)\Delta y + \left(v_n^* - v_s^*\right)\Delta x\right]$$

  - For single phase flow, the coefficients in the PPE are fixed → computationally cheaper than the original MPS.

# MPPM approach

- Face velocities can be interpolated from the neighbouring moving particles using Shepard's method or Moving Least-Square (MLS) techniques.

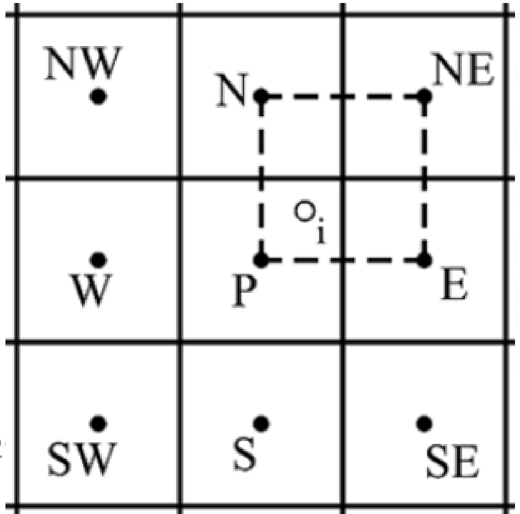


# MPPM approach

- Step 3: From the new pressure field, correct the particle velocities and positions.

$$\vec{u}_p^{n+1} = \vec{u}_p^{*} - \Delta t \frac{\nabla p_p^{n+1}}{\rho} \qquad \vec{r}_p^{n+1} = \vec{r}_p^{n} + \Delta t \vec{u}_p^{n+1}$$

  - The pressure gradient force acting on moving particles is determined via the simple shape function:

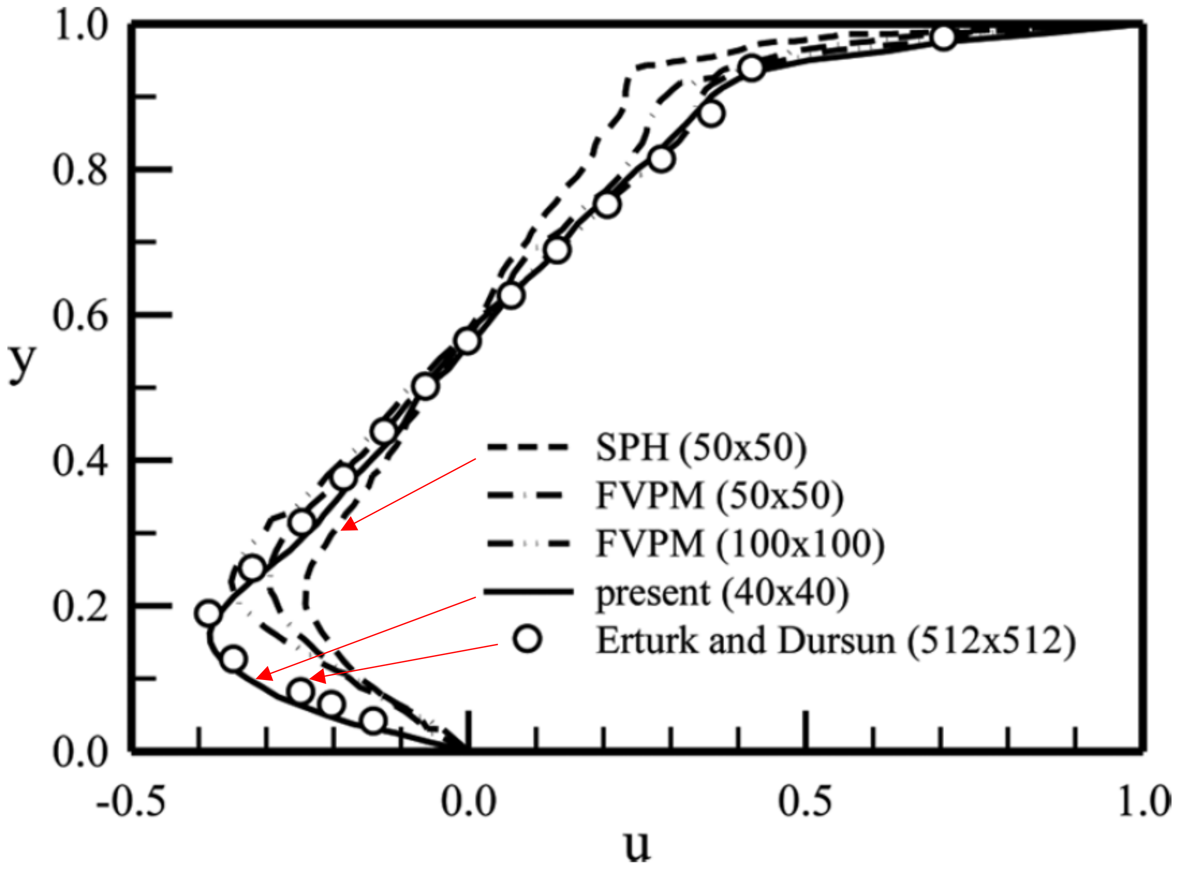



$$\left(\frac{\partial p}{\partial x}\right)_p = \frac{\partial p}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial p}{\partial \eta}\frac{\partial \eta}{\partial x} = \frac{p_E - p_P}{\Delta x}\left(1 - \frac{y_p - y_P}{\Delta y}\right) + \frac{p_{NE} - p_N}{\Delta x}\frac{y_p - y_P}{\Delta y}$$

$$\left(\frac{\partial p}{\partial y}\right)_p = \frac{\partial p}{\partial \xi}\frac{\partial \xi}{\partial y} + \frac{\partial p}{\partial \eta}\frac{\partial \eta}{\partial y} = \frac{p_N - p_P}{\Delta y}\left(1 - \frac{x_p - x_P}{\Delta x}\right) + \frac{p_{NE} - p_E}{\Delta y}\frac{x_p - x_P}{\Delta x}$$

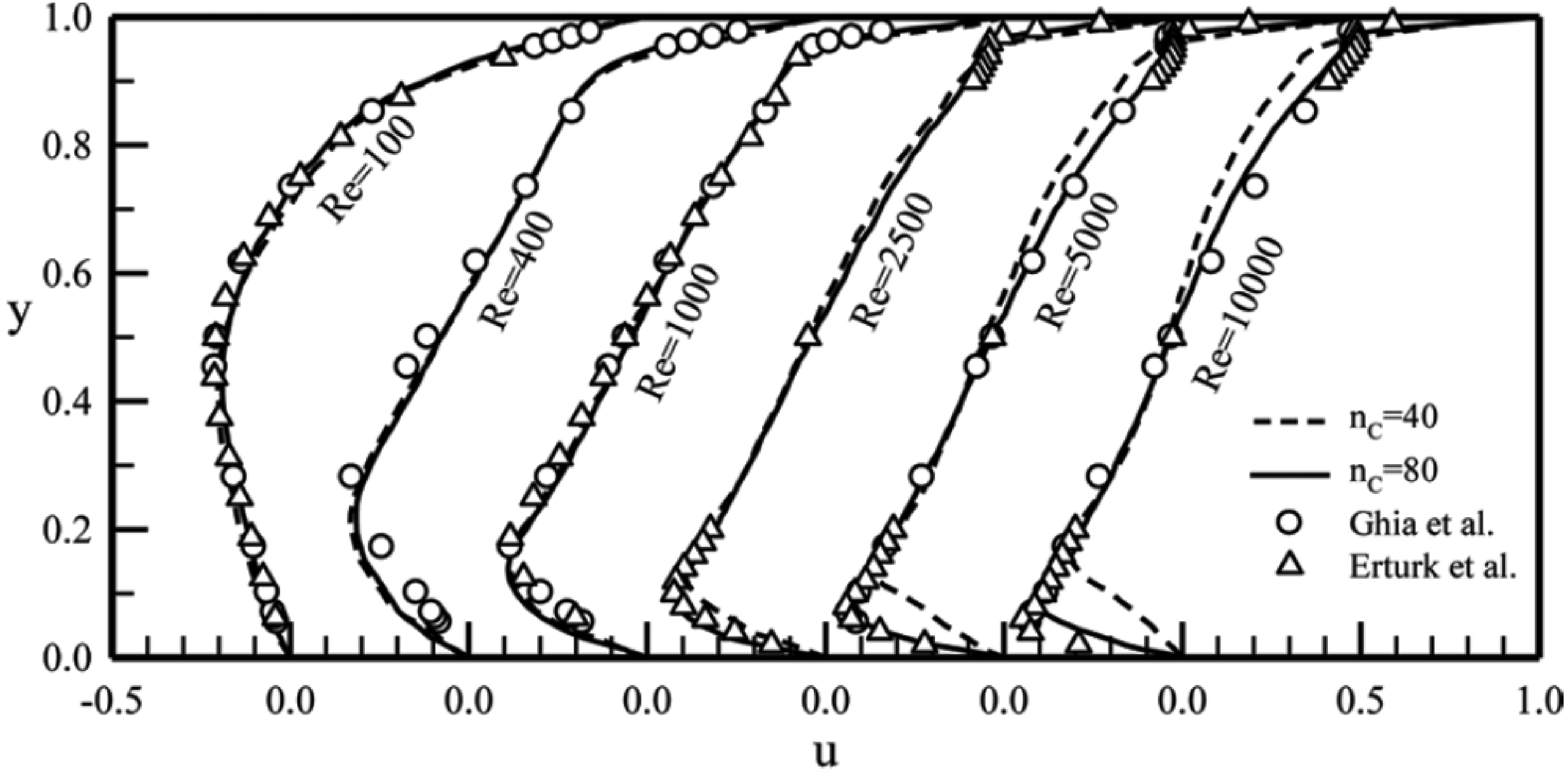
# MPPM results (single phase)

- Lid-driven flow (Re = 1000)- Taken from Hwang (2011)



# MPPM results (single phase)

- Lid-driven flow at various Re and mesh spacing - Taken from Hwang (2011)

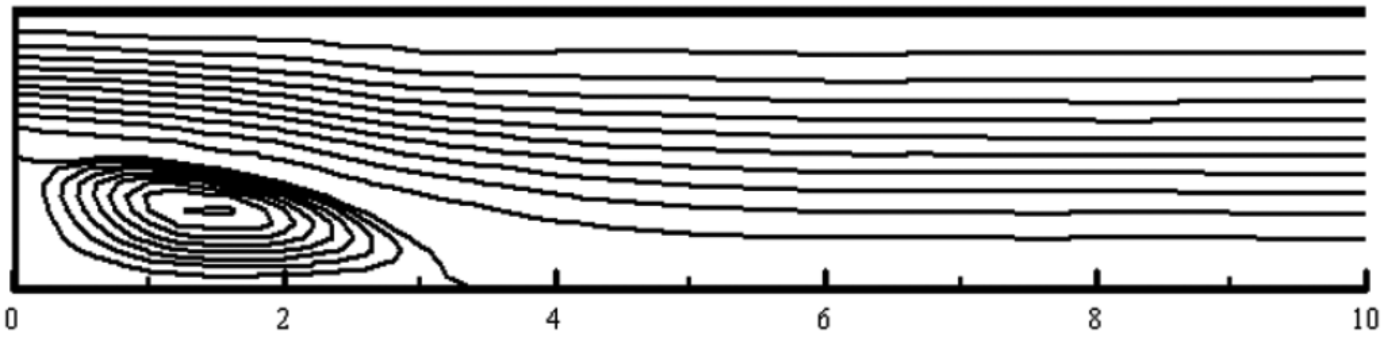


# MPPM results (single phase)

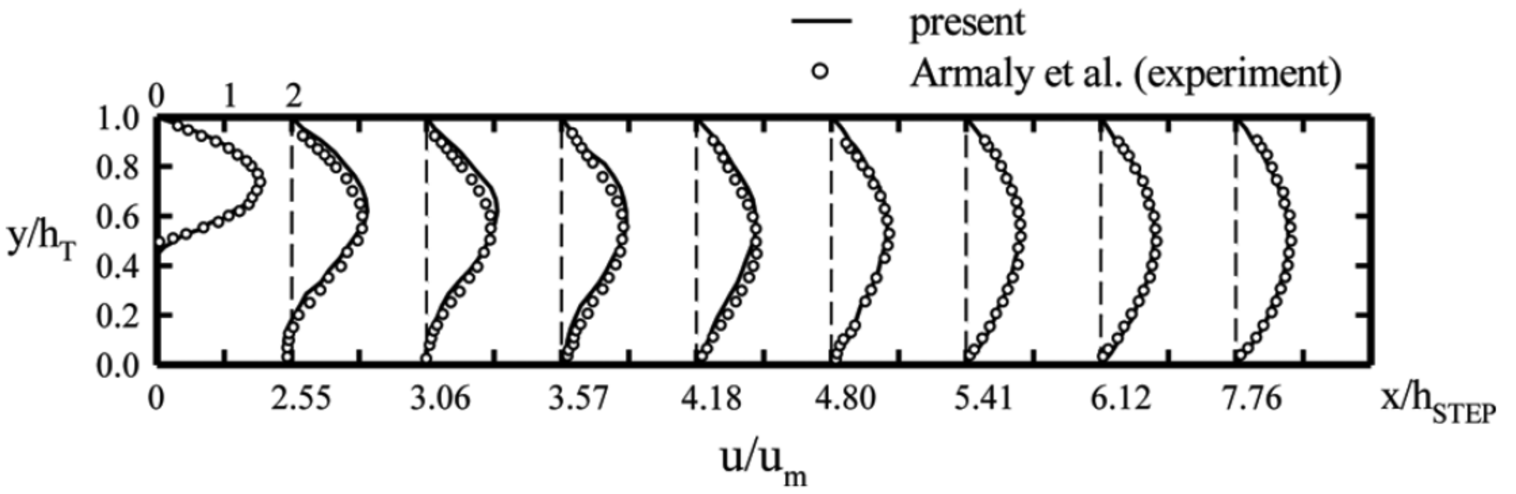
- Backward facing step

  (Re = 100)

- Taken from Hwang (2011)



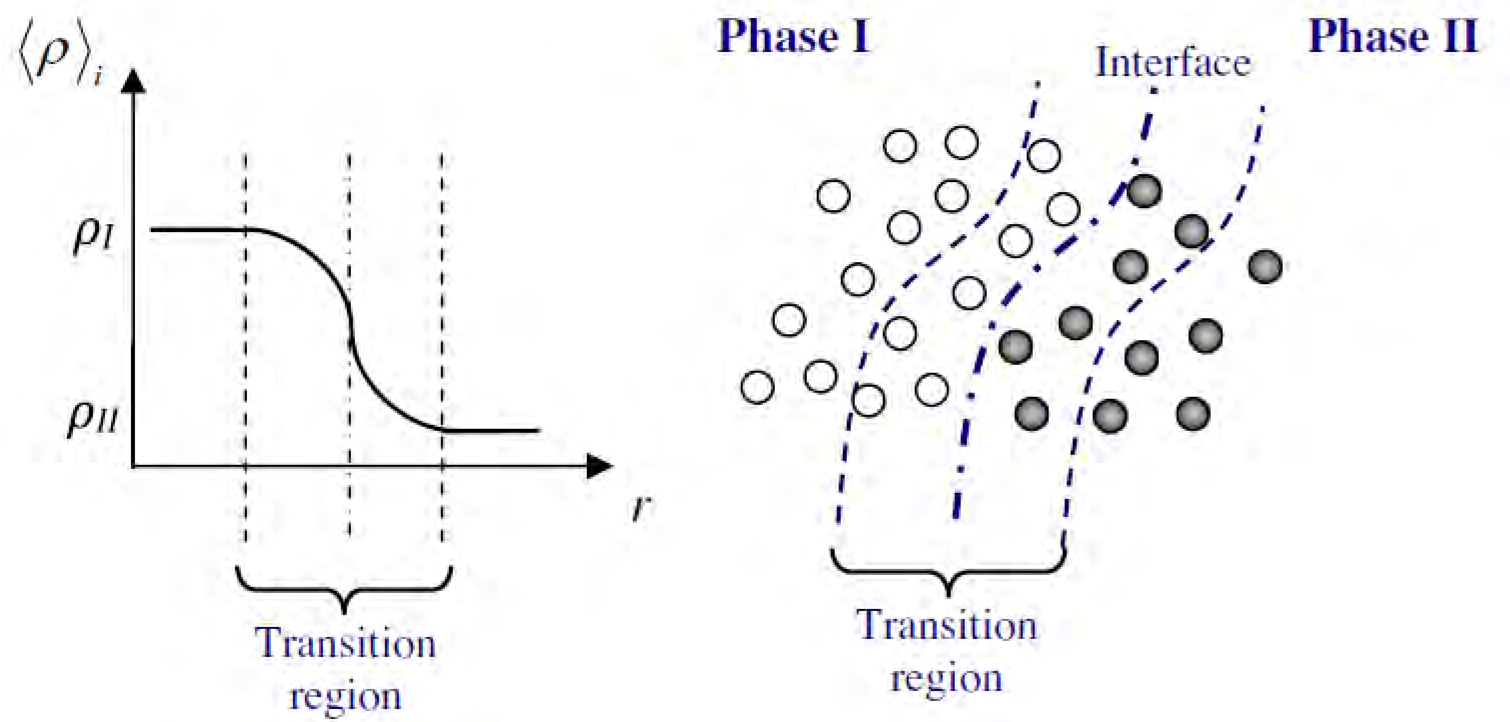

(d)



# Extension to Multiphase Flow

# Extension of MPPM to handle multiphase flows

- The success of multiphase flow in particle method → a proper interfacial density interpolation scheme for interfacial fluid particle.




Pictures taken from Shakibaeinia and Jin (2012)

# Extension of MPPM to handle multiphase flows

- Some commonly used density interpolation scheme employ simple averaging (Khayyer and Gotoh 2013):
  - **Shepard interpolation****:

$$\rho_i = \frac{1}{\sum_{j \in I} W_{ij}} \sum_{j \in I} \rho_j W_{ij}$$

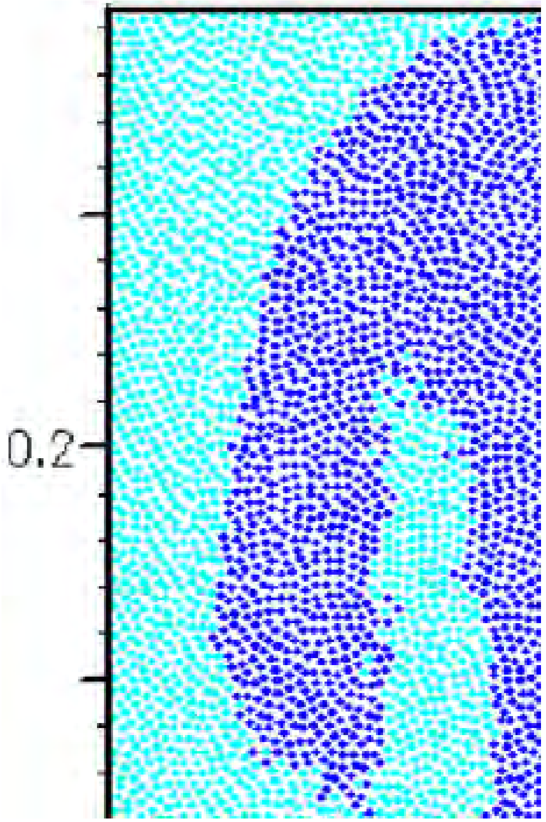
  - Taylor series

$$\rho_i = \frac{1}{\sum_{j \in I} W_{ij}} \sum_{j \in I} \left( \rho_j - \frac{\partial \rho_i}{\partial x_{ij}} x_{ij} - \frac{\partial \rho_i}{\partial y_{ij}} y_{ij} \right) W_{ij}$$

**** We never succeed in simulating fluid with density ratio > 10.**

# Extension of MPPM to handle multiphase flows

- Intrusion of particles into different fluid region:
  - Degrade the accuracy of the interfacial density calculation.
- E.g.: RTI case (density ratio 1:3)
  - Taken from Shakibaeinia and Jin (2012)



# Extension of MPPM to handle multiphase flows – A Proposal

- To secure a smooth fluid interface, we propose to determine the interfacial particle fluid density via a level-set function :
  - Good accuracy on surface normal/curvature calculation.
- Again, the level-set function is solved in the background pressure mesh.
- We employ the conservative level-set method by Olsson and Greiss (2005) for good mass conservation.

# CLS-MPPM Method

From the divergence-free velocity field obtained from MPPM,

- Step 1: Advance the level set function in time via a 3rd order TVD-RK method (Jiang and Peng 2000). Spatial terms are approximated by an upwind scheme with SuperBee limiter.

$$\frac{\partial \phi}{\partial t} = L(\phi) \quad Where,\ L(\phi) = -\nabla \cdot (\phi \vec{u})$$

$$\phi^1 = \phi^n + \Delta t L(\phi^n)$$

$$\phi^2 = \phi^1 + \frac{\Delta t}{4}\left(-3L(\phi^n) + L(\phi^1)\right)$$

$$\phi^{n+1} = \phi^2 + \frac{\Delta t}{12}\left(-L(\phi^n) - L(\phi^1) + 8L(\phi^2)\right)$$

# CLS-MPPM Method

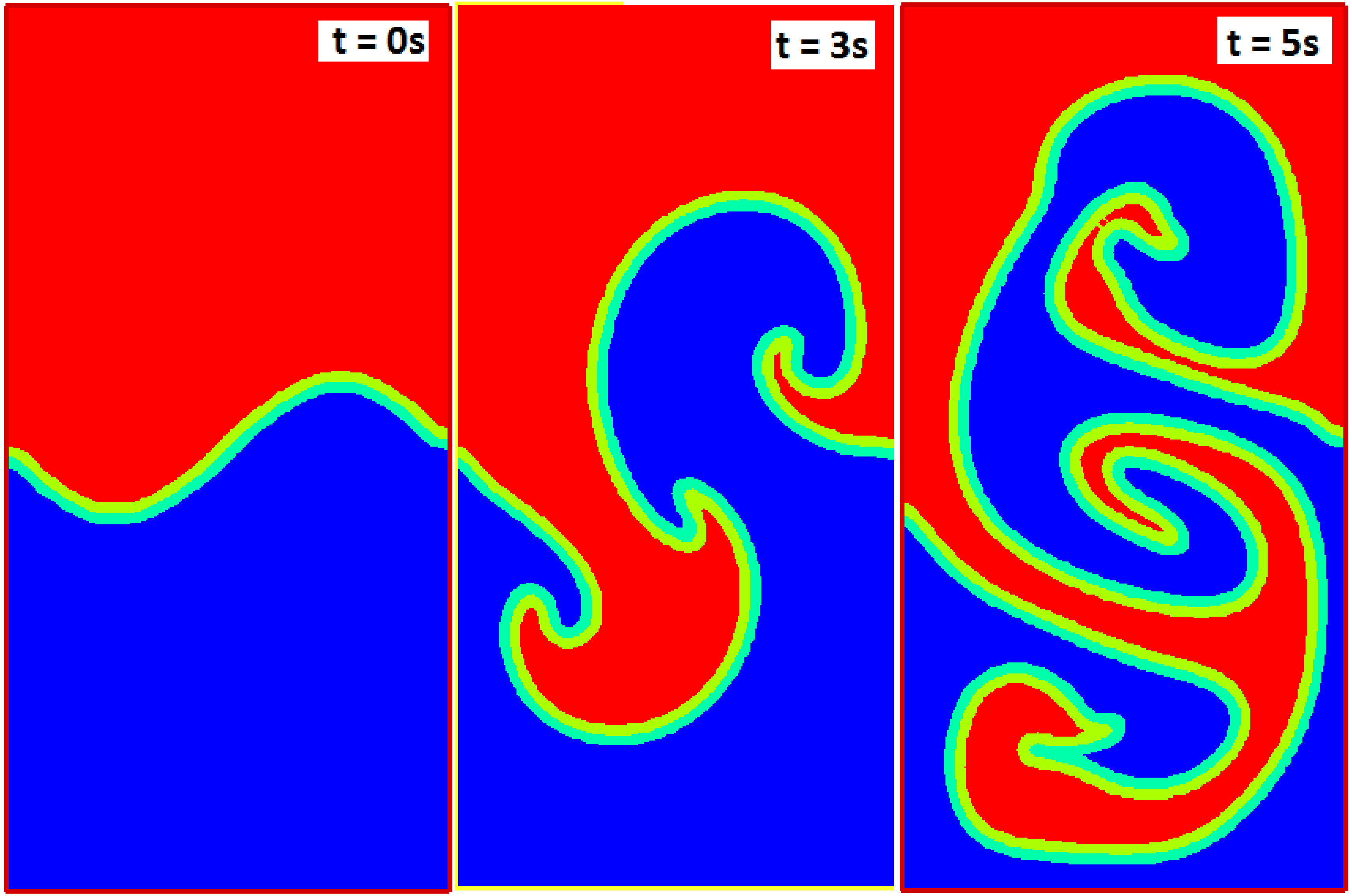
- Step 2: Reinitialize the MESH level-set function using the artificial compression.

$$\Phi_\tau + \nabla \cdot (\Phi(1-\Phi)\underline{n}) = \bar{\mu}\nabla \cdot (\nabla \Phi).$$

  - $\mu$ to control the thickness of interface (~3 cell width if $\mu$ = h/2)
  - Ensure uniform interface thickness as time progresses.
    - Accurate interfacial particle density.

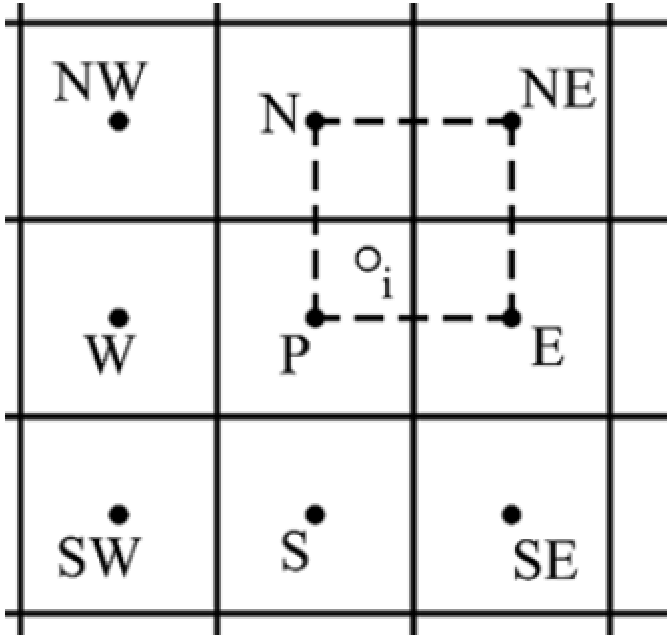
# Outcome of Level-Set reinitialization

- RTI problem
  - Density ratio 1:1.8
  - Contour lines of Level-Set = 0.05, 0.5, 0.95 are plotted on background mesh



# CLS-MPPM Method

- Step 3: Interpolate the PARTICLE level-set from the MESH level-set using bi-linear interpolation.




$$\Phi_i = \Phi_P(1-\xi)(1-\eta) + \Phi_E \xi(1-\eta) + \Phi_N(1-\xi)\eta + \Phi_{NE}\xi\eta$$

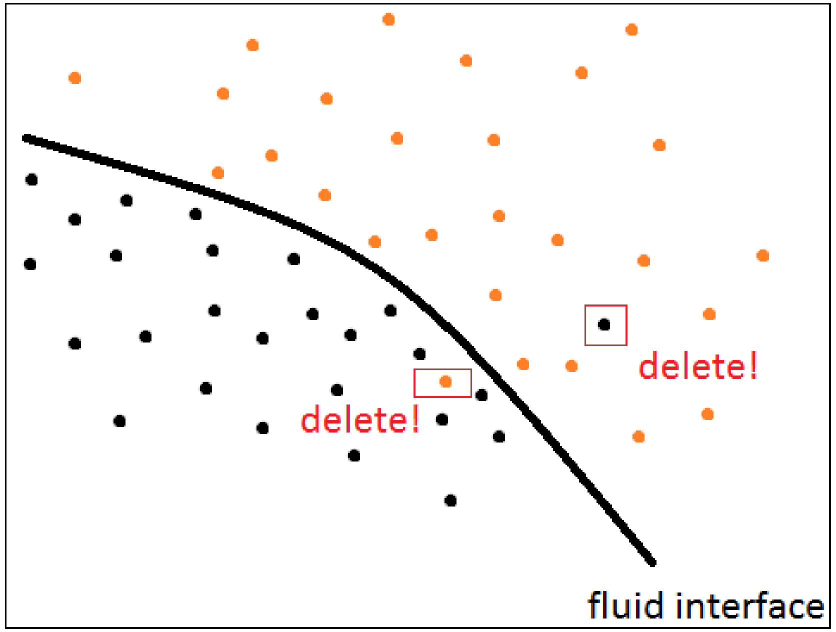
$$\xi = (x - x_P)/\Delta x$$

$$\eta = (y - y_P)/\Delta y$$

$$(\rho)_i = \rho_1 + (\rho_2 - \rho_1)\cdot \Phi_i$$

# CLS-MPPM Method

- In MPPM, moving particles are merely deployed for velocity interpolation purpose, they can be simply deleted if they reside in the wrong regime.



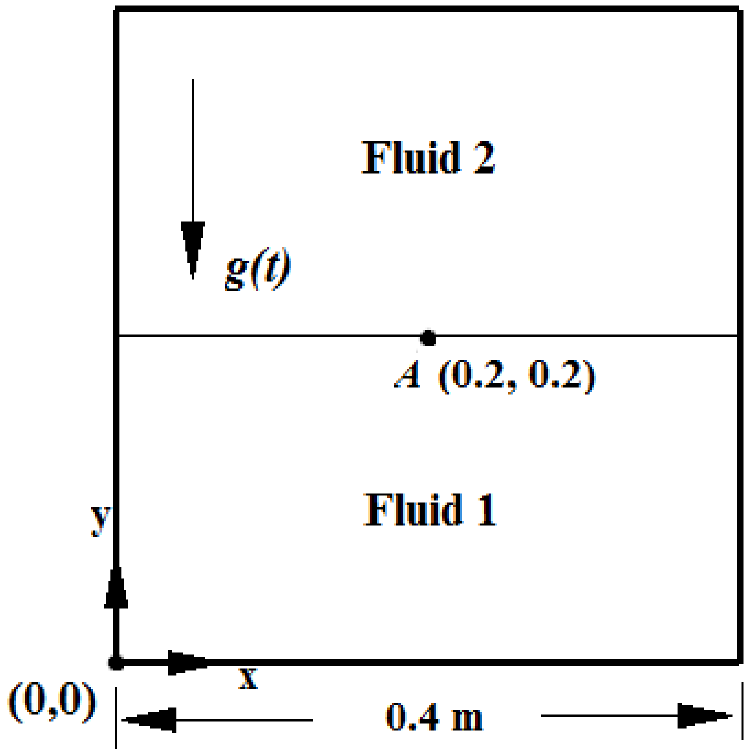

- Thus, the smoothness of the fluid interface can be retained via the smooth level set function.

# Test Cases

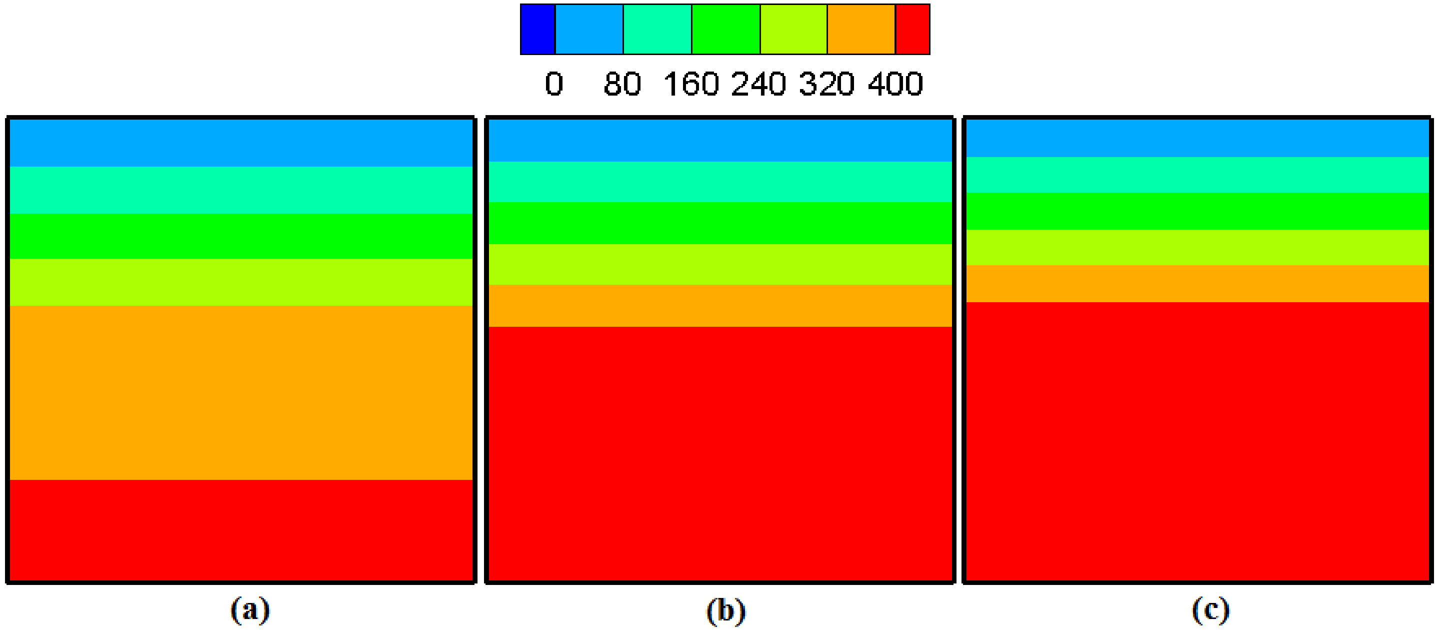
# Multiphase Flow using CLS-MPPM(1)

- Hydrostatic problem subjected to varying gravitational field
  - $\rho_1$ = 1.0 kg/m$^3$
  - $\rho_2$ = 50.0 kg/m$^3$

$$g(t) = 10 + 10\cos\left(200\pi t\right)\exp(5\pi t)$$

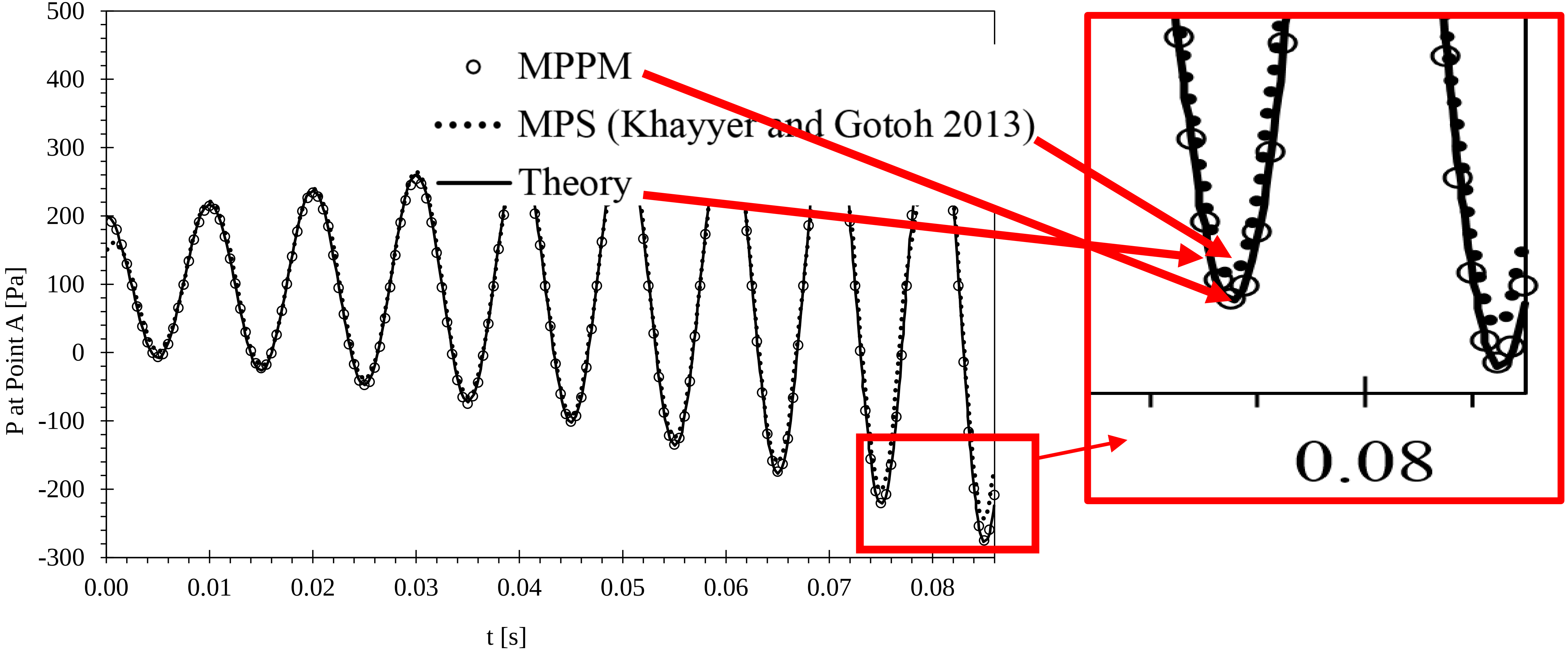


# Hydrostatic – varying gravity




Pressure field at $t$ = (a) 0.07s; (b) 0.08s and (c) 0.09s for a static multi-fluid problem subjected to external acceleration.

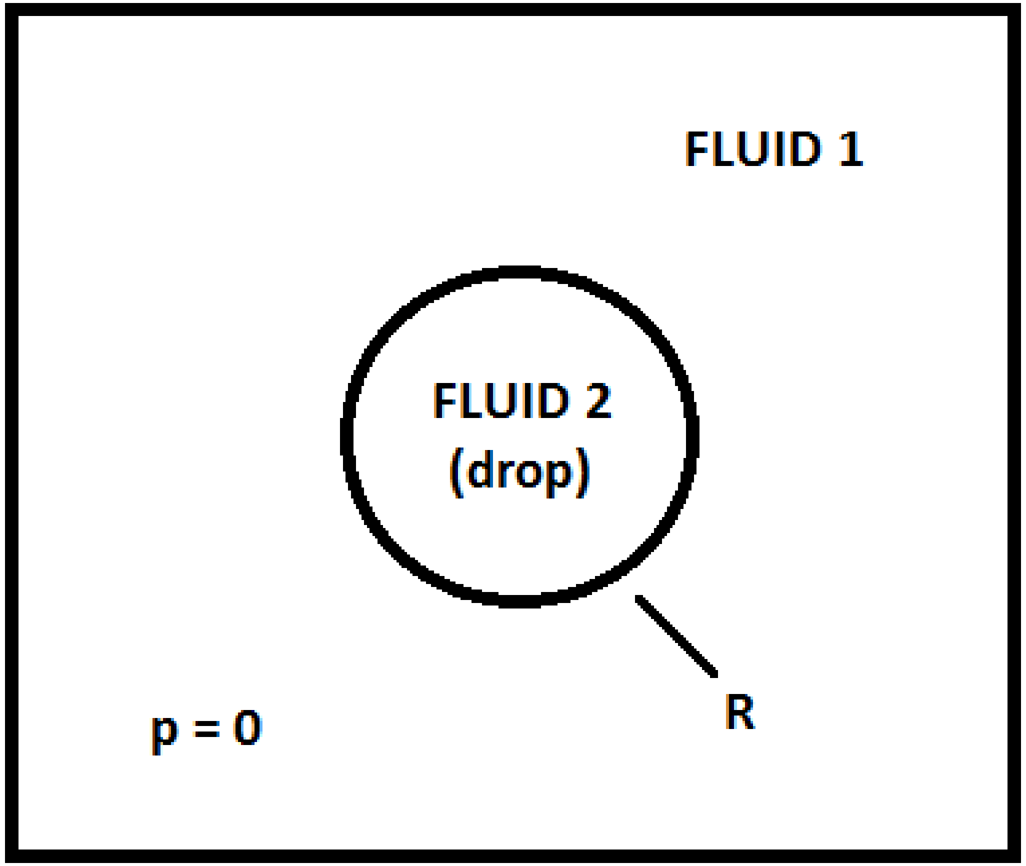
# Hydrostatic – varying gravity

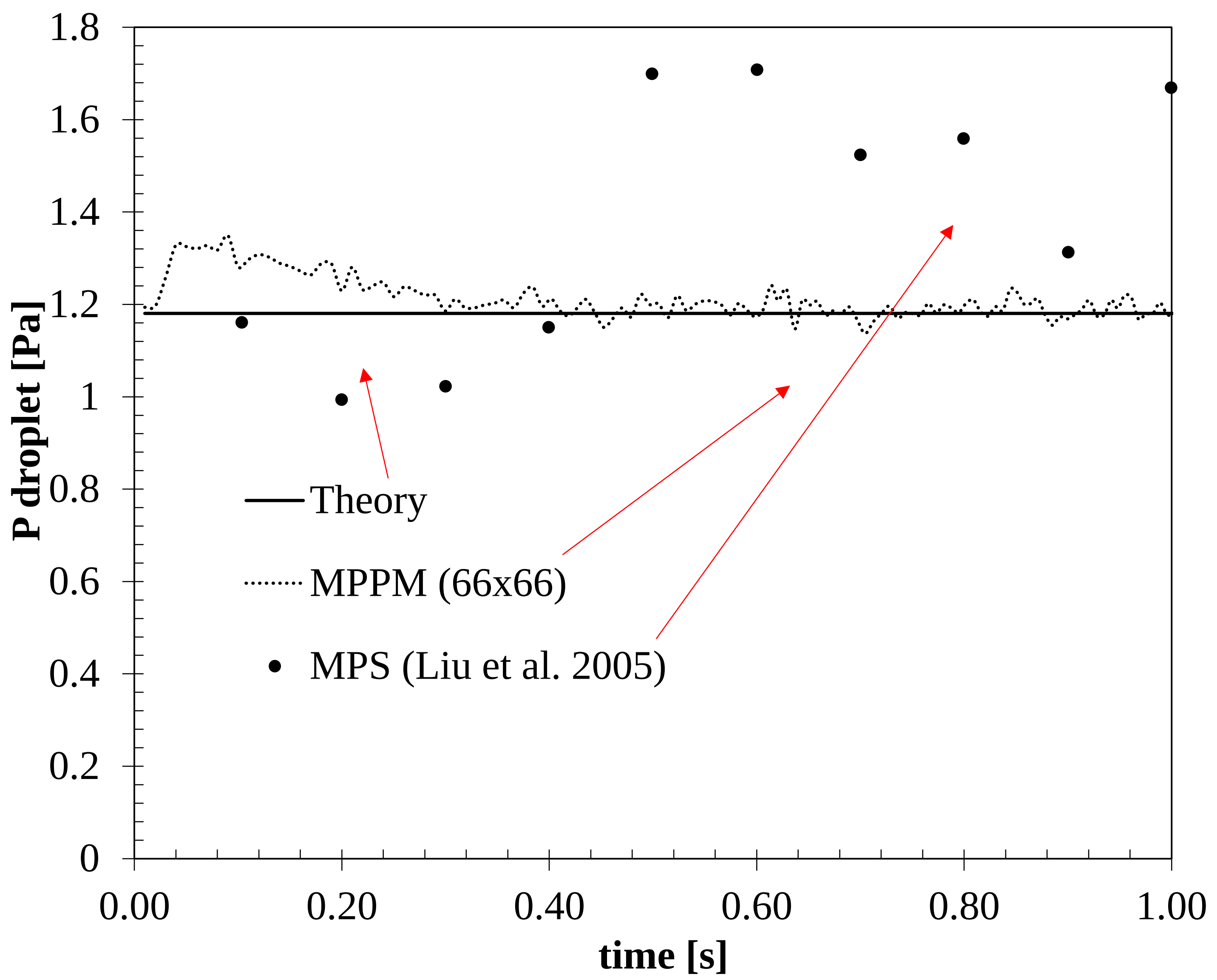


# Multiphase Flow using CLS-MPPM(2)

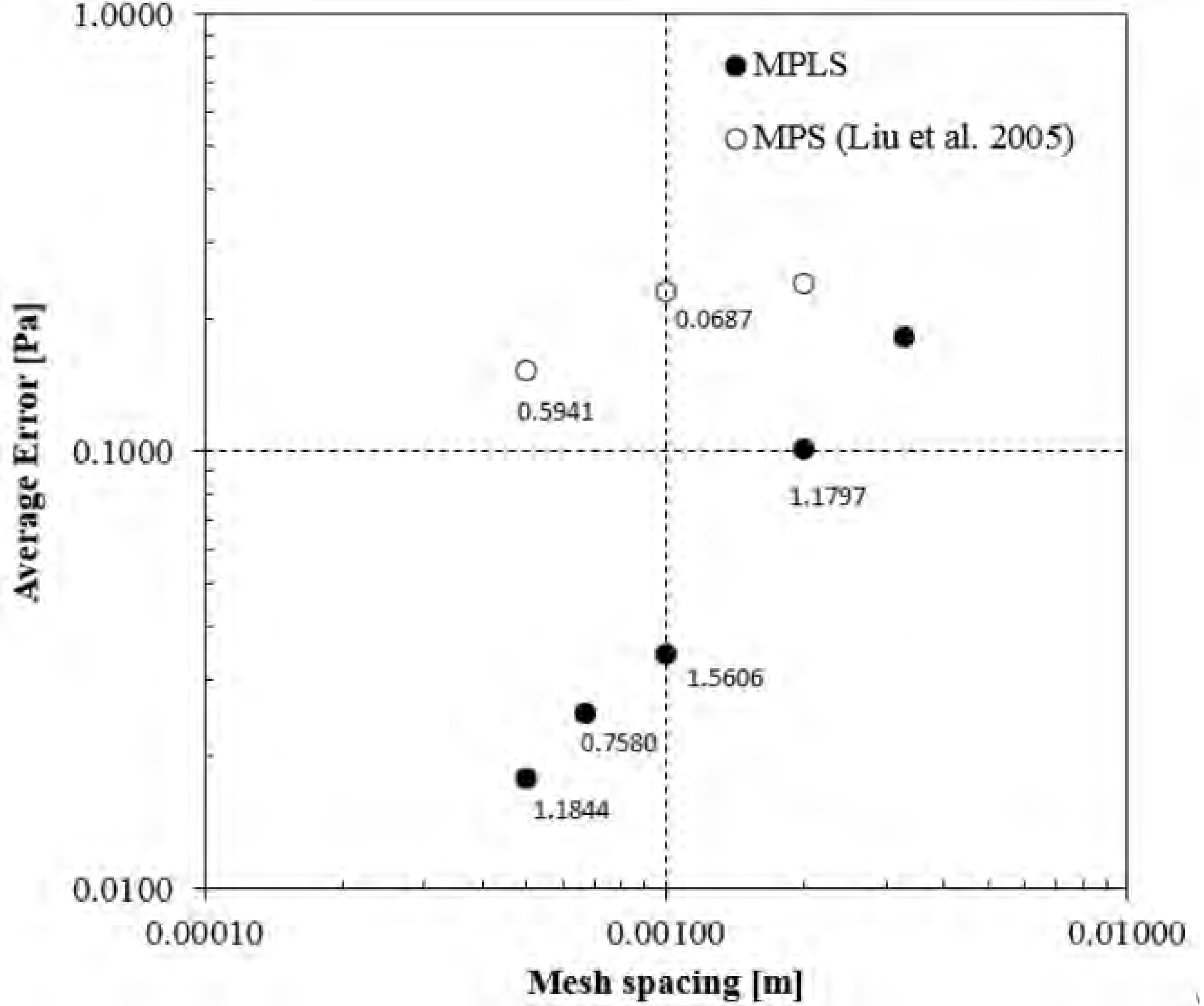
- Equilibrium Bubble
  - $\rho_1$ = 500.0 kg/m$^3$
  - $\rho_2$ = 1000.0 kg/m$^3$
  - σ = 0.02361 N/m
  - R = 0.02m
  - g = 0 m/s$^2$, inviscid.

$$p_{\mathrm{drop}} = \sigma\kappa = \sigma / R$$




1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
P droplet [Pa]
0.00
0.20
0.40
0.60
0.80
1.00
time [s]
Theory
MPPM (66x66)
MPS (Liu et al. 2005)

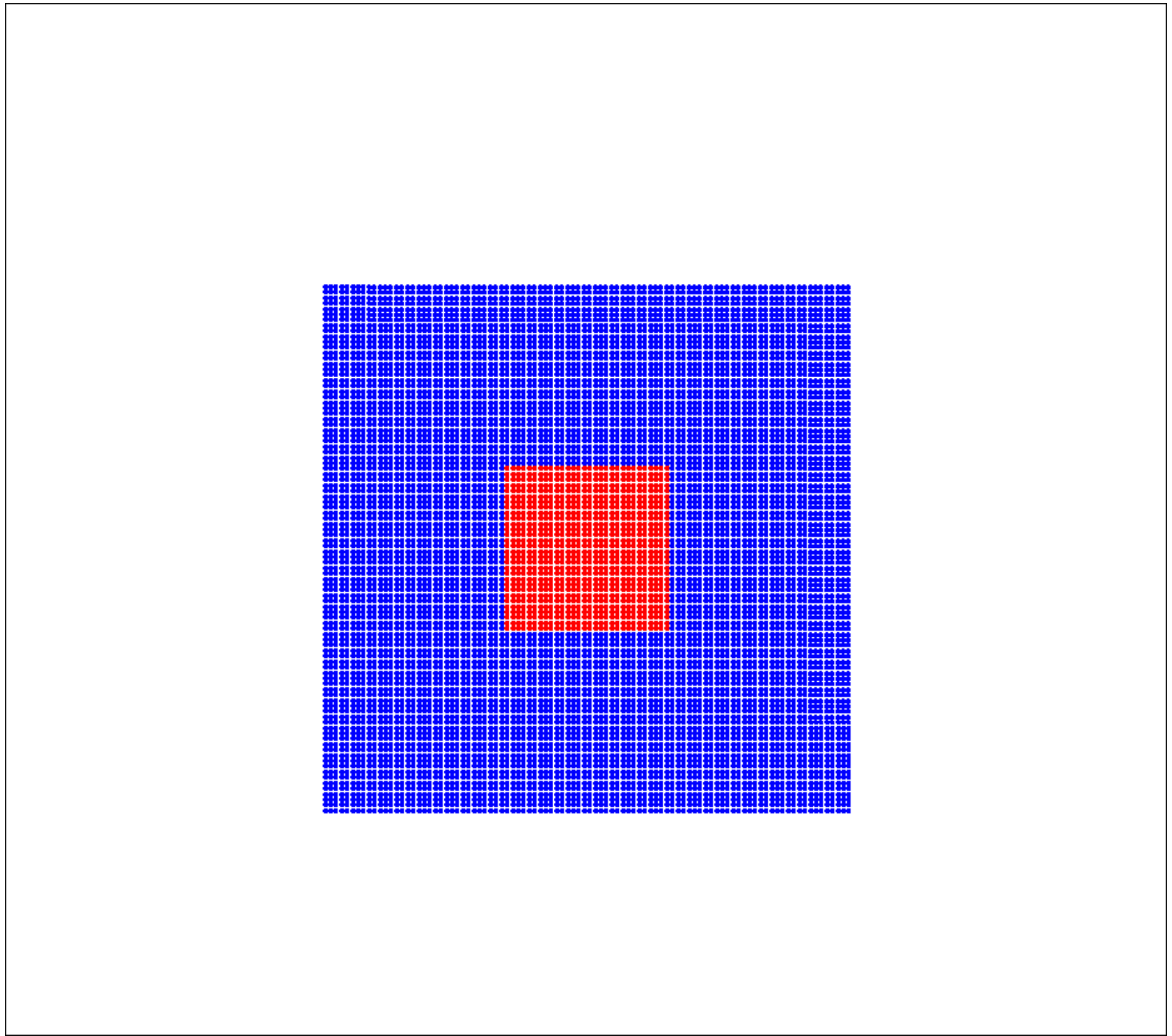
# Grid convergence test



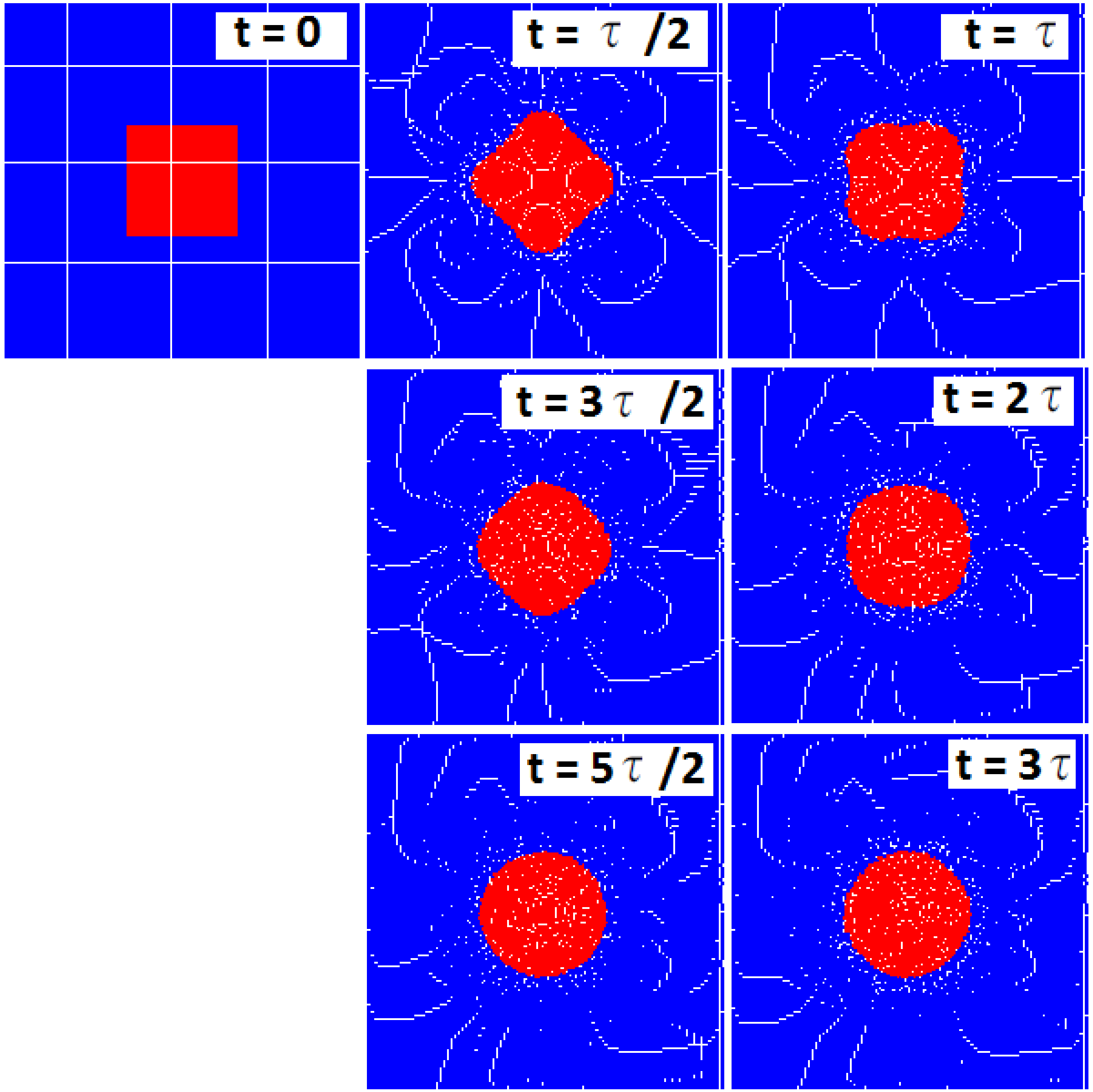
# Multiphase Flow using CLS-MPPM(3)

- Oscillating Bubble
  - Droplet
    - fluid: Ethanol (surrounded by blue Particles with small dens and visc.)
    - side length = 7.5cm (n=4 sides)
  - $\sigma$ = 0.02361 N/m
  - g = 0 m/s$^2$
- Theoretical period of oscillation:

$$\omega_n^2 = \frac{(n^3 - n)\sigma}{(\rho_d + \rho_e)R_0^3}, \qquad \tau = 2\pi/\omega_n = 1.299 \text{ s}$$



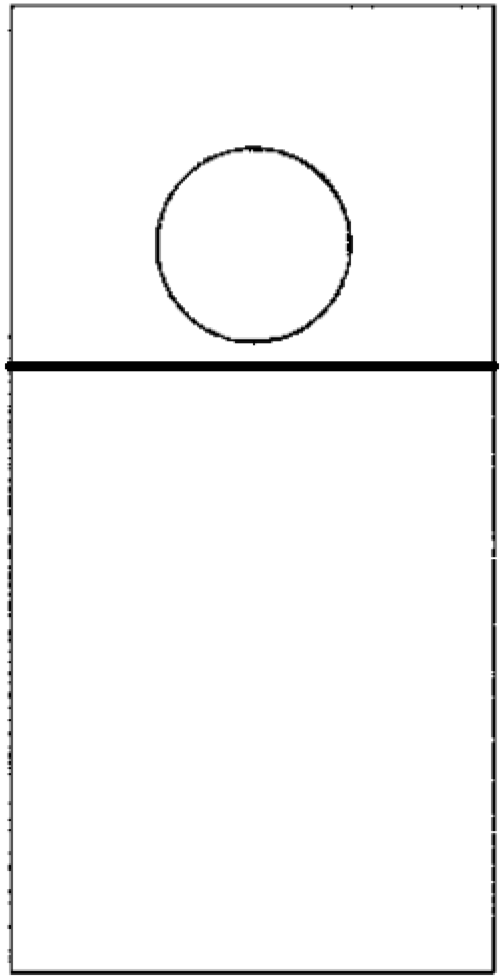
- Change of fluid interface

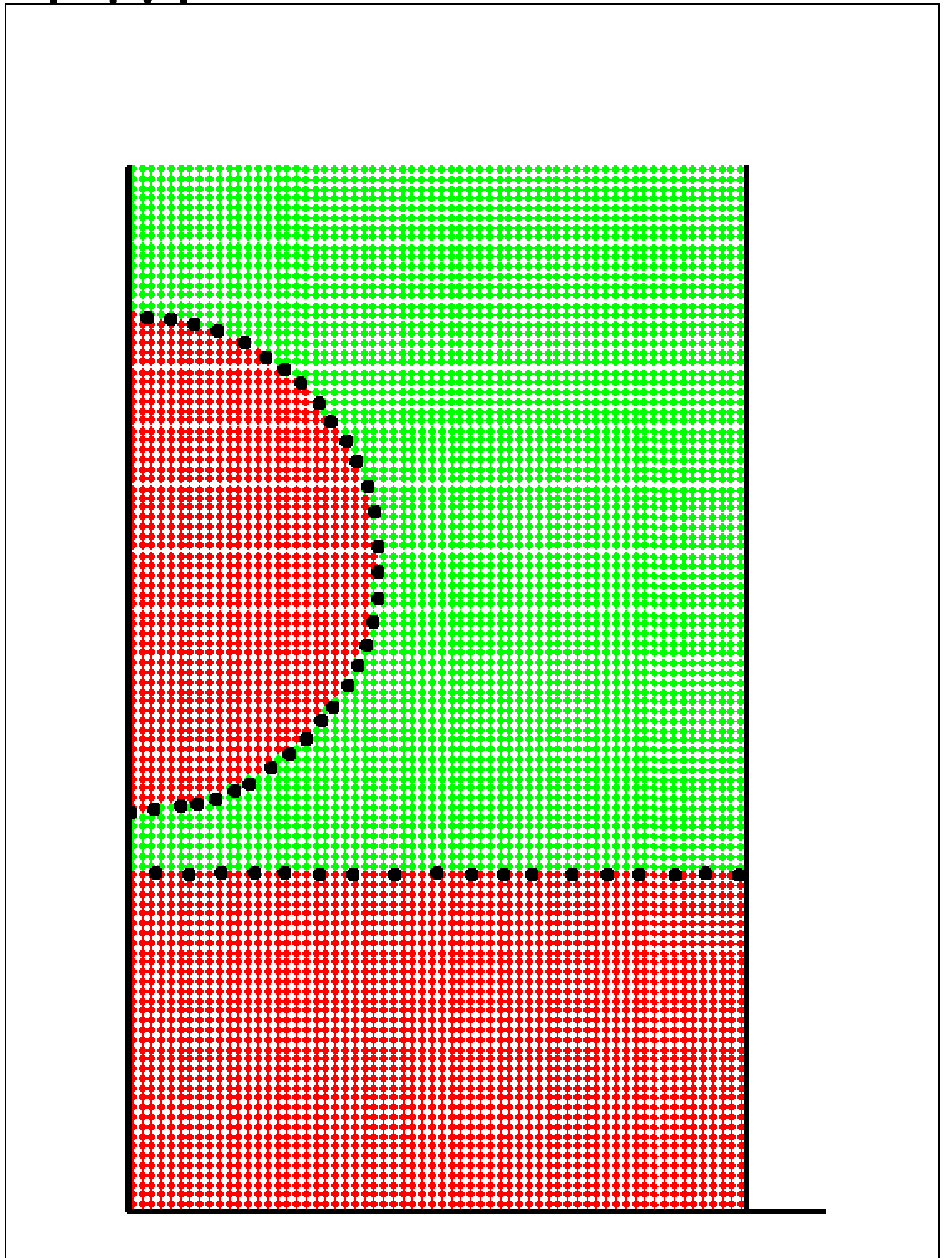


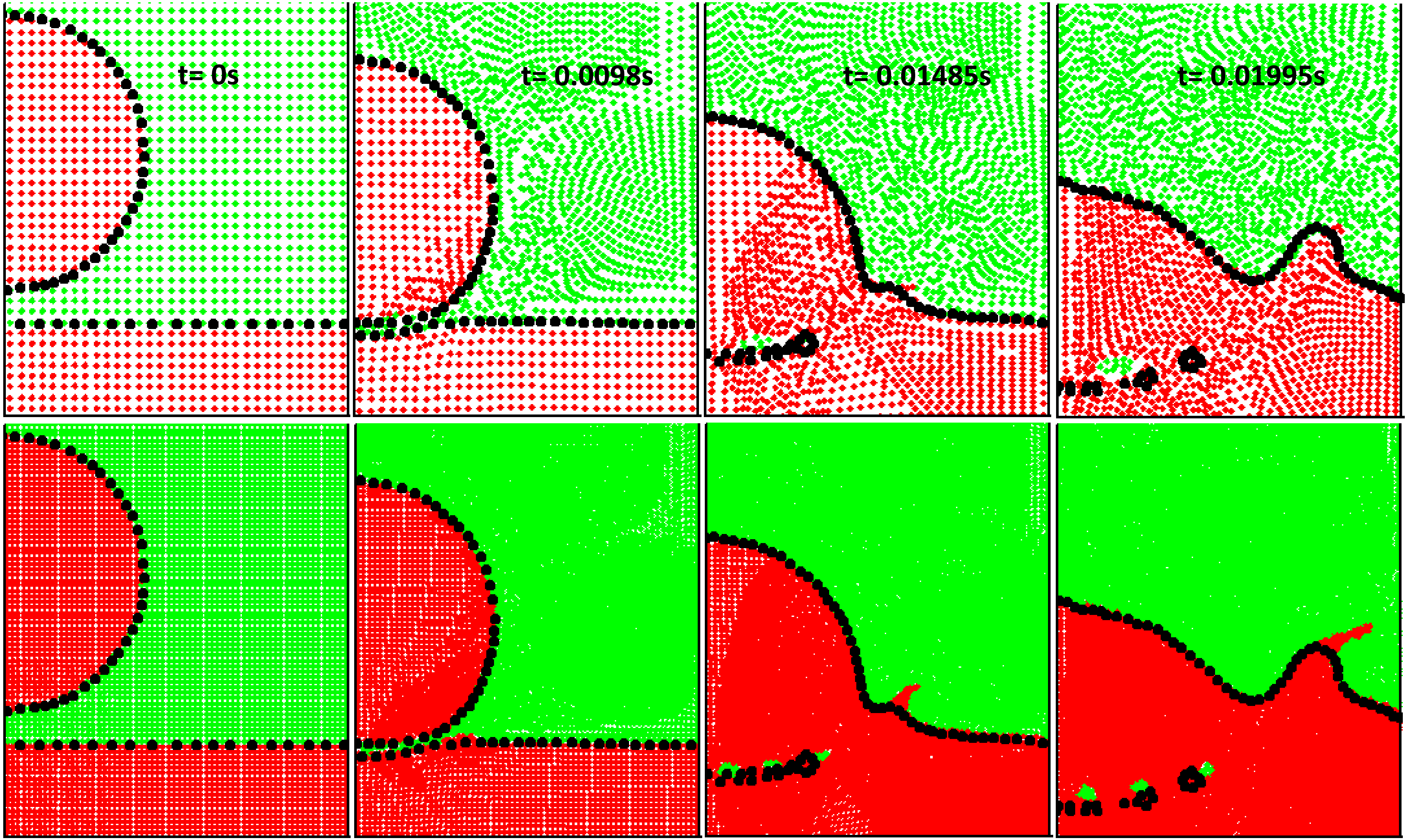
# Multiphase Flow using CLS-MPPM (4)

- Droplet Splash
  - $\rho_{water}$ = 999.2kg/m$^3$
  - $\rho_{air}$ = 1.225kg/m$^3$
  - $\mu_{water}$ = 1.1377 x 10$^{-3}$ Pa.s
  - $\mu_{air}$ = 1.77625 x 10$^{-5}$ Pa.s

- Symmetric BC is imposed.
- Domain: 3.5mm x 14mm



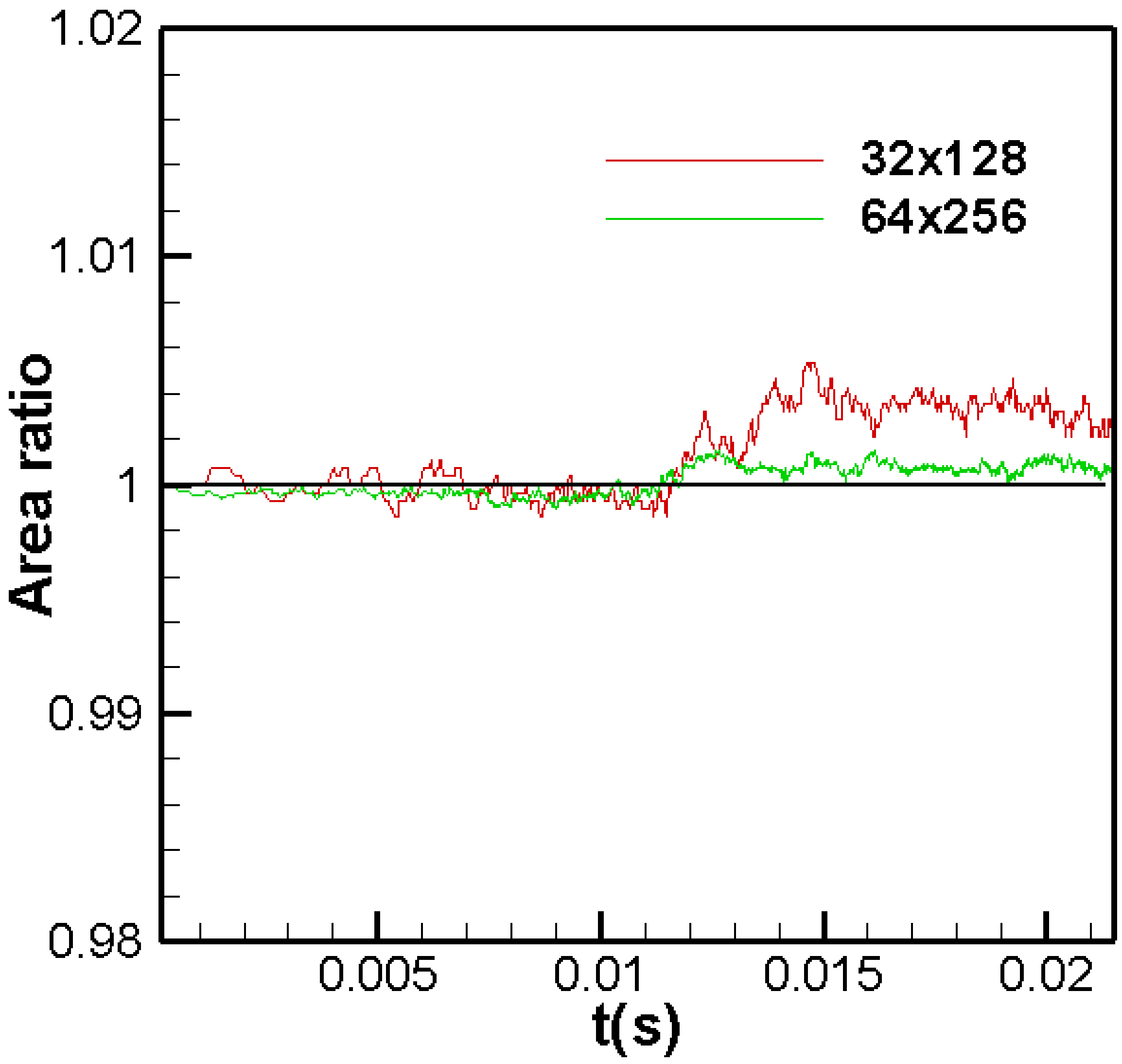







Interfaces predicted by 32x128 (upper) and 64x256 (lower) pressure mesh. • : VOF solutions from Puckett et al. (1999) on 32x128 grid

# Droplet Splash (Mass conservation)

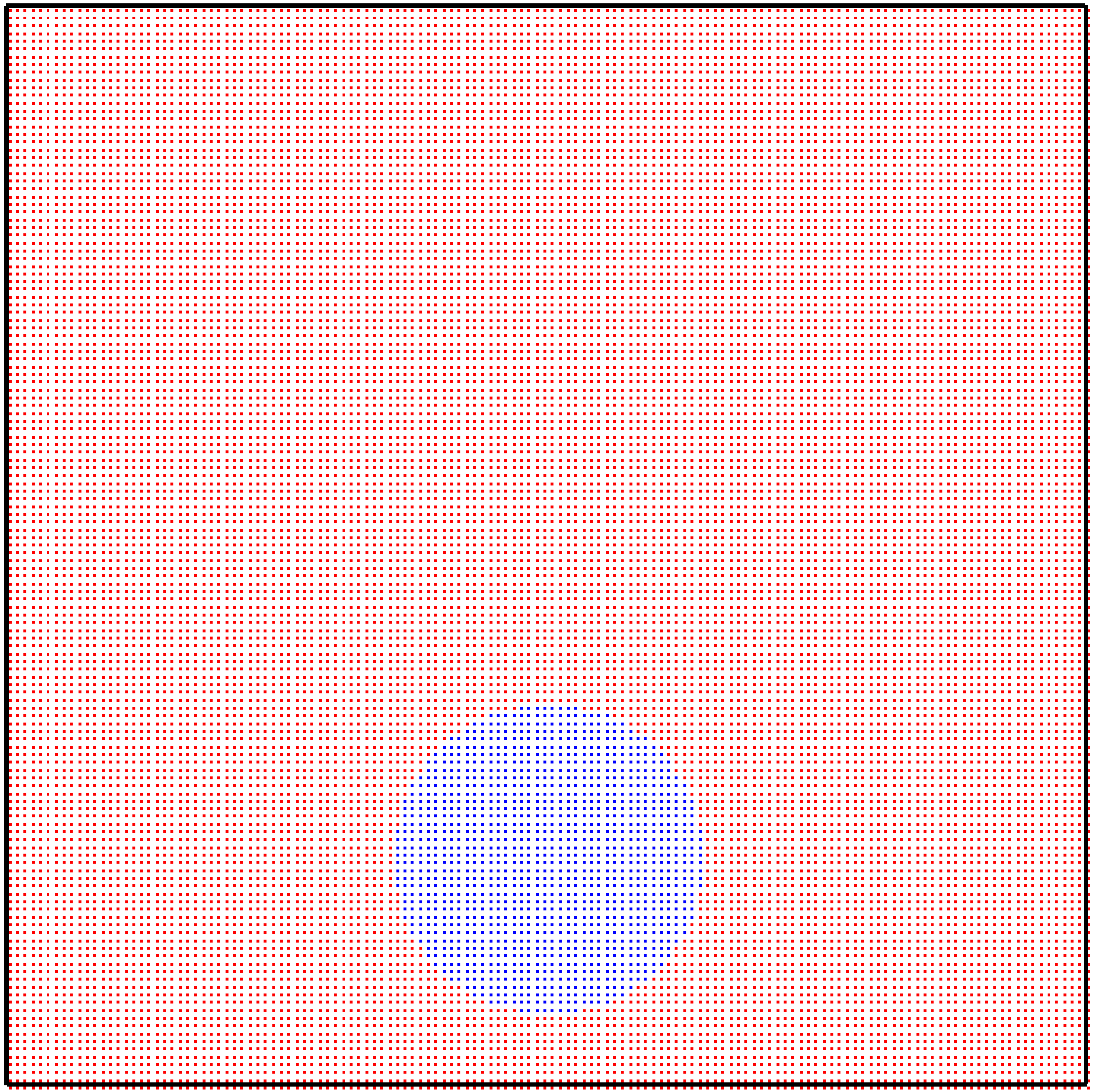


# Multiphase Flow using CLS-MPPM (5)

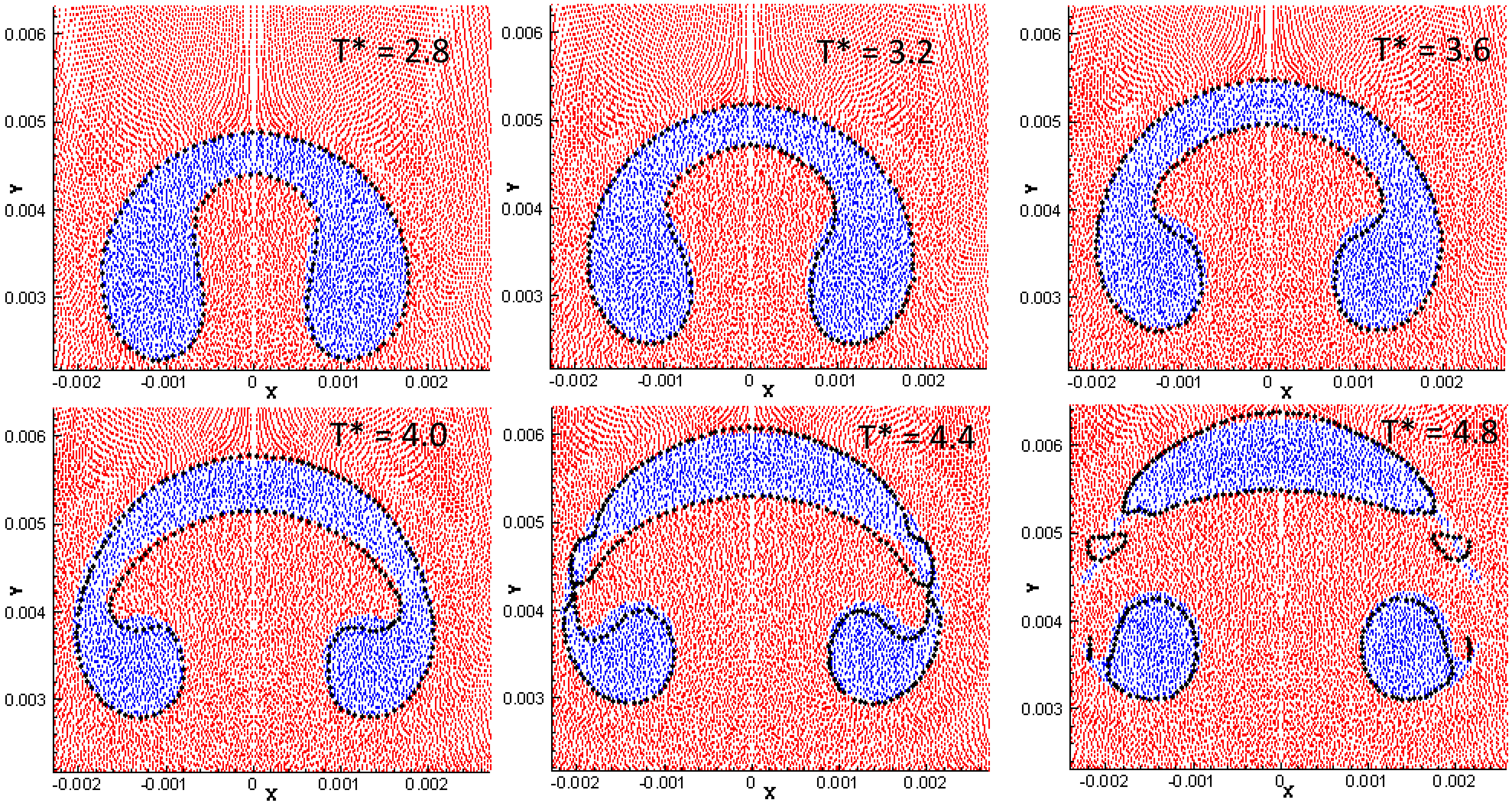
- Rising bubble

  ($Re$ = 1000; $B$ = 200)

  - $\rho_H$ = 1000.0 kg/m$^3$
  - $\rho_L$ = 1.0 kg/m$^3$
  - $\mu_H$ = 3.91511 x 10$^{-4}$ Pa.s
  - $\mu_L$ = 3.91511 x 10$^{-6}$ Pa.s
  - $\sigma$ = 3.0656 x 10$^{-4}$ N/m

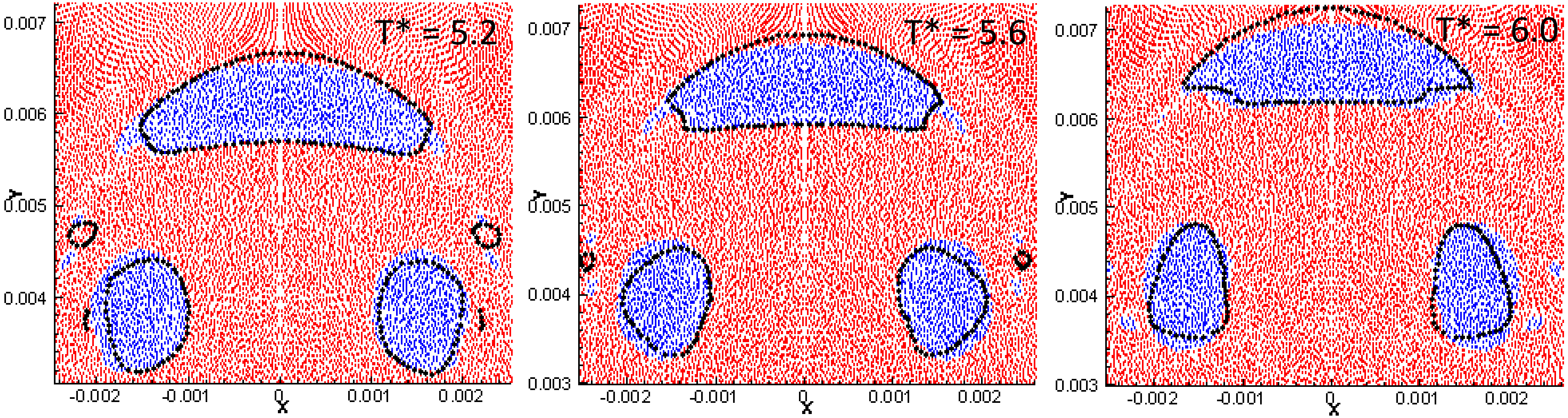


# Rising bubble ($Re$ = 1000; $B$ = 200)



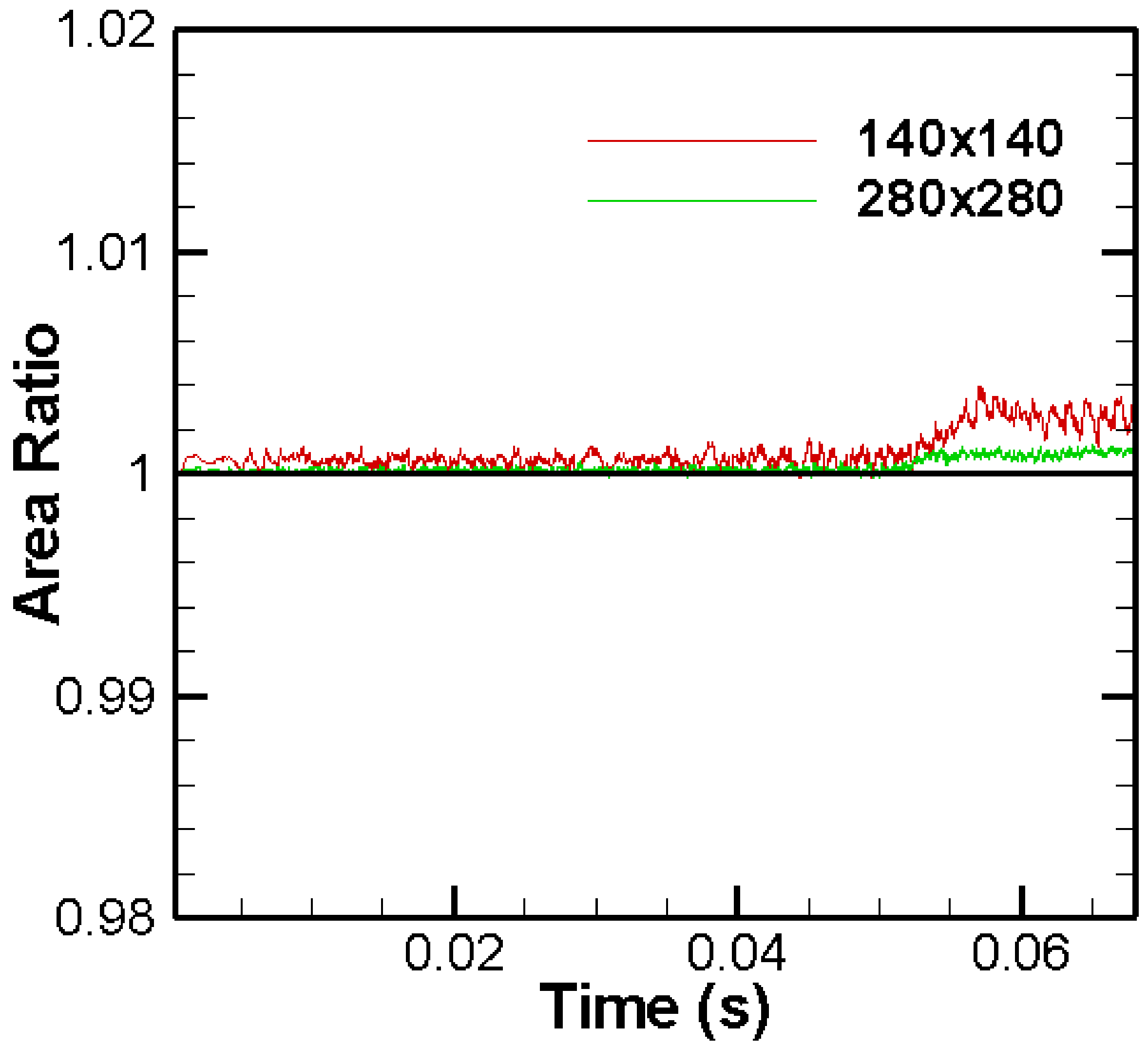

- Level-set solutions (140x140) from Sussmann et al. (1994)

# Rising Bubble (*Re* = 1000; *B* = 200)




- Level-set solutions from Sussmann et al. (1994)

# Rising Bubble(Mass conservation)



# Multiphase Flow using CLS-MPPM (6)

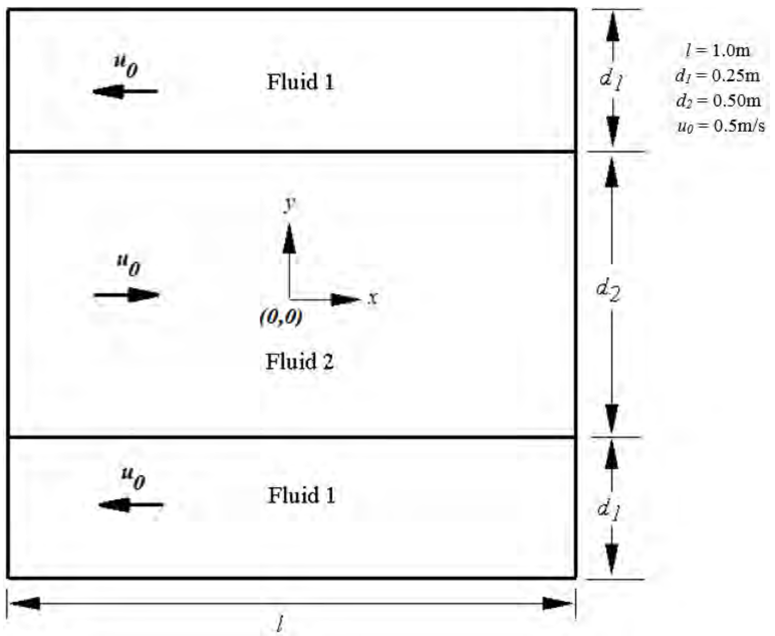
- KH Instability
- Density Ratio 1:2

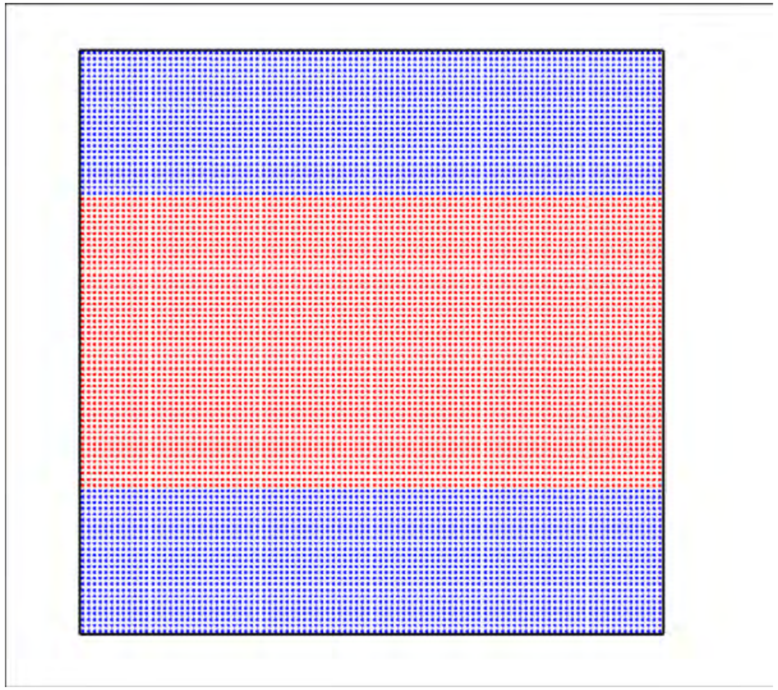
$$v_0 = \begin{cases} A_0 \sin[-2\pi(x+0.5)/\lambda] & |y-0.25| < 0.025 \\ A_0 \sin[2\pi(x+0.5)/\lambda] & |y+0.25| < 0.025 \end{cases}.$$

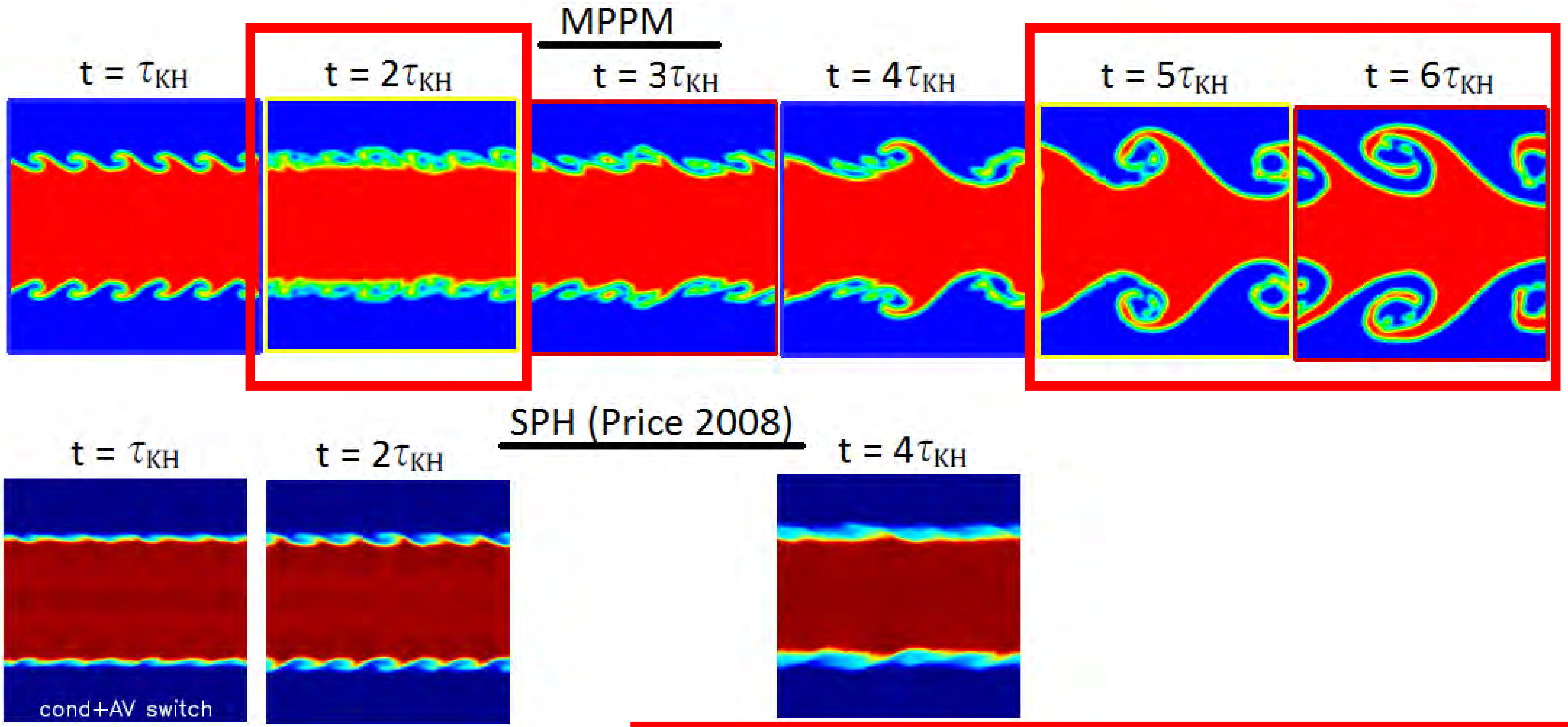
$$A_0 = 0.025\text{m/s}$$
$$\lambda = 1/6 \text{ m}$$

$$\omega = \frac{2\pi}{\lambda}\frac{(\rho_1\rho_2)^{1/2}(2u_0)}{\rho_1+\rho_2}.$$

$\tau_{KH}$ =0.3536s



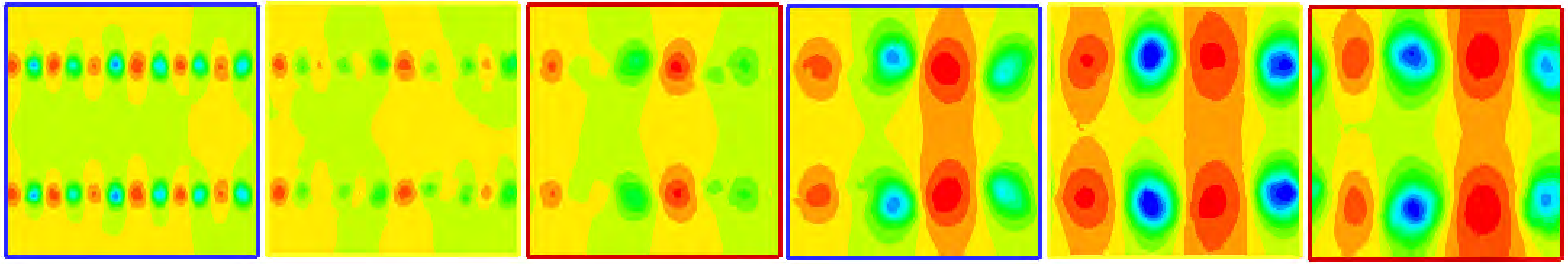






- Mode change from 1/6 to ½ by a factor ~3 (comply with theory)
- Growth is delayed in SPH.

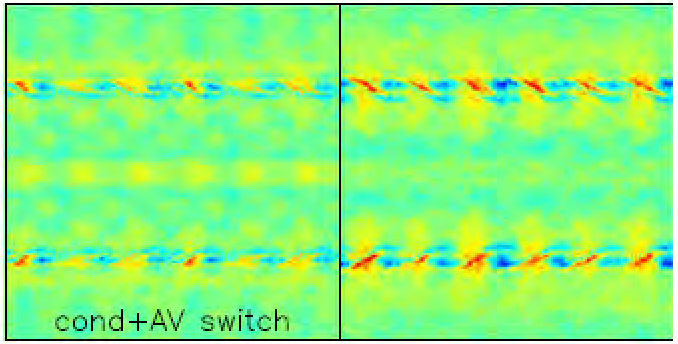
## MPPM

$t = \tau_{KH}$ $t = 2\tau_{KH}$ $t = 3\tau_{KH}$ $t = 4\tau_{KH}$ $t = 5\tau_{KH}$ $t = 6\tau_{KH}$

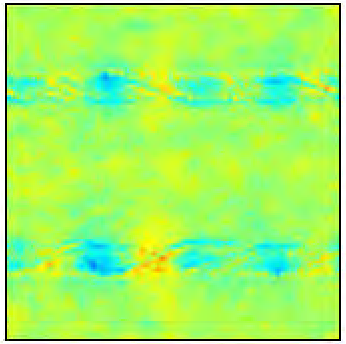


## SPH (Price 2008)

$t = \tau_{KH}$ $t = 2\tau_{KH}$




$t = 4\tau_{KH}$



Static pressure distribution

# Conclusion

- Improvements have been made to the existing MPS-based particle method:
  - A relatively smooth pressure field can be secured.
  - Particles are subjected to “actual” pressure gradient without artificial repulsive force.
  - No collision model is employed.
- A level-set method is used for interfacial density evaluation.
  - Smooth fluid interface can be secured.
  - More accurate surface normal and curvature can be attained.
  - Enable multiphase flow computation with high density ratio.

# ON-GOING WORKS

- An accurate and consistent Laplacian model for scattered distribution of moving particles.
- Higher-order time integration scheme for moving particles.
- Better mass conservation → VOF + Level set
- 3D extension and parallelization.

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