# HPC-LEAP Mid-Term Meeting: ESR4

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# Outline

# Academic background and training during HPC-LEAP

## Academic background

- Bachelor of Science in Physics at University of Bayreuth
- Master of Science in Theoretical Physics at Leiden University

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## HPC-LEAP Workshops/Secondment

- HPC-LEAP workshop series in numerical analysis and algorithms (CoS-1) in Wuppertal and Juelich
- HPC-LEAP workshop series in HPC architetctures and numerical methods (CoS-2) in Juelich and Dublin
- HPC-LEAP workshop "HPC technologies in complex and turbulent flows" in Rome (oral presentation)
- planned secondment at University of Wuppertal (BUW) in preconditioning methods

## Other venues

- JMBC course "Turbulence" in Delft
- CISM school "Multiscale Modeling of Flowing Soft Matter and Polymer Systems" in Udine
- conference "Lattice Boltzmann 2016" in Rome
- DSFD 2017 conference in Erlangen, oral presentation: "Multi-scale LBM simulations of droplets in time-dependent flows"

# Droplets in turbulence

## Carreer Development Plan (CDP)

- Optimal algorithms for modelling finite size particles with internal dynamics in turbulent flows
- Two-way coupling approach (Eulerian-Lagrangian) via a combined LBM-pseudo-spectral algorithm

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# The meso-scale: between fields and particles

## Navier-Stokes equations

$$\nabla \cdot \mathbf{v} = 0$$

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v}$$

## Hamilton's equations

$$\dot{\mathbf{q}}_i = \frac{\partial H(\{\mathbf{q}_i, \mathbf{p}_i\})}{\partial \mathbf{p}_i}$$

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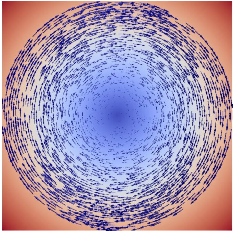
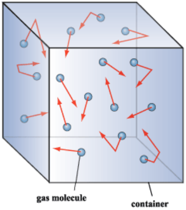


**Meso-scale**



# The meso-scale: the Lattice Boltzmann Method

## Boltzmann equation and Lattice Boltzmann Equation (LBE)

$$\partial_t f(\mathbf{x}, t) + \mathbf{v} \cdot \nabla f(\mathbf{x}, t) = \mathrm{Coll}(f(\mathbf{x}, t))$$

$$\underbrace{f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t)}_{\textbf{Streaming}} = \underbrace{\Delta t \, \mathrm{Coll}(f_i(\mathbf{x}, t))}_{\textbf{Collision}}$$

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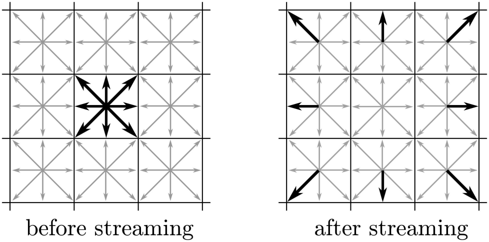
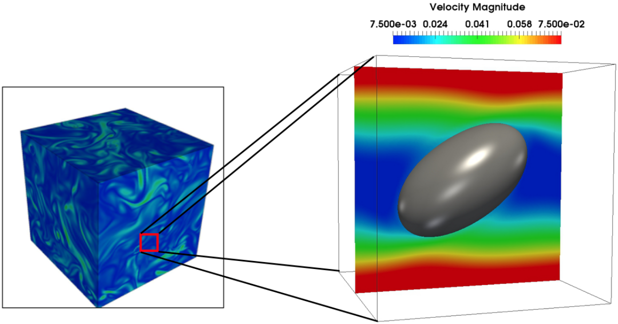


# LBM simulations of droplets in time-dependent flows




Scale separation: turbulent flow $\leftrightarrow$ droplet size

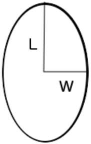
# Quantitative analysis

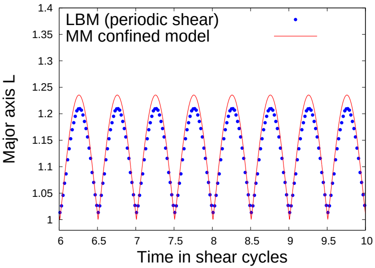
## Maffettone-Minale model

$$\frac{dM}{dt} = \underbrace{[f_2(Ca)(S \cdot M + M \cdot S) + \Omega \cdot M - M \cdot \Omega]}_{\textbf{droplet stretching}} - \underbrace{f_1(Ca)R(M)}_{\textbf{droplet relaxation}}$$

$M$: Droplet deformation tensor $S$, $\Omega$: Shear tensor parts

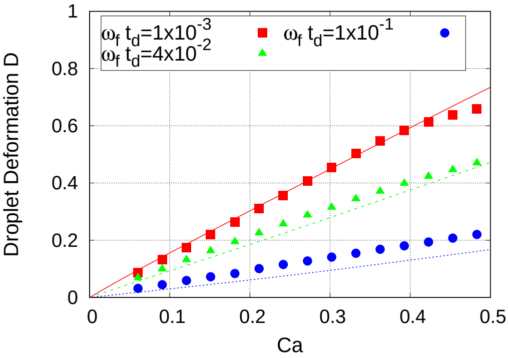
$Ca$: Capillary number (shear / surface forces)



## Parameters

$t_d$ : Droplet relaxation time $\omega_f$: shear frequency




Deformation $D$ for droplet response factors $\omega_f t_d$

# Conclusion and outlook

Accomplished tasks:

- **LBM algorithm** modelling a **time-dependent boundary condition** for an external flow field implemented and tested
- successful benchmark of the deformation of a **finite size particle with internal dynamics** in a **synthetic shear flow**

Future plans:

- replacement of the external synthetic flow with a turbulent signal produced via a **pseudo-spectral** code
- quantitative **multi-scale** analysis of droplet morphology in a **turbulent flow**

# Acknowledgements

HPC-LEAP
EUROPEAN JOINT DOCTORATES

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Tor Vergata

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**Eindhoven**
University of Technology
**Where innovation starts**