Presentation for EAGRE Kick-off Meeting

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- **Self-introduction**
- **Research Background**
- **Progress Review**

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Self-introduction

Yang Lu, from Nanjing, China

Education

- Nov. 2017 – Present University of Leeds New PhD candidate in School of Mathematics
- Sept. 2017 – Jun. 2020 Xi'an Jiaotong University Master of Engineering (Power engineering and engineering Thermophysics)
- Sept. 2013 – Jun. 2017 Xi'an Jiaotong University Bachelor of Engineering (Energy and Power Engineering)

Research Experience

- Numerical simulation on droplet dynamics
- Multiphase lattice Boltzmann method
- Parallel programming via OpenMP/MPI

Interests

- Reading, badminton, swimming…

Research Background

Lattice Boltzmann Colour-Gradient Model for Ternary Fluid Flows and its Applications in Compound Droplet Dynamics

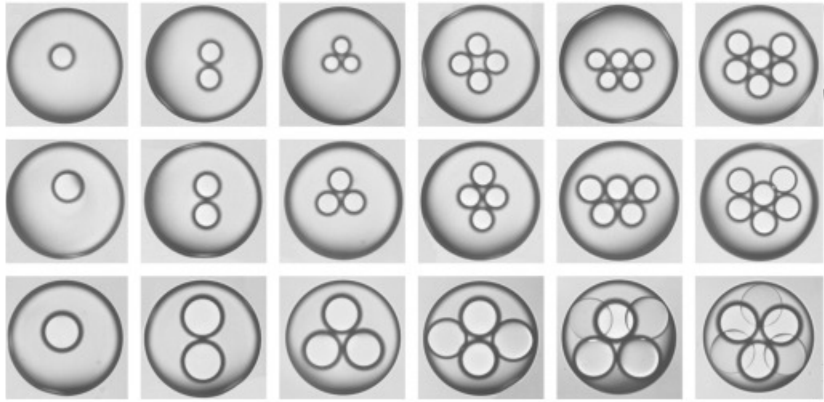
- Deformation and breakup of a compound droplet in three-dimensional oscillatory shear flow
- Numerical simulation of immiscible three-phase flows with contact-line dynamics on curved substrates

Deformation and breakup of a compound droplet in three-dimensional oscillatory shear flow

1. Introduction
2. Problem statement and numerical method
3. Oscillatory deformation of a compound droplet
4. Breakup of a compound droplet

Introduction

Compound droplets (double emulsions): highly structured fluids consisting of emulsion drops that contain a single or a collection of smaller drops.



[1]

Applications: materials processing, drug delivery, food processing, pharmaceuticals, personal care products and cosmetics

→ A thorough understanding of the deformation and breakup of compound droplets in external flow fields is of great significance.

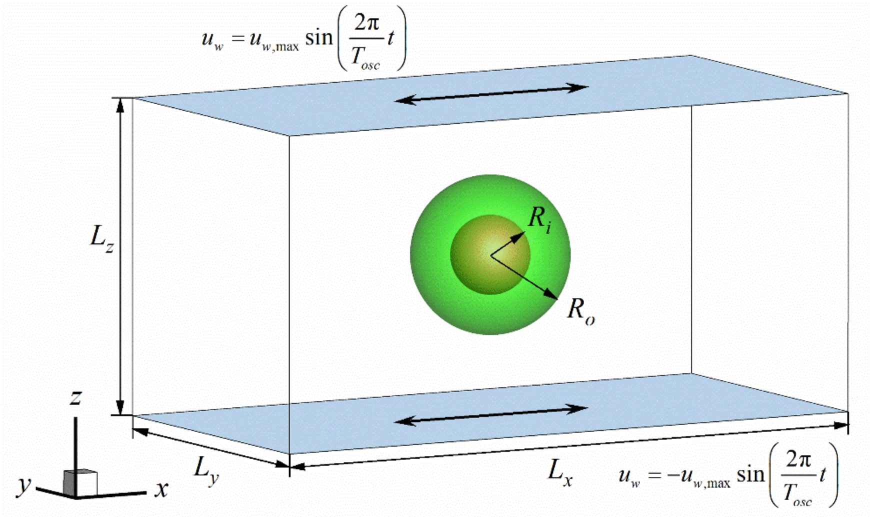
- flow through confined geometries
- deformation and breakup in extension flow/ steady simple shear flow
- impact and spreading…

→ It is necessary to put effort into the case of **deformation and breakup of compound droplets in oscillatory shear**, which is largely unexplored.

[1] Chu, L. , Utada, A. , Shah, R. , Kim, J. and Weitz, D. (2007) Angew. Chem. Int. Ed., 46: 8970-8974.

Problem statement and numerical method (1)

Problem statement



$Re = \rho_1 \dot{\gamma}_{\max} R_o^2 / \mu_1$

$Ca = \mu_1 \dot{\gamma}_{\max} R_o / \sigma_{12}$

$\boxed{\dot{\gamma}_{\max} = 2u_{w,\max}/L_z}$

radius ratio R_i/R_o

wall confinement ratio $2R_o/L_z$

viscosity ratios $\lambda_{21} = \mu_2/\mu_1,\ \lambda_{31} = \mu_3/\mu_1$

matrix fluid 1, outer droplet fluid 2, inner droplet fluid 3

$\mu_k \quad \sigma_{kl} \quad \rho_k$ (equal densities)

G.E.

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

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot \mu \boldsymbol{S} + \boxed{\boldsymbol{F}_s}$$

interfacial tension force

I.C. $\boldsymbol{u} = \boldsymbol{0}$

the compound droplet is spherical at the centre of the box

B.C. the x and y directions: periodic

top plate: $u_{w,\max} \sin(2\pi t/T_{osc})$

lower plate: $-u_{w,\max} \sin(2\pi t/T_{osc})$

Problem statement and numerical method (2)

Numerical method

A lattice Boltzmann colour-gradient model for simulating immiscible ternary fluids with a full range of interfacial tensions[1]

- collision step $f_i^{\dagger}(\boldsymbol{x},t) = f_i(\boldsymbol{x},t) + \boxed{\Omega_i(f_i(\boldsymbol{x},t))} + \boxed{\Phi_i(\boldsymbol{x},t)}$ the perturbation term

$$\Omega_i(f_i(\boldsymbol{x},t)) = -\frac{1}{\tau_f}\left[f_i(\boldsymbol{x},t) - f_i^{eq}(\boldsymbol{x},t)\right]$$

$$\Phi_i(\boldsymbol{x},t) = w_i\left(1-\frac{1}{2\tau_f}\right)\left[\frac{\boldsymbol{e}_i-\boldsymbol{u}}{c_s^2}+\frac{(\boldsymbol{e}_i\cdot\boldsymbol{u})\,\boldsymbol{e}_i}{c_s^4}\right]\cdot\boldsymbol{F}_s(\boldsymbol{x},t)\,\delta_t$$

interfacial force: $\boldsymbol{F}_s = \sum_i \sum_{l,l\neq k} \nabla\cdot\left[\frac{\sigma_{kl}C_{kl}}{2}|\boldsymbol{G}_{kl}|(\boldsymbol{I}-\boldsymbol{n}_{kl}\boldsymbol{n}_{kl})\right]$

- recolouring step $f_{i,k}^{\ddagger}(\boldsymbol{x},t) = \frac{\rho_k}{\rho} f_i^{\dagger}(\boldsymbol{x},t) + \sum_{l,l\neq k} \boxed{\beta_{kl}}\, w_i \frac{\rho_k\rho_l}{\rho}\boldsymbol{n}_{kl}\cdot\boldsymbol{e}_i$

segregation parameter $\beta_{kl} = \beta^0 + \beta^0 \min\left(\frac{35\rho_r\rho_g\rho_b}{\rho^3}, 1\right) g(X_{kl})$

- propagation step $f_{i,k}(\boldsymbol{x}+\boldsymbol{e}_i\delta_t, t+\delta_t) = f_{i,k}^{\ddagger}(\boldsymbol{x},t)$

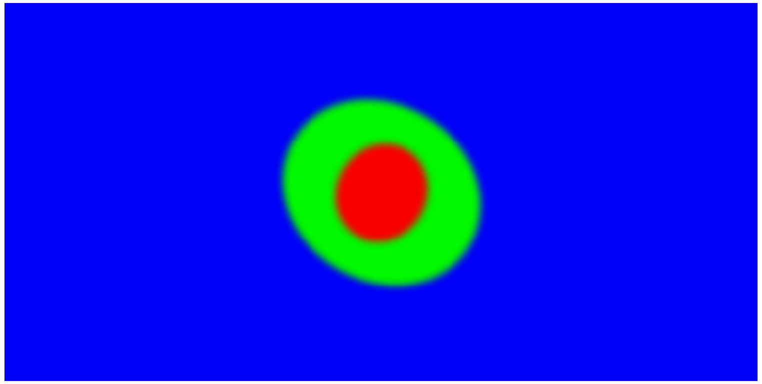
[1] Yu, Y. , Liu, H. , Liang, D. and Zhang, Y. (2019) Phys. Fluids 31, 012108

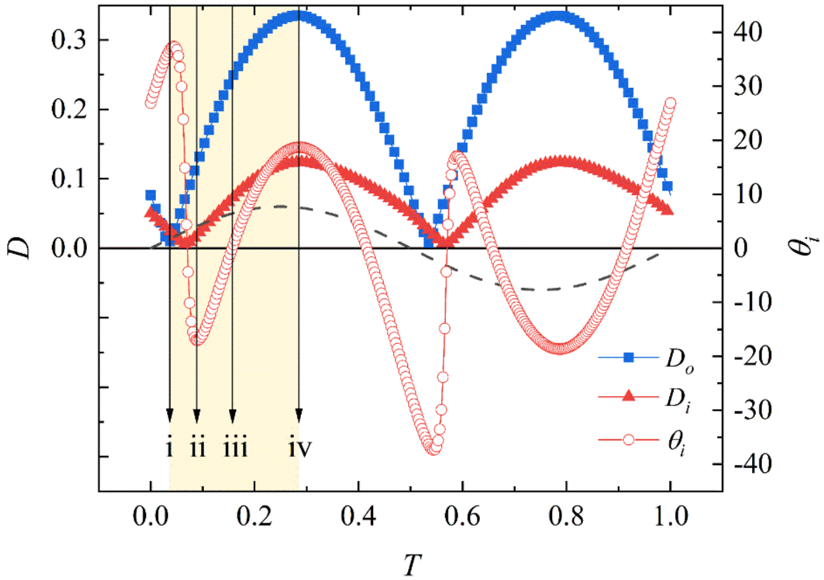
Oscillatory deformation

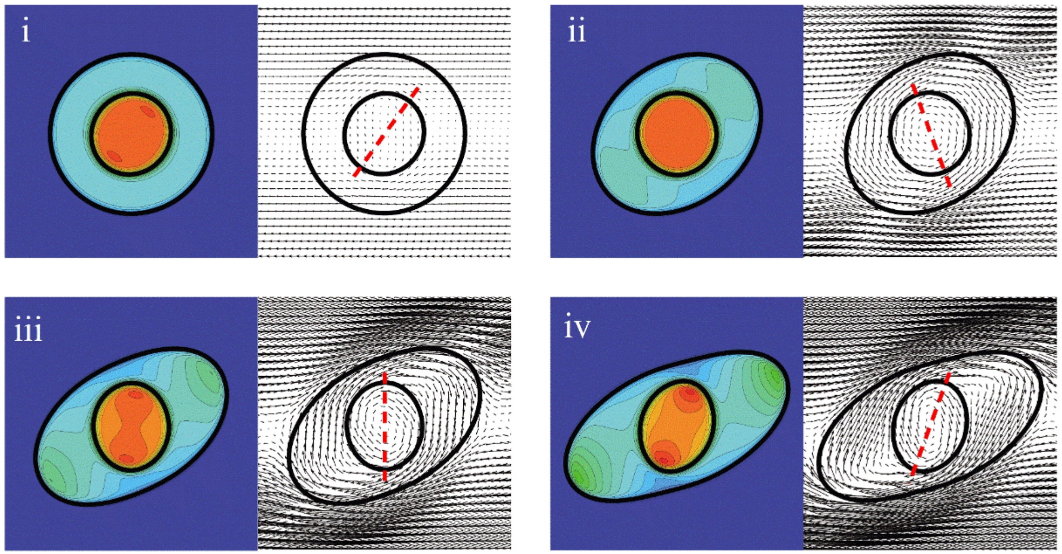
Effect of shear flow period T_{osc}

$\alpha = 10$

$$T_{osc} = \alpha L_x / u_{w,\max}$$



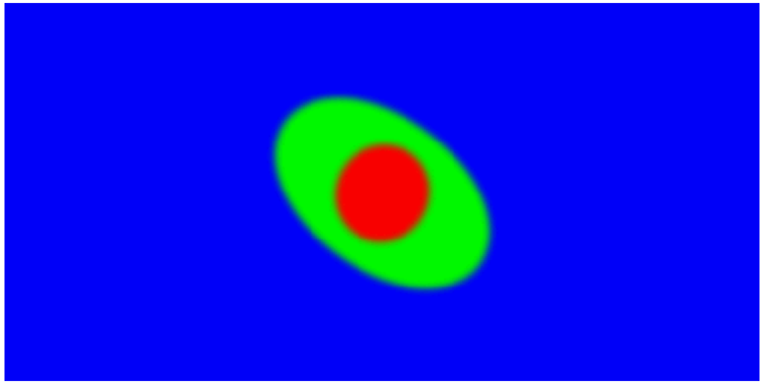




In one oscillatory cycle, the dynamic behaviour of the **inner droplet** is mainly controlled by **viscous shear force** arising from the closed vortical flow interior to the outer droplet, but it is also affected by the **pressure force** especially during flow reversal.

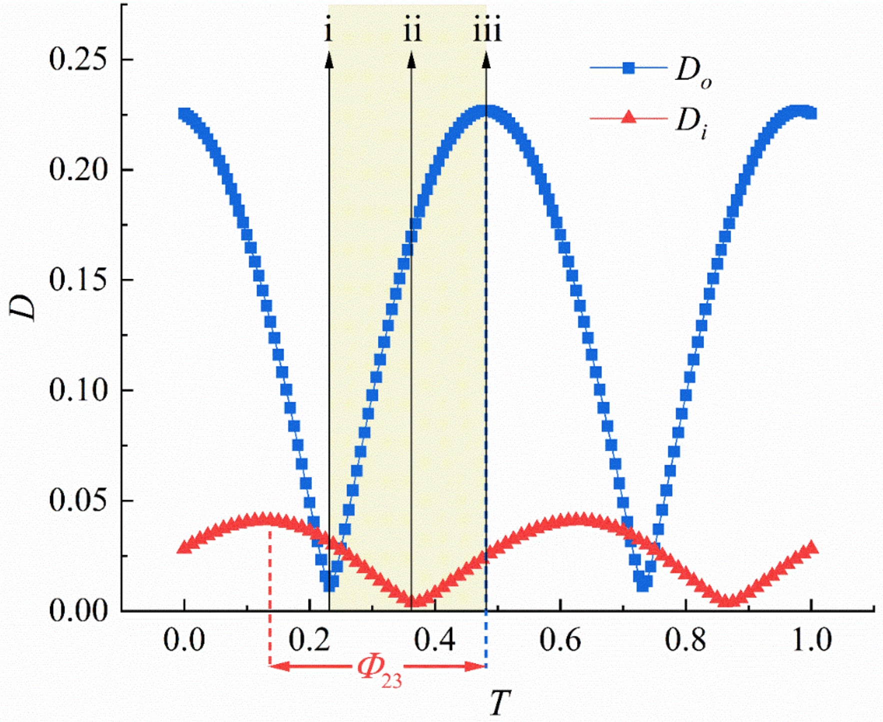
Oscillatory deformation

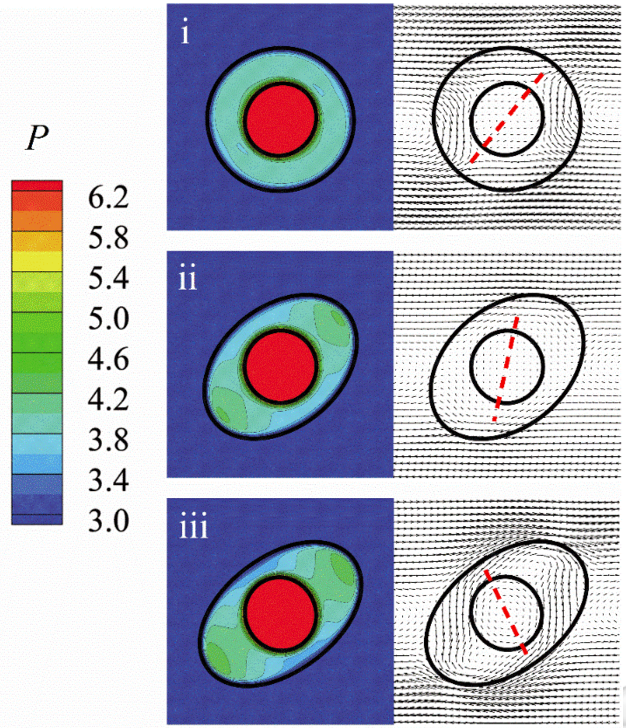
Effect of viscosity ratios



$\lambda_{21} = 0.1$

$\alpha = 1$

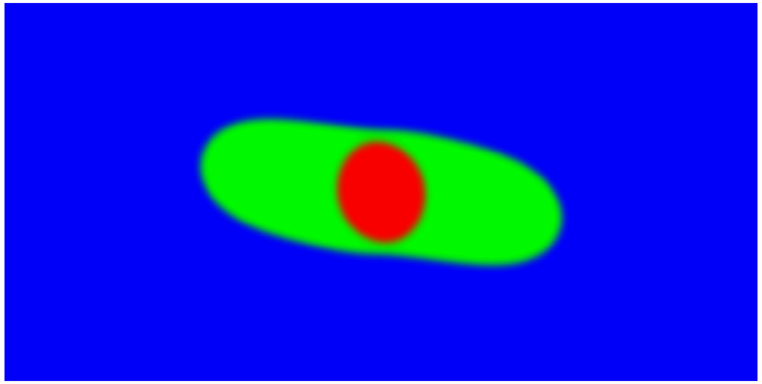


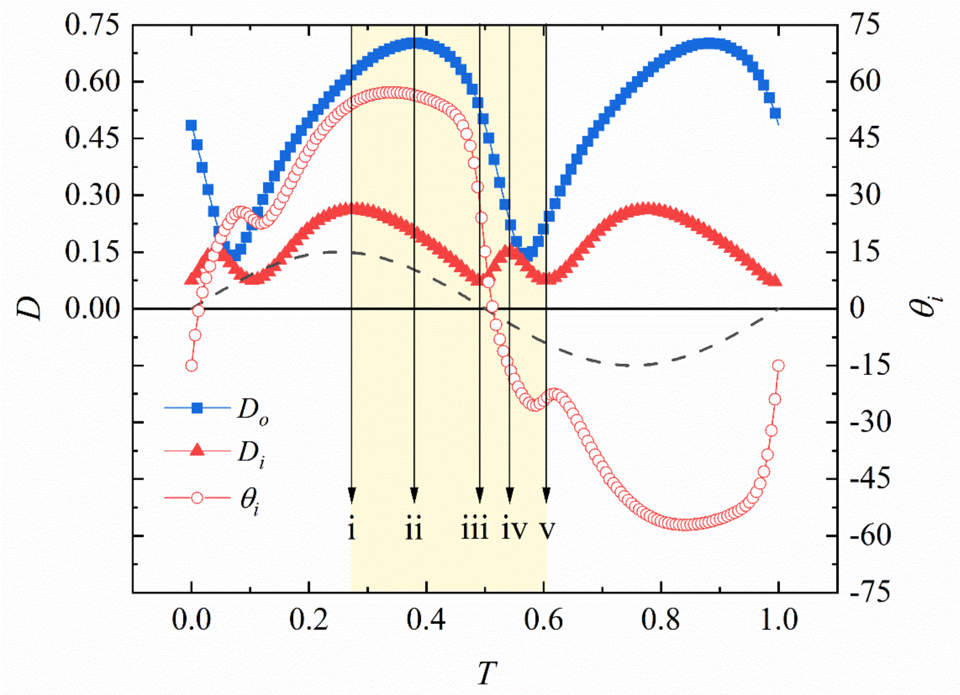


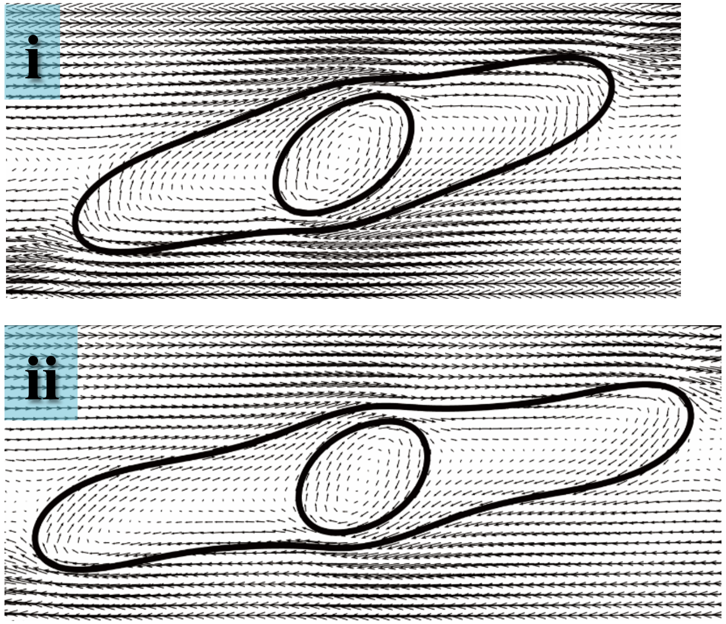
The pressure force has considerable impact on the dynamic behaviour of the inner droplet to suppress deformation against the viscous shear force. Combining the two **opposite mechanism** results in phase advance between the core and shell.

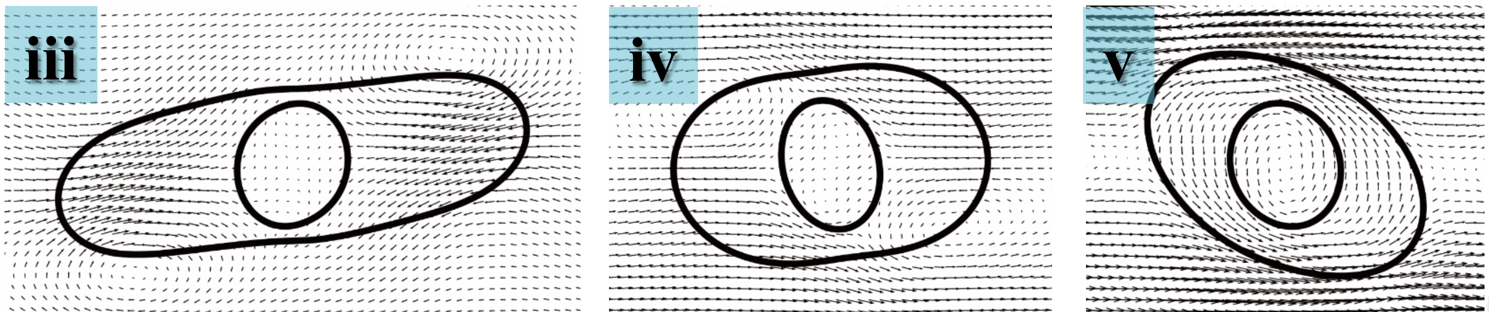
Oscillatory deformation

Effect of the capillary number *Ca*





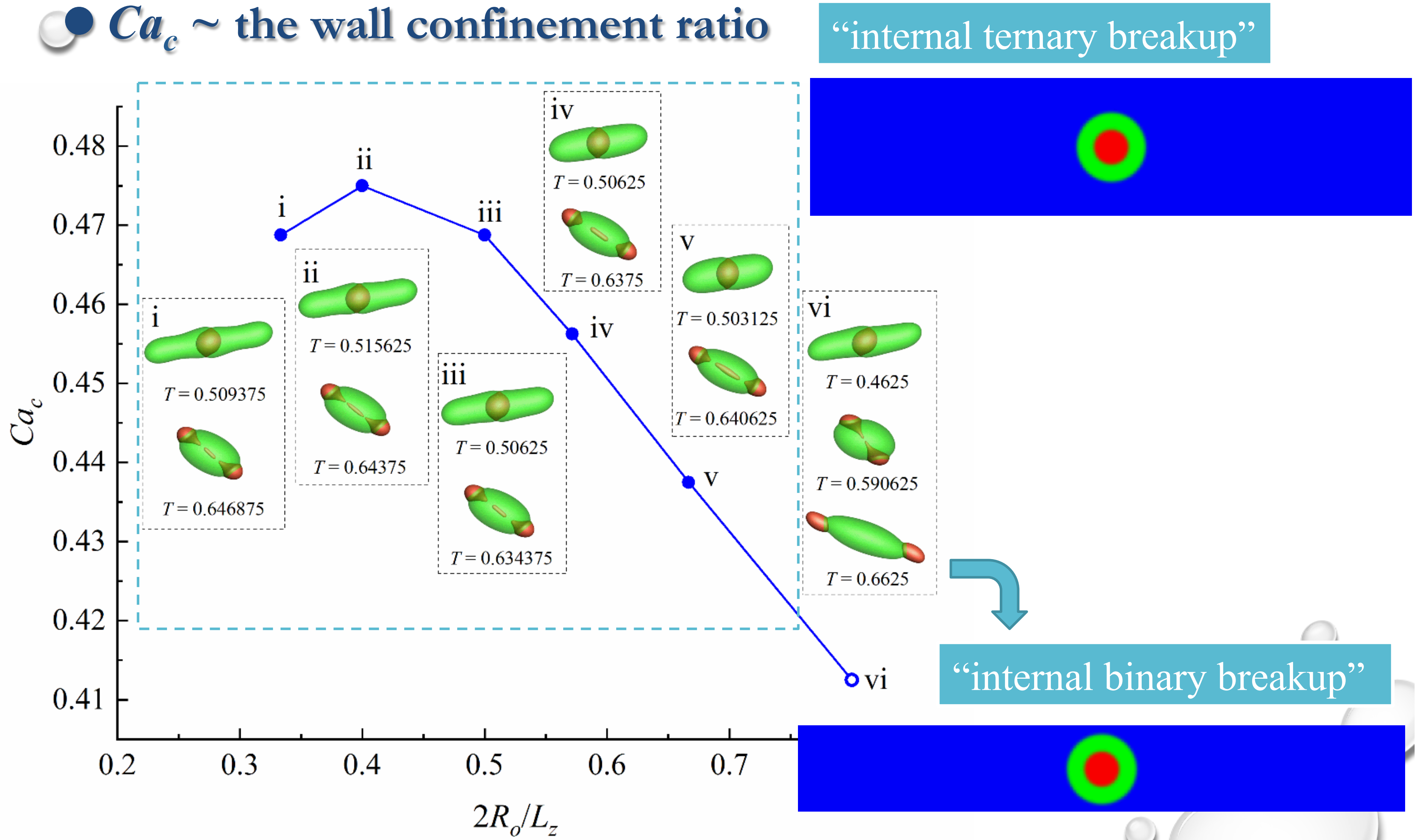




$Ca = 0.4625$ multipeaked oscillations

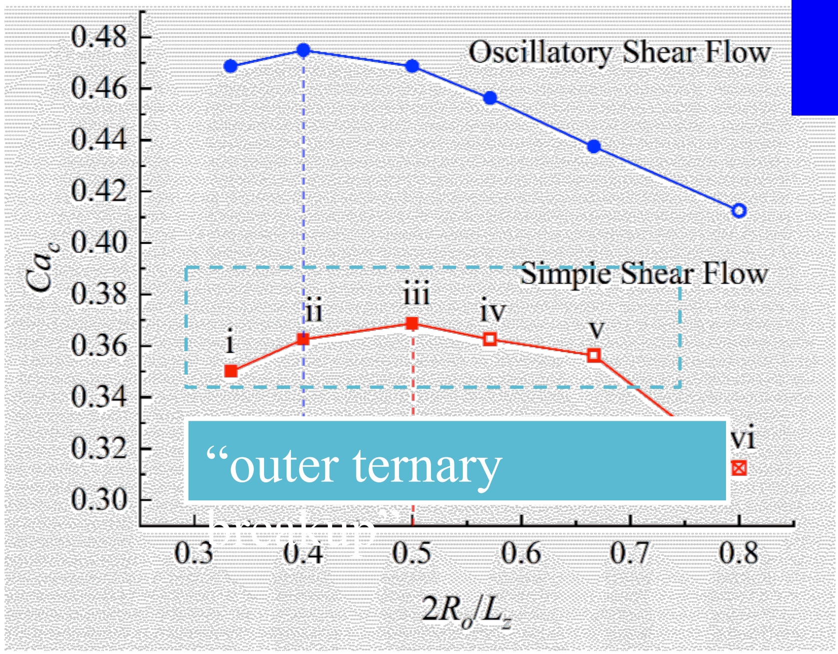
Breakup of a compound droplet

- Ca_c ~ the wall confinement ratio

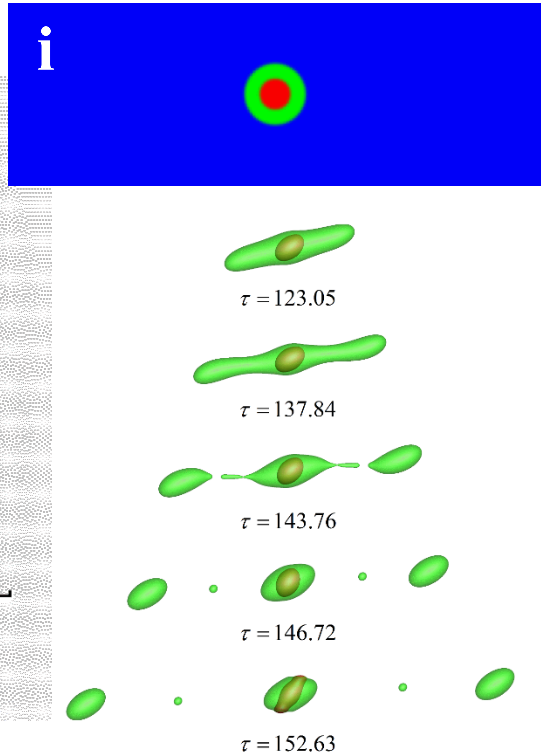


Breakup of a compound droplet

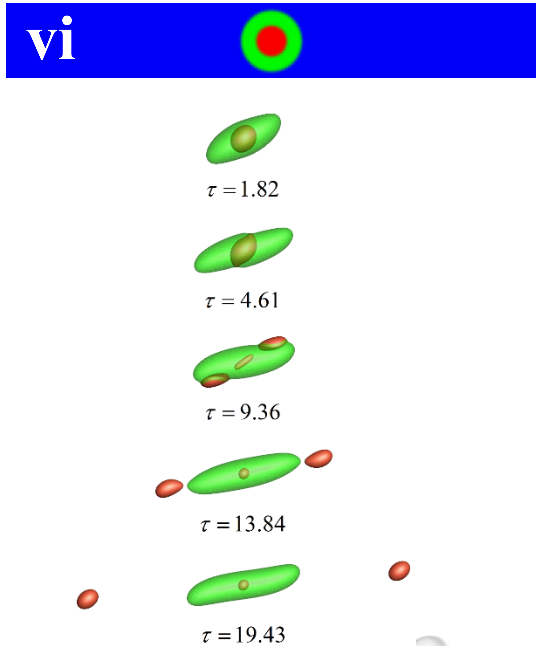
Oscillatory shear vs Simple shear



“outer ternary breakup”



“inner ternary breakup”

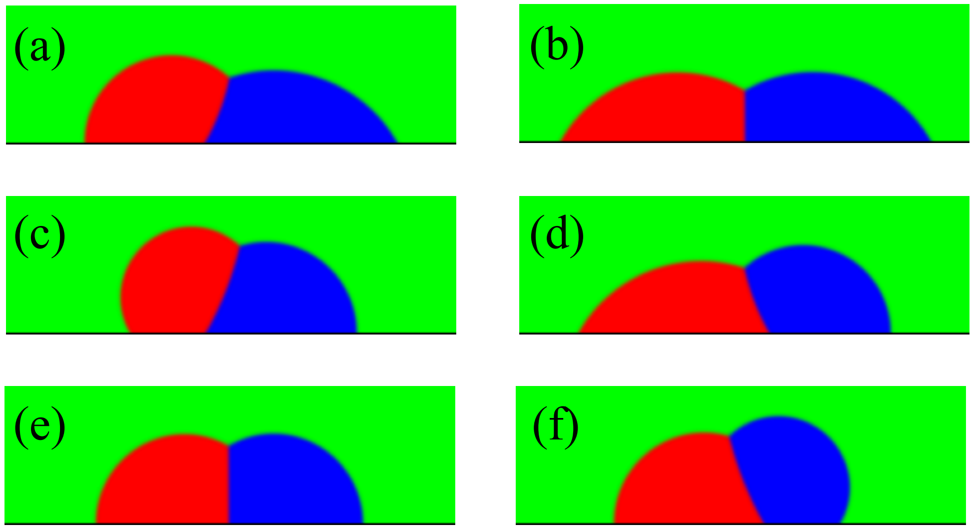


- ✓ The variation trend for Ca_c is quite similar between the two.
- ✓ Ca_c for breakup in oscillatory shear is found to be higher.
- ✓ Two breakup modes are identified for either shear flow, and their transition occurs at a high confinement ratio.

Numerical simulation of immiscible three-phase flows with contact-line dynamics on curved substrates

Extended a multiple-relaxation-time colour-gradient LB model to the simulation of immiscible three-phase flows with contact-line dynamics on curved substrates through the implementation of a characteristic moving-contact-line model.[1]

- **Janus droplet on a flat surface**



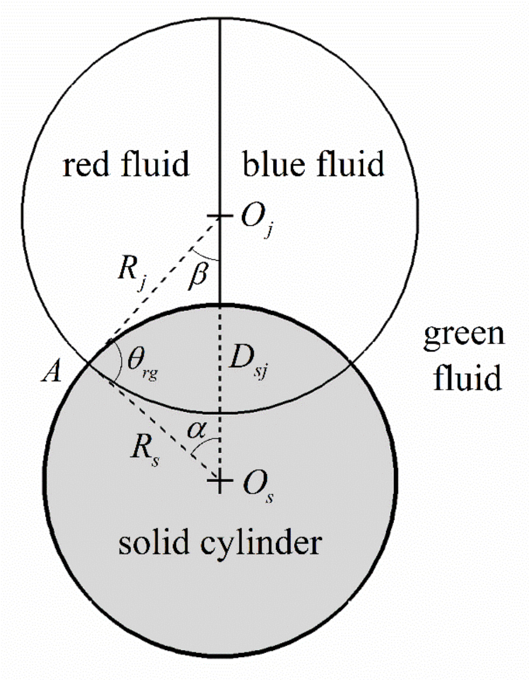
	θ_{rg}	θ_{br}	θ_{gb}
(a)	**90°**	**60°**	**120°**
	89.1°	61.0°	120.0°
(b)	**60°**	**90°**	**120°**
	59.7°	90.0°	119.9°
(c)	**120°**	**60°**	**90°**
	118.2°	60.8°	90.9°
(d)	**60°**	**120°**	**90°**
	60.0°	119.1°	90.9°
(e)	**90°**	**90°**	**90°**
	89.1°	90.0°	90.9°
(f)	**90°**	**120°**	**60°**
	89.1°	119.2°	61.8°

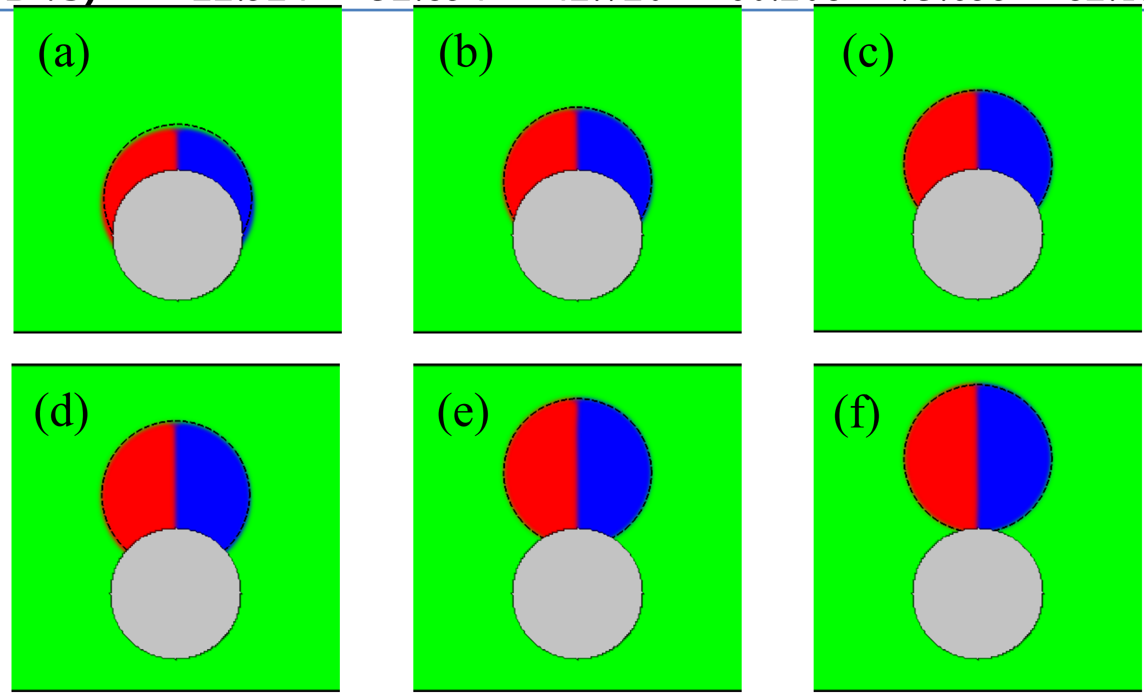
[1] Liu, H.-R., Ding, H. (2015) J. Comput. Phys., 294:484-502.

● Perfect Janus droplet on a cylinder

$$\begin{cases} \sigma_{rg} = \sigma_{gb} \quad \sigma_{br} = 0 \\ \theta_{rg} = \theta_{bg} \quad \theta_{br} = 90^\circ \end{cases}$$

	(a)	(b)	(c)	(d)	(e)	(f)
$\theta_{rg} = \theta_{bg}$	**30°**	**45°**	**60°**	**90°**	**120°**	**150°**
D_{sj}	22.524	32.854	42.720	60.208	73.655	82.114

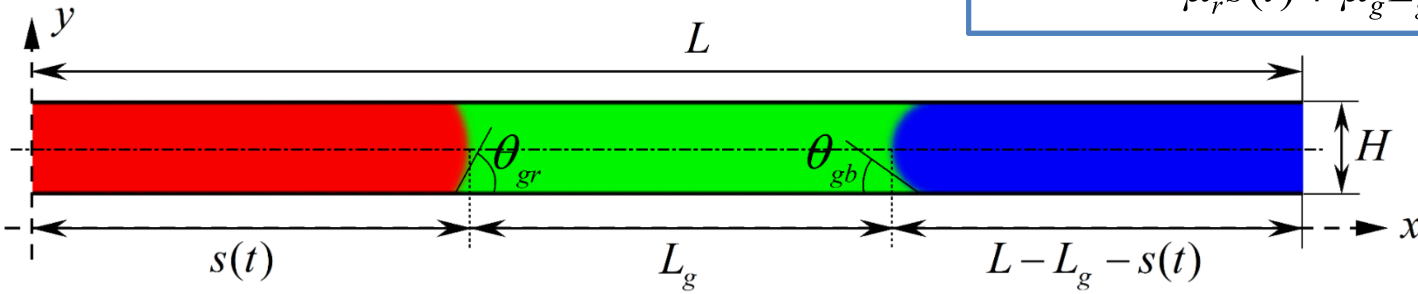




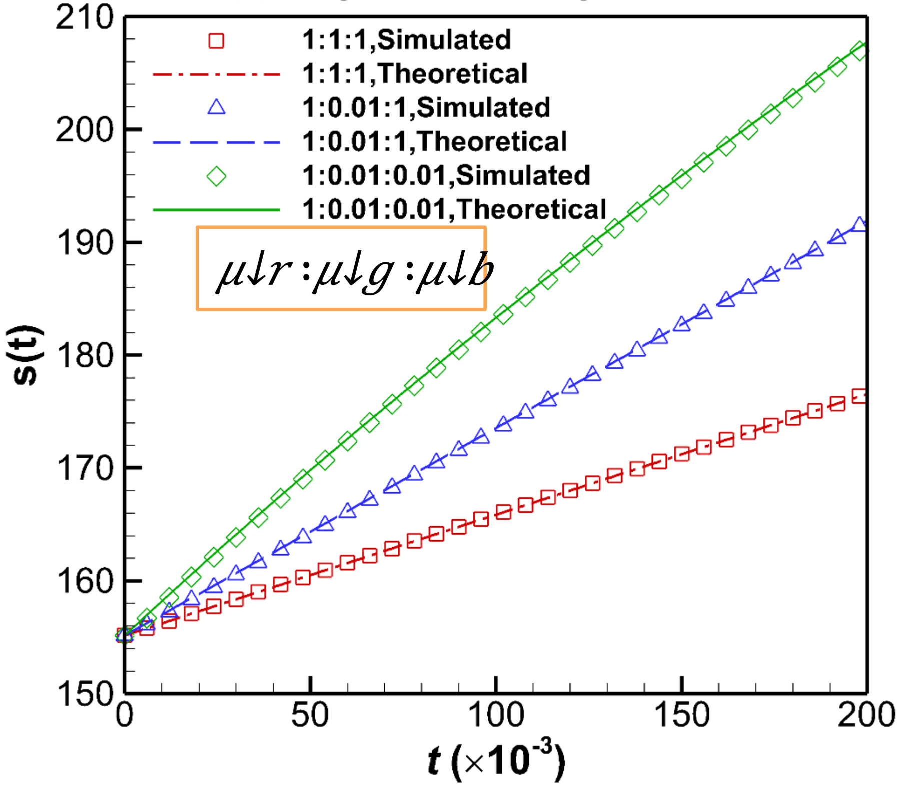
$R_s = 40,\ R_j = 45$

Capillary filling of ternary fluids

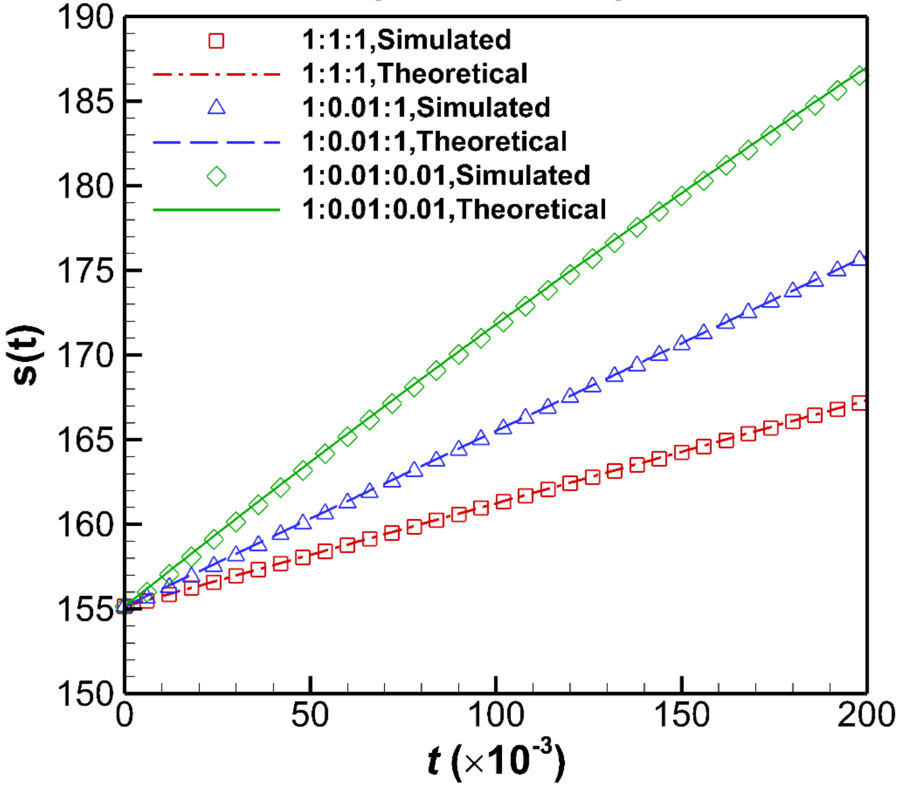
$$\frac{\mathrm{d}s(t)}{\mathrm{d}t}=\frac{H}{6}\frac{\sigma_{gb}\cos\theta_{gb}-\sigma_{gr}\cos\theta_{gr}}{\mu_r s(t)+\mu_g L_g+\mu_b\left[L-L_g-s(t)\right]}$$



(a) $\theta_{gr}=60°$, $\theta_{gb}=30°$



(b) $\theta_{gr}=60°$, $\theta_{gb}=45°$



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Deformation and breakup of a compound droplet in three-dimensional oscillatory shear flow

Haihu Liu [a], Yang Lu [a], Sheng Li [a], Yuan Yu [b], Kirti Chandra Sahu [c]

Sheng Li, Yang Lu, Fei Jiang, et al. Lattice Boltzmann simulation of three-phase flows with moving contact lines on curved surfaces. (submitted to *Physical Review E*, under review)

As a Marie Curie Early-Stage Researcher, I participate in the project “**ExtremeWaves**”, which focuses on better numerical and computational modelling of extreme water wave.

Progress Review

Training Plan

- **MATH5453M Foundations of Fluid Dynamics** (Semester 1, 30 credits)

  Theoretical part: fundamental theoretical concepts of fluid dynamics and their application on solving engineering and scientific problems. (T1, T2, T3, T4 and Final Exam)

  Numerical part: Finite Difference, Finite Volume and Finite Element Methods (N1, N2, N3)

- **COMP5454M Fluid-Structure Interactions** (Semester 2, 15 credits)

Or

- **MATH5458M Advanced Geophysical Fluid Dynamics** (Semester 2, 20 credits)

  Depending on whether the two workshops at MARIN can be added.

Constructing social media and personal webpage…

https://www.linkedin.com/in/yang-lu-902438200/

Thank you!

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