固気流動層内での物体浮沈挙動の離散粒子シミュレーション

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@環境資源工学会第40回シンポジウム
「 乾式分離精製のための粉体工学研究の最前線 」
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Difficulty of granular problems and discrete particle numerical simulation

- Co-existence of fluid-like & solid-like state
- High particle concentration ※invisible
- High degree of freedom: Large number of particles
- Multi-scale: micro → macro
- Multi-physics：Various physics exist
  （※hydrodynamics effects by surrounding fluid）

"粉は魔物"

＝ A world still highly depending on experience and intuition

Prediction and physical elucidation by discrete particle numerical simulation

Dense gas-solid flows

Dense gas-solid flows
= gas + highly-concentrated
solid particles

e.g.) Fluidized bed, spouted bed, pneumatic conveyer

Gas-Solid hydrodynamic interactions
+
Solid-solid contact interactions

- Very complex flows
- Emergence（創発）of mesoscopic structures dominating the flows (e.g., Bubbles, clusters)

Gas-solid bubbling fluidized bed

Governing equations for DEM-CFD

Fluid(CFD)

Spatially-averaged equations

- **Equation of continuity**

$$\frac{\partial}{\partial t}\varepsilon + \nabla \cdot (\varepsilon \boldsymbol{u}) = 0$$

- **Equation of motion**

$$\frac{\partial}{\partial t}(\varepsilon \boldsymbol{u}) + \nabla \cdot (\varepsilon \boldsymbol{u}\boldsymbol{u}) = -\frac{\varepsilon}{\rho_f}\nabla p + \boldsymbol{f}_{p\to f}$$

(Anderson & Jackson, 1967)

ε	: void fraction
$\boldsymbol{u}$	:fluid velocity
$\boldsymbol{f}_{p\to f}$	:fluid-particle force
p	:pressure

Particle(DEM)

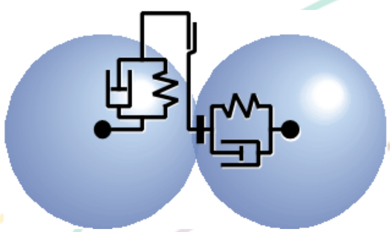
- **Translational equation of motion**

$$m_i \dot{\boldsymbol{v}}_i = \sum_j \boldsymbol{f}_{Cij} + \boldsymbol{f}_{f\to p_i} + m_i \boldsymbol{g}$$

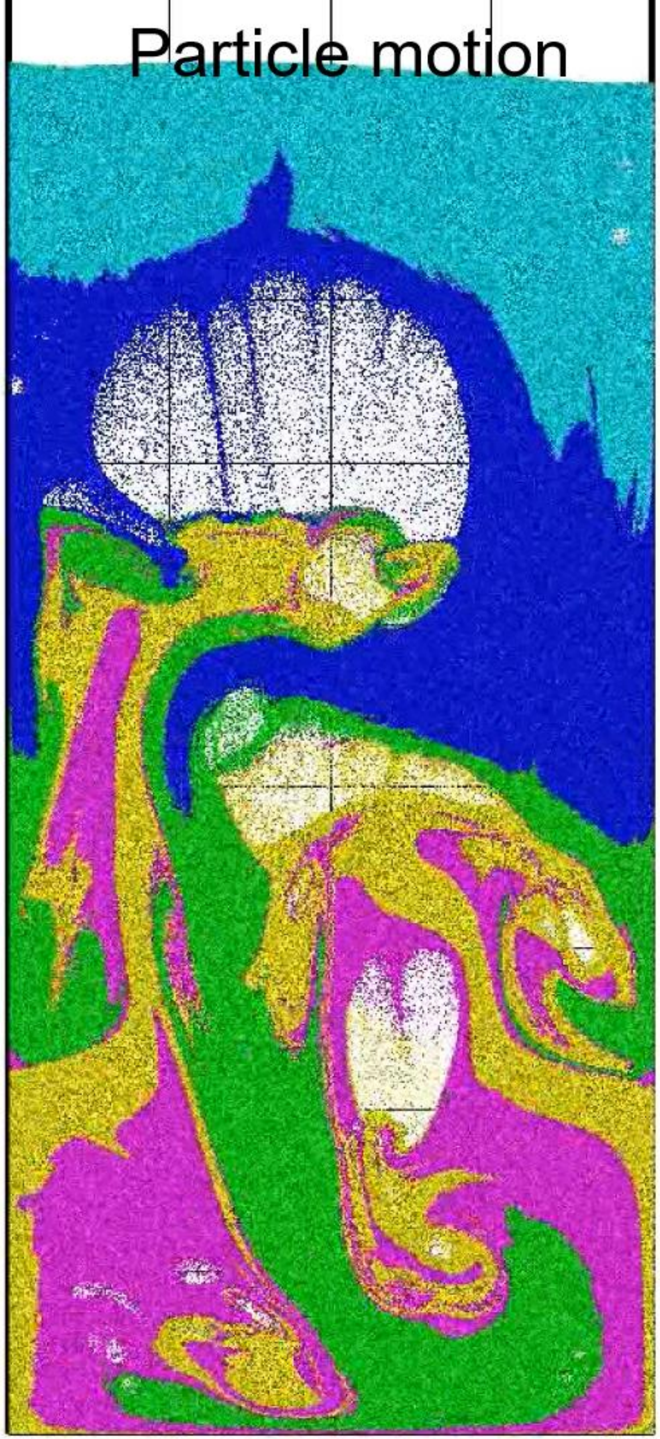
- **Rotational equation of motion**

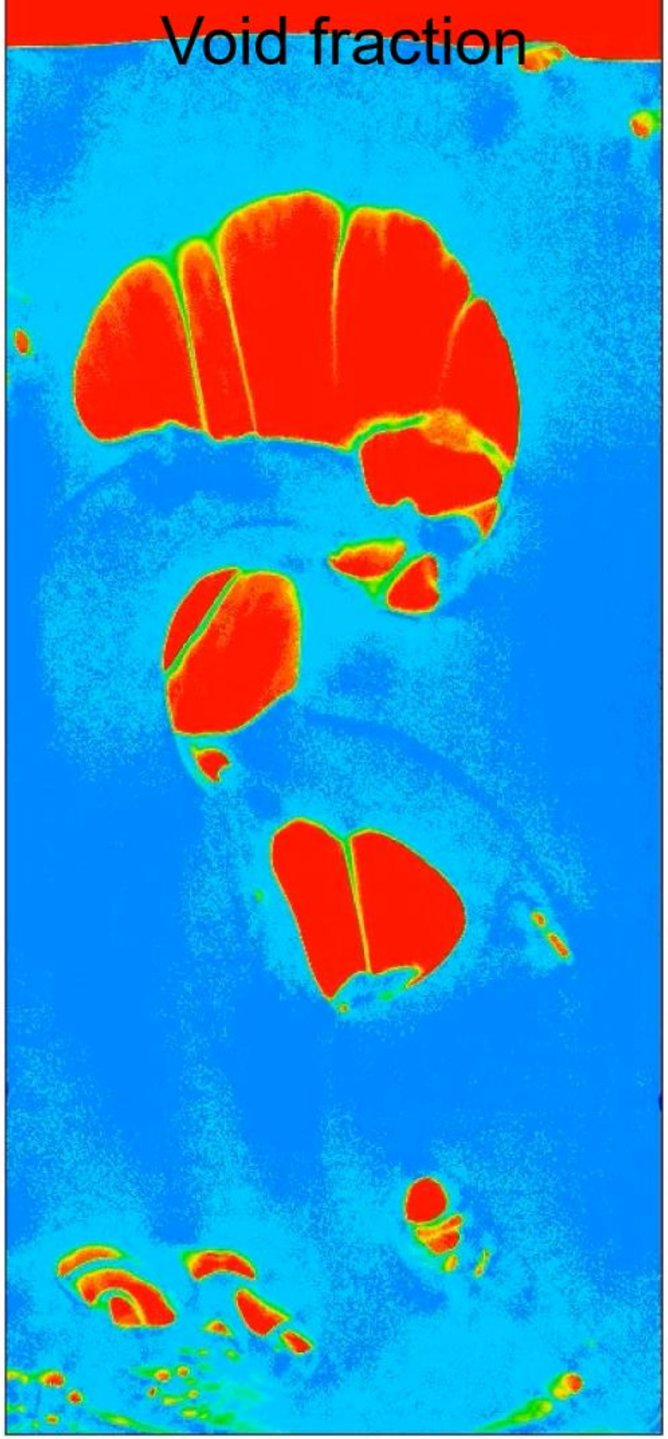
$$I_i \dot{\boldsymbol{\omega}}_i = \sum_i \boldsymbol{M}_{ij}$$

$\boldsymbol{v}_i$	: particle velocity
$\boldsymbol{f}_{Cij}$	: contact force
$\boldsymbol{f}_{f\to p_i}$	: fluid-particle force
I_i	: moment of inertia
$\boldsymbol{\omega}_i$	: angular velocity
$\boldsymbol{M}_{ij}$	: torque



Particle motion is considered individually





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DEM-CFD of bubbling fluidized bed

N_p= 20 million

d_p= 2mm

$\Delta x / d_p$= 2.5

L / d_p = 10^3

Large solid objects in FBs

In a number of fluidized bed applications, large solids are coexisting with small emulsion particles

Gasification, Combustion, Separation, Granulation

***O*(10μm－1mm)**

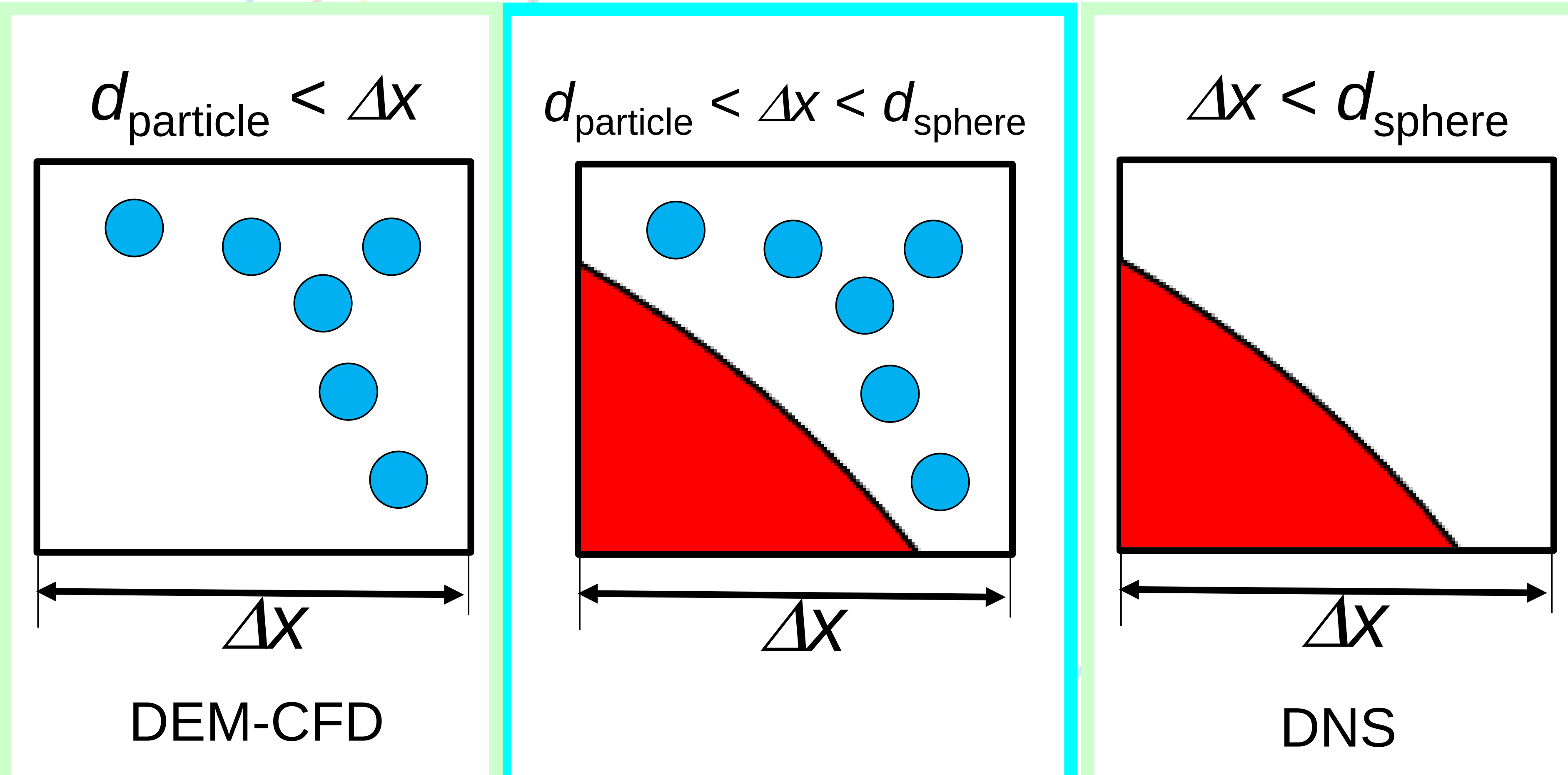
Sand

＋ ***O*(1－10mm)**

Large solid objects
(Wooden biomass, incombustibles)

$$\frac{\text{Large object}}{\text{sand}} = \frac{O(1 \sim 10\text{mm})}{O(10\mu\text{m} \sim 1\text{mm})} = O(1 \sim 1000)$$

Momentum exchange between solids and fluid



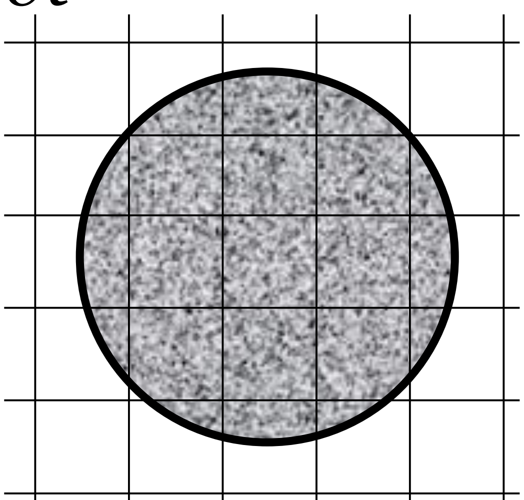
How to treat the momentum exchange especially for cells including both small and large solids?

Volume penalization method

Kolomenskiy & Schneider (J. Comput. Phys., 2009)

- A resolved DNS method for solid-fluid interactions
- Solid is assumed to be a porous media, fictitiously. When the permeability η goes to zero, the object will be a solid
- Penalization term which expresses the resistance due to the existence of porous media is added to N-S eq.

$$\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot (\boldsymbol{u}\boldsymbol{u}) = -\frac{\nabla p}{\rho_f} + \nu \nabla^2 \boldsymbol{u} + \frac{\chi(\boldsymbol{x})}{\eta}\left(\boldsymbol{U}_{\text{solid}} - \boldsymbol{u}\right)$$



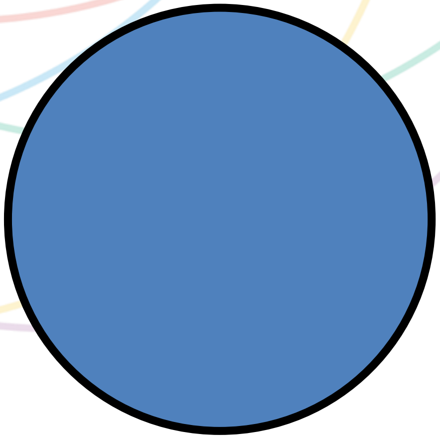
η : permeability

$$\chi(\boldsymbol{x}) = \begin{cases} 1 & \boldsymbol{x} \in \overline{\Omega}_{solid} \\ 0 & \boldsymbol{x} \in \Omega_{fluid} \end{cases}$$

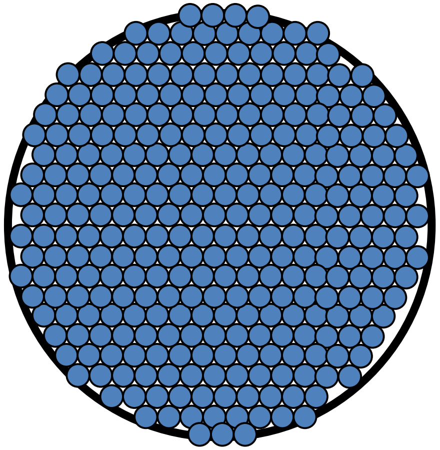
:mask function

Fictitious particle method(FPM)

Tsuji et al. (AIChE J., 2014)

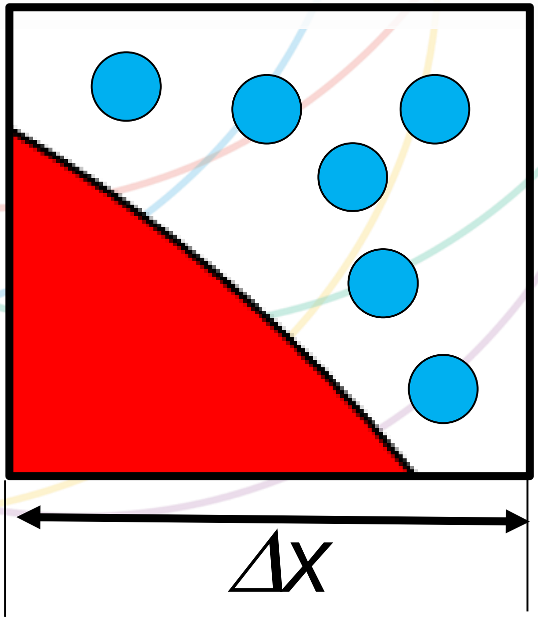


Only when the momentum exchange between solids and gas is considered, sphere is assumed to be an agglomerate of small particles, FICTITIOUSLY



Sphere would be a solid when the fictitious particles are small enough and highly packed

Fictitious particle method (cont.)

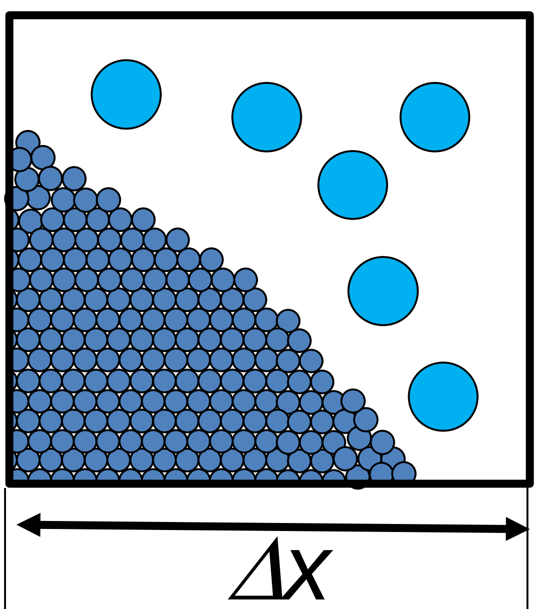


cells including both particles & small fictitious particles

↑ Local homogeneity

use conventional drag correlations as a binary system (particle & small fictitious particle)

$$\beta = \begin{cases} \dfrac{\mu(1-\varepsilon)}{\langle d \rangle^2 \varepsilon}\left[150(1-\varepsilon)+1.75Re\right] & (\varepsilon \le 0.8) \quad \text{Ergun} \\[2ex] \dfrac{3}{4} C_D \dfrac{\mu(1-\varepsilon)}{\langle d \rangle^2} \varepsilon^{-2.7} Re & (\varepsilon > 0.8) \quad \text{Wen \& Yu} \end{cases}$$



$\langle d \rangle$: Sauter mean diameter

Governing equations of fluid

- Eq. continuity

$$\frac{\partial}{\partial t}\varepsilon + \nabla\cdot(\varepsilon\boldsymbol{u}) = 0$$

- Eq. momentum

same term with conventional DEM-CFD model

$$\frac{\partial}{\partial t}(\varepsilon\boldsymbol{u}) + \nabla\cdot(\varepsilon\boldsymbol{u}\boldsymbol{u}) = -\frac{\varepsilon}{\rho_f}\nabla p + \varepsilon\nu\nabla^2\boldsymbol{u} + \frac{\beta}{\rho_f}(\bar{\boldsymbol{U}} - \boldsymbol{u})$$

ρ_f/β corresponds to permeability η in VP method

VP method:

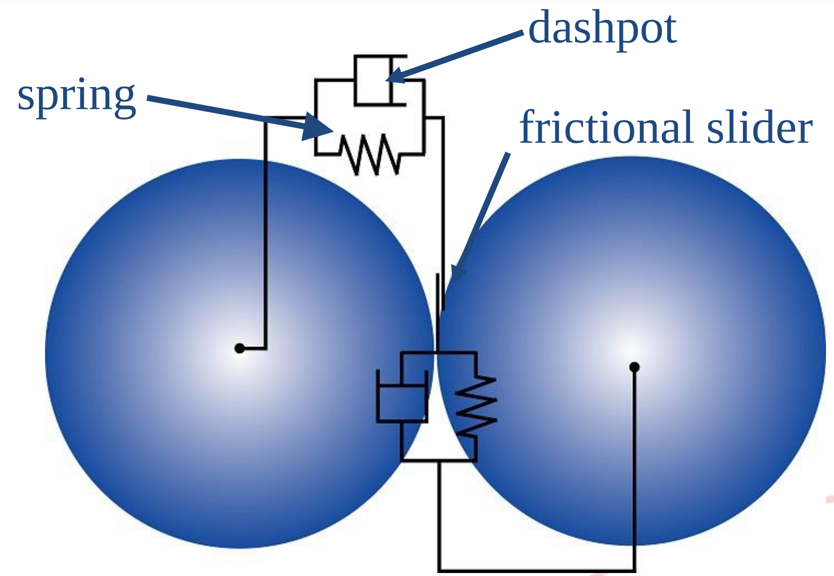
$$\frac{\partial\boldsymbol{u}}{\partial t} + \nabla\cdot(\boldsymbol{u}\boldsymbol{u}) = -\frac{\nabla p}{\rho_f} + \nu\nabla^2\boldsymbol{u} + \frac{\chi(\boldsymbol{x})}{\eta}(\boldsymbol{U}_{\mathrm{solid}} - \boldsymbol{u})$$

Governing eq. of particle & sphere

- Translational motion:

$$m\dot{\boldsymbol{v}}_i = \sum_j \boldsymbol{f}_{Cij} + \boldsymbol{f}_{Di} + m\boldsymbol{g}$$

contact force **fluid force** **gravity**



contact force model

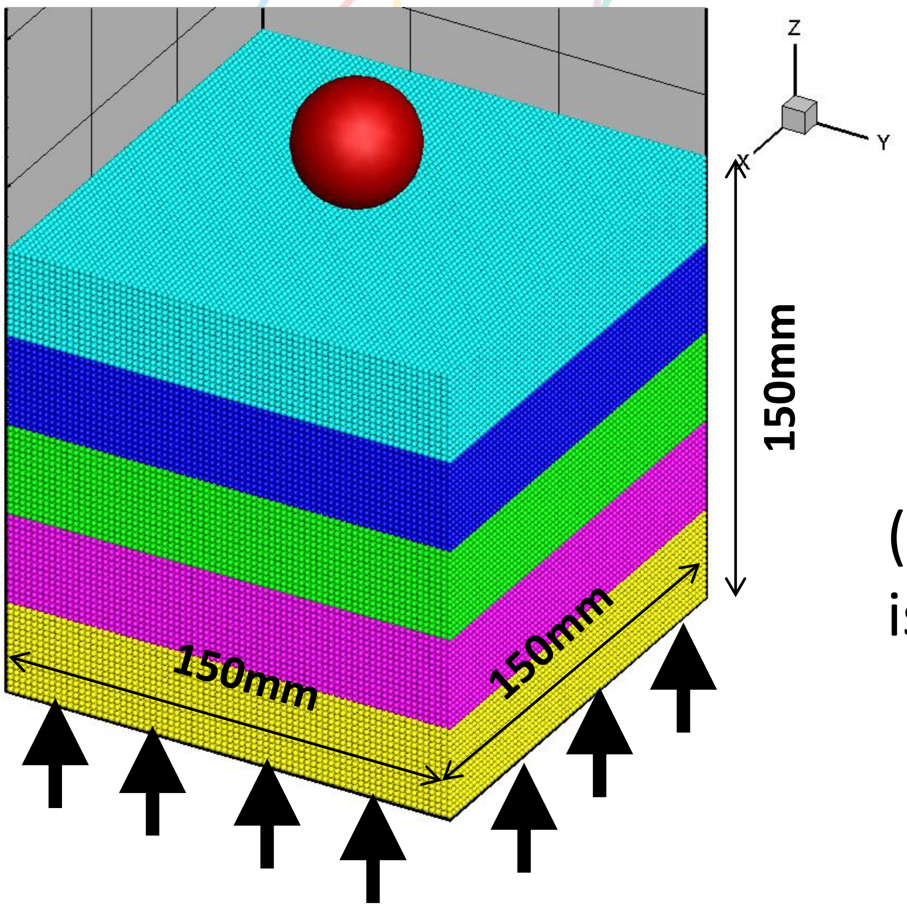
- Rotational motion:

$$I\dot{\boldsymbol{\omega}}_i = \sum_j \boldsymbol{M}_{ij}$$

fluid force working on particle: $$\boldsymbol{f}_{Dpi} = \left\{ \frac{\beta}{1-\varepsilon} \left(\boldsymbol{u} - \boldsymbol{U}_{pi} \right) - \nabla p \right\} V_p$$

fluid force working on sphere: $$\boldsymbol{f}_{Dsi} = \int_{sphere} \left\{ \beta \left(\boldsymbol{u} - \boldsymbol{U}_{si} \right) - \left(1 - \varepsilon_s \right) \nabla p \right\} dV$$

Single sphere in bubbling FB



Uniform air inflow
(superficial velocity 1.4 m/s $>u_{mf}$)

particle :
$d_{particle}$ =2.3mm glass particle
$\rho_{particle}$=2430 kg/m^3

sphere :
d_{sphere} = 40mm
$\rho_{sphere}/\rho_{bulk}$=0.75,1.01,1.61

(apparent density of particle bed is ρ_{bulk}=1530kg/m^3)

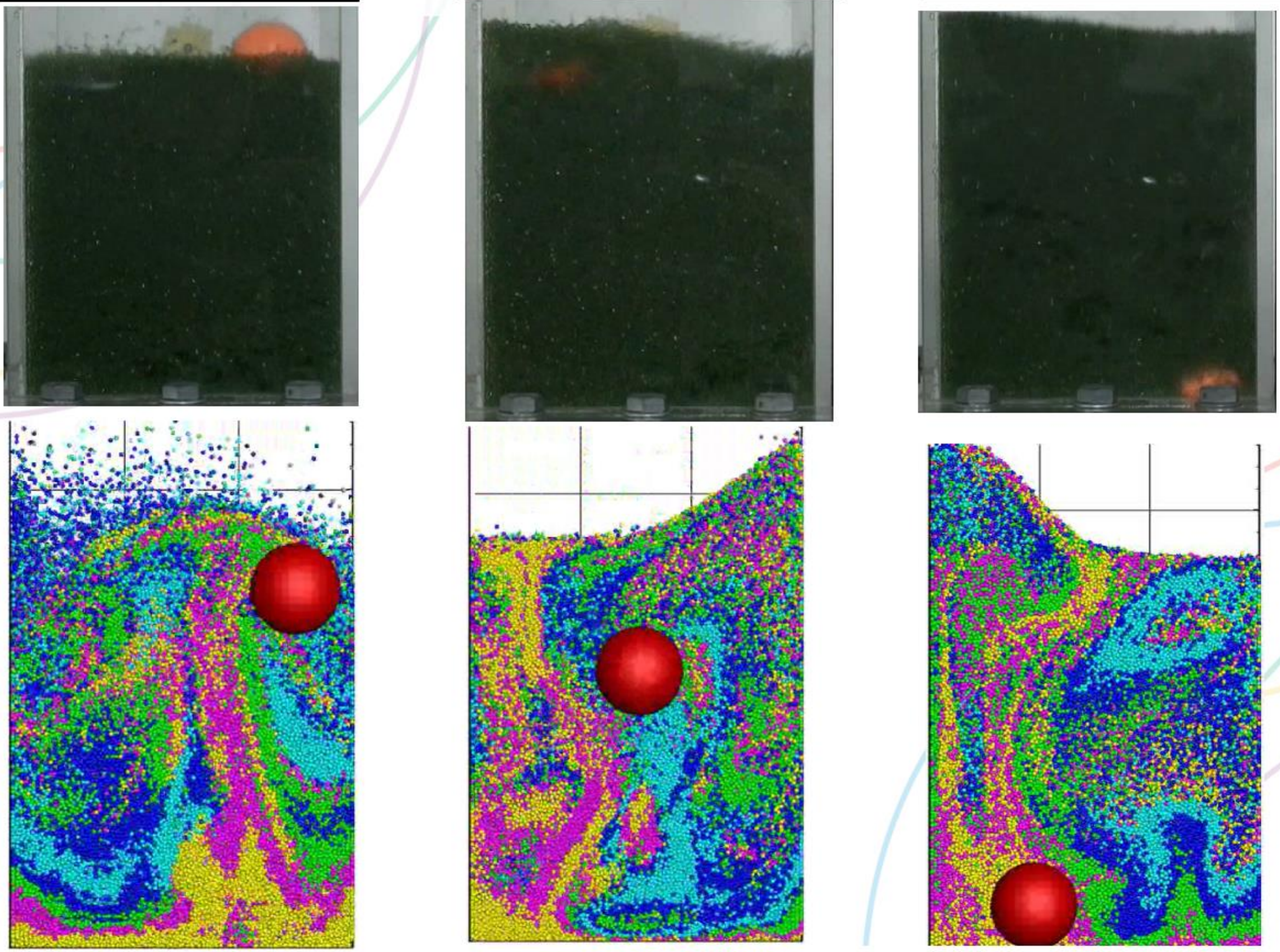
$d_{particle} : d_{sphere}$ = 1: 17.2

model parameters

$d_{fic}=d_{particle}/2$, α_{fic}=0.74

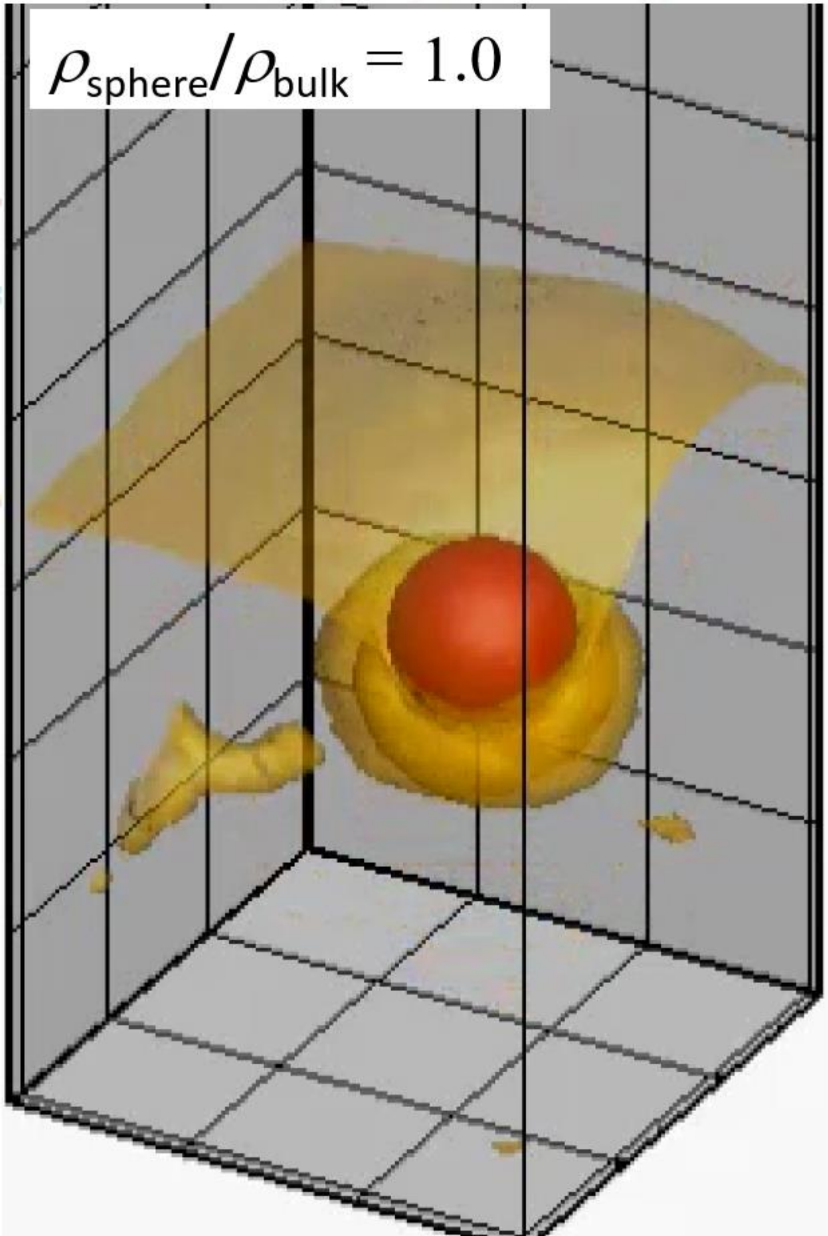
Motion of solids

$\rho_{sphere}/\rho_{bulk}$=0.75 | $\rho_{sphere}/\rho_{bulk}$=1.00 | $\rho_{sphere}/\rho_{bulk}$=1.61

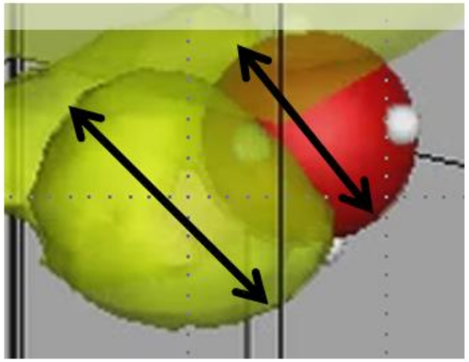


Tsuji et al. (*AIChE J.*, 2014)

Bubble observation (ε =0.8 iso-surface)



$d_{\text{bubble}} \approx d_{\text{sphere}}$



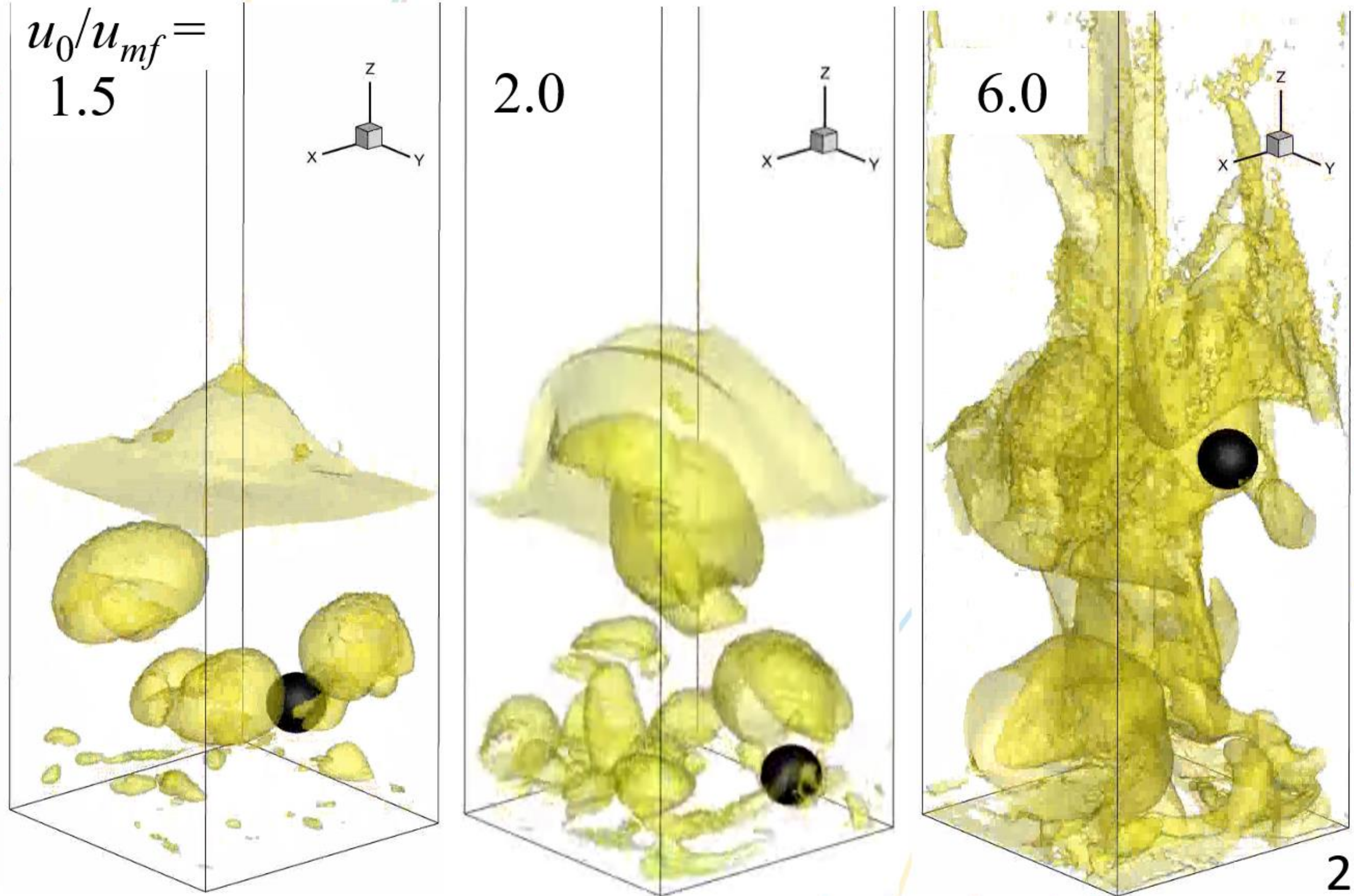
Sphere motions are largely influenced by bubbles

Sphere is NOT small comparing to bubbles. It is impossible with conventional DEM-CFD

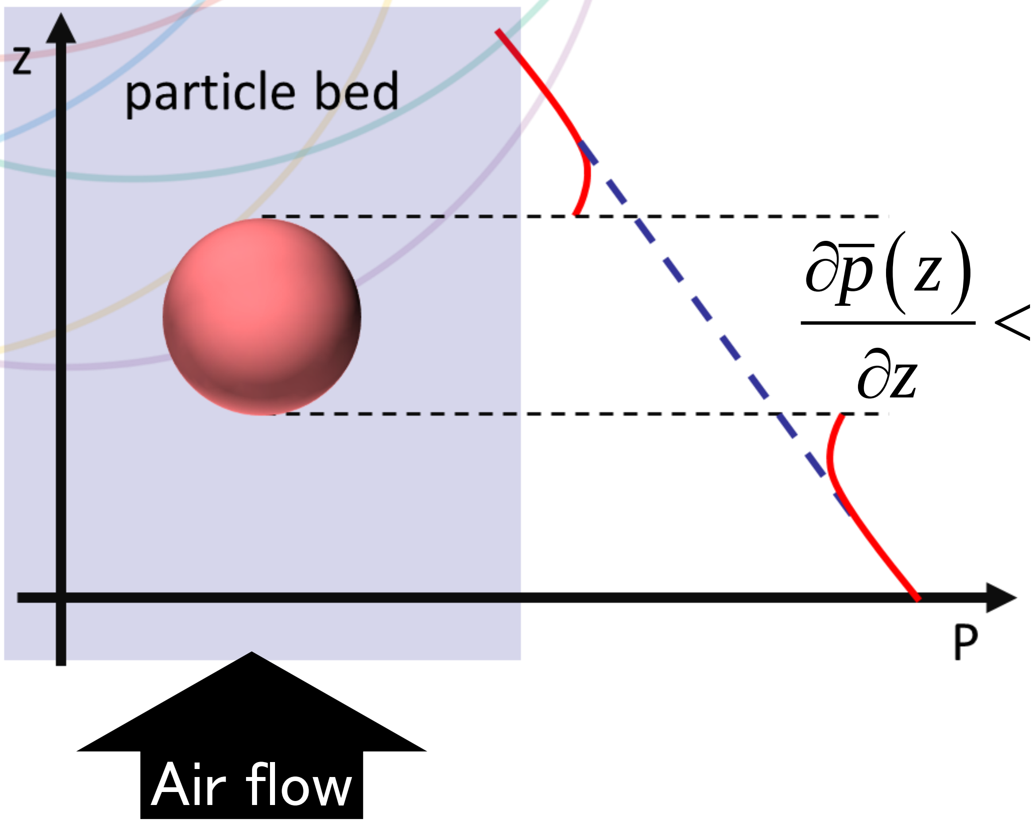
Bubble structure

$\varepsilon = 0.8$ iso-surface

Playspeed x1/10



Upward force due to gas pressure gradient



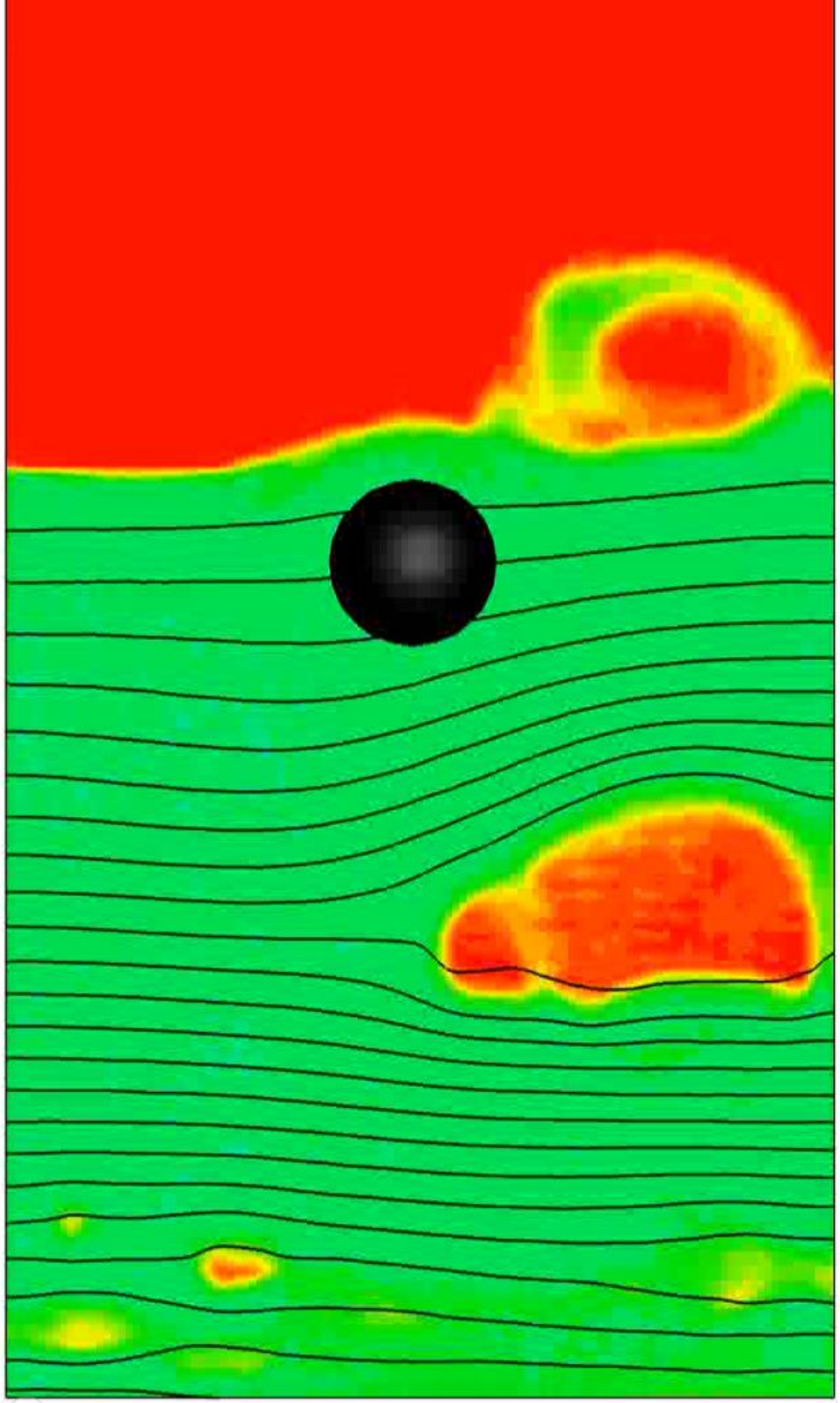
$$\frac{\partial \overline{p}(z)}{\partial z} < 0$$

$$F_{fluid}$$

$$= F_{viscous} + F_{pressure}$$

$$\approx F_{drag\_pressure} + F_{buoyancy}$$

$$= -\int \nabla p dV$$

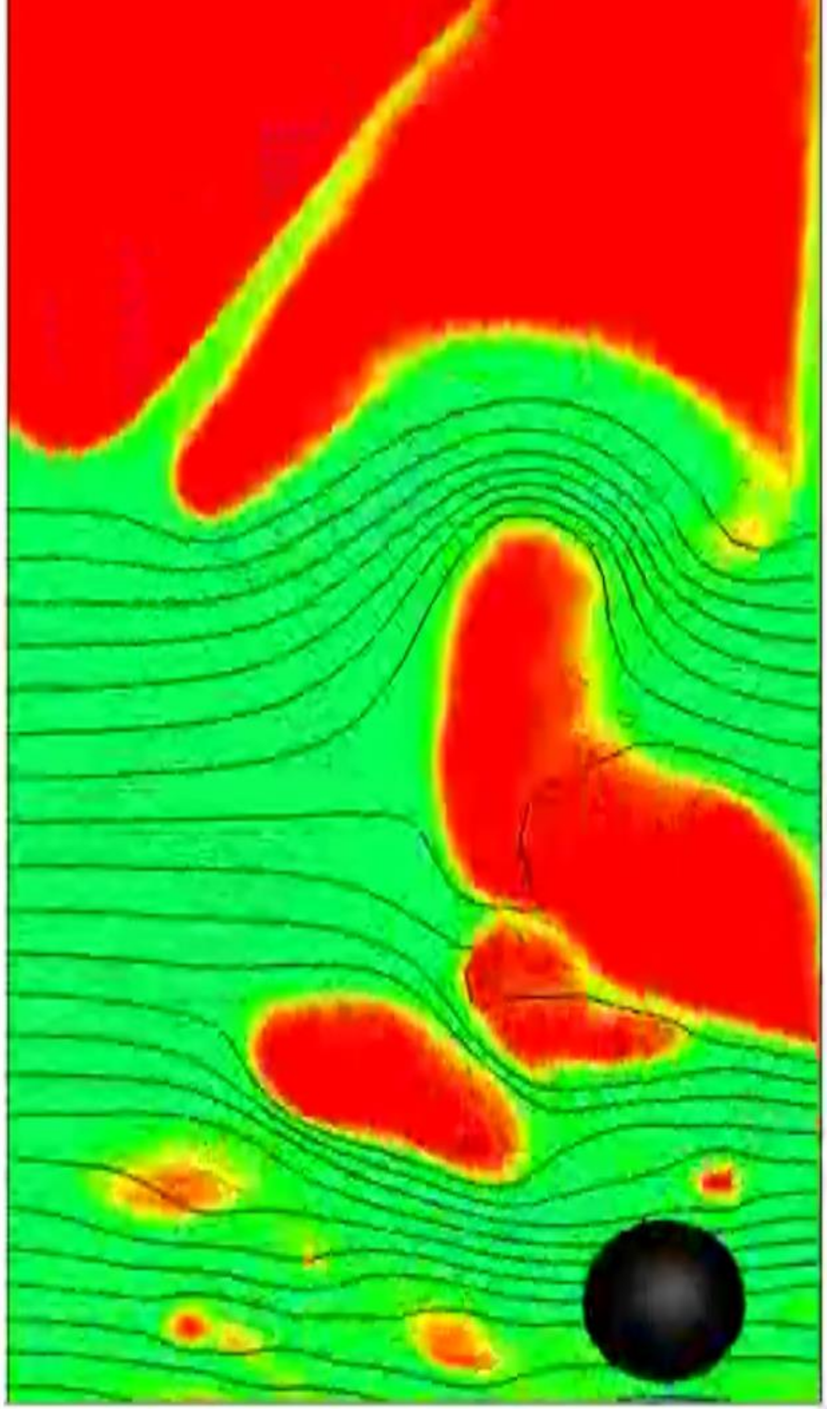


$u_0/u_{mf} = 1.5$

Δp=100 Pa for successive iso-lines

- Moderate bubbling fluidization

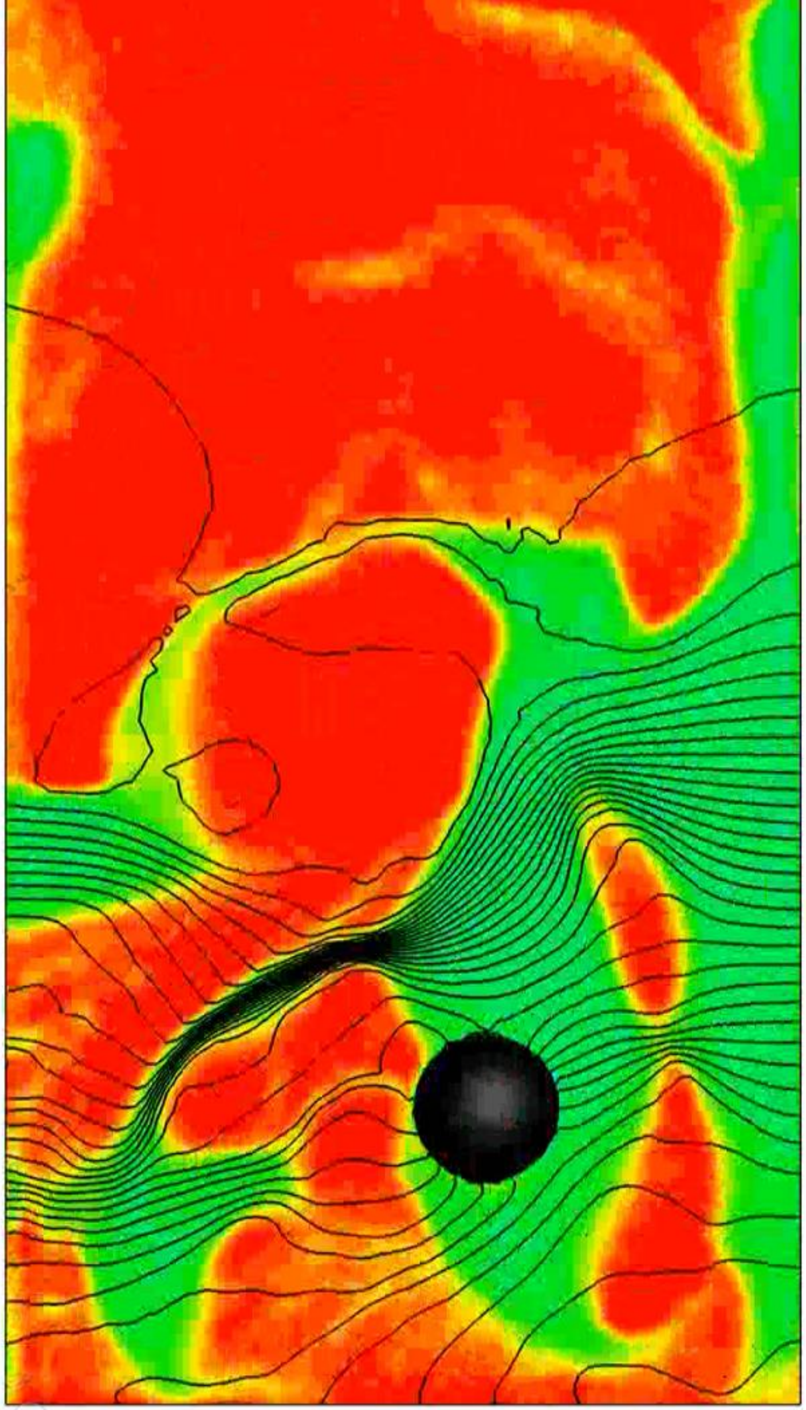
- Pressure gradient is almost uniform in the bed excepting the vicinity of bubbles



u_0/u_{mf} =2.0

Δp=100 Pa for successive iso-lines

- Inhomogeneity is enhanced
- Large bubble nucleation just above the distributer



$u_0/u_{mf}=6.0$

Δp=100 Pa for successive iso-lines

1. Gas pressure gradient force is dominant for the floating of large objects in FBs
2. Sphere is at rest in higher gas velocity (U_0/U_{mf} = 6.0). Floating is is due to occasional formation of dense phase and sudden large gas pressure gradient.
3. Floating at higher gas velocity cannot be explained by an AVERAGED PICTURE (e.g., apparent density of the bed)

Real-time MRI measurement (center slice)

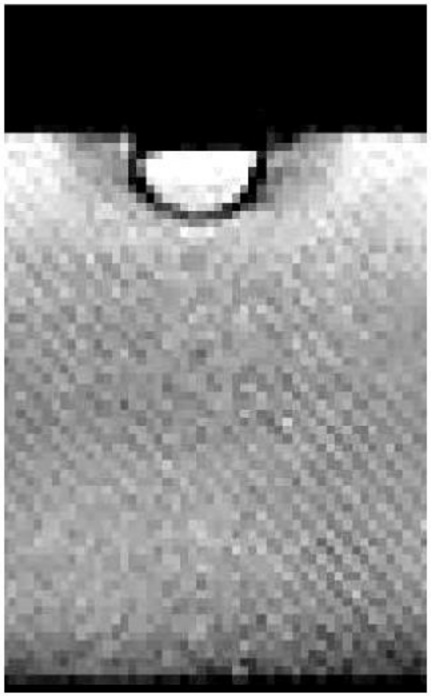
$U_0/U_{mf} = 0.95$

Temporal resolution: 45 msec

Spatial resolution: 2.5x2.5x10 mm

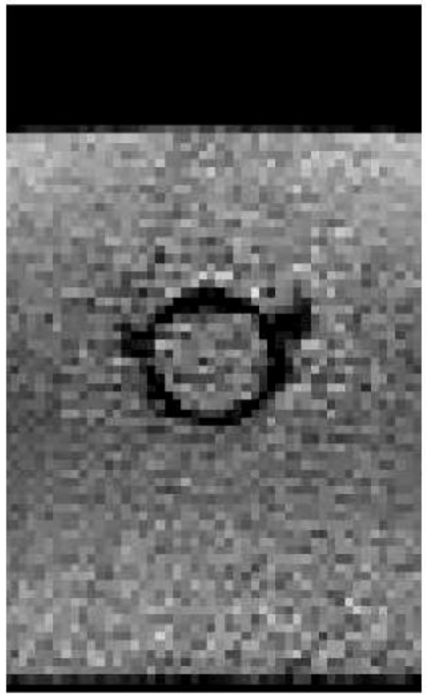
$\rho_{sphere}/\rho_{bulk}$ =

0.65



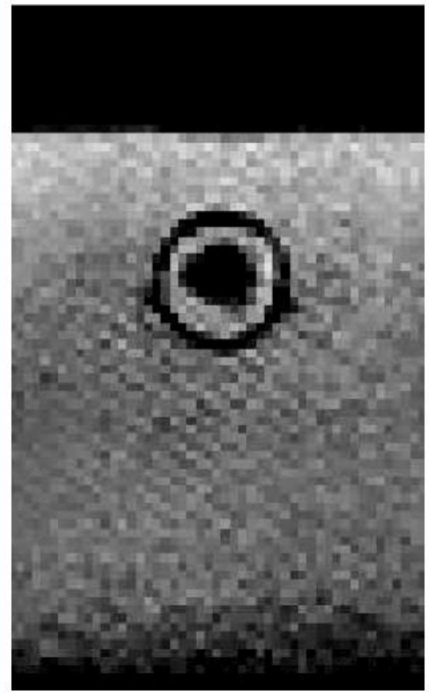
- Local bubbling
- Half-immersed & Floating

1.00



- Local bubbling and detachments
- Slow sinking
- Stopped at a deep depth

1.20



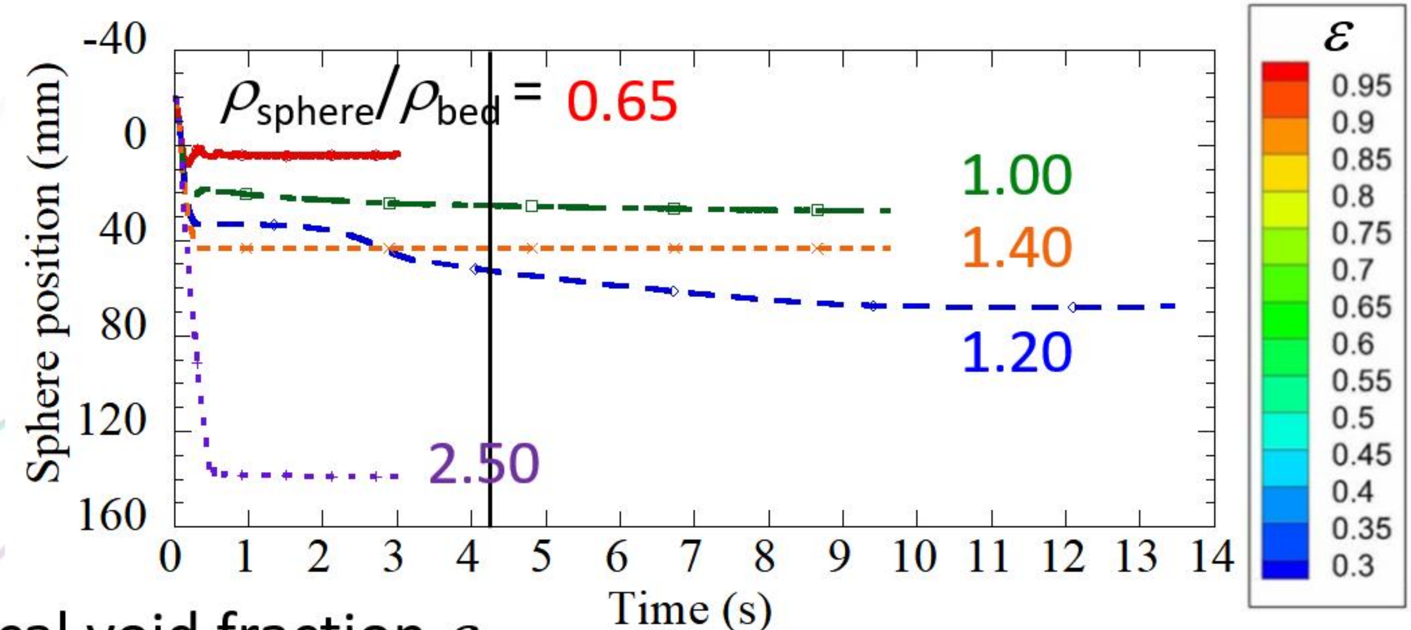
2.50

- No bubble detachments
- Fast sinking
- Stopped at a certain depth

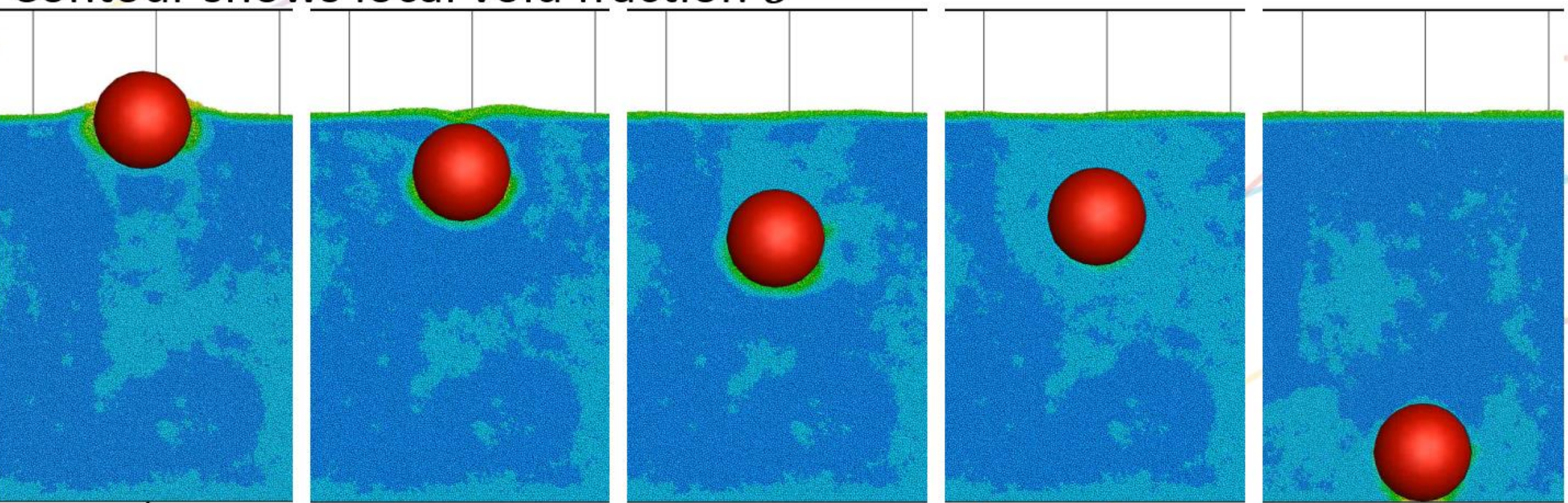
(Penn et al., *Sci. Adv.*, 2017; Tsuji et al., *Phys. Fluids*, 2021)

Numerical results

U_0/U_{mf} =0.95



Contour shows local void fraction ε

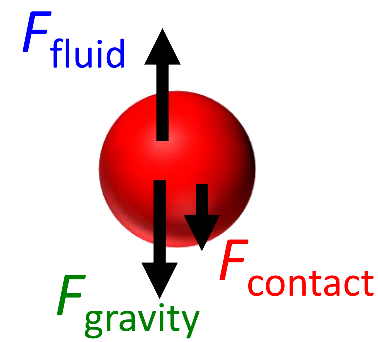


ρ_{sphere}/ρ_{bed} =

0.65 1.00 1.20 1.40 2.50

(Tsuji et al., *Phys. Fluids*, 2021)

1. Anomalous sinking at $\rho_{sphere}/\rho_{bulk} \approx 1.0$ is due to the attenuation of pressure gradient force caused by bubble detachments from the surface of large object
2. It cannot be explained by an AVERAGED PICTURE (e.g., the bed is at a solid-like state under $U_0/U_{mf} \approx 0.95$)



Influence of non-sphericity

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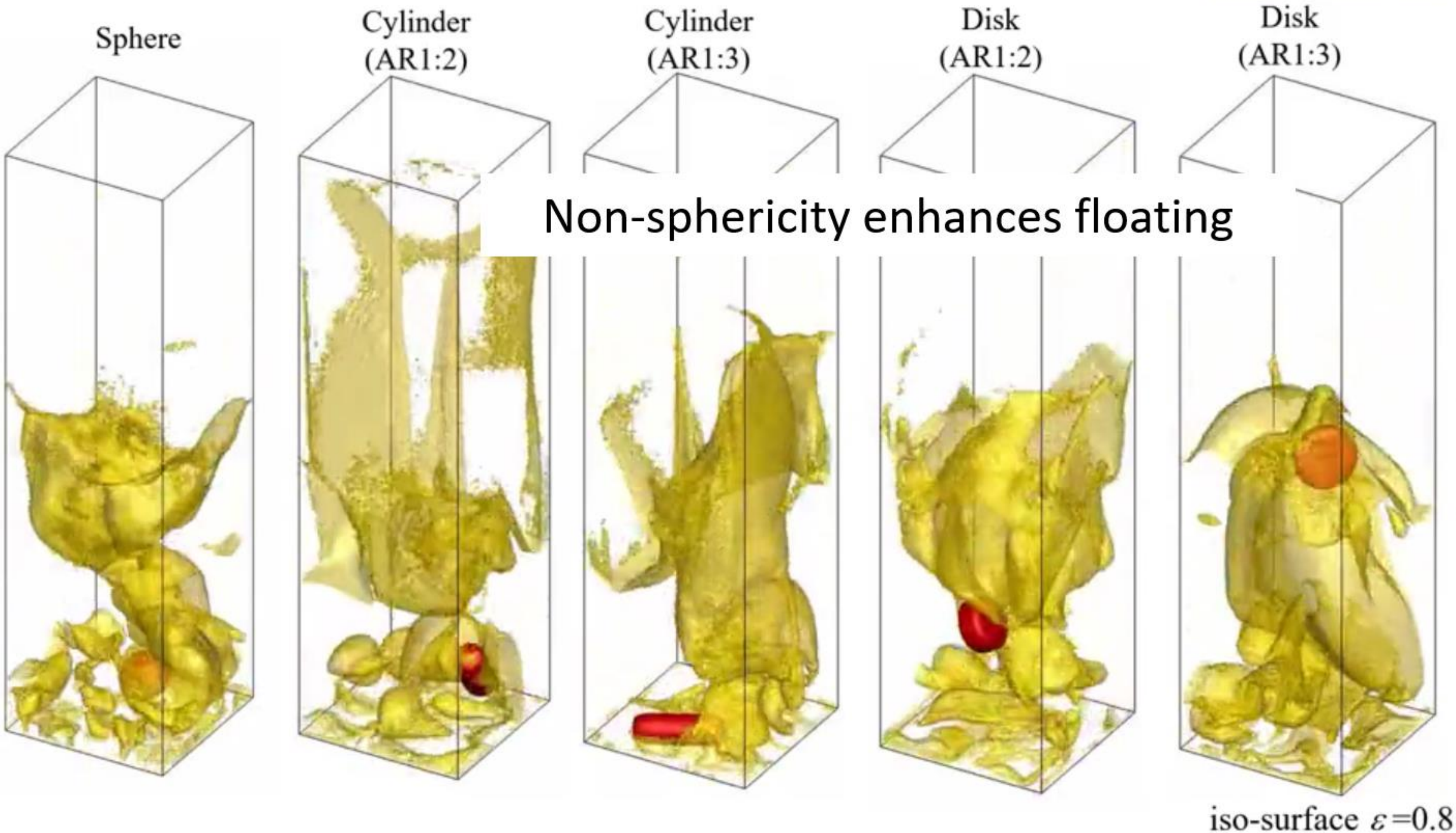
All shapes keep the same volume and mass



Non-sphericity enhances floating

It is not explainable by the buoyancy effect only

(Tsuji et al., *Chem. Eng. Sci.*, 2022)

Summary

1. DEM-CFD simulation based on cutting-edge models with modern computers is a powerful tool to explore complex granular flows
2. Fictitious particle model (FPM) is good for large particle size difference:
   - reproduced counterintuitive sinking/floating behaviors
   - enhanced essential understanding of flow physics
3. Floating/sinking of large objects in FBs cannot be described only by an averaged picture
4. A lot of unknows still remain for granular problems

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