4th Workshop on Advances in CFD, LB and MD Modeling of Capillary Two-Phase Flows and Experimental Validation

May 16th-19th, 2019, Rio de Janeiro, Brazil

The Workshop precedes ICMF 2019 (May 19th-24th, Rio de Janeiro)

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Workshop description

We are happy to present this Workshop on the latest advances in the computational modelling of the interfacial dynamics of capillary two-phase flow phenomena using Computational Fluid Dynamics (CFD), Lattice Boltzmann (LB) and Molecular Dynamics (MD) methods. The Workshop is now at its 4th edition, following the 2016-2017 editions at the EPFL in Lausanne, Switzerland, and the 2018 edition at Kobe University, Japan.

The international team of lecturers is as follows: Prof. A. Tomiyama, S. Hosokawa and Prof. K. Hayashi (Kobe University), Prof. J.R. Thome (University of Edinburgh), Prof. G. Anjos (Federal University of Rio de Janeiro), Prof. N. Mangiavacchi (State University of Rio de Janeiro), Prof. G. P. de Oliveira (Federal University of Paraiba), Prof. P. Theodorakis (Polish Academy of Sciences) and Dr. M. Magnini (Imperial College London).

Direct numerical simulation of two-phase flows is an active field of research since the beginning of the computational fluid dynamics in the early sixties. However, thanks to the exponential increase of the computer performance observed in the latest decades, the computational modelling of two-phase flows is advancing rapidly towards more complex and heterogeneous approaches, thus yielding unprecedented insight into the essential aspects of the flow. CFD techniques model the flow at the continuum-scale and consider a sharp gas/liquid interface with zero thickness. Intermolecular forces determining the interface physics are not directly captured, but their effect is modelled by introducing a surface tension force concentrated at the sharp interface. This Workshop tackles in detail the most popular CFD techniques to capture the interface dynamics across a fixed computational mesh, i.e. Volume Of Fluid and Level Set method, and a novel Arbitrary Lagrangian-Eulerian moving mesh methodology. LB methods adopt a meso-scale description of the flow based on the discrete Boltzmann equation and collision models to simulate the fluid flow. This allows simple numerical codes, easy parallel implementations, and fast computation of the multiphase flows with complicated boundary conditions. MD predicts the evolution of individual, but interacting, molecules. As a more fundamental model, MD captures a much greater range of phenomena with no additional assumptions and therefore it yields a more detailed molecular level exploration of the interfacial region thermophysics. The Workshop also focuses on quantitative experimental flow visualization techniques which are pertinent to the experimental validation of numerical methods. The global tendency towards miniaturization driven by micro-electronics, as well as by the pharmaceutical and fuel cell industries, to name a few, is bringing ever greater attention to microscale two-phase flows. In this context, surface tension and phase change represent important aspects that require ad-hoc numerical modelling and are encompassed in this course.

The present Workshop is addressed to PhD students, postdoctoral researchers and industrial specialists involved in both experimental and numerical investiga-
tion of two-phase flows, i.e. all those who wish to get acquainted with the traditional background and the most recent developments on the heterogeneous interface modelling strategies mentioned above for capillary two-phase flows. These will be elaborated by the leading scientists who will lecture on the field of CFD, LB and MD modelling of interfacial flows. The Workshop is designed to promote interaction during and after the lectures: the participants are invited to present their research in a dedicated session which will take place on the first day of the course; practical “hands-on” sessions are scheduled on three afternoons, where the participants will apply and develop the codes provided by the lecturers to simulate benchmark flow configurations.

Workshop location and travel information

The Workshop will be held at the Federal University of Rio de Janeiro (UFRJ), Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia (COPPE/UFRJ), Cidade Universitaria, Bloco G, Mechanical Engineering Department (Google Maps): the room number will be communicated before the Workshop. The end of the Workshop coincides with the beginning of the 10th International Conference on Multiphase Flow (ICMF 2019), which will take place in Rio de Janeiro on May 19th-24th, 2019.

Workshop registration and inscription fee

The Workshop does not have any registration fee in order to promote the participation of students/researchers. The link to the registration page can be found on the website of the Virtual International Research Institute of Two-Phase Flow and Heat Transfer (VIR2AL). When registering, participants will be invited to submit a brief personal overview of their research and interests in two-phase flow. The registration deadline is April 1st, 2019. You are encouraged to register as soon as possible. A maximum number of 40 participants will be accepted. As this is an advanced course, it is expected that participants already have a working knowledge of numerical fluid mechanics.

Schedule and contents of the lectures

THURSDAY, 16 May
8:30-10:00, 10:30-12:00 – Introduction and ALE-FEM formulation for two-phase flow, Prof. N. Mangiavacchi and Prof. G. P. de Oliveira. The first lecture will start with a brief introduction to the numerical simulation of flows with interfaces. Afterwards, the principles behind the Arbitrary Lagrangian-Eulerian Finite Element Method formulation (ALE-FEM) for solving two-phase flows with a moving interface will be presented. An overview of the conservation equations for two-phase flows written in a generalized formulation and the modelling of the interfacial forces will be explained, followed by an introduction to the FEM theory and the solution of a practical handmade 1D test case.

13:00-16:30 – Hands-on session, Prof. G. Anjos. The participants will follow a demonstration with the lecturer’s 2D ALE-FEM code for two-phase flows (based on the JCP’s article “A 3D Moving Mesh Finite Element Method for Two-Phase Flows”).

16:30-18:00 – “My research in 150 s” and apero. Participants are invited to present their research in 150 seconds (timing will be strictly enforced) in front of the class in a clear, concise and straightforward manner, with the support of two slides preloaded on our computer.

FRIDAY, 17 May
8:30-10:00 – Molecular dynamics simulation of fluid flows, Prof. P. Theodorakis. This lecture presents the underlying theory of molecular dynamics (MD) simulation and the basic structure of an MD code along with the most popular force-fields and numerical schemes. Material for different flavours of MD simulation will be provided and discussed with respect to their advantages and disadvantages. Particular examples will be discussed in the context of fluid dynamics, which can be used as a template for building your own MD simulation. The most important literature and state-of-the-art of MD will also be presented.

10:30-12:00 – Phase change modelling in interface capturing frameworks, Dr. M. Magnini. This lecture presents an overview of the most popular models for including phase change (evaporation/condensation) within interface capturing frameworks. The background theory, temperature boundary condition at the interface, and numerical implementation which are peculiar of each model are discussed. The differences between microscale and macroscale oriented formulations are debated. Mathematical techniques for the smoothing of the phase change source terms are introduced. Some typical validation benchmarks to assess the phase change models accuracy are illustrated. Results of CFD simulations aimed to investigate flow boiling within microchannels are described.

13:00-16:30 – Hands-on session, Dr. M. Magnini. This practical session shows how to set-up and run a two-phase flow simulation using the VOF method implemented in the open-source CFD toolbox OpenFOAM. The solver is first introduced; two benchmark configurations will be simulated by the participants: (1) the breaking of a dam and (2) the rise of a Taylor bubble in a vertical tube.

SATURDAY, 18 May
8:30-10:00, 10:30-12:00 – Fundamentals of lattice Boltzmann method and its application to two-phase flows, Prof. K. Hayashi. This lecture presents the fundamentals of the Lattice Boltzmann (LB) method, i.e. the solution algorithm of the LB equation for single phase flows, the numerical treatments for boundary conditions, and the multi-scale expansion of
the LB equation to deduce the continuity and Navier-Stokes equations. Numerical techniques for two-phase flows in the LB framework will then be given.

13:00-16:30 – Hands-on session, Prof. K. Hayashi. Several LB simulations will be demonstrated in this hands-on session to enhance understanding of the LB modeling given in the morning lecture.

SUNDAY, 19 May

8:30-9:30 – Mathematical bases of two-phase flow models, Prof. A. Tomiyama. Fundamental equations for predicting multiphase flows within the context of continuum dynamics are introduced in this lecture. Local instantaneous mass, momentum and energy equations and jump conditions at interfaces are derived from conservation laws and some integral theorems, and kinematic equations for interface tracking are deduced from a geometric equation of surface, and averaged field equations for multi-fluid and Euler-Lagrange models are derived from the local instantaneous equations and phase-definition functions. A simple method to derive semi empirical correlations and relevant dimensionless groups from local instantaneous equations and jump conditions is also introduced as a useful tool for developing a correlation from experimental or numerical data.

9:45-10:45 – Optical measurements for validation of numerical simulation of two-phase flow, Prof. S. Hosokawa. Experimental data are required for validation of models used in numerical predictions of two-phase flows. Since optical measurement methods such as laser Doppler velocimetry and image processing methods are not invasive and do not affect flow characteristics, they are frequently used for the validation. In this lecture, fundamentals of the measurement methods are explained and examples of validations of numerical predictions are presented. Advanced methods such as a small LDV probe and spatiotemporal filter velocimetry are also introduced to demonstrate their potential for validating numerical simulations.

11:00-12:00 – Measurement and image processing techniques for quantifying two-phase flows, Prof. J. R. Thome. This lecture will give an overview of several experimental techniques developed at the Lab. of Heat and Mass Transfer at EPFL for two-phase flow visualization and image processing. The 1st technique is for the measurement of dynamic void fractions in stratified and slug flows in horizontal tubes, using a laser sheet and high speed camera together with image processing to overcome the refractive index effect of the channel to the test liquid (refrigerants). The 2nd technique is for characterizing micro channel two-phase flows to determine: flow pattern, bubble frequency, bubble length, bubble velocity, bubble coalescence rates and indirectly the void fraction (bubbly and slug flows only), using a pair of lasers and diodes with signal processing. The 3rd technique is referred to as the “time-strip” method, that is an image post-processing method for high speed videos of two-phase flows, particularly suited for characterizing bubbly and slug flows. The 4th technique is micro-Particle Shadow Velocimetry, in which the shadows of particles are tracked from behind using LED lighting, rather than micro-PIV with front lighting by a laser requiring fluorescent particles, to obtain: bubble shapes, velocity flow fields, etc. Quantitative measurements are obtained for creating test cases for numerical validations and for the building of mechanistic models.

The lecturers

Prof. G. Anjos is Professor of Mechanical Engineering at the Federal University of Rio de Janeiro (UFRJ/COPPE), Brazil. He received his Ph.D. degree at the Swiss Federal Institute of Technology (EPFL). His doctoral thesis has been nominated for the EPFL best thesis award of 2012 and it has been published in the renowned Journal of Computational Physics in 2014. Additionally, Prof. Anjos has worked as Post-Doc at the Massachusetts Institute of Technology (MIT). His research interests include two-phase flows, scientific computing, fluid dynamics and heat and mass transfer. He is member of the Brazilian Society of Mechanical Sciences and Engineering (ABCM).

Prof. G. P. de Oliveira holds a D.Sc. degree in Mechanical Engineering from the State University of Rio de Janeiro (UERJ) and a post-doc in Computational Modelling. His expertise covers Applied Mathematics, Numerical Methods and Multiphase CFD. Currently, he is Adjunct Professor at Federal University of Para´ıba, Brazil, and member of the Management Committee of LaMEP - Petroleum Engineering Modelling Laboratory.

Prof. K. Hayashi is Associate Professor at the Graduate School of Engineering, Kobe University, Japan, since 2012. He was formerly Assistant Professor (2007-2008) and then Lecturer (2008-2009) at the Kobe City College of Technology, and Assistant Professor at the Kobe University (2009-2012). His research focuses on developing numerical methods for simulating complicated motions of bubbles and drops and correlations based on the bubble and drop mechanics.
Prof. S. Hosokawa is Associate Professor at the Graduate School of Engineering, Kobe University, Japan, since 1998. He was formerly Assistant Professor at the Kobe University (1993-1998). His research interests include development of optical measurements for single and multiphase flows, turbulence in dispersed two-phase flows, motion of fluid particles, mass and momentum transfer at an interface and generation method and application of microbubbles.

Dr. M. Magnini is a postdoc research associate at Imperial College London. He received a M. Sc. degree in Mechanical Engineering in 2007 from the Alma Mater Studiorum - Università di Bologna, Italy, and a Ph.D. degree in Energy Engineering in 2012 from the same institution. Before joining Imperial College, he was a post-doc at EPFL from 2013 to 2017. His research focuses on numerical simulations of two-phase flows with phase change within macro and microchannels, theoretical modelling of thin film dynamics and evaporation in microchannel flows.

Prof. N. Mangiavacchi received his Ph.D. in Mechanical Engineering and Scientific Computing at The University of Michigan, Ann Arbor, USA in 1994. He is currently Associate Professor of the Mechanical Engineering Department at the State University of Rio de Janeiro (UERJ). He directs the GESAR laboratory, an interdisciplinary group that is concerned on numerical and experimental modeling of complex flow phenomena, applied to environmental problems. Interest includes numerical simulation of multiphase flows.

Prof. P. Theodorakis is Assistant Professor at the Polish Academy of Sciences (Institute of Physics). He received his PhD from the University of Ioannina and carried out postdoctoral research in Germany (Max Planck Institute for Polymer Research), Austria (University of Vienna), and the United Kingdom (Imperial College London). He has also been a Marie Sklodowska-Curie and a Max Planck Fellow. His expertise lies within computer simulation in the areas of soft matter, polymer and statistical physics, biophysics, and fluids physics. Recent research in the area of fluids physics includes the superspreading of surfactant-laden flows, the directed fluid motion on gradient substrates, and the study of surface nanobubbles.

Prof. J. R. Thome is visiting Professor at the University of Edinburgh and Professor Emeritus at the Swiss Federal Institute of Technology in Lausanne (EPFL), Switzerland. His primary research interests are two-phase flow and heat transfer, covering both macro-scale and micro-scale heat transfer (boiling and condensation). He is chair of the Virtual International Research Institute on Two-Phase Flow and Heat Transfer (VIR2AL). He was also the Director of the ERCOFTAC European Coordination Center (European Research Community On Flow, Turbulence And Combustion) with about 180 affiliated universities, research centers and industrial companies, resigning this position in 2011.

Prof. A. Tomiyama is Professor at the Graduate School of Engineering, Kobe University, Japan, since 2003. He was formerly researcher at the Energy Research Laboratory at Hitachi Ltd. between 1984 and 1988, then Assistant Professor (1988-1991) and Associate Professor (1991-2002) at the Kobe University. In 2011 he became Vice Dean at the Graduate School of Engineering, Kobe University, and Dean since 2015. His research interests are experimental and numerical investigation of multiphase flows in nuclear reactors, chemical plants, fuel injectors and environmental systems.