Technische Universiteit Eindhoven University of Technology

Where innovation starts

Università di Roma Tor Vergata

HPC-LEAP Mid-term Meeting ESR 7

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HPC-LEAP
EUROPEAN JOINT DOCTORATES

Contents

- Introduction
- Career development plan
- Current progress:
  - *Influence of thermal fluctuating on ligaments break-up*
  - *Wettability of particle in multicomponent fluid*
- Future research plan

Introduction about myself

Education:

Bachelor : Control Science and Engineering

***Harbin Institute of Technology*, Harbin, China**

Boston University, Boston, **U.S.A.** (Summer semester)

Master: Computational Science and Engineering

***Technical University of Munich*, Munich, Germany**

ETH Zurich, Zurich, **Switzerland** (Master thesis)

Ph.D.: Physics

Eindhoven University of Technology, Eindhoven, **the Netherlands**

University of Rome Tor Vergata, Roma, **Italy**

Innsbruck, 2017

Secondments:

Eurotech: M27 – M30

Scaling and performance tests of novel algorithms

Experience in HPC-LEAP

Experience in HPC-LEAP:

Workshops:

1. Numerical analysis and algorithms towards exascale, *Wuppertal, Germany* (COS-1); *Juelich, Germany* (COS-2)
2. School on HPC architectures and large-scale numerical computation, *Juelich, Germany* (COS-1); *Dublin, Ireland* (COS-2)
3. JBMC course on computational fluid dynamics in turbulence, *Delft, The Netherlands*
4. Lattice Boltzmann 2016, *Rome, Italy*
5. HPC Applications to complex and turbulent flows, *Rome, Italy*

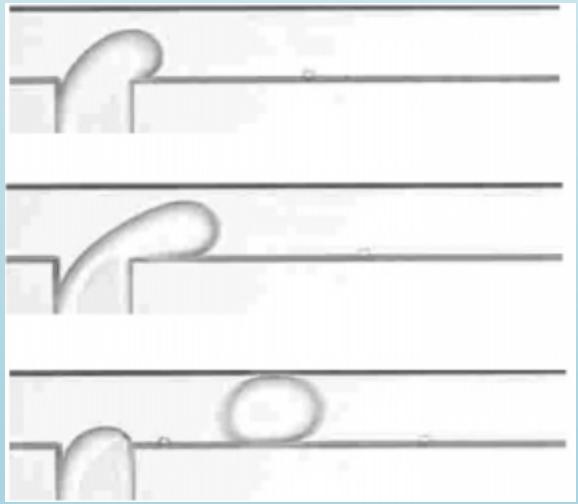
Conferences & talks:

1. Talk: *Applications of fluctuating lattice Boltzmann*, **HPC Applications to complex and turbulent flows**, Rome, Italy, Oct, 2016
2. Talk: *Influence of thermal fluctuations on a ligament breaks up: a fluctuating lattice Boltzmann study*, **FLOWING MATTER 2017**, Porto, Portugual, Jan 2017
3. Talk: *Influence of thermal fluctuations on ligaments break-up: a fluctuating lattice Boltzmann study*, **International DSFD conference 2017**, Erlangen, Germany, July 2017
4. Attend: **FOM physics conference**, Veldhoven, the Netherlands, Jan 2017

Career Development Plan & motivation

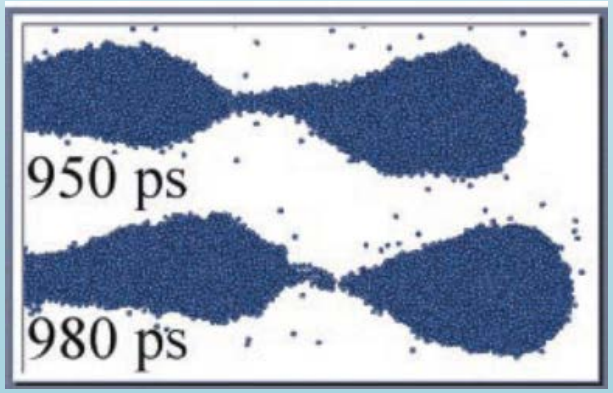
CDP:

1. *High Performance computing in novel LBM algorithm*
2. *Applications of Fluctuating hydrodynamics*
3. *Finite size particles in Micro-nano fluidics*



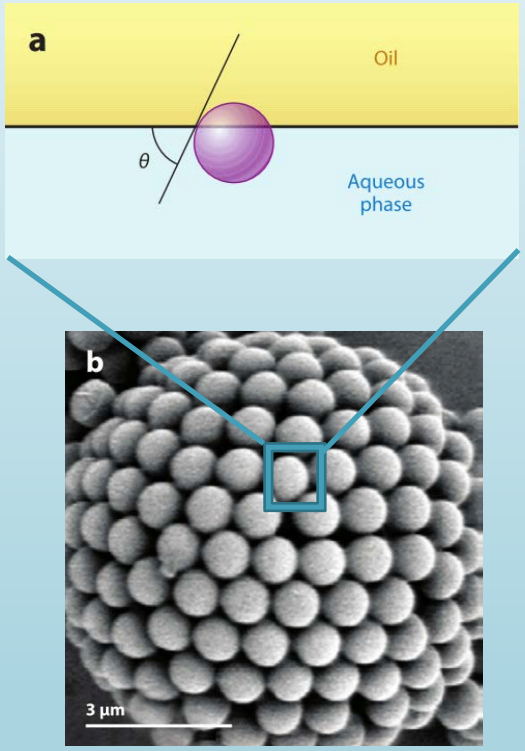
Droplet formation in T-shaped microchannel[1]

1. S Van der Graaf, et al. Langmuir,2006



Breakup of nanojets[2]

2. Michael Moseler and Uzi Landman, Science, 2000



Pickering emulsions[3,4,5]

3. CC Berton-Carabin, et al. Annual review of food science and technology, 2015

4. Aveyard et al. (2003)

5. Dinsmore et al. 2002).

The methodology of FLBM

Optimum for parallelization

Local update

lattice Boltzmann model [1,2](ESR 1, 4)

Fluctuation Dissipation Theorem

Essential at the small scale

Brownian motion

1. R

2. X

Fluctuating Multicomponent Lattice Boltzmann Model

D. Belardinelli,[1,*] M. Sbragaglia,[1,†] L. Biferale,[1,‡] M. Gross,[2,3,§] and F. Varnik[4,¶]

[1] *Department of Physics, University of Rome "Tor Vergata", Via della Ricerca Scientifica 1, 00133, Rome, Italy.*

[2] *Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, Germany*

[3] *Institut für Theoretische Physik IV, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany*

[4] *Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Universitätsstr. 150 44780 Bochum, Germany*

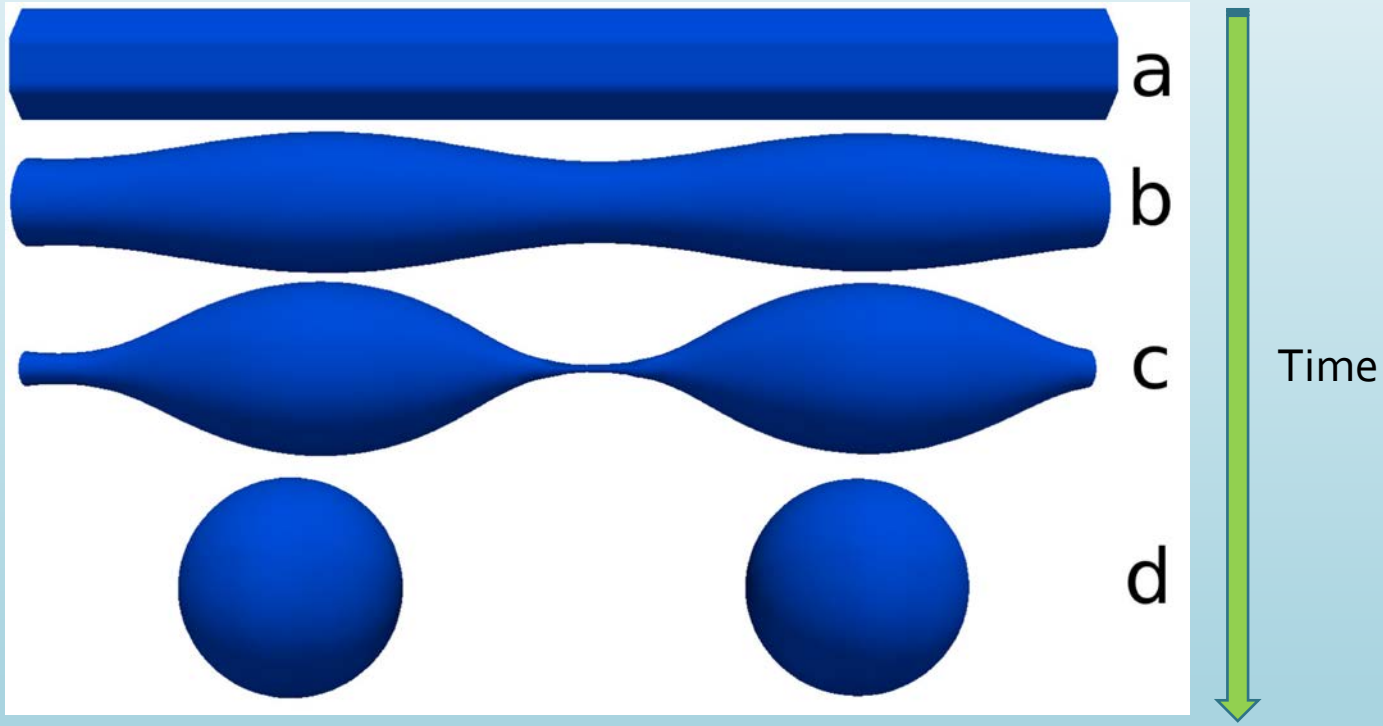
(Dated: November 16, 2016)

Phys. Rev. E

Study of ligament breaks up

Ligament breaks up

- Periodic boundary condition
- Measurement: marching tetrahedron algorithm



Evolution of ligament break-up dynamics

Study of ligament breaks up

Axisymmetric Lubrication theory ⟺ **lattice Boltzmann model**

Axisymmetric Lubrication theory

$$\partial_t h^2 + (h^2 v)' = 0, \qquad (1)$$

$$\partial_t (h^2 v) + (h^2 v^2)' = -G' + 3(h^2 v')' + D(hN)', \qquad (2)$$

T= 4.8090

T= 9.1809

T is **dimensionless** time unit

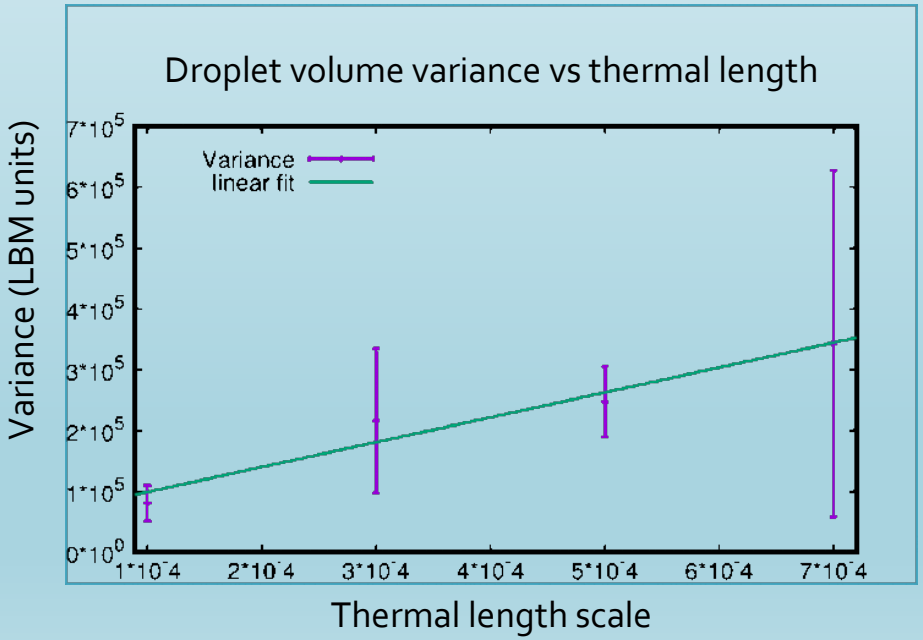
Study of ligament breaks up

ligament breaks up without thermal fluctuations

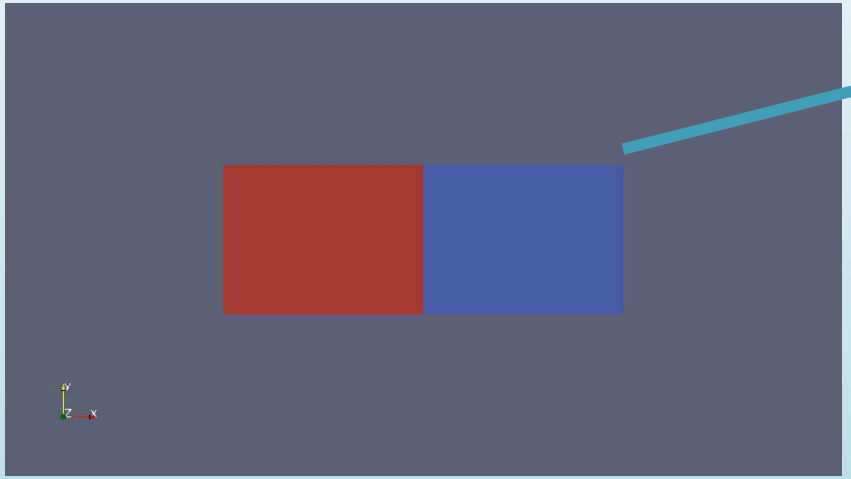
ligament breaks up with thermal fluctuations

Thermal length: L_t = 0.1

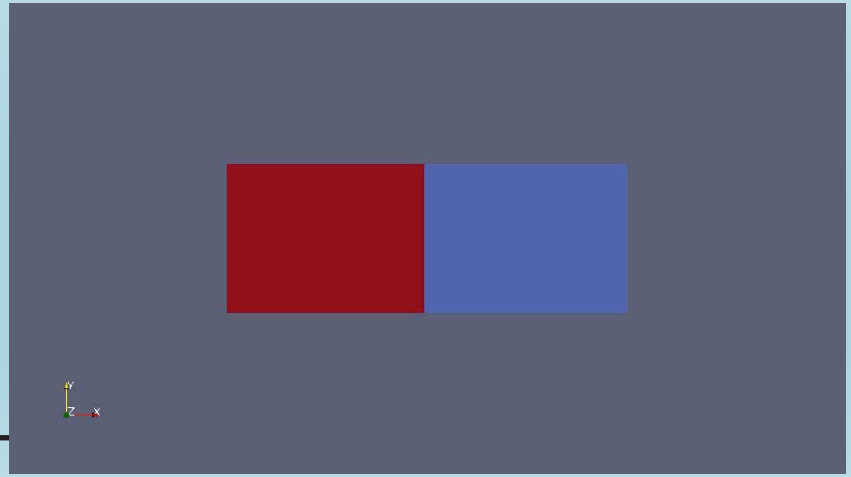
- Domain size: N_x X N_x X N_x - 96X96X256
- Simulation timesteps: 20,000
- Number of simulations for each data sets: > 200
- Volume measurement: marching tetrahedron algorithm



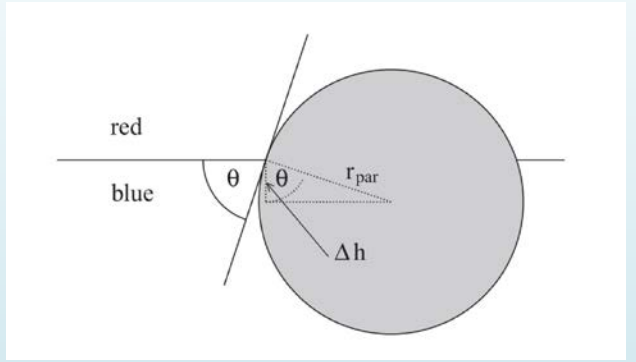
Wettability of Particle

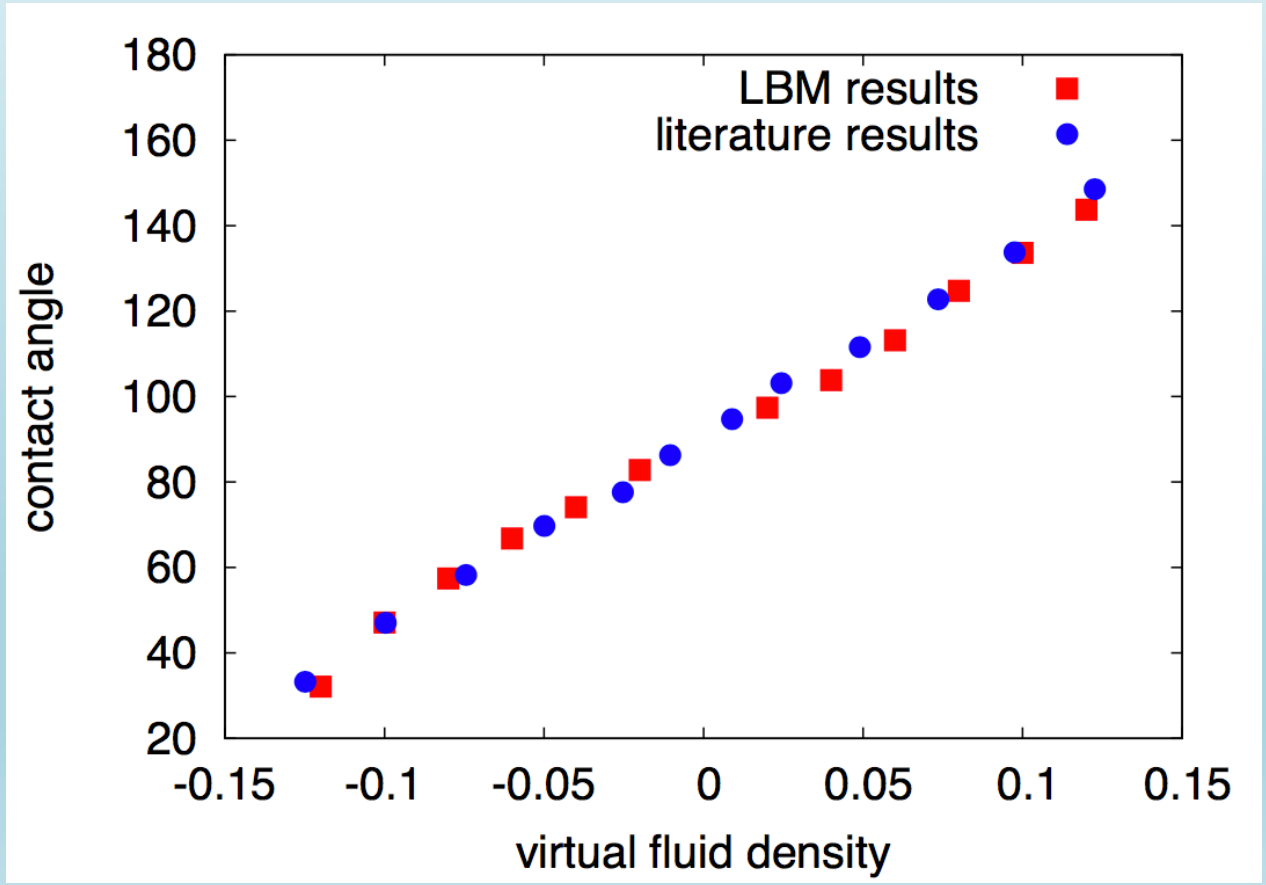


Particle virtual density 0.02



Particle virtual density 0.1





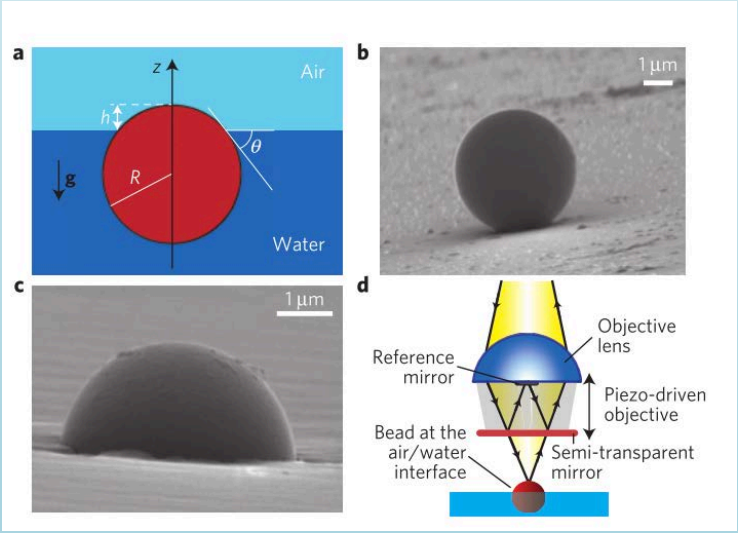
Future research plan

Ligaments break-up and stochastic lubrication theory

- Modeling multicomponent axisymmetric stochastic lubrication equations (SLE)
- Comparison of SLE-theory: for both multiphase or multicomponent
- Explore on **HPC supercomputing resource** for statistical purpose

Particle at fluctuating interface

- Brownian diffusion of a partially wetted colloid
- Influence of capillary force to the **finite-size particle** at **fluctuating** interface



1. Giuseppe Boniello, et al. Nature material, 2015

Acknowledgement

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Thank you for your attention!

Questions?

Reference

[1] D Belardinelli, M Sbragaglia, L Biferale, M Gross, and F Varnik. Fluctuating multicomponent lattice boltzmann model. *Physical Review E*, 91(2):023313, 2015.

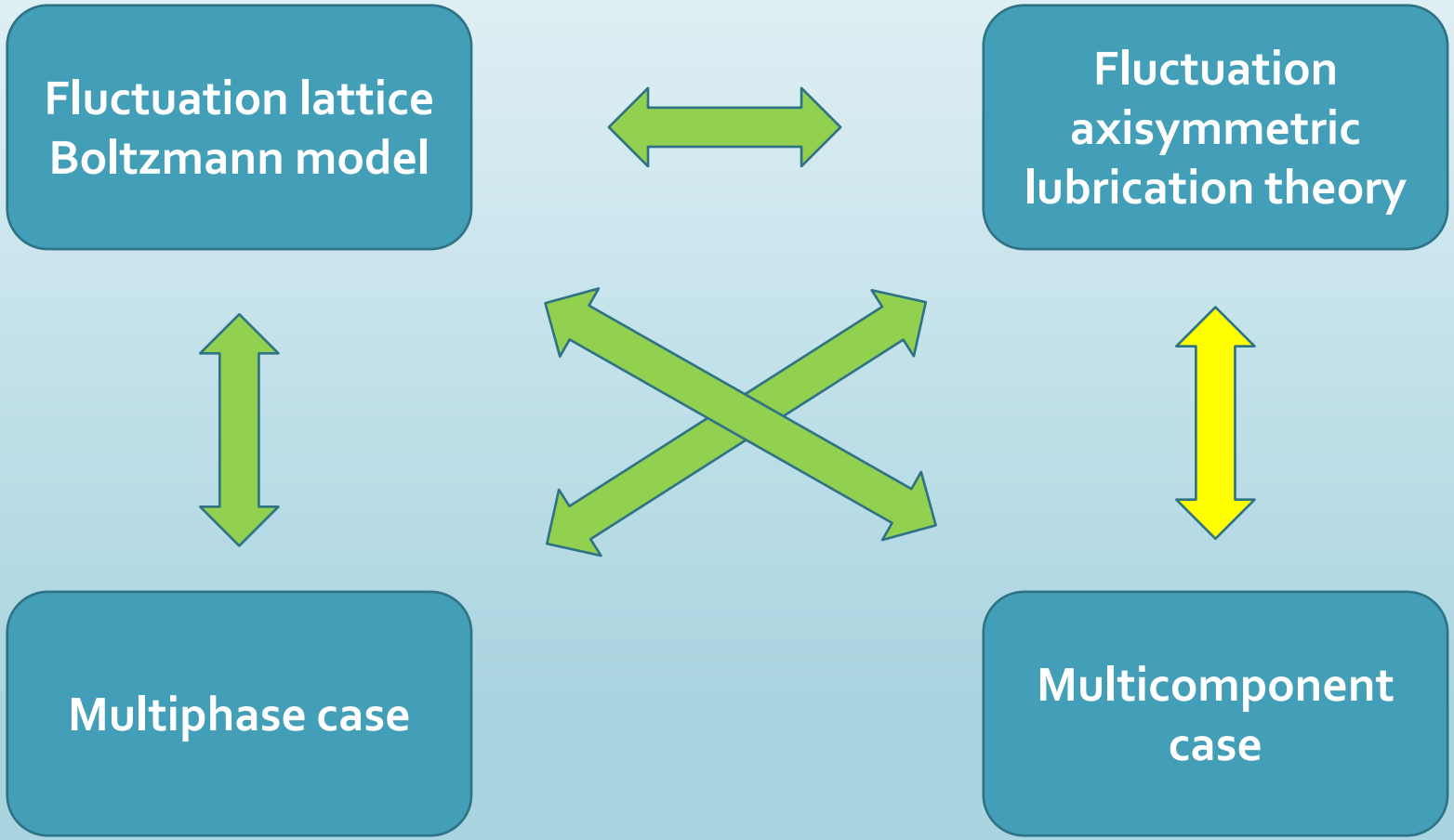
[2] Sudhir Srivastava, JHM ten Thije Boonkkamp, and Federico Toschi. The lattice boltz- mann method for contact line dynamics. 2011.

[3] Sauro Succi. *The lattice Boltzmann equation: for fluid dynamics and beyond*. Oxford university press, 2001.

[4] S Van der Graaf, T Nisisako, C Schroen, RGM Van Der Sman, RM Boom. Lattice Boltzmann simulations of droplet formation in a T-shaped microchannel, Langmuir 22 (9), 4144-4152, 2006

[5] K van Dijke, G Veldhuis, K Schroën, R Boom, Parallelized edge-based droplet generation (EDGE) devices, Lab on a Chip 9 (19), 2824-2830, 2009

Study of ligament breaks up



Summery

- ✓ **Introduction and research interests**
- ✓ **Current research progress**
  - ➢ **Ligaments break-up**
    - The FLBM model can be use to study the fluctuating multicomponent fluid: eg. ligament break-ups
    - The droplet distribution with different KbT has been measured
    - We have measured the relationship between KbT and variance of droplet size.
  - ➢ **Wettability of single particle**
    - Contacted angles are matched with Jens 2011 for different wettability of the particle
- ✓ **Future plan**