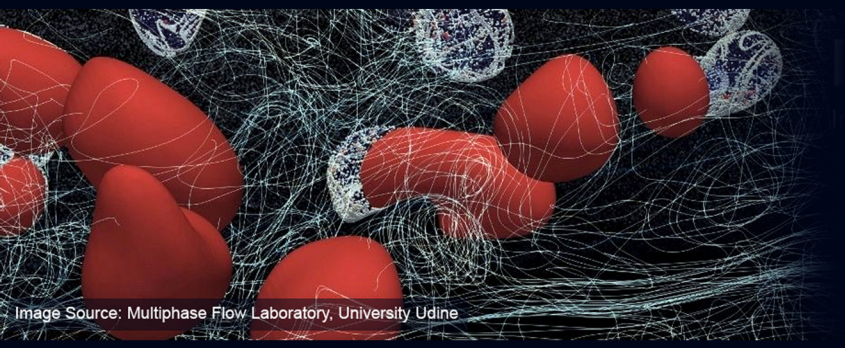
4th International Conference on Numerical Methods in Multiphase Flows

September 28-30, 2022
Venice, Italy



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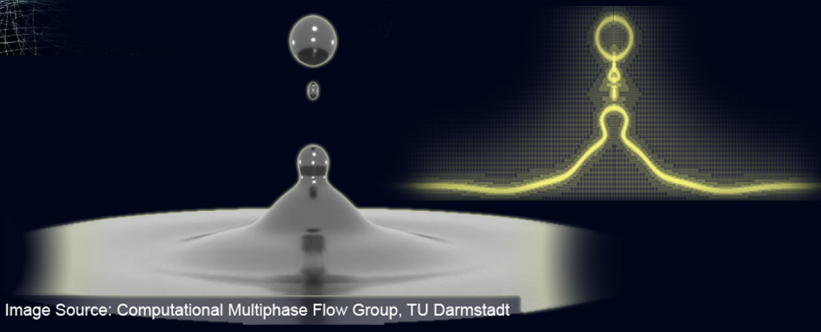

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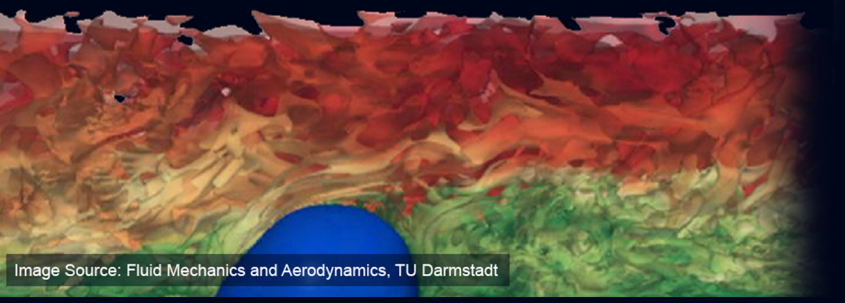

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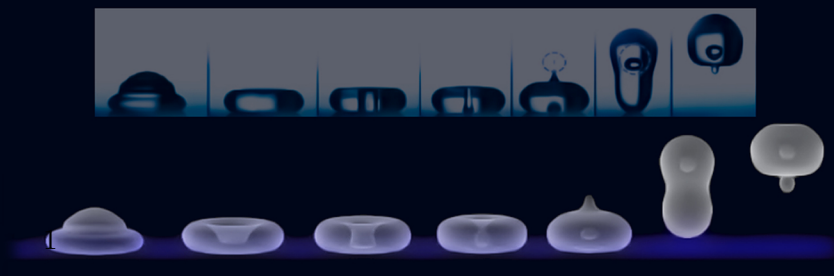

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The Nucleation Process and its Coupling to the Macroscale

Carlo Massimo Casciola, University of Rome

Abstract: Bubble nucleation is a ubiquitous phenomenon whose prediction proved a formidable task, particularly in the case of water. Here a self-contained model is discussed which is shown able to accurately reproduce data for bulk water over the most extended range of temperatures for which accurate experiments are available [1]. The computations are based on a Ginzburg-Landau model which, as only inputs, requires a reliable equation of state for the bulk free energy and the interfacial tension of the water-vapor system. Rare event techniques borrowed from statistical mechanics allow the determination of the free-energy barrier and the nucleation rate. By consistently including thermal fluctuations [2] in the spirit of Fluctuating Hydrodynamics, the approach is extended to dynamic conditions in presence of solid walls of different wettability [4] to allow coupling with fluid motion [4]. The talk will focus on the wall wettability in compliance with the fluctuation-dissipation balance, a crucial point in the context of the fluctuating hydrodynamics theory. Depending on time availability, new, still unpublished results concerning the coupling of nucleation and fluid flow, the effect of micro-confinement, and time-changing thermodynamic conditions will also be addressed.

[1] F. Magaletti, M. Gallo, C.M. Casciola, Water cavitation from ambient to high temperatures, Scientific Reports 2021, 11 1.

[2] M. Gallo, F. Magaletti, C.M. Casciola, Thermally activated vapor bubble nucleation: the Landau Lifshitz/Van der Waals approach, Phys. Rev. Fluids. 2018, 3, 053604.

[3] M. Gallo, F. Magaletti, C.M. Casciola, Heterogeneous bubble nucleation dynamics, Journal of Fluid Mechanics 2021, 906 10.

[4] M. Gallo, F. Magaletti, D. Cocco, C.M. Casciola, Nucleation and growth dynamics of vapor bubbles, Journal of Fluid Mechanics 2020, 883.

Bio: Carlo Massimo Casciola leads a research group based at the Mechanical and Aerospace Department of the La Sapienza University of Rome, working on the dynamics of complex flows and the coupling of macroscopic flows with a microstructure. He has given contributions to turbulence, particulate, polymers-laden, and multiphase flows, micro/nanofluidics through molecular dynamics simulations and free-energy methods, and mesoscale methods (phase field methods and fluctuating hydrodynamics). In 2013 received the prestigious ERC Advanced Grant, BIC – Following Bubbles from Inception to Collapse, and developed a novel microfluidic chip to study cavitation enhanced blood vessel permeability thanks to the ERC Proof of Concept grant INVICTUS, IN VItro Cavitation Through UltraSound.

From Close-Packed to Dilute Conditions: Well-Posed Eulerian Two-Fluid Models For High-Speed Polydisperse Fluid–Particle Flows

Rodney Fox, Iowa State University

Abstract: High-speed gas–particle flows arise in many applications, and almost always involve polydisperse particles (size, composition, etc.) over a wide range for the solids volume fractions. In this presentation, I will describe how to combine quadrature-based moment methods (QBMM) [1] with a well-posed compressible Eulerian two-fluid model derived from the kinetic theory of granular flows to model such flows. Our approach relies on first formulating a particle-phase kinetic model valid for close-packed to dilute particulate suspensions, coupled to a modified Euler equation for the compressible fluid phase. A critical component of our computational approach for treating polydispersity is the formulation of the numerical fluxes for the size-velocity moments found from the kinetic model. Using the hyperbolic quadrature method of moments (HyQMOM) [2] and size-conditioned velocity moments (CQMOM) [3] for the particle phase, we compute the flux eigenvalues needed for hyperbolic flow solvers, which are real-valued for all physically relevant conditions. Finally, through numerical examples, we demonstrate that by including added mass and fluid-phase pseudoturbulence [4], our modeling approach extends to fluid–particle flows with arbitrary material-density ratios (e.g., bubbly flows). In particular, we show that due to the combined effect of the particle-fluid-particle stress tensor and added mass, the compressible two-fluid model is well posed for all physically relevant flow conditions.

[1] D. Marchisio, R. O. Fox, Computational Models for Polydisperse Particulate and Multiphase Systems, Cambridge University Press, Cambridge, 2013.

[2] R. O. Fox, F. Laurent, Hyperbolic quadrature method of moments for the one-dimensional kinetic equation, SIAM Journal of Applied Mathematics, 82(2), pp. 1–21, 2022.

[3] C. Yuan, R. O. Fox, Conditional quadrature method of moments for kinetic equations, Journal of Computational Physics, 230(22), pp. 8216–8246, 2011.

[4] R. O. Fox, F. Laurent, A. Vié, A hyperbolic two-fluid model for compressible flows with arbitrary material-density ratios, Journal of Fluid Mechanics, 903(A5), pp. 1–39, 2020.

Bio: Professor Fox joined Iowa State University as the Glenn Murphy Professor of Engineering in 1999, and was the Herbert L. Stiles Professor of Chemical Engineering from 2003-2012. Since 2001, he has been Associate Scientist at the US-DOE Ames Laboratory. He was promoted to Distinguished Professor in Engineering in 2010. Fox has held visiting professorships in Belgium, Denmark, France, Italy, Switzerland and The Netherlands. From 1987-88, he was a NATO Postdoctoral Fellow at LSGC in Nancy, France working under the guidance of Prof. Jacques Villermaux. His numerous professional awards include a NSF Presidential Young Investigator Award in 1992 and the ISU Outstanding Achievement in Research Award in 2007. Professor

Fox was elected Fellow of the American Physical Society in 2007 and of the AIChE in 2020. From 2012-14, he was a Marie-Curie Senior Fellow at the Ecole Centrale in Paris, France.

In 2015 he was selected as an International Francqui Professor by the Francqui Foundation in Belgium, and awarded a Chaire d'Attractivité at the Université Fédérale Toulouse Midi-Pyrénées, France. In 2016 he was selected for the North American Mixing Forum Award for Excellence and Sustained Contributions to Mixing Science and Practice, and the Shell Particle Technology Forum Thomas Baron Award. In 2022 he was named the Fulbright-Tocqueville Distinguished Chair at the University of Paris-Saclay, CentraleSupélec.

Professor Fox has made numerous ground-breaking contributions to the field of multiphase and reactive flow modeling. The Fox group spearheaded many fundamental advances in the development of novel computational fluid dynamics (CFD) models to overcome specific scientific challenges faced in the chemical and petroleum industries. He developed powerful quadrature-based moment methods (CQMOM, EQMOM, HyQMOM) for treating distribution functions (particle size, bubble size, velocity, etc.). The impact of Fox's work extends far beyond chemical engineering and touches every technological area dealing with turbulent flow and chemical reactions. His first book, Computational Models for Turbulent Reacting Flows, published by Cambridge University Press (CUP) in 2003, offers an authoritative treatment of the field. His second CUP book in 2013, Computational Models for Polydisperse Particulate and Multiphase Systems, provides a comprehensive treatment of CFD model for disperse multiphase flows. His current research is focused on well-posed multifluid models for polydisperse systems and multiphase turbulent flows.

Multi-Scale Simulation of Two-Phase and Three-Phase Flows

Hans Kuipers, Eindhoven University of Technology

Abstract: Dispersed multiphase flows with deformable interfaces are frequently encountered in industrial processes involving large scale synthesis of synthetic fuels and base chemicals. In addition to formation, coalescence and break-up of bubbles, mass and heat transfer in the presence of chemical transformations prevail. These complex processes significantly influence the specific interfacial area, mixing of chemical species as well as the large scale circulation patterns and ultimately the performance (conversion/selectivity) of multiphase chemical reactors.

For such complex flows involving mass, momentum and heat transfer a multi-scale modeling approach is adopted in which the interactions between the phases can be properly accounted for. The idea is essentially that detailed models are used to generate closures for the interphase mass, momentum and heat transfer coefficients to feed coarse-grained (such as stochastic Euler-Lagrange) models which can be used to compute the system behavior on a much larger (industrial) scale. In this contribution recent advances in the area of multi-scale simulation of dispersed two-phase and three-phase flows will be highlighted with emphasis on coupled mass, momentum and heat transfer. In addition, areas which need substantial further attention will be discussed.

Bio: Hans Kuipers graduated in 1985 at the department of Chemical Engineering of the University of Twente. In December of the same year he started with his Ph.D. study at the Reaction Engineering group of University of Twente on detailed micro balance modeling of gas-fluidized beds. In June 1990 he received his Ph.D. degree in Chemical Engineering and was appointed as assistant professor in the Reaction Engineering group headed by Prof. W.P.M. van Swaaij. In 1994 he was appointed as associate professor in the same group. In 1999 he became full-time professor in Fundamentals of Chemical Reaction Engineering at the University of Twente. From 2006 until 2010 he was Scientific Director of the Institute of Mechanics Processes and Control (IMPACT) at the University of Twente. Since August 2010 he is a fulltime professor at Eindhoven University of Technology and heads the group Multiphase Reactors. He teaches amongst others introductory and advanced courses on transport phenomena and multiphase reactors. His research interests are in the area of multiphase chemical reactors. He participates in the Gravitation Program Multi-scale Catalytic Energy Conversion (MCEC) and acts as program director Process Technology and member of the Executive Board (EB) of the Advanced Research Center (ARC) Chemical Building Blocks Consortium (CBBC). In 2015 he was elected as member of the Royal Dutch Academy of Sciences (KNAW) and in 2019 he was invited as Honorary Professor of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences. He has published more than 450 papers in peer reviewed journals with H-index (Scopus) of 74.

High-Fidelity Simulations of Interfacial Two-Phase Flows on Unstructured Grids

Vincent Moreau, CORIA

Abstract: With the steady increase of the power of parallel super-computers, 3D unsteady simulations offer a great potential to study interfacial two-phase flows. However, the simulation of highly non-linear phenomena such as primary atomization requires very accurate numerical methods and high resolution to capture interface dynamics. While most direct numerical simulations of interfacial two-phase flows are carried out with structured grids or Cartesian-based Adaptive Mesh Refinement, recent advances in numerical methods for tetrahedron-based meshes and parallel mesh adaptation strategies raise the attractiveness of unstructured grids. The use of tetrahedra has two advantages for practical configurations: complex geometries are easily meshed and the mesh is locally more isotropic than Cartesian grids. The presentation will detail recent numerical improvements to the Accurate Conservative Level Set method [Janodet et al., JCP 2022] in terms of interface distance, curvature calculation and profile reinitialization. The presentation will also discuss how to include more physics in such simulations such as static contact angles [Pertant et al., JCP 2021] or scalar transport in order to widen the scope of these methods. Finally, the presentation will be focused on the development of highly-efficient dynamic adaptation of tetrahedron-based unstructured grids. The proposed methodology, which heavily relies on the remeshing library MMG (www.mmgtools.org) has been thoroughly optimized to reach good performances with grids of several billion cells on more than 10.000 cores. This dynamic mesh adaptation strategy has been implemented in the YALES2 code (www.coria-cfd.fr) and applied to the modeling of primary atomization in many configurations: liquid jet in cross flow, pressure swirl atomizers, triple disk pressure injector, oil scavenging systems... In these applications, the local mesh adaptation enabled a drastic reduction of the CPU cost compared to the fixed-grid approach and enabled to reach unprecedented mesh resolutions at the interface.

Bio: Vincent Moureau is a CNRS researcher at CORIA in the combustion modeling group. Since 2009, his research is focused on turbulent combustion and spray modeling, and on the development of the YALES2 solver for Large-Eddy Simulation and Direct Numerical Simulation of turbulent flows in complex geometries using massively parallel computers. He received the Yves Chauvin award for his PhD thesis in 2005, the 3rd prize of the Bull Joseph Fourier award for the promotion of numerical simulation in 2010, an IBM faculty award in 2011, and the aeronautical and aerospace science award of the French Academy of Science in 2018.

Multiphase Flows of Complex Fluids

Outi Tammisola, KTH

Abstract: Complex non-Newtonian fluids' transport and flow over surfaces governs the production of many industries, along with natural hazards. Numerous multiphase flows in everyday life occur in non-Newtonian carrier fluids, from food products (chocolate, mayonnaise, yoghurt) to biological flows (blood, saliva), process industries, ink jet printing, oil drillings, mud flows. Unability to predict and control such flows leads to technological barriers for novel applications, and traditional process industries waste energy when trying to improve mixing and prevent clogging. In this lecture, we show how constitutive equations including both viscoelasticity and yield stress of the carrier fluid can be coupled with efficient direct numerical simulation algorithms [1,2] which for the first time enabled large-scale simulations of three-dimensional systems in such fluids [3,4,5]. Numerical challenges associated with viscoelasticity and yield stress, and ways to overcome them, will be discussed. We will present recent progress in simulating flows of elastoviscoplastic fluids in the inertial regime, including droplets, particles, and wetting problems.

[1] D. Izbassarov, M. Rosti, M. Niazi Ardekani, M. Sarabian, S. Hormozi, L. Brandt, O. Tammisola Computational modeling of multiphase viscoelastic and elastoviscoplastic flows, International Journal of Numerical Methods for Fluids 2018, 88(12), 521-543.

[2] Z. Ge, J. C. Loiseau, O. Tammisola, L. Brandt An efficient mass-preserving interface-correction level set/ghost fluid method for droplet suspensions under depletion forces. Journal of Computational Physics 2018, 353,435-459.

[3] D. Izbassarov, M. E. Rosti, L. Brandt, O. Tammisola, Effect of finite Weissenberg number on turbulent channel flows of an elastoviscoplastic fluid. Journal of Fluid Mechanics 2021, 927, A45.

[4] D. Izbassarov, O. Tammisola, Dynamics of an elastoviscoplastic droplet in a Newtonian medium under shear flow, 2020, Phys. Rev. Fluids 5(11), 113301

[5] E. Chaparian, M. Niazi Ardekani, L. Brandt, O. Tammisola, Particle migration in channel flow of an elastoviscoplastic fluid. Journal of Non-Newtonian Fluid Mechanics 284, 104376.

Bio: Outi Tammisola is associate professor in fluid dynamics at Dept. Of Engineering Mechanics, KTH Royal Institute of Technology. She received her PhD at KTH 2011, held a postdoctoral position in Univ. of Cambridge 2011-2014, assistant professor position in Univ. of Nottingham 2014-2017, and returned to KTH 2017. Her research interests are in numerical simulations of non-Newtonian fluids (especially yield-stress fluids), multiphase flows, flow instability and control, and interfacial flows. She received the prestigious ERC Starting Grant 2019 (MUCUS) on the project MUCUS – Modelling of complex fluid flows over surfaces and walls. Furthermore, she is the main coordinator of the YIELDGAP EU project 2020, 3.2M€ on "YIELD-stress fluid flows beyond Bingham: closing the GAP in modelling real-world yield-stress materials",

involving 9 universities, 5 companies, and 12 PhD students, and has several grants as a PI from the Swedish Research Council. She is an associate editor for Theoretical and Computational Fluid Dynamics, and has published more than 40 peer-reviewed journal papers, whereof 15 in Journal of Fluid Mechanics and 3 in Journal of Computational Physics.

On the Modelling and Simulation of Electrically Charged Particle-Laden Flows

Olivier Simonin, Institut de Mécanique des Fluides de Toulouse (IMFT)

Abstract: Turbulent particle-laden flows are encountered in many practical applications such as geophysical flows, engineering processes or health/medicine studies. The modelling and simulation of particle transport and dispersion is complex due to the multiphysical nature of particle-laden flows. A non-exhaustive list includes particle-turbulence interaction, inter-particle collisions or particle bouncing on smooth or rough walls. In addition, although long neglected in modelling approaches, the effect of electrical charges on the dynamics of particle flow can be very important. The objective of this talk is to present some recent advances in modelling and simulation of electrically charged particle flows for two very different particle-laden flow regimes.

The first part of the presentation is devoted to the effect of electrostatic forces on the dynamic of small inertial particles, with the same charge, transported by a homogeneous isotropic turbulent flow, for very dilute configurations. This phenomenon is analyzed from direct numerical simulation (DNS) of gas turbulent flows coupled with Lagrangian tracking of discrete solid particles. The simulation results show that the self-dispersion and segregation of the particles decrease with increasing electric charge. In contrast, the kinetic energy of the particles can increase or decrease with respect to the electric charge effect depending on the particle turbulent Stokes number. Statistical analysis of the simulation results is carried out in the frame of the fluid-particle joint PDF approach and shows that the change in the kinetic energy of the charged particles is only due to a change in the efficiency of entrainment by the fluid turbulence characterized by the fluid-particle velocity covariance modification by electrostatic effects.

The second part of the presentation is devoted to the statistical modelling of the mean electric charge transport with triboelectric effects in mono-dispersed gas-particle flows for kinetic and collisional regimes. The kinetic theory of granular flows is used to derive the transport equations for the mean particle electric charge and for the second-order moments: charge-velocity correlations and charge variance. The collision terms in these equations are closed by assuming that the electrostatic interaction does not modify the collision dynamics and without presuming explicitly the form of the dependence of the joint charge-velocity PDF on the particle electric charge. The proposed derivation shows that the dispersion phenomenon has two contributions: a kinetic contribution due to the electric charge transport by the random motion of particles and a collisional contribution due to the electric charge transfer during particle–particle collisions. Another phenomenon that contributes to the mean electric charge transport is a triboelectrical current density due to the tribocharging effect by particle–particle collisions in the presence of a global electric field. A gradient approximation model and a full second-moment transport equation model are tested in a periodic box with non-uniform initial mean charge distribution. The results show that the full second moment transport model is able to capture some important mechanism that are neglected in the gradient dispersion modelling approach

and, in particular, allows to account for the coupling of the mean electric charge transport with the charge variance production and dissipation.

[1] Boutsikakis, A., Fede, P., Simonin, O., 2022, "Effect of electrostatic forces on the dispersion of like-charged solid particles transported by homogeneous isotropic turbulence", J. Fluid Mech., Vol. 938, A33.

[2] Montilla, C., Ansart, R., Simonin, O., 2020, "Modelling of the mean electric charge transport equation in a mono-dispersed gas-particle flow", J. Fluid Mech., Vol. 902, A12.

Bio: Olivier Simonin obtained a PhD on environmental turbulence in 1981 before joining EDF R&D to work on the modelling and simulation of water-vapour and reactive gas-solid flows in the power industry. In 2001, he joined Toulouse-INP/ENSEEIHT to become a full professor of fluid mechanics. His research at the Institut de Mécanique des Fluides de Toulouse (Université de Toulouse / CNRS) focuses on the modelling and simulation of very dilute to dense particle-laden reactive flows using a multi-scale approach based on : direct simulations of particle-resolved flows, Euler-Lagrange mesoscale simulations (DPS/LES or DEM/CFD) and the development of the N-Euler multiphase approach from a joint fluid-turbulent-particle PdF modelling approach and the kinetic theory of rapid granular media. Finally, he is making a major contribution to the development and application of a multi-fluid HPC numerical code, `neptune_cfd`, for the prediction of industrial reactive fluidized beds in support of new processes for reducing the greenhouse effect.

DAY 1	Wednesday, September 28, 2022				
08:30	09:00	Registration			
09:00	09:15	Opening			
09:15	09:55	Keynote lecture	**H. Kuipers - Multi-scale simulation of two-phase and three-phase flows** Chair: R. Kunz, Room: Auditorium		
10:00	*11:00*	*Regular talks*	*Session: Methods for incompressible two-phase flow* *Chair: H. Kuipers, Room: Auditorium*	*Session: Advanced algorithms and solution techniques for coupled multiphase systems* *Chair: A. Roccon, Room: Aula Magna 1-E*	*Session: Adaptive, dynamic and multiscale techniques* *Chair: Y. Hoarau, Room: Aula 1-G*
10:00	10:15	RT1	An unstructured collocated finite-volume Level Set method with a geometrical phase indicator (T. Marić, D. Jurić, Jalel Chergui, S. Shin)	Extension of the multi-regime two-fluid model towards wall-bounded multi-scale liquid films (P. Porombka, J.Schlottke)	An octree-adaptive immersed boundary-lattice Boltzmann method for 3D simulation of fluidrigid particle interactions (Z. Cheng, A. Wachs)
10:15	10:30	RT2	Adjoint-based optimisation of interfacial flows in the sharp interface limit (T. Fullana, A. Q. Rodrıguez, V. Le Chenadec, T. Sayadi)	A phase-change model for diffusion-driven mass transfer problems in incompressible two-phase flows (G. Gennari, R. Jefferson-Loveday, S.J. Pickering)	A subgrid-scale modeling frame-work for convection-dominated interfacial species transport applied to modeling mass transfer in a metallurgical refining ladle (J. Maarek, S. Zaleski, S. Popinet)
10:30	10:45	RT3	A conservative Cartesian cut-cell method for accurate predictions of mass, heat and momentum transfers (A.Q. Rodriguez, T. Fullana, V. Le Chenadec)	Investigation of droplet motion on chemically heterogeneous surfaces using a Phase-Field approach (F. Bodziony, H. Marschall)	An adaptive sharp interface method for detailed simulations of collective bubble growth and collapse dynamics (R.K. Shukla, M. Sawardekar, P. Das, J.B. Freund)
10:45	11:00	RT4	Lattice Boltzmann simulation of a turbulent pipe flow laden with spherical particles (F. Gharibi, S.A. Hosseini, D. Thevenin)	Interface-retaining coarse models for complex multiphase flows (X. Chen, J. Lu, G. Tryggvason)	Large-eddy simulations of spur gear lubrication by oil jets using an interface capturing method and dynamic mesh adaptation (M. Cailler, R. Mercier, I. Tsetoglou, P. Benard, P. Benez, G. Lartigue, V. Moureau)
11:00	11:30	Coffee Break			
11:30	*13:00*	*Regular talks*	*Session: Methods for compressible two-phase flow* *Chair: J. Lindau, Room: Aula 1-G*	*Session: Methods for particulate flows* *Chair: F. Evrard, Room: Auditorium*	*Session: Interfacial instabilities and multiphysics* *Chair: M. Pelanti, Room: Aula Magna 1-E*
11:30	11:45	RT5	Large eddy simulations of primary breakup in metal melt gas atomization (D. P. L. Thuy, J. J.C. Remmers, N. G. Deen, G. Finotello)	Dominant mechanisms of secondary flows in horizontal particle-laden pipe flows (X.M. Zhang, G.J. Nathan, Z.F. Tian, R.C. Chin)	Physical accuracy and numerical stability of the Lattice Boltzmann color gradient multicomponent model for the jetting of micro-droplets (K.P.N. Datadien, G. di Staso, H.M.A. Wijshoff, F. Toschi)
11:45	12:00	RT6	Investigating 3-D effects on flashing cryogenic jets with highly resolved LES (J. W. Gartner, A. Kronenburg, A. Rees, M. Oschwald)	A wavelet-based kinematic simulation for turbulent dispersed two-phase flows (R. Letournel, F. Laurent, M. Massot, A. Vié)	Interface-resolved direct numerical simulation of the breakup of solid fibers in turbulence (F. Dalla Barba, F. Picano, U. Galvanetto, M. Zaccariotto)
12:00	12:15	RT7	Modeling and simulation of stiff two-phase tube problems (Y. Hoarau, E. Goncalves da Silva)	Accurate Lagrangian subgrid-scale models for turbulent particle-laden flow (M. Herzog, A. Lattanzi, J. Wakefield, S. Subramaniam, J. Capecelatro)	Particle capture by deformable drops in three-phase turbulent channel flow (K. Miranda, A. Hajisharifi, C. Marchioli, A. Soldati)
12:15	12:30	RT8	Hyperbolic Solvers for the modeling of Compressible Two-Phase Flows (J. Paris, A. Vié, T. Schmitt)	The behavior of elongated non-spherical particles in wall-bounded turbulent flow: Detailed model validation (M. A. Taborda, L. Pasternak, M. Sommerfeld)	The Chaotic Life of Mayonnaise (I. Girotto, R. Benzi, A. Scagliarini, G. di Staso)
12:30	12:45	RT9	Contact line treatment for boiling flows using a weakly compressible diffuse interface framework (N. Scapin, A. Shahmardi, L. Brandt, A. D. Demou, M. Pelanti)	A numerical strategy for Particle-Resolved Direct Numerical Simulation of gas-solid reactive flows (I. Girault, M.-A. Chadil, E. Masi, S. Vincent, O. Simonin)	Influence of density and viscosity on deformation, breakage and coalescence of bubbles in turbulence (F. Mangani, G. Soligo, A. Roccon, A. Soldati)
12:45	13:00	RT10	A compressible hybrid model for cavitating flows (A. Madabhushi, K. Mahesh)	A robust numerical scheme for simulating heterogeneous reactions in particle-laden flows in the N-Euler framework (G. Pierre, J. Laviéville, B. Bédat, O. Simonin)	Water-lubricated channel flow (A. Roccon, F. Zonta, A. Soldati)
13:00	14:30	Lunch Break			

14:30	15:10	Keynote lecture	**R. Fox - From close-packed to dilute conditions: Well-posed Eulerian two-fluid models for high-speed polydisperse fluid–particle flows** Chair: A. Soldati, Room: Auditorium		
15:15	*16:15*	*Regular talks*	*Session: Critical assessment and numerical benchmark of method development* *Chair: M. Fricke, Room: Aula 1-G*	*Session: Progress in Eulerian-Lagrangian & Eulerian-Eulerian modeling of dispersed flow* *Chair: R. Fox, Room: Auditorium*	*Session: Methods for interface advection* *Chair: S. Tanguy, Room Aula Magna 1-E*
15:15	15:30	RT11	A comparative benchmark of four Volume-of-Fluid solvers by means of advection and capillary test cases (A. Lippert, A. Dorr, R. Bosch, T. Tolle, T. Marić)	A hybrid method between sectional and moment method for the description of a population of soot (F. Laurent, J.Y. Xing, C.P.T. Groth)	On the numerical approximation and transport of the mean curvature in Volume-of-Fluid methods (M. Fricke, J. Kromer, D. Bothe)
15:30	15:45	RT12	A coupled VOF-fictitious domain technique for the simulation of interfacial flows interacting with moving particles (M. Saeedipour)	Application of a morphology adaptive multifield model towards a plunging jet considering entrainment (R. Meller, B. Krull, F. Schlegel, M. Tekavčič)	Pointwise divergence-free cutfem for the Darcy interface problem (T. Frachon, P. Hansbo, E. Nilsson, S. Zahed)
15:45	16:00	RT13	Limitations and perspectives of phase-change modelling based on interface capturing methods for evaporation simulations (V. Boniou, T. Schmitt, A. Vié)	Multi-Euler/Lagrange simulation of gas/liquid/solid multiphase flows (F. Baraglia, J. Laviéville, N. Mérigoux, O. Simonin)	Maximum gradient based compression algorithm for interface capturing (A. Yadav)
16:00	16:15	RT14	An extended numerical model for the Direct Numerical Simulation of evaporating droplets : Applications to Leidenfrost droplets (S. Tanguy, G. Mialhe. D. Legendre)	Algebric momentum preserving method with a fully coupled 3D parallel solver for the simulation of two-phase incompressible flows (M. El Ouafa, S. Vincent, V. Le Chenadec, B. Trouette)	Enabling accurate interface advection with iso-Advector at larger time steps (K. Missios, J. Roenby)
16:15	16:45	Coffee Break			
16:45	*17:45*	*Regular talks*	*Session: Numerical benchmarks (verification & validation) for method development* *Chair: B. Motta, Room: Aula Magna 1-E*	*Session: Progress in Eulerian-Lagrangian & Eulerian-Eulerian modeling of dispersed flow* *Chair: C. Marchioli, Room: Aula 1-G*	*Session: Phase transition & numerical modeling of interfacial heat & mass transfer* *Chair: H. Kuhlmann, Room: Aula 1-G*
16:45	17:00	RT16	Turbulent Poiseuille flow of two immiscible liquid layers inside a channel (G. Giamagas, F. Zonta, A. Roccon, A. Soldati)	A multi-fluid Large-Eddy Simulation framework based on the Conservative Level Set approach for predicting two-phase heat transfer (F. Pecquery, V. Moureau, M. Cailler, C. Merlin)	Volume-of-Fluid method with phase change in water jet cooling (K. Nabbout, M. Sommerfeld)
17:00	17:15	RT17	Droplet deformation and breakup in shear-thinning viscoelastic fluid under simple shear flow (D. Wang, N. Wang, H. Liu)	Numerical simulation of spraying systems using the Euler/Lagrangian method with an advanced stochastic droplet collision model (M. Sui, M. Sommerfeld)	Large-eddy simulation of cavitating tip leakage vortex (M.H. Arabnejad, H. Nilsson, R.E. Bensow)
17:15	17:30	RT18	Analysis of the dynamics of an isolated cavitating vortex (A. Savio,M. Cianferra, V. Armenio, R. Bensow)	Numerical simulation of gas atomization process for metal powder production (J. Hua, D. Mortensen, J.O. Odden)	Multicomponent droplet evaporation in a geometric Volume of Fluid framework (E. Cipriano, A. Frassoldati, T. Faravelli, A. Cuoci)
17:30	17:45	RT19	Finite Volume Computation of Journal Bearing Cavitation (J. Lindau, D. Leonard, A. Metrz, R. Campbell)	Stochastic sprays in the under-resolved turbulence (M. Gorokhovski , S. Oruganti)	Modeling of droplet condensation on walls based on the adaptation of the Ranz-Marshall correlation for two-phase turbulent flow with CFD approach (S. Benteboula, F. Dabbene)
18:00	19:30	Poster session with Welcome Aperitif (offered by the International Journal of Multiphase Flow)			

LIST OF POSTER PRESENTATIONS:

- An eXtended Discontinuous Galerkin Method for three-dimensional two-phase flows: Application to viscous droplet oscillations (M. Smuda, D. Zrnić, F. Kummer, G. Brenn, M. Oberlack)
- Algebric momentum preserving method with a fully-coupled 3D parallel solver for the simulation of two-phase incompressible flows (M. El Ouafa, S. Vincent, V. Le Chenadec, B. Trouette)
- Direct Numerical Simulation of Bubble Formation and Dynamics in Water Electrolysis Using a Phase-Field Method (N. Bordbar, D. Bothe, Holger Marschall)
- Simulation of reservoir dynamics (B. Oualid)
- Non-Coaxially Rotating Motion in Casson Martial along with Temperature and Concentration Gradients via First-order Chemical Reaction (N. Jabbar)
- Spreadsheet modelling of temperature and hydraulic profile of an uninsulated subsea pipeline with insufficient data (B. O. Bassey)
- Simulation of rigid and flexible objects immersed in a fluid-drop system (K. Miranda, C. Marchioli)

DAY 2	Thursday, September 29, 2022			
09:00	09:40	Keynote lecture	**V. Moureau - High-fidelity simulations of interfacial two-phase flows on unstructured grids** Chair: S. Balachandar, Room: Auditorium	
09:45	*11:00*	*Regular talks*	*Session: Advanced Computational and Numerical Method Developments* *Chair: V. Moureau, Room: Auditorium*	*Session: Simulation of complex multiphase flows – Applications* *Chair: F. Denner, Room: Aula Magna 1-E*
9:45	10:00	RT1	A numerical model for two-phase liquid-vapor flows with arbitrary-rate heat and mass transfer (M. Pelanti)	On the effect of in-plane solidity on the different regimes of canopy flows (S. Nicholas, M. Omidyeganeh, A. Pinelli)
10:00	10:15	RT2	A Discontinuous Galerkin Method for compressible gas/liquid interfacial flows (W. White, E. Johnsen)	Numerical assessment of cavitation erosion in a high-pressure fuel injector (M. Ozgunoglu, M.H. Arabnejad, G. Mouokue, R.E. Bensow)
10:15	10:30	RT3	An analytical wall function for turbulent wall condensation in the presence of noncondensable gas with buoyancy, suction and inter-diffusion convection (A. Iziquel, S. Benteboula, C. Josserand)	An investigation of rain-droplet interaction for re-entry vehicles (R. Forehand, M. Kinzel)
10:30	10:45	RT4	A unified multiphysics framework for multi-region coupling and its application to ALE interface-tracking (H. Alkafri, M. E. Fadeli, H. Marschall)	Direct Numerical Simulation of CMAS particles and their deposition on aircraft components (B. Cavainolo, M. Kinzel)
10:45	11:00	RT5	A particle-center-averaged Euler-Euler model for bubbly flow simulations (H. Lyu, D. Lucas, R. Rzehak, F. Schlegel)	An eXtended Discontinuous Galerkin Method for three-dimensional two-phase flows: Application to viscous droplet oscillations (M. Smuda, D. Zrnić, F. Kummer, G. Brenn, M. Oberlack)
11:00	11:30	Coffee Break		
11:30	*13:00*	*Regular talks*	*Session: Numerical multiphysics modeling of surfactants & interfacial transport* *Chair: V. Le Chenadec, Room: Auditorium*	*Session: Machine-learning and data-driven techniques for multiphase flow simulations* *Chair: S. Sasic, Room: Aula Magna 1-E*
11:30	11:45	RT6	Coupled Level-Set Volume-of-Fluid solver for thermo-capillary applications (H. Valdez, J. Cousin, J.C.B. de Motta)	Data-assisted simulations of recurrent multiphase flows: the benefits and the drawbacks of simplicity (T. Lichtenegger)
11:45	12:00	RT7	A 2D hybrid method for interfacial transport of passive scalars (Y. Fan, X. Hu, N. Adams)	Parametric high-fidelity data generation for multiparticle flow systems using physics-informed operator networks (B. Siddani, Y. Yang, S. Balachandar)
12:00	12:15	RT8	Quadratic interface reconstruction from volume fractions on arbitrary polyhedral meshes (F. Evrard, R. Chiodi, A. Han, B. van Wachem, O. Desjardins)	Universal closure models of drag, lift, torque, and pseudo turbulence using physics-guided deep learning (S. Balachandar, B. Siddani)
12:15	12:30	RT9	Fully-coupled algorithm for viscoelastic interfacial flows (F. Denner, C. Gorges, F. Evrard, B. van Wachem)	Two-phase flow reduced-order model : a two-scale model of polydisperse oscillating droplets (A. Loison, T. Pichard, S. Kokh, M. Massot)
12:30	12:45	RT10	Nano- and microscale simulations of water boiling on heterogeneous surfaces (A. Mokos, K. Karalis, P.A. Patel, S.V. Churakov, N.I. Prasianakis)	Simplified erosion modeling in gas dominant flow with enhanced learning from CFD models (J. Zhang, F. Darihaki, R. Vieira, S. Shirazi)
12:45	13:00	RT11	Direct numerical simulation of the gas-liquid mass transfer around a rising bubble in the presence of surfactants (K. Kentheswaran, N. Dietrich, B. Lalanne)	Development of an automated framework for data-based modeling of filtered drag for coarse-grained simulations of fluidized beds based on Artificial Neural Networks and Bayesian optimization (G. D'Alessio, M. Solaiman, S. Sundaresan, M. Mueller)
13:00	14:30	Lunch Break		
14:30	15:10	Keynote lecture	**O. Simonin - On the modelling and simulation of electrically charged particle-laden flows** Chair: G. Tryggvason, Room: Auditorium	
15:15	*16:15*	*Regular talks*	*Session: Advanced Computational and Numerical Method Developments* *Chair: O. Simonin, Room: Auditorium*	*Session: DNS/LES of two-phase flows* *Chair: J. Capecelatro, Room: Aula Magna 1-E*
15:15	15:30	RT12	Effect of gravity term discretisation on spurious velocities at the fluid interface (J. Roenby, K. Møller, H. Scheufler)	Drop impact onto a thin liquid film: extension from two to three phase scenarios using phase-field method (M. Bagheri, M. Worner, H. Marschall)
15:30	15:45	RT13	A microstructure-based model to predict fluid-particle forces in random particle arrays (B. Hardy, O. Simonin, J. De Wilde, G. Winckelmans)	Water droplet impact on thin oil film and bubble entrapment: Three phases simulation (P.-A. Maes, A. Amirfazli, C. Josserand)
15:45	16:00	RT14	Splitting schemes for phase-field models (V. Calo, P. Minev, V. Puzyrev)	The mechanisms behind a shear-induced lift force on deformable bubbles - a DNS study (N. Hidman, H. Strom, S. Sasic, G. Sardina)
16:00	16:15	RT15	Neuroevolution-enabled adaptation of the Jacobi method for non-symmetric pressure equation with density discontinuities (X. Yang, T.-R. Xiang ,Y.-P. Shi)	Direct Numerical Simulation of the collapse of a bubble in contact with a wall (D. Fuster, M. Saini)
16:15	16:45	Coffee Break		

16:45	*17:45*	*Regular talks*	*Session: Simulation of complex multiphase flows - Applications* *Chair: D. Lucas, Room: Auditorium*	*Session: DNS/LES of two-phase flows* *Chair: A. Vié, Room: Aula Magna 1-E*
16:45	17:00	RT16	A three-phase cavitation solver for the simulation of ventilated cavitating flow in OpenFOAM (B. C. Khoo, C. Xu, X. Zhao)	The velocity jump discontinuity for single bubbles rising in a viscoelastic fluid: Insights from direct numerical simulations (M. Niethammer, G. Brenn, D. Bothe)
17:00	17:15	RT17	Simulation of oil-water core-annular flow through an inclined pipe (E. Yaghoubi, S. Passoni, I.M. Carraretto, R. Mereu, L.P.M. Colombo)	Energy balance in lubricated drag-reduced turbulent channel flow (A. Roccon, F. Zonta, A. Soldati)
17:15	17:30	RT18	On the effect of Dean vortices on particle focusing in micro-fluidic applications (D. De Marinis, A. Coclite, M.D. de Tullio)	Numerical investigation of the in-nozzle flow dynamics in pressure-swirl atomizers (J. Carmona, G. Lartigue, V. Moureau)
17:30	17:45	RT19	Numerical simulation of dust deposition on fixed-tilt solar arrays in a desert environment (C.T. Moustaph, O. Simonin, P. Fede, M. Pallud, P. Maheshwari)	Dynamics and wakes of a fixed and freely moving tetrahedron in an inertial flow (G. Gai, A. Wachs)
20:00	22:30	Social Dinner		

DAY 3	Friday, September 30, 2022			
09:00	09:40	Keynote lecture	**O. Tammisola - Multiphase flows of complex fluids** Chair: S. Zaleski, room: Aula Magna 1-E	
09:45	*11:00*	*Regular talks*	*Mini-Symposium: Dynamic wetting and numerical treatment of moving contact lines* *(Chair: D. Bothe, Room: Aula Magna 1-E)*	*Session: High Performance Computing and parallel computing methods, techniques for large-scale simulations of multiphase systems* *(Chair: O. Tammisola, Room: Aula 1-G)*
9:45	10:00	RT1	Volume-of-Fluid based simulation of dynamic wetting processes based on the generalized Navier boundary condition (Y. Kulkarni, M. Fricke, T. Fullana, S. Zaleski)	Numerical study of particle suspensions in elastoviscoplastic (EVP) duct flows (S. Habibi, M. Niazi, K.T. Iqbal, E. Chaparian, L. Brandt, O. Tammisola)
10:00	10:15	RT2	Improvement of VOF two-phase flow method in a collocated Finite Volume framework (V.-Q. Hoang, G. Vinay, O. Laget, F. Plourde)	Subgrid-scale modeling of droplet bag breakup (A. Han, O. Desjardins)
10:15	10:30	RT3	A coupling VOF/embedded boundary to model arbitrary contact angles on solid surfaces (M. Tavares, C. Josserand, A. Limare, J. M. Lopez, S. Popinet)	A fast and highly scalable Direction splitting algorithm to solve momentum and heat transfer in flow laden with non-spherical rigid bodies (A. Goyal, A. Wachs)
10:30	10:45	RT4	A thermodynamically consistent phase-field model for moving contact line problems and its application in vesicle motions (P. Lin)	High performance computing of the collapse of a bubble array near a wall (E.G. da Silva, P. Parnaudeau)
10:45	11:15	Coffee Break		
11:15	11:55	Keynote lecture	**C.M. Casciola - The nucleation process and its coupling to the macroscale** Chair: F. Picano, Room: Aula Magna 1-E	
12:00	*13:15*	*Regular talks*	*Mini-Symposium: Dynamic wetting and numerical treatment of moving contact lines* *Chair: H. Marschall, Room: Aula Magna 1-E*	*Session: Advanced algorithms and solution techniques for coupled multiphase systems* *Chair: C.M. Casciola, Room: Aula 1-G*
12:00	12:15	RT6	Simulating wetting of geometrically complex surfaces using the plicRDF-isoAdvector unstructured Volume-ofFluid method (M.H. Asghar, M. Fricke, D. Bothe, T. Marić)	Time-implicit multilayer modelling of gravity and capillary waves (S. Popinet, C. Robert, A. Antkowiak)
12:15	12:30	RT7	Adhesion in coalescence-induced jumping droplets - relevant or not? (K. Kontantindis, J. Göhl, A. Mark, S. Sasic)	Front-Tracking approaches for the modelling of breakup and coalescence (P. Regnault, S. Vincent, E. Chenier)
12:30	12:45	RT8	To coalesce or not to coalesce Understanding sessile droplets subject to surface tension gradients (S. Zitz, J. Roenby)	Front tracking with surface normal propagation restriction (C. Gorges, F. Evrard, B. van Wachem, A. Hodzic, C. M. Velte, F. Denner)
12:45	13:00	RT9	Wettability pattern mediated trapped bubble removal from an immiscible liquid-liquid interface (I.U. Chowdhury, P.S. Mahapatra, A.K. Sen)	FastRK3P*: a fast and stable pressure-correction method for two-fluid incompressible homogeneous shear turbulence (P. Trefftz-Posada, A. Ferrante)
13:00	13:10	Closure		
13:10	14:30	Lunch Break		

Wednesday – 2022-09-28

Session I

- **Methods for incompressible two-phase flow**
  (Chair: H. Kuipers, Room: Auditorium)
- **Advanced algorithms and solution techniques for coupled multiphase system**
  (Chair: A. Roccon, Room: Aula Magna 1-E)
- **Adaptive, dynamic and multiscale techniques**
  (Chair: Y. Hoarau, Room: Aula 1-G)

An unstructured collocated finite-volume Level Set method with a geometrical phase indicator

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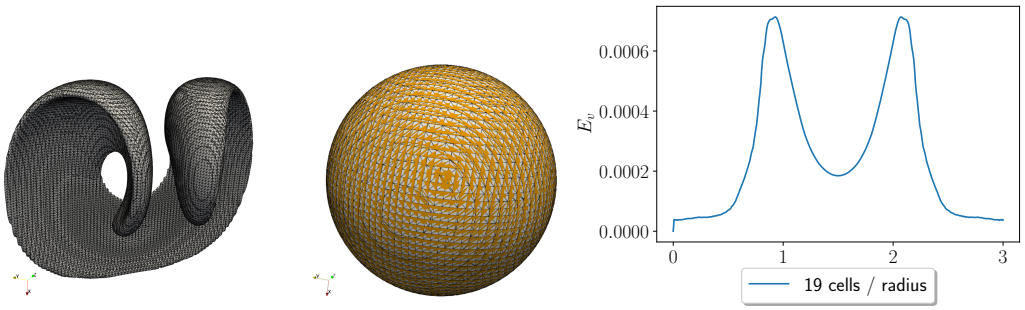
The Level Set method for simulating multiphase flows [1, 2] (see [3] for a recent review) relies on re-distancing to ensure the signed-distance nature of the level-set field. The signed distance is advantageous for the phase indicator and curvature computation, and the numerical errors in the Level Set transport are not amenable to numerical differentiation [4, sec. 7.1]. However, it turns out that a geometrical approximation of the zero level-set renders numerical differentiation unnecessary for the phase-indication and the curvature approximation, and, for incompressible flows, the unstructured collocated discretization renders the differentiation unnecessary for the Level Set equation. This approach, therefore, successfully disregards re-distancing (that amplifies mass loss) and higher-order (W)ENO schemes (that complicate parallel programming). There is a similarity to the hybrid coupled Level Set / VOF method; however, only in one direction - the phase indication is borrowed from the VOF method. The proposed method demonstrates acceptable volume conservation on finer mesh resolutions - easily usable because the method's simplicity ensures very high serial and parallel computational efficiency.



(a) Extreme at $t = 1.5$ s.

(b) Initial (gray) vs advected (orange) interface ($t = 3$ s).

(c) Volume conservation.

Figure 1: 3D deformation [5], ran with $CFL \approx 1$ on a 128^3 mesh, 573 seconds with 4 CPU cores.

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Adjoint-based optimisation of interfacial flows in the sharp interface limit

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The flows encountered in energy conversion systems consist of a wealth of complex phenomena, including interfaces, reactions and turbulence. While the past decades have seen remarkable progress in computing capabilities, allowing computational fluid dynamics to become an ever more present tool in describing and predicting such multi-physics flows, these state-of-the-art computational resources still provide limited insight towards a robust optimization framework for technological applications. Targeted manipulation of such flows by enhanced designs or active control strategies is indeed crucial for improvements in performance and robustness and venturing beyond standard operating conditions. The transition from model-based numerical simulations to model-based optimal control requires an alternative approach, which allows access to inverse information. In the fields of external aero-dynamics and aero-acoustics for example, the introduction of such an approach has led to improved airframe designs and reduced noise production levels, with considerable economical, environmental and health-related implications.

The multi-physics aspects of interfacial two-phase flows however constitute a far larger step in complexity, due to the presence of discontinuities across the interface, and to the highly unsteady nature of the flow. As far as two-phase flows are concerned, to date, inverse information has been extracted from simulations of simplified configurations with additional unrealistic assumptions, or from low-fidelity models.

In this work, gradient based optimisation is performed on a Stefan problem, where the motion of the interface is a function of the jump in the temperature gradient. In particular, we study the growth or retraction of crystal shapes by taking into account the curvature effects at the boundary. In order to capture the movement of the interface, the one-fluid formulation is used, where the sharp interface is represented using a level set method. The gradient is extracted using an adjoint-based formulation and specifically defined tracking-type objective functions are minimized to control the final shape of the crystal.

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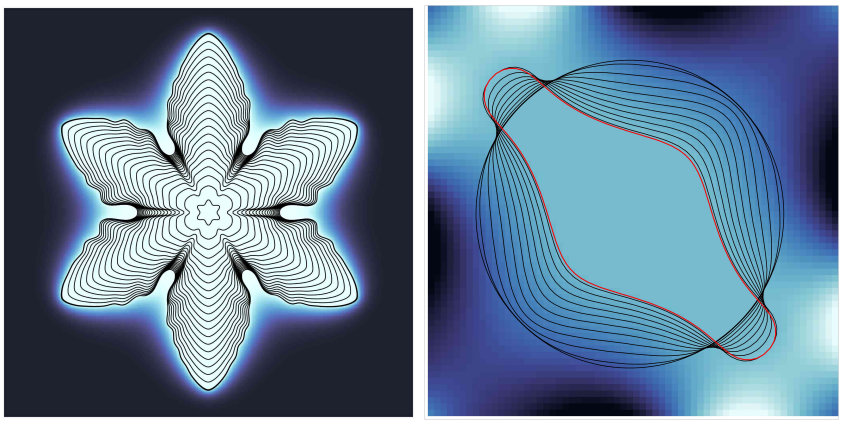

Figure 1: Left : crystal growth in an under-cooled liquid bath with anysotropic effect.
Right : final iteration of the optimization algorithm where the red curve is the desired shape.

A Conservative Cartesian Cut Cell Method for Accurate Predictions of Mass, Heat and Momentum Transfers

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The cut cell method provides an excellent tool to perform high-fidelity simulations of flows in complex geometries due to its reliance on Cartesian grids, which greatly reduces the complexity of the mesh generation process.

An energy-conservative cut cell method [1] is proposed based on the discrete calculus of Morinishi [2] to discretize the transport equations, including the incompressible Navier-Stokes equations, by means of the Marker-And-Cell (MAC) method where vector field components are located at face centers and scalar fields at cell centers. The solid boundary is specified using the level set method, where the boundary is defined as the zero-contour of a scalar field. The discrete operators obtained with this cut cell method retain the structure of their continuous counterparts, i.e. the symmetry and skew-symmetry of the diffusive and convective transport operators, respectively, and local and global energy conservation.

Validation of the operators is performed for cell-centered and face-centered fields for Neumann and Dirichlet boundary conditions. Fields obtained with the discrete operators are compared with analytical solutions to check the convergence rates of the operators.

A pressure projection method [3] is implemented to solve the incompressible Navier-Stokes equations. Time-advancement is performed with an implicit-explicit Runge-Kutta scheme. The accuracy of the transfers is investigated by analyzing the pressure trace and the viscous drag in flows around rigid solids, e.g. a cylinder and a NACA airfoil, at low Reynolds numbers and comparing them to the results obtained using with the Immersed Boundary Projection Method [4], which also works on Cartesian grids and where a set of Lagrangian points defines the solid boundaries.

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Lattice Boltzmann simulation of turbulent pipe flow laden with spherical particles

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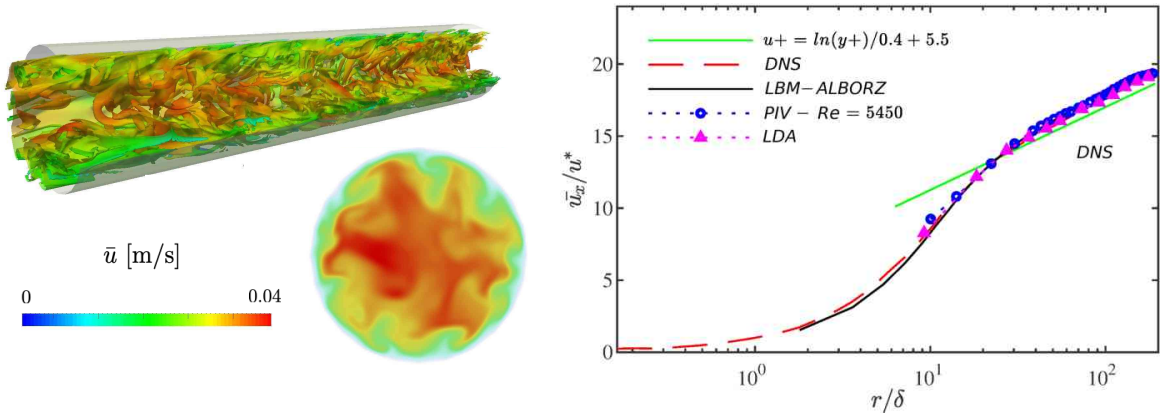
Particle-laden flows are ubiquitous in a wide range of natural and industrial systems. For instance it is well known that one can modulate turbulence characteristics of the carrier phase flow via finite-sized solid particles. In the present contribution we look into the effect of the introduction of solid spherical particles to a turbulent pipe flow. The study is conducted by performing direct numerical simulations of: a) single-phase and b) particle-laden two-phase turbulent pipe flows. The carrier phase dynamics is modeled using the lattice Boltzmann method while fully resolved solid particles are coupled to the flow via a direct forcing immersed boundary method. All simulations are carried out using the extensively validated in-house solver ALBORZ [1].



(a) (b)

Figure 1: a) Snapshot of the instantaneous velocity field obtained with ALBORZ, b) Radial distribution of average stream-wise velocity for turbulent pipe flow at $\mathrm{Re}_\tau = 180$. DNS data from [2], PIV and LDA from [3], compared to LBM results of ALBORZ.

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Extension of the multi-regime two-fluid model towards wall-bounded multi-scale liquid films

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Multiregime closure models for the two-fluid model often focus on continuous-dispersed and large-scale interface flow morphologies [1, 2, 3]. Thin liquid films at solid walls, e.g. in annular flow or film condensation, so far have not been considered in a multiregime two-fluid (MTF) model. Rather, thin liquid films are currently treated as large-scale interfaces. The film interface thus has to be resolved, which is conflicting with the two-fluid model approach and increases computational cost. For the interface resolving volume-of-fluid method, coupling to a liquid film (LF) model was previously proposed to treat subgrid size liquid films [4]. Here, we adapt this approach to the framework of the MTF model. A film thickness transport equation and film momentum equation are solved in a shell region of the two-fluid model volume domain. Mass- and momentum transfer between both models is included depending on a critical film volume fraction in the first cell at the wall. Thus a hybrid representation of liquid films depending on the local film thickness is obtained in the proposed LF-MTF model. The implementation in the CFD solver STAR-CCM+ is outlined and a basic verification case is presented. Validation results of LF-MTF model simulations against X-ray microtomographic data of horizontal annular flow [5] show qualitative agreement and outline paths for further model improvement. Finally, simulation results of droplet separators demonstrate the applicability of the LF-MTF model to industrial CFD.

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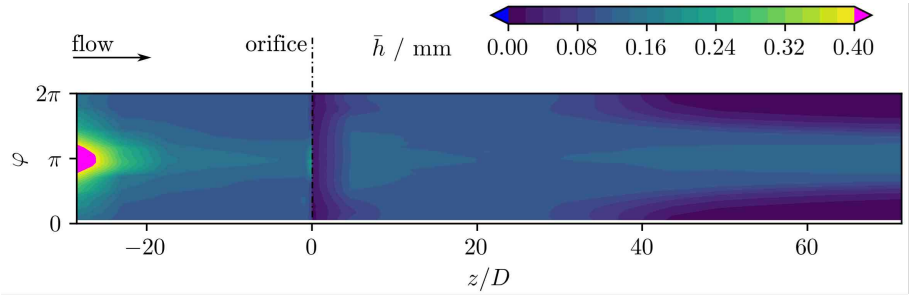

Figure 1: Liquid film thickness on pipe wall obtained from LF-MTF model simulation of horizontal annular flow through orifice.

A phase-change model for diffusion-driven mass transfer problems in incompressible two-phase flows

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We present a VOF-based numerical method for incompressible Direct Navier-Stokes (DNS) equations for diffusion-driven phase-change flows. The interface is tracked with a geometric (PLIC) scheme and special emphasis is placed on the treatment of velocity discontinuities across the interface. A novel algorithm is presented to smoothly extend the liquid velocity field across the interface in a way that the interface can be transported by a divergence-free velocity field. Our methodology requires minimum computational effort and is readily implementable in existing VOF codes. The transport of species is treated with a two-scalar approach [1] and special attention is paid to the advection and diffusion steps which must be consistent with the position of the interface to avoid artificial mass transfer. Henry's Law is used to compute the jump in species concentration across the interface. The methodology is implemented in the open-source code Basilisk [2] and is validated against analytical and semi-analytical models (2D and 3D). Benchmarks include the Stefan problem for a planar interface, suspended bubbles in under- and super-saturated solutions and a rising bubble in a creeping flow (Fig. 1). The relative errors on the relevant quantities are generally below 1% for the finest grids. The method is finally applied to study the growth of electrochemically generated bubbles on planar electrodes and the effect of contact angles and number of nucleation sites is investigated; results are compared against experiments available in the literature [3].

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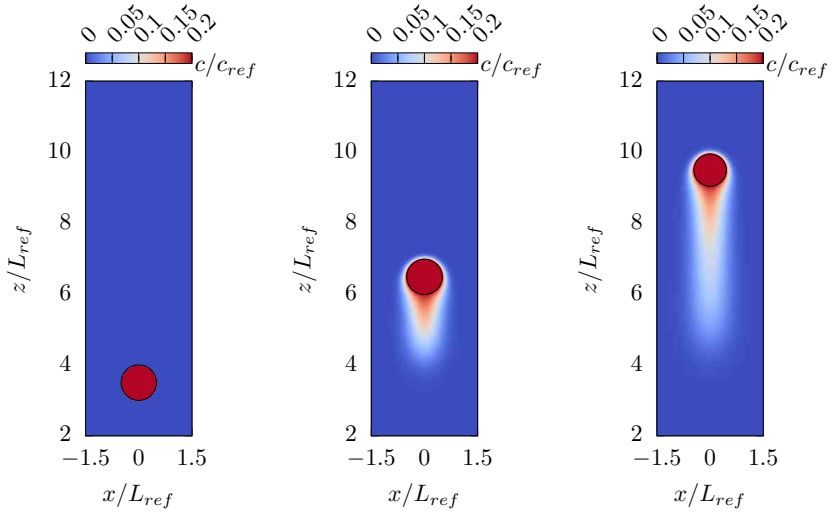

Figure 1: DNS of mass transfer from a rising bubble in a creeping flow.

Investigation of Droplet Motion on Chemically Heterogeneous Surfaces using a Phase-Field Approach

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In this work, 3D Direct Numerical Simulations (DNS) of droplets on chemically non-homogeneous surfaces are investigated [1]. The simulations are performed using our diffuse interface phase-field solver `phaseFieldFoam` (implemented in OpenFOAM, FOAM-extend 4.0 and 4.1). The solver has been enhanced to use a load-balanced adaptive mesh refinement technique and a moving reference-frame technique, to refine the mesh at the interface and to follow the droplet's center of mass, respectively. This substantially reduces computational costs.

Validation is done against several test cases including the equilibrium shape of a droplet spreading on a spherical substrate by comparison to analytically derived solutions, as well as comparison with experimental results of the droplets' velocity profiles as they slides down a chemically homogeneous substrate. We also detail on the benchmark of a capillary rise of liquid column driven by wettability gradient, which serves as a validation case for chemically heterogeneous surfaces [2].

Finally, we set out how chemical heterogeneities influence droplets, detailing the effects on droplet shape, internal flow, droplet velocity and viscous dissipation (cp. Fig. 1).

Acknowledgements

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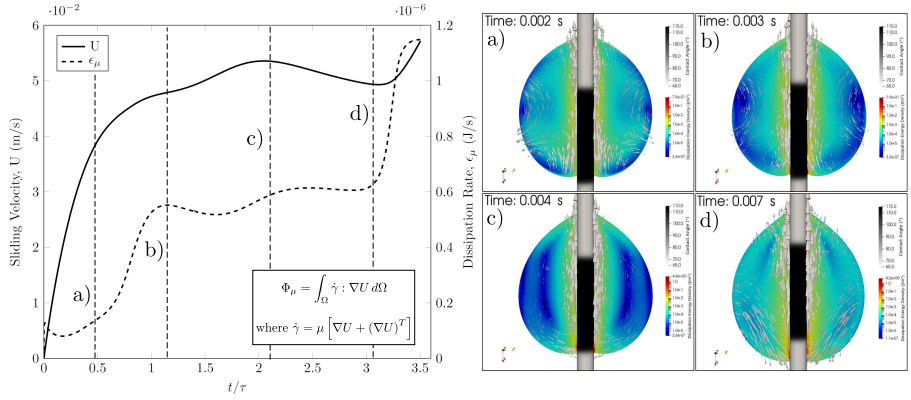

Figure 1: Droplet moving on a chemically heterogeneous fibre strand ($\theta_0 \in \{65°, 115°\}$). Velocity and dissipation rate (left) dissipation energy density profile and internal velocity field of the droplet (right).

Interface Retaining Coarse Models for Complex Multiphase Flows

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Multiphase flows are characterized by the presence of a sharp interface. In many situations such flows also consists of a large range of scales, making fully resolved numerical simulations expensive or unfeasible [1]. For predictions of the behavior of systems of practical interest it is therefore necessary to use coarse models where large scales are evolved deterministically and small scales are represented statistically. We describe a systematic process to coarsen fully resolved numerical solutions for multiphase flows while retaining a sharp interface [2]. The different phases are identified by an index function that takes different values in the different phases and is coarsened by solving a constant coefficient diffusion equation, while tracking the interface contour. Small flow scales of one phase, left behind when the interface is moved, are embedded in the other phase by solving another diffusion equation with a modified diffusion coefficient that is zero at the interface location to prevent diffusion across the interface, along with a pseudo pressure equation to preserves the incompressibility of the coarsened volumetric velocity field. See the figure below. The dynamics of the small scales in the mixed regions can be modeled in many different ways, including using homogeneous mixture, drift flux, and two fluid Euler-Euler models, as well as Euler-Lagrange models. We discuss current efforts in modeling the coarse evolution, using simple homogeneous mixture models.

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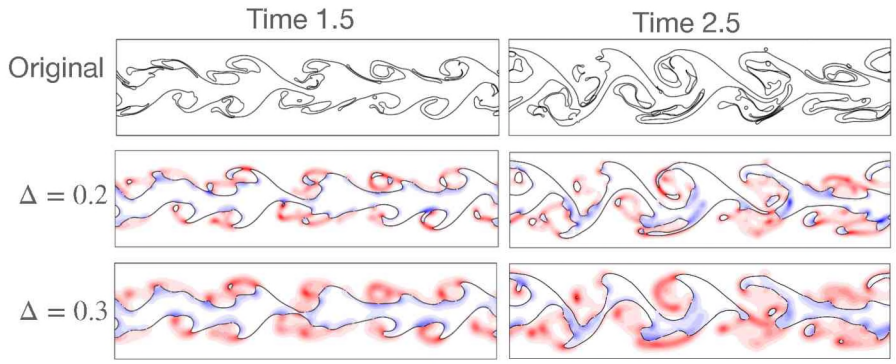

Figure 1: A fully resolved flow with an interface separating two fluids (top) and filtered flow field for two filtering levels (middle and bottom. For the filtered solutions the mixture fractions are also show.

An octree-adaptive immersed boundary-lattice Boltzmann method for 3D simulation of fluid-rigid particle interactions

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We present an immersed boundary-lattice Boltzmann method (IB-LBM) with adaptive mesh refinement (AMR) for simulating three-dimensional fixed/moving rigid particle dynamics immersed in a fluid. The incompressible flow field is solved by a finite-difference LB model with a multi-relaxation-time collision operator to improve stability and accuracy of simulations. Fluid-solid interactions are handled by an improved explicit feedback IBM which employs the smoothed Dirac delta functions [1] and compensates internal fluid mass effect. To save computing costs, the coupled method is implemented on adaptive octree grid in the open-source software *Basilisk* [2], which dynamically reconstructs meshes based on various adaptivity criteria and enables MPI parallel computing. We carry out a series of validations on single-particle system, including flow past a fixed sphere at a Reynolds number $0 \leq Re \leq 300$ and sphere sedimentations in a closed box with different sizes at a Galileo number $0 \leq Ga \leq 255.35$. A good agreement has been achieved through comparison between our results and reference data, which demonstrates high accuracy and robustness of the present method. With simulation interest in many-particle system, we finally investigate the flow past a random array of spheres with different volume fractions.

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A subgrid-scale modeling framework for convection-dominated interfacial species transport applied to modeling mass transfer in a metallurgical refining ladle

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We consider the numerical simulation of interfacial mass transfer between liquid steel and slag in a metallurgical ladle. The transport of a passive scalar along a liquid–liquid sheared interface is dominated by two transport phenomena: convection in the stream-wise direction and diffusion in the interface normal direction. In the problem considered, the large Schmidt number leads to the formation of a thin concentration boundary layer potentially orders of magnitude smaller than the smallest hydrodynamic length scales. As such, fully resolving both hydrodynamic and mass transfer length scales results in infeasible computational costs. Previous approaches to solve this problem resolve the concentration boundary layer at small Schmidt numbers and use boundary layer theory to extrapolate the results to the experimental number of 1480 [1]. In the current work, we use a subgrid-scale (SGS) modeling framework developed in [2] to precisely model the advective and diffusive fluxes in the thin boundary layer, allowing us to consider boundary layers much thinner than the grid size. Consequently, we simulate the problem by fully resolving the hydrodynamics and modeling the mass transfer, allowing us to accurately model much larger Schmidt numbers than is done with traditional numerical methods at comparable computational costs. The framework developed is published in the open-source Free Software library Basilisk [3], allowing others to use the framework to model interfacial heat and mass transport in complex flows.

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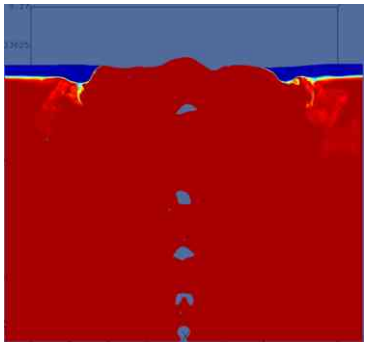

Figure 1: DNS of interfacial mass transfer of a reduced scale experiment of a metallurgical ladle.

An adaptive sharp interface method for detailed simulations of collective bubble growth and collapse dynamics

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The aspherical growth and jetting collapse of acoustically excited bubbles is an important mechanism for tissue damage in biomedical applications such as burst wave lithotripsy and histotripsy. The short timescales and the particularly strong intensity of the jetting collapse challenges simulation-based investigations of collective bubble collapse in a tissue-mimicking medium. Here, we present a novel sharp interface free-surface tracking method for performing large scale detailed simulations of jetting collapse of bubbles in non-Newtonian fluids. The method employs a high-order implicit description of the gas-medium interface on an adaptively refined structured mesh for an accurate and robust treatment of the large variations in the interface topology. The bubble contents are taken to be homogeneous and inviscid, and they are represented through a polytropic gas equation of state, as in the case of well-established Rayleigh-Plesset model for radially symmetric bubble dynamics. Comparisons to Rayleigh-Plesset on a coarse rectangular mesh show how the formulation can accurately track multiple bubble collapse and rebound events. The robustness and accuracy of our adaptive free-surface interface tracking implementation is demonstrated on a range of test configurations consisting of bubbles that undergo collective growth and jetting collapse. Figure 1 depicts the axisymmetric near-wall growth and jetting collapse of a bubble that is initially placed at a stand-off of twice the initial bubble diameter. Demonstration simulations to be presented at the conference will include fully three-dimensional runs of multiple bubbles undergoing collective oscillations and jetting collapse in the vicinity of rigid boundaries.

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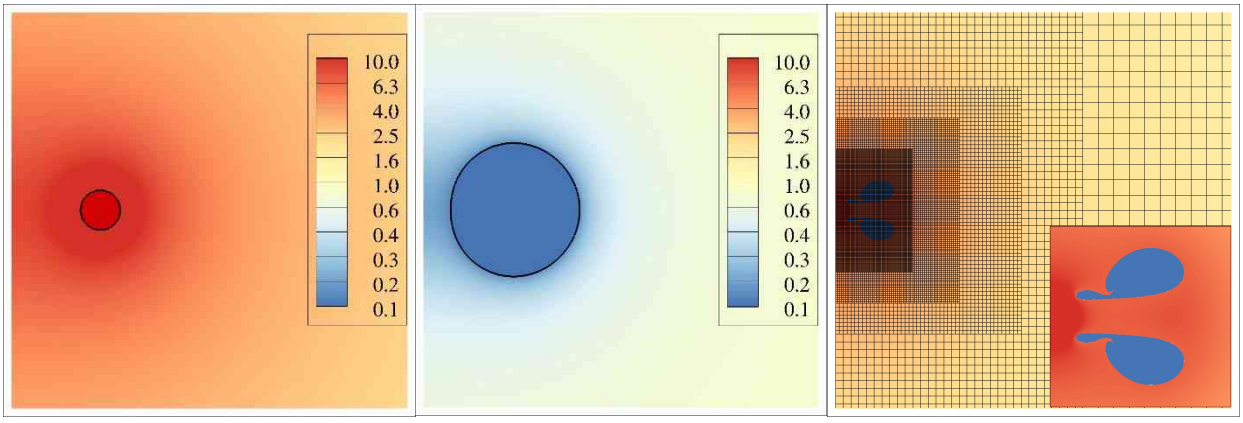

Figure 1: Growth and collapse of an initially spherical bubble placed next to a rigid wall. Colored contours illustrate the pressure field normalized with respect to the initial far-field ambient pressure, with the solid black line representing the bubble-medium interface. The left frame shows the initial spherical bubble and the corresponding pressure distribution. The middle frame illustrates a fully expanded state in which the bubble attains its maximum volume. The right frame corresponds to a state in which bubble collapse leads to a strong jet that pierces through the bubble. The inset in the right frame illustrates a zoomed-in view of the collapsed bubble. The overlaid dark lines show the adaptive mesh used in the calculation. The rigid wall coincides with the left boundary in all the three frames. The initial bubble pressure is twenty-fold the far-field ambient pressure.

Large-Eddy Simulations of spur gear lubrication by oil jets using an Interface Capturing Method and Dynamic Mesh Adaptation

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Mastering lubrication and cooling in aeronautic gearboxes is a major design challenge for efficient and reliable turbofans. At all operating conditions, appropriate lubrication of the gears is imperative to reduce heating due to mechanical friction, while lubricant-induced losses must be minimized for optimal performances. 3D unsteady simulation of the turbulent two-phase flow encountered in such complex geometries is very difficult to perform as the range of time and space scales is broad. The moving mechanical parts and the discontinuous physical properties of oil and air also contribute largely to the numerical difficulties. In this paper, an unsteady 3D Finite-Volume approach is described and used to bring a fine understanding of the complex non-linear liquid/gas interface dynamics. The approach relies on i) a Conservative Level-Set method [1] for an accurate description of the liquid/gas topology, ii) Dynamic Mesh Adaptation [2] to automatically refine the mesh at the interface vicinity and iii) an Immersed Boundary method to account for the fluid domain deformation due to gears motion [3]. This High-Fidelity approach is used to study the oil jet interaction with a rotating spur gear. The simplified gearbox studied experimentally by Massini et al., [4, 5] is considered. This configuration is a rectangular casing enclosing a driven spur gear which is lubricated by a radial oil jet generated by a spraybar. Large-Eddy Simulations are performed to assess the impact of the spur gear rotation speed on the lubrication quality and on power losses. In particular, the oil jet coherence, potential deviation, and oil penetration in the gear teeth spacing are investigated. The power losses due to windage and oil lubrication are analyzed and compared with correlations from the literature. Preliminary comparison between the numerical results and high-speed visualizations, shown in Fig. 1 are very promising.

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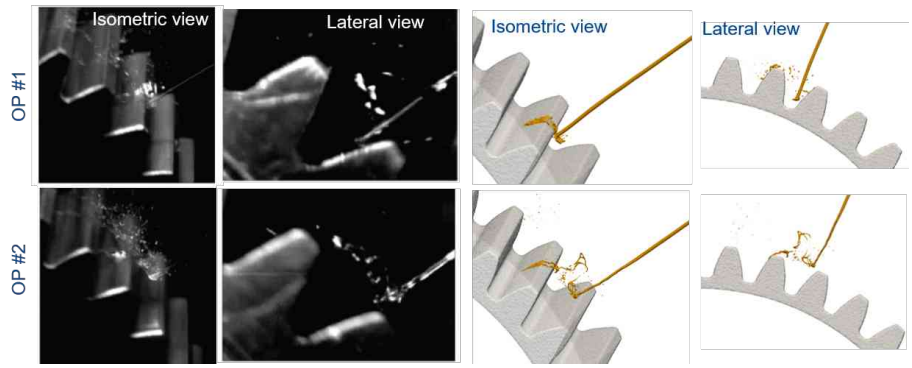

Figure 1: Comparison of air-oil interface snapshots obtained from high-speed visualization [4] (left) and evaluated numerically (right) for two spur gear rotational speed.

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Wednesday – 2022-09-28

Session II

- **Methods for compressible two-phase flow**
  (Chair: J. Lindau, Room: Aula 1-G)
- **Methods for particulate flows**
  (Chair: F. Evrard, Room: Auditorium)
- **Interfacial instabilities and multiphysics**
  (Chair: M. Pelanti, Room: Aula Magna 1-E)

Large eddy simulations of primary breakup in metal melt gas atomization

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Bed-based techniques for additive manufacturing (AM), in which thin layers of metal powder are melted locally by a laser, allow for the production of components with complex designs. While the metal AM technology is relatively matured, flexible production of metal powder on a small scale is lagging behind. A common process for the production of this powder is gas atomization, in which high pressure gas jets are used to rupture a molten metal stream into fine droplets, which subsequently solidify into a powder. Currently, the production of metal powders by gas atomization takes place in bulk, limiting the flexibility of the feedstock. It is acknowledged that a small scale batch process for the production of high-quality metal powder will be beneficial to the versatility and sustainability of powder bed AM techniques [1].

This work focuses on the modelling of the initial breakup of the metal melt in gas atomization, known as primary breakup. In this stage, the metal melt stream breaks up into large droplets and ligaments. High local Weber and Reynolds numbers are encountered as a result of supersonic gas jets impinging on the metal melt stream. Large velocity and temperature gradients increase the computational complexity of the breakup process. While in previous studies mainly the gas dynamics were studied [2, 3], the current modeling strategy is aimed at understanding the primary breakup process for both the melt and gas phase. To this end, the gas-melt interface is modeled using a Volume-of-Fluid (VOF) method for compressible flow in the open-source OpenFOAM software.

In previous studies of primary atomization, a Reynolds-Averaged Navier-Stokes (RANS) approach is often employed to represent the turbulent behaviour of the flow [4, 5]. However, due to the highly transient nature of the atomization and the dependence of the breakup on local flow conditions, it is questionable whether the averaged nature of the RANS formulation is able to represent the details of the melt breakup accurately. In this work, Large Eddy Simulations (LES) are applied instead, in order to be able to partially resolve the local turbulent flow structures. Special attention is devoted to the local resolution of the computational grid, with respect to the fraction of turbulent kinetic energy resolved in the LES. In order to increase the understanding of the primary breakup, statistics of the breakup behavior are related to process variables, such as atomization pressure and turbulent intensity of the melt phase.

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Investigating 3-D effects on Flashing Cryogenic Jets with highly resolved LES

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For the development of upper stage rocket engines with laser ignition, the transition of oxidizer and fuel from the pure cryogenic liquid streams to an ignitable mixture needs to be better understood. Due to the near vacuum conditions that are present at high altitudes and in space, the injected fuel rapidly atomizes in a so-called flash boiling process. To investigate the behavior of flashing cryogenic jets under the relevant conditions, experiments of liquid nitrogen have been performed at the DLR Lampoldshausen. The experiments are accompanied by a series of computer simulations and here we use a highly resolved, fully compressible LES to identify 3D effects and to better interpret results from the experiments and existing 2D RANS. It is observed that the vapor generation inside the injector and spray kinetics differ significantly between the two simulation types due to missing 3D effects and the difference in resolution of turbulent structures. Still, the observed 3D spray dynamics suggest a suitable location for laser ignition that could be located in regions of relative low velocity and therefore expected low strain rates. Further, measured droplet velocities are compared to the velocities of notional Lagrangian particles with similar inertia as the measured droplets. Good agreement between experiments and simulations exist and strong correlation between droplet size and velocity can be demonstrated.

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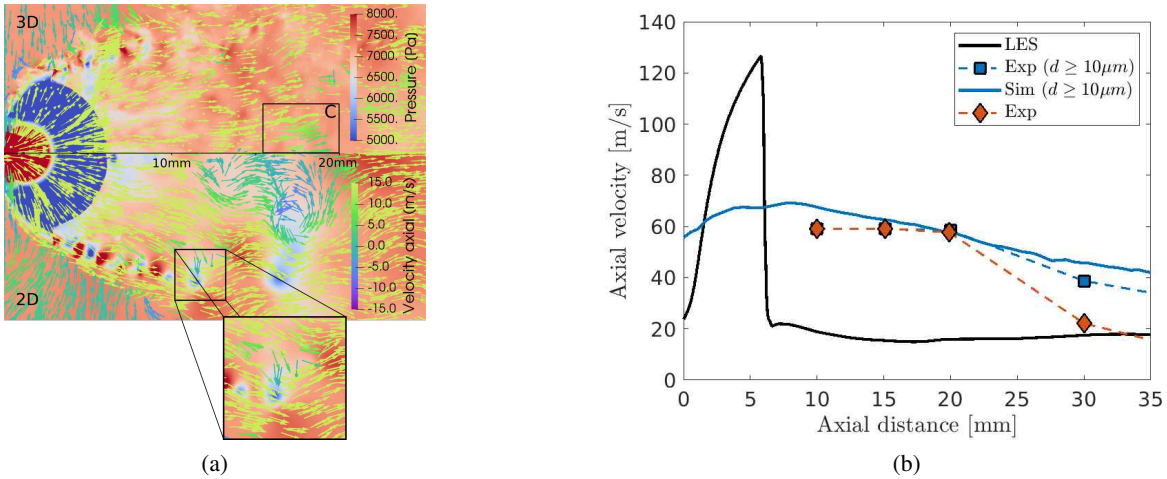

(a) (b)

Figure 1: (a) Pressure and axial velocity displayed as vector glyphs for 3D and 2D simulations with a suitable location for laser ignition in area C. (b) Axial velocity of the one fluid solution (LES), the experimental data (Exp), as well as a conditioned velocities for droplets larger than $10\,\mu\mathrm{m}$ in the experiment and of Lagrangian particles in the simulation.

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Modeling and simulation of stiff two-phase tube problems

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Several physical and numerical models have been developed to investigate cavitating flows within the framework of the continuum modelling method. In its implementation, there are different approaches according to the assumptions made (2-fluid, 1-fluid…). A major problem for the modelling is linked to the metastable states for pure phases and the non equilibrium thermodynamic path during the phase transition. A hierarchy of models exists, with the numbers of equations ranging from seven to three only.

In the present paper, the simplicity of the model is privileged in view of its use in realistic applications. We tested and compared various two-phase models: 4-equation model involving different source term for the mass transfer between phase [1,2] and a 5-equation model based on the Kapila formulation [3]. Various tube cases involving shock-waves, expansion waves and phase transition are considered for the validation.

4-equation model

The governing equations are written for a single fluid model. The formulation is composed by three conservation law for mixture quantities plus an equation for the void ratio α.

$$\frac{\partial \rho}{\partial t}+\frac{\partial \rho u}{\partial x}=0 \tag{1}$$

$$\frac{\partial \rho u}{\partial t}+\frac{\partial \left(\rho u^2+P\right)}{\partial x}=0 \tag{2}$$

$$\frac{\partial \rho E}{\partial t}+\frac{\partial \left(\rho H u\right)}{\partial x}=0 \tag{3}$$

$$\frac{\partial \alpha}{\partial t}+u\frac{\partial \alpha}{\partial x}=\alpha\left(1-\alpha\right)\left(\frac{\rho_l c_l^2-\rho_v c_v^2}{\alpha\rho_l c_l^2+\left(1-\alpha\right)\rho_v c_v^2}\right)\frac{\partial u}{\partial x}+\frac{\dot{m}}{\rho_I} \tag{4}$$

The mass transfer between phases $\dot{m}$ can be evaluated by different ways. A first formulation involves contributions for the vaporization and condensation processes, with constants related for each process. A second one involves the divergence of the mixture velocity.

Results

Various test cases are considered: double rarefaction tube with phase transition, shock tubes with different fluid (dodecane and CO2). Validation is done by comparing results against exact solution and reference solution from the literature [4,5].

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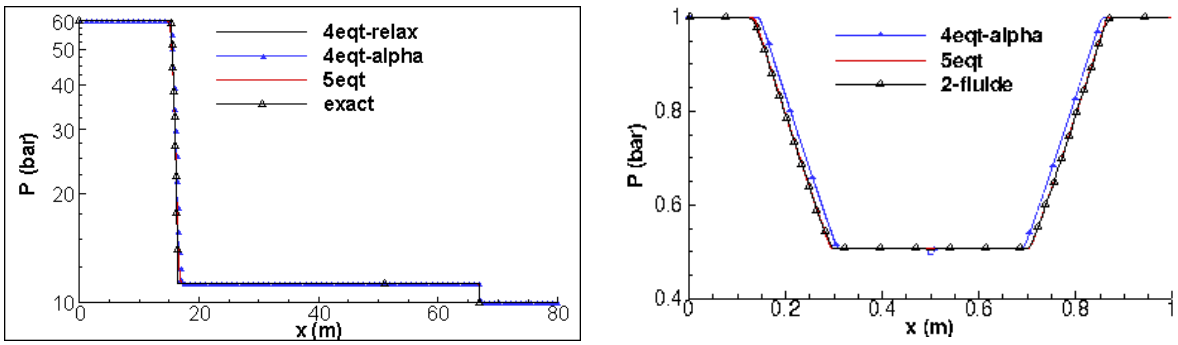

Figure 1: Pressure profile shock-tube problem CO2 (left) and pressure profile expansion-tube problem with cavitation (right)

Hyperbolic Solvers for the modeling of Compressible Two-Phase Flows

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Multifluid models offer a wide range of potential applications when it comes to modeling compressible two-phase flows, giving access to various disequilibriums between each phase. Derived from Drew's averaging of the phases' transport equations [1], they represent phase interfaces as physical discontinuities, allowing for a continuous Eulerian description. These models can be designed as hyperbolic, given convexity of the equation of state.

This however poses two main difficulties : thermodynamic closure and numerical methods for the non-conservative terms that appear in those systems. Here we will focus on this second aspect. From the 7-equation model [2] with complete disequilibrium between phases, various asymptotic limits were introduced, such as Kapila's five-equation model [3], adding velocity and pressure equilibrium and thus reducing the amount of non conservative terms. Interesting findings on a 6-equation model as good compromise between the 5 and 7-equation systems are also considered [6].

For each of these models, a variety of solutions exist to evaluate the numerical flux at each finite volume cell boundary. For example, the Rusanov, HLL, Roe and HLLC fluxes are the most frequently used ones, the latter posing the most difficulties [2, 4, 5, 7]. Our objective is to provide an investigation on these models, studying their accuracy and robustness when implemented on different hyperbolic solvers. Particular attention will be given to the treatment of non conservative terms.

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Contact-line treatment for boiling flows using a weakly compressible diffuse interface framework

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Nucleate boiling, as one of the most efficient mechanisms for heat transfer and energy conversion, has been widely used in many industries requiring substantial energy transfer within a short period of time (solar energy, thermal power, nanoelectronics, to name a few). During the last decades, theoretical studies together with the experimental tests and numerical simulations confirm the complex physics behind the nucleate boiling problem. Given the limitations of the theoretical approaches, especially for non-ideal working fluids, and difficulties in experimental measurements, performing a successful numerical simulation of the problem is a demanding task worth pursuing. In this study, we propose a novel mathematical framework, based on the diffuse interface method, able to incorporate not only phase change, compressibility but also wettability over complex surfaces. The governing equations are based on the Baer-Nunziato two-fluid formulation [1] and extended with the approach proposed in [2] to include contact angles treatment (both static and dynamic) and wall roughness. The method is first validated with simple benchmarks of increasing complexity, and then employed in the more challenging configuration of three-dimensional nucleate boiling.

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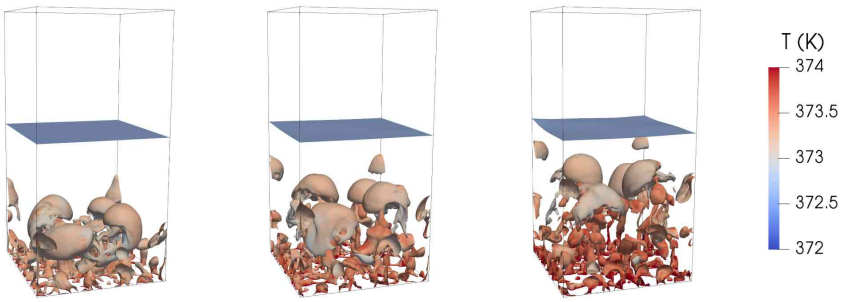

Figure 1: Instantaneous snapshots of volume fraction 0.5 iso-surfaces, colored using the temperature field for the three-dimensional nucleate boiling in water for time $0.40 - 0.45 - 0.50\ s$ (left-center-right).

A compressible hybrid model for cavitating flows

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Cavitating flows have a wide range of vapor length scales, ranging from massive cavities to micro-bubbles. We develop a compressible hybrid multi-scale model that captures the dynamics of both massive cavities (or resolved vapor) and micro-bubbles (or unresolved vapor) and accounts for medium compressibility.

Past work has shown that resolved vapor behavior can be accurately captured when tracked in an Eulerian sense [1, 2, 3], and the unresolved vapor dynamics is best captured when tracked in a Lagrangian sense [4]. The key idea behind our hybrid model is to split the net vapor mass, momentum and energy in the compressible homogeneous mixture equations into constituent resolved and unresolved components to ensure their independent treatment. The resolved vapor is then tracked in an Eulerian sense using the transport equation, and the micro-bubbles are tracked in a Lagrangian sense using the novel 'generalized RP equation' developed in this work. An important point to note is that the hybrid model reduces to the homogeneous mixture model (HMM) in the absence of unresolved vapor and the Euler-Lagrangian (EL) model in the absence of resolved cavities.

Integrating the spherical momentum equation from the bubble surface (R) to a finite distance (kR) and coupling it with the linear wave equation yields the generalized RP equation. Such an approach results in $p(kR)$, the resolved phase pressure at a finite distance, being the external pressure experienced by the bubble. Accounting for local external pressure ($p(kR)$) via first principles allows the model to capture inter-bubble interactions without additional modelling. The generalized RP equation yields the Keller-Miksis equation when k become infinitely large, and the incompressible RP equation when both speed of sound and k become infinitely large.

The hybrid model has been validated for unresolved and resolved single bubbles as well as for bubble-bubble interaction problems. The bubble behavior is shown to be independent of the parameter k. The ability to account for interaction between a resolved and an unresolved gas bubble is demonstrated. Results are shown for a cloud of micro-bubbles exposed to an acoustic pulse.

Acknowledgements

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Dominant mechanisms of secondary flows in horizontal particle-laden pipe flows

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The present study is concerned with numerical simulations of secondary flows in horizontal particle-laden pipe flows. Direct numerical simulations coupled with a four-way coupling discrete particle model were employed using a Euler-Lagrange approach, considering the drag, lift and gravitational forces on particles, together with the collisions of particles with the wall and with other particles. A nearly elastic coefficient of restitution, $e = 0.97$, was employed for both particle-wall and inter-particle collisions. The Reynolds number, Stokes number and particle-to-fluid density ratio were fixed at $Re = 20000$, $Sk = 11.2$ and $\rho_r = 1000$, respectively. The single variable was the particle mass loading, which varied from $\Phi_m = 0.4$ to 0.9, 1.2, and 1.8 to assess its influence on the flow and particle behaviour. These four values of Φ_m result in four different flow regimes characterised by various combinations of secondary flow structures of the fluid and particle phases, shown in Fig. 1(a) and (b), respectively. With the increase in Φ_m, the fluid secondary flow structure varies from a centre-upward two-cell to a four-cell, and a centre-downward two-cell structure. This coincides with a transition of the particle secondary flow structure from a reversed four-cell to a six-cell, and a centre-downward two-cell structure. To investigate the driving mechanisms for these secondary flow motions, the forces exerted on the fluid phase, including the pressure gradient force, the interaction force exerted by the particles, and the resultant force, were examined to identify the contribution of each of these forces to the fluid secondary flow motions. A similar analysis was also applied to the drag, lift, gravitational and resultant forces exerted on the particle phase for the particle secondary flow motions. The force analyses explain the secondary flow directions and the interaction between fluid and particle phases. Finally, sketches summarising the dominant mechanisms are also presented to advance the understanding of secondary flows in such flows.

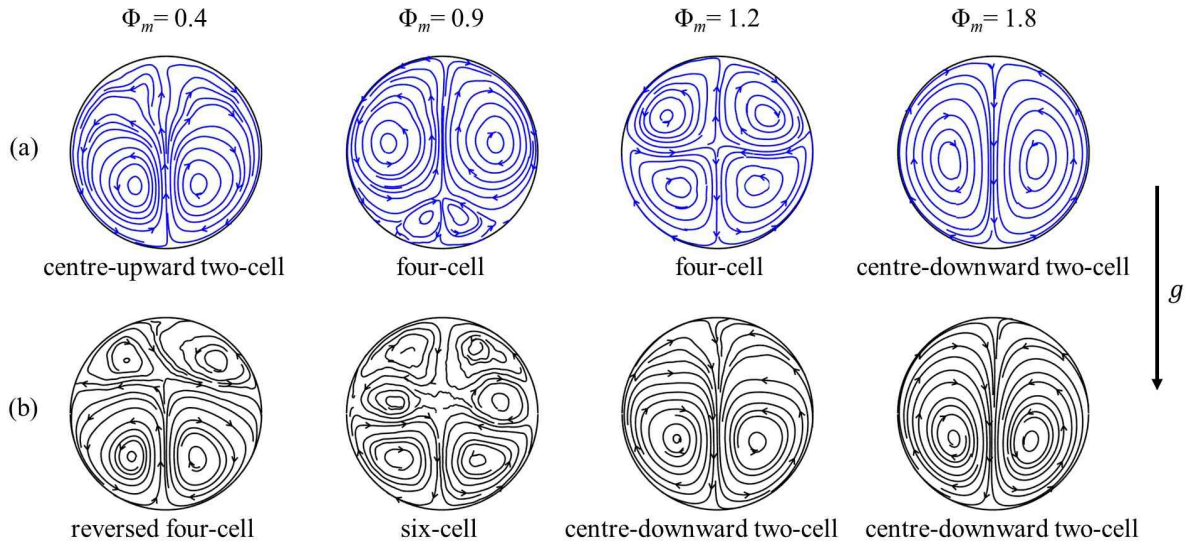

Figure 1: Secondary flow structures of (a) the fluid phase and (b) the particle phase, for various values of particle mass loading.

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A wavelet-based kinematic simulation for turbulent dispersed two-phase flows

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Lagrangian simulations are today widely used for simulating aeronautical chambers. The way droplets are spatially distributed strongly affects the combustion, and accurate modeling and simulation strategies are required. The objective of the present contribution is to investigate how to correctly reproduce preferential concentration in Large Eddy Simulation (LES) of particle-laden flows. We suggest a new strategy in the spirit of kinematic modeling of turbulence [1], based on divergence-free wavelets [2]. This formalism has the same advantages as a Fourier-based kinematic simulation [3], namely its analytic formulation, its numerical simplicity, and its similarity with the Kolmogorov picture of turbulence. By controlling the model characteristic length and time scales, we can reproduce the flow statistics and the particles segregation obtained by DNS with a better agreement than with Fourier-based kinematic simulation [4]. Moreover, the compacity of wavelets modes allows preserving the locality of the information, and the versatility of the model offers many perspectives for more complex flow configurations with strong heterogeneities.

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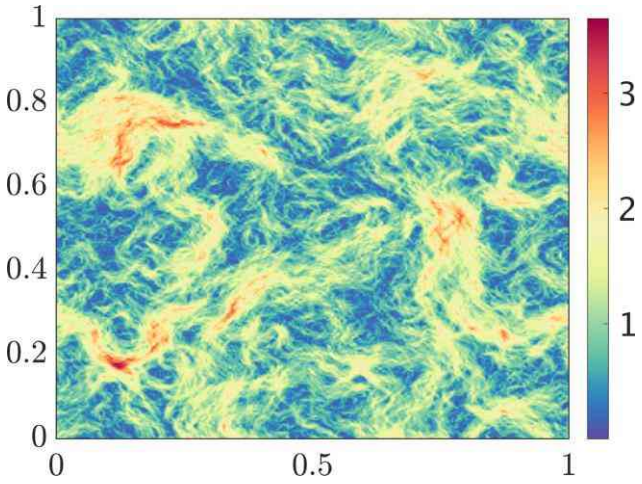

Figure 1: Snapshot of a wavelet-based kinematic velocity field

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Accurate Lagrangian subgrid-scale models for turbulent particle-laden flows

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Particle dynamics in turbulent flows are complex and involve significant interaction between scales. In the dilute limit, particles may respond to length and time scales present within an intrinsically turbulent flow (i.e., a flow that would exhibit finite turbulent kinetic energy (TKE) even in the absence of the disperse phase). At higher concentrations, particles may respond to the dynamic boundary layers generated by neighboring particles (pseudo-turbulent kinetic energy, PTKE). In the context of large-eddy simulation (LES) and Reynolds-averaged Navier–Stokes (RANS), models are needed to account for subgrid-scale (SGS) fluid velocity fluctuations (TKE or PTKE) on particle dispersion.

Stochastic models are commonly employed for dilute particle-laden flows (TKE) but are far less established for dense suspensions that exhibit PTKE. Despite their pervasive application, existing stochastic models are incapable of capturing the correct instantaneous spatial distribution of particles (e.g., preferential concentration). So-called structural SGS models aim to capture two-point particle statistics through reconstruction of the fluid velocity field. Such examples include approximate deconvolution, fractal and spectrally optimized interpolation, and stochastic vortex structure models. However, such approaches are limited in their ability to accurately reconstruct SGS motion and remain relatively unexplored [1]. Marchioli (2017) [1] notes that an ideal SGS model would combine the strengths of structural and stochastic models; allowing for accurate predicting of one-point and two-point statistical moments and geometric particle dispersion. Here, we propose a stochastic model for PTKE and examine a correlated stochastic model for the prediction of one-point *and* two-point statistics.

We first introduce a system of Langevin equations that form a hierarchy in terms of the physics they are capable of resolving [2]. Two canonical flow configurations are then considered: (i) flow through dense homogeneous suspensions of particles (PTKE-driven homogeneous heating/cooling) and (ii) the classical situation of a dilute concentration of inertial particles in homogeneous isotropic turbulence (TKE). In the former case, we employ a force Langevin model to describe neighbor-induced hydrodynamic interactions. The inclusion of a fluctuating drag force, modeled as an Ornstein-Uhlenbeck (OU) process, allows for accurate predictions of granular temperature evolution. In the latter case, particles spontaneously cluster due to non-linear interactions with carrier-phase turbulence. We present a new framework that embeds two-point statistics into the stochastic increment of the fluid velocity "seen" by a particle. A covariance matrix is assembled using particle-pair information that is readily available in LES and RANS. Decomposition of this covariance matrix allows for it to be applied in the OU process, transforming the independent random increments into spatially correlated random increments. The construction and decomposition of the covariance matrix presents several challenges, as its size scales with the number of particles. Because the two-point statistics decay rapidly with particle pair separation, the covariance matrix is sparse. We explore methods for exploiting the sparsity to allow for an efficient implementation in LES and RANS.

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The behavior of elongated non-spherical particles in wall-bounded turbulent flow: Detailed model validation

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Powder handling in industrial processes is a wide-spread unit operation in many industrial areas involving particle transport in gas or liquid in numerous types of devices, such as conveying in channels and pipes, particle separators, mixing vessels, paper making devices, and sediment transport. These types of multiphase flows are wall bounded and mostly highly turbulent. The particles found in these processes are rarely spherical but may have various shapes, from regular (e.g., fibers, rods, and plates) to irregular (i.e., agglomerates). Although for many years research is related to the behavior of regular non-spherical particles in turbulent flows, a conclusive description is, even today, not yet available. For many design rules and also in numerical computations of dispersed multiphase flows by computational fluid dynamics (CFD) methods the most common assumption is that the particles are spherical. This applies to the relevant fluid dynamic forces in a confined flow and to the interactions between particles (i.e., collisions and lubrication) as well as the particle-wall interactions, which of course yields a non-realistic treatment of the problem.

The numerical calculation of particle-laden flows by point-particle Euler/Lagrange type methods is based on tracking each non-spherical particle's translational and rotational motion, so that the center position and the orientation of the particles is known. For the calculation of non-spherical particles in turbulent flows, the translational motion is calculated in world space (laboratory frame of reference) and the rotational motion in body space (centered at the particle mass center), where the relevant forces, considering the corresponding angle of incidence, such as drag, gravity, shape lift, slip shear lift, slip rotational lift, and added mass were included. The models were derived based on first principles, which builds on available literature [1,2]. In addition, the hydrodynamic torques and the moments of inertia about the particle principal axis are also considered. To calculate the fluid flow and model the turbulence in the continuous phase, different RANS models were considered.

Model validation using the Euler/Lagrange point-particle framework for elongated, inertial fibers was completed using two different experimental data, one obtained by Marchiolli's research group [3] in which a turbulent channel flow (also with DNS validation) was considered, and the other experimental data was obtained by the Multiphase Flow Systems (MPS)-OVGU research group using imaging techniques such as the classical PIV (particle image velocimetry) and PTV (particle tracking velocimetry) under turbulent conditions in a fully water channel test facility, resolving their size, shape and orientation. Good agreement with the experimental results was observed when the proper fiber dynamics was included in the simulations, and particularly the hydrodynamic wall interaction (e.g., lubrication) was studied.

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A numerical strategy for Particle-Resolved Direct Numerical Simulation of gas-solid reactive flows.

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This work is part of a project (ANR MIMOSAH), which aims to model hydrogen combustion in fluidized beds. The project relies on a multiscale approach, from a very fine characterization of the combustion at microscopic scale to derive macroscale models. To this end, fully resolved simulations of a reactive, multi-species and weakly compressible mixture seeded with *partially inert* spherical rigid particles are performed; the particles are not consumed by heterogeneous combustion, but their surface is considered to undergo potential adsorption / recombination / desorption of gaseous radical.
The starting point of this work is the code RESPECT, that is able to simulate particle-laden flows with an unreactive and incompressible carrier fluid. The code is based on a method named Viscous Penalty Method (VPM) [1]: a One-Fluid model is solved on a fixed Cartesian grid, with the rigid-body motion enforced in the solid zone by viscous penalization.
To account for the proper boundary conditions at the solid-gas interface in presence of surface reactions, a rigorous One-Fluid model has been developed. It is based on an extension of Kataoka's single-field representation [2] that is then filtered in space, following a commonly applied methodology in the VOF community [3]. This filtering procedure enables to model the numerical smearing out of the interface. The resulting One-Fluid model extends the compressible model of Caltagirone *et al.* [4], with additional new terms requiring a proper numerical treatment:

- singular source terms at the solid-gas interface, essentially due to the presence of surface reactions.
- unresolved interfacial terms, caused by variables that are discontinuous across the solid-gas interface (such as species mass fractions).

As a first step, we discretize the One-Fluid reactive system of PDEs without these additional terms (that corresponds to a single-phase multi-species reactive flow); its implementation is compared against benchmark tests. Then we will present the numerical strategy implemented to take into account the first type of additional terms, that leverages on the geometrical approach of Min & Gibou [5] for discretizing the surface Dirac distribution. Finally, numerical prospects for the second type of terms will be outlined.

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A robust numerical scheme for simulating heterogeneous reactions in particle-laden flows in the N-Euler framework

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In reactive flows, the chemical time scales are often many orders of magnitude lower than other flow time scales. When simulating reactive flows, one must at least verify that i) species mass fraction takes physical values, that is greater or equal to zero and ii) their sum should add up to unity in each phase. Simonin and Laviéville [1] have built an adaptively implicit scheme for the numerical integration of species mass fractions that verify those two properties for any time step size during gaseous homogeneous reactions in multiphase flows.

The present work extends this scheme for heterogeneous reactions in multiphase flows. We implement this numerical scheme in the neptune_cfd code, a multiphase flow solver within the framework of N-Euler developed for the nuclear industry as part of a collaboration between EDF, CEA and IRSN and extended to reactive gas-particle flows with the support of IMFT. We exhibit properties i) and ii) with a test case consisting of the pyrolysis of biomass particles followed by heterogenous and homogeneous oxidation reactions in a perfectly stirred reactor. Fig. 1 shows the mass fraction of each species over time. Consistent results are obtained for time step size up to two order of magnitude greater than chemical time scale. A 3D fluidized bed simulation with the same reactive mixture is being carried out.

We note that this numerical scheme does not strictly verify the conservation of the mass of each atomic elements which can lead to a significant error on the mass fraction of each species and, consequently, on the predicted temperature. This error becomes more important when the ratio between the time step of the simulation and the time scale of the chemistry becomes larger. We have shown that this error can be significantly reduced by adapting our numerical scheme into an iterative method during homogenous reaction. Further investigations will be conducted to extend and confirm this result to heterogenous reactions.

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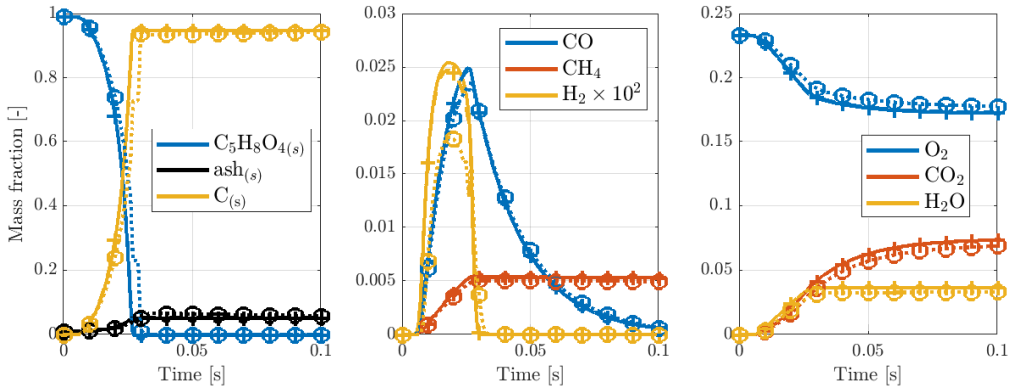

Figure 1: Mass fractions of all species (except N_2) over time obtained from simulations using three different constant time step: i) 10^{-5} s ($\sim$ minimum chemical time scale), full lines, ii) 10^{-4} s, dashed lines and crosses (1 every 100) and iii) 10^{-3} s, dotted lines and circles (1 every 10).

Physical accuracy and numerical stability of the Lattice Boltzmann color gradient multicomponent model for the jetting of microdroplets

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The performance of the Color-Gradient (CG) multicomponent Lattice Boltzmann model is quantitatively assessed on several physical flow problems where breakup, coalescence and contraction of fluid ligaments are important. Specifically we consider droplet oscillation, ligament contraction and the jetting of microdroplets as seen in inkjet printing. Our results show that the CG model is a suitable choice for challenging simulations of droplet formation, due to numerical stability, physical accuracy and wide range of accessible parameters. A jetting simulation with typical fluid parameters found in industrial applications, including a high density ratio, correct surface tension, viscosity values and tunable nozzle wetting boundary conditions, is shown to be achievable using the model. We show that the model can be used to investigate imperfect and asymmetric jetting as a consequence of asymmetric nozzle wetting, as illustrated in Fig. 1.

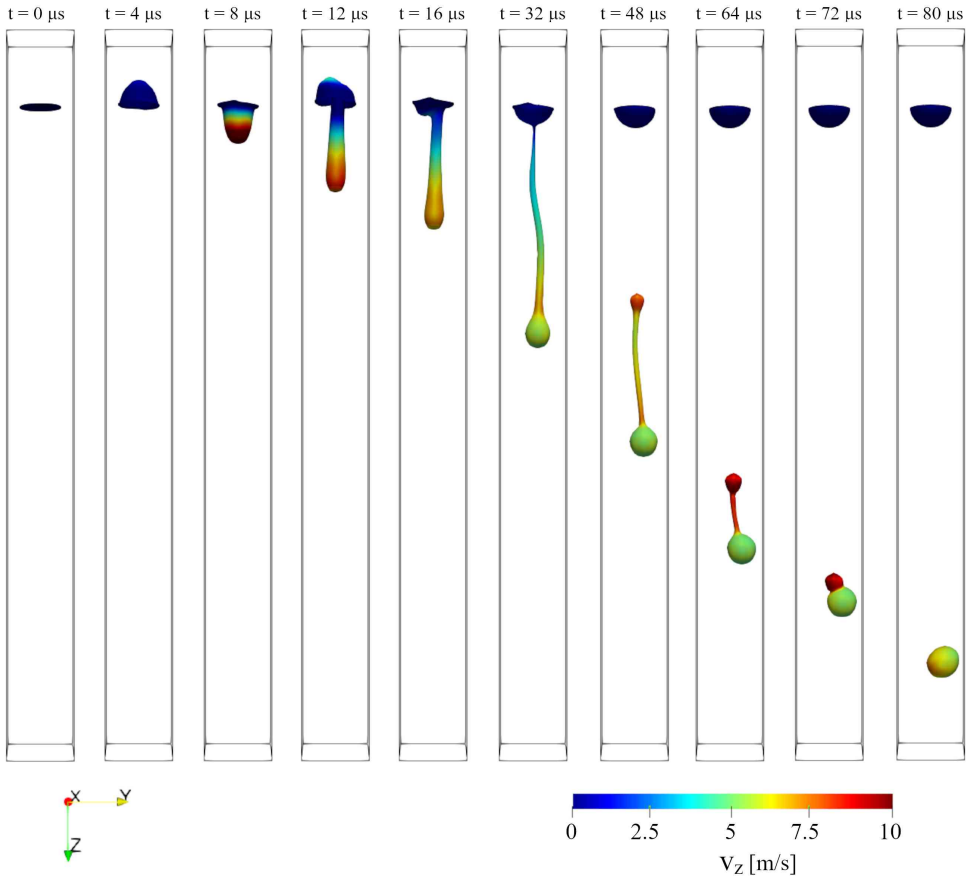

Figure 1: Example of asymmetric jetting due to non-homogeneous nozzle wetting, simulated in full 3D using a CG-LBM model.

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Interface-resolved direct numerical simulation of the breakup of solid fibers in turbulence

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The breakup of solid fibers transported in turbulent flows is a problem of crucial relevance in chemical engineering. The process occurs due to the peaks of stress exerted by the turbulent fluctuations on the solid fibers that may overcome the ultimate strength of the material causing a fracture [1]. This peculiar problem can be generally enclosed within the macro category of Fluid-Structure Interaction (FSI), a strongly non-linear problem that involves the intricate coupling between the governing equations of fluid dynamics and solid mechanics. The problem becomes even more complex if fracture mechanics is taken into account. Advancing our capability in the modeling of this class of problems, with a focus on fiber breakup, is of crucial relevance, but presents many challenges related to the complexity of the phenomena involved, their multiphysics nature and the high demand for computational resources. In this context, we aim to present a novel methodology for simulating generic, three-dimensional fluid-structure interaction problems involving fracturing. Peridynamics is used to describe the mechanical behavior of the solid phase and coupled via a multi-direct immersed boundary method with the incompressible formulation of the Navier-Stokes equations, which are used to resolve the dynamics of the fluid phase. The synchronization of the solution is achieved with a fully explicit, weak-coupling strategy that allows for fast and efficient computations. We tested our methodology against different benchmarking test cases whose results were compared to well-referenced and independent data available in the literature [2]. Finally, the proposed methodology was applied to the numerical simulation of the breakup of brittle fibers in Homogeneous Isotropic Turbulence (HIT). Some qualitative results of the simulation are presented to show the potential of the proposed approach.

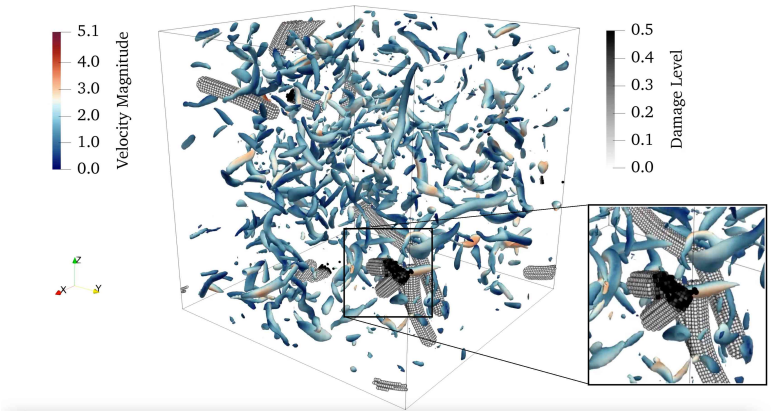

Figure 1: A snapshot of the break up of brittle fibers in HIT. Vortical structures are highlighted by Q-criterion and colored according to velocity magnitude.

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Particle capture by deformable drops in three-phase turbulent channel flow

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The capture of neutrally buoyant, sub-Kolmogorov particles at the interface of deformable drops in turbulent flow and the subsequent evolution of particle surface distribution are investigated. Direct numerical simulation of turbulence, phase-field modelling of the drop interface dynamics and Lagrangian particle tracking are used. Particle distribution is obtained considering excluded-volume interactions, i.e. by enforcing particle collisions. Our results show that particles are transported towards the interface by jet-like turbulent motions and, once close enough, are captured by interfacial forces in regions of positive surface velocity divergence. These regions appear to be well correlated with high-enstrophy flow topologies that contribute to enstrophy production via vortex compression or stretching. The rate at which particles get trapped at the interface is observed to scale with the turbulent kinetic energy of the fluid measured within one Kolmogorov length scale from the drop: This scale corresponds to a distance slightly longer than the particle stopping distance, chosen as reference scaling length for the selection of the volume-averaging thickness. This finding can be explained by considering that in our flow configuration, particle capture is driven by the turbulent fluctuations in the vicinity of the drop interface. Once captured by the interfacial forces, particles disperse on the surface. Excluded-volume interactions bring particles into long-term trapping regions where the average surface velocity divergence sampled by the particles is zero. These regions correlate well with portions of the interface characterized by higher-than-mean curvature. This finding is relevant for the understanding of the effect that particles may have on the drop surface properties, in particular surface tension. The convex portions of the interface will be those where changes of the surface tension and, hence, of drop deformability induced by the presence of very small particles will be larger.

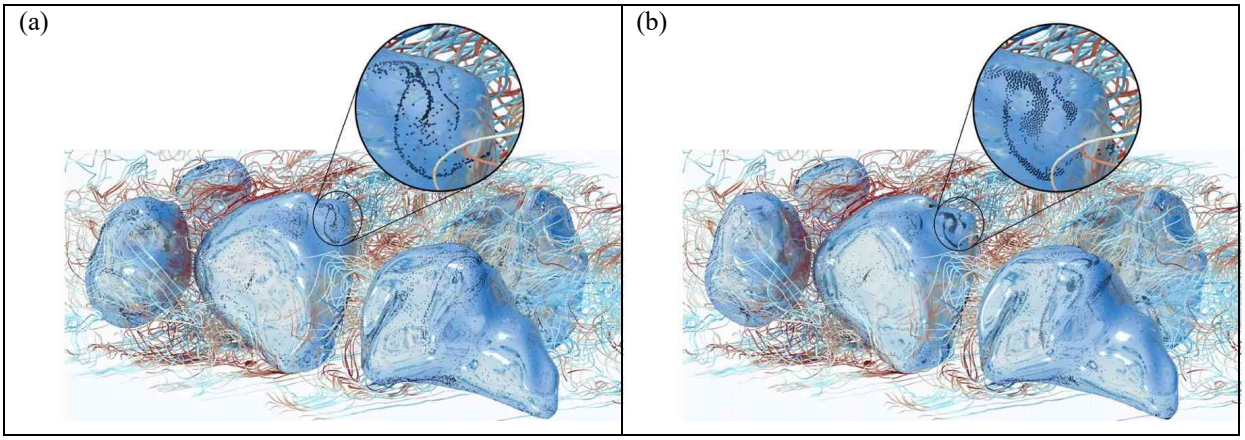

Figure 1: Snapshot of particle distribution on the drop surface. Trapped particles form highly-concentrated filamentary clusters without EVE (a), but appear more evenly distributed when EVE are included (b). From [1].

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The Chaotic Life of Mayonnaise

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Emulsions are important ingredients of many foods and cosmetics and, as such, common to our daily life, additionally, emulsions are also extremely interesting physical systems due to their rich phenomenology. In this talk we present how we achieved highly dense emulsions via high-resolution computer simulations on high-end massively parallel HPC systems. We employ a highly optimized Lattice Boltzmann [1] code, based on the Shan-Chen multicomponent modelling for immiscible binary fluids [2,3], supplemented with a model of long-range interaction to introduce frustration in the system, allowing for a stabilization mechanism that mimics disjoining pressure [4]. In figure 1(a) we graphically show how such an emulsion looks like for a concentration of about 80% and for a small resolution run (512^3). Such a concentrated emulsion is shown to possess a non-zero yield-stress and still be able to flow when the intensity of the large-scale stirring force is above a critical threshold. We will report on the validation of the numerical simulations and on the statistical analysis of dispersion in order to demonstrate the usefulness of fully-resolved numerical simulations for the study of dense emulsions.

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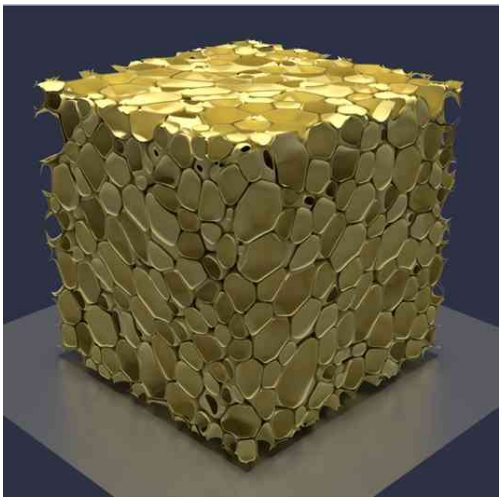

Figure 1: High-resolution rendering of a dense emulsion obtained via computer simulation.

Influence of density and viscosity on deformation, breakage and coalescence of bubbles in turbulence

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Giovanni Soligo
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We numerically investigate the effect of density and viscosity differences on a swarm of large and deformable bubbles dispersed in a turbulent channel flow. For a given shear Reynolds number, $Re_\tau = 300$, and a constant bubble volume fraction, $\Phi \simeq 5.4\%$, we perform a campaign of direct numerical simulations (DNS) of turbulence coupled with a phase-field method (PFM) accounting for interfacial phenomena. For each simulation, we vary the Weber number (We, ratio of inertial to surface tension forces), the density ratio (ρ_r, ratio of bubble density to carrier flow density) and the viscosity ratio (η_r, ratio of bubble viscosity to carrier flow viscosity). Specifically, we consider two Weber numbers, $We = 1.50$ and $We = 3.00$, four density ratios, from $\rho_r = 1$ down to $\rho_r = 0.001$ and five viscosity ratios from $\eta_r = 0.01$ up to $\eta_r = 100$. Our results show that density differences have a negligible effect on breakage and coalescence phenomena, while a much stronger effect is observed when changing the viscosity of the two phases. Increasing the bubble viscosity with respect to the carrier fluid viscosity damps turbulence fluctuations, makes the bubble more rigid and strongly prevents large deformations, thus reducing the number of breakage events. Local deformations of the interface, on the contrary, depend on both density and viscosity ratios: as the bubble density is increased, a larger number of small-scale deformations, small dimples and bumps, appear on the interface of the bubble. The opposite effect is observed for increasing bubble viscosities: the interface of the bubbles become smoother. We report that these effects are mostly visible for larger Weber numbers, where surface forces are weaker. Finally, we characterize the flow inside the bubbles; as the bubble density is increased, we observe, as expected, an increase in the turbulent kinetic energy (TKE) inside the bubble, while as the bubble viscosity is increased, we observe a mild reduction of the TKE inside the bubble and a strong suppression of turbulence.

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Water-lubricated channel flow

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We use direct numerical simulation (DNS) to study the problem of drag reduction in a lubricated channel, a flow instance in which two thin layers of a lubricating fluid (density ρ_1, viscosity η_1, thickness h_1) are injected in the near-wall region of a plane channel, so to favor the transportation of a primary fluid (density ρ_2, viscosity η_2, thickness h_2). To cover a meaningful range of possible oil/water configurations, we consider two different viscosity ratios in the range $0.1 < \lambda < 0.01$ and for each viscosity ratio, we consider a surfactant-free case (clean) and a surfactant-laden interface. All DNSs are performed using the constant power input (CPI) approach, which prescribes that the flow rate is adjusted according to the actual pressure gradient so as to keep constant the power injected into the flow. The CPI approach has been purposely extended here to the case of multiphase flows. A phase-field method is used to describe the dynamics of the liquid-liquid interface. We unambiguously show that a significant drag reduction (DR) can be achieved for all the four configurations considered. Upon a detailed analysis of the turbulence activity in the two lubricating layers and of the interfacial wave dynamics, we are able to characterize the effects of surface tension forces, surfactant concentration and viscosity contrast on the drag reduction performance.

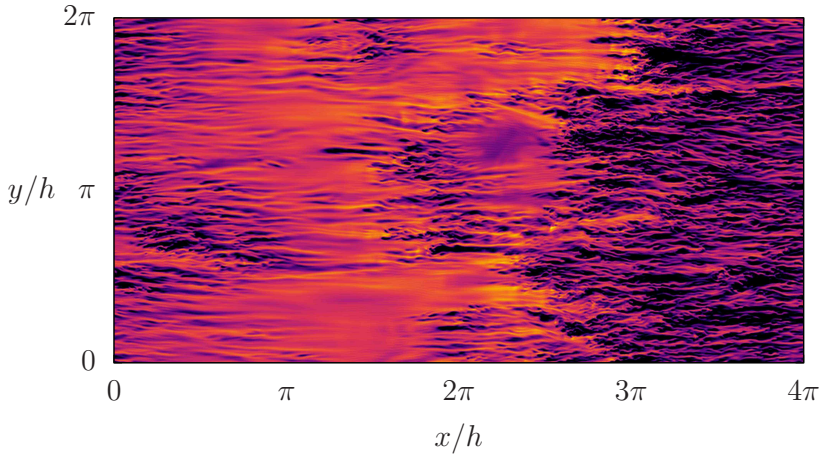

Figure 1: Visualization of the instantaneous streamwise velocity on a $x - y$ plane. The plane is located inside the top lubricating layer and is located at $\simeq 10w.u.$ from the top wall.

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Wednesday – 2022-09-28

Session III

- **Critical assessment and numerical benchmark of method development**
  (Chair: M. Fricke, Room: Aula 1-G)
- **Progress in Eulerian-Lagrangian & Eulerian-Eulerian modeling of dispersed flow**
  (Chair: R. Fox, Room: Auditorium)
- **Methods for interface advection**
  (Chair: S. Tanguy, Room Aula Magna 1-E)

A comparative benchmark of four Volume-of-Fluid solvers by means of advection and capillary test cases

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Tobias Tolle
Robert Bosch GmbH, Renningen

Aaron Dörr
Robert Bosch GmbH, Renningen

Tomislav Marić†
Technical University Darmstadt

Numerical simulations of two-phase flows are increasingly used as tools in the development process of technical applications and products.They can provide a more comprehensive understanding of the processes involved or guidance for design improvement. Yet, the underlying numerical methods for two-phase flows are still very actively researched; for the Volume-of-Fluid (VoF) method alone the published literature is substantial, see [1] for a recent review. Especially surface tension and large density differences (see e.g. [2]), characteristic for gas-liquid systems, are still numerically challenging. Consequently, these challenges have to be considered when performing simulations and interpreting the results.
In the light of ongoing research and numerical challenges, four state-of-the-art VoF based solvers, *interFoam* [3], *interIsoFoam* [4], *Ansys® Fluent* [5], and *Basilisk* [6], are compared. This comparison is motivated by the observation that while there are several VoF solvers available - both closed and open source - demonstrating impressive capabilities, fundamental benchmark data is scarce and often not comparable due to different test case set-ups. To close this gap to some extent and provide a basis for future benchmarks, advection accuracies are analyzed using canonical advection test cases first. Second, capillary verification test cases, e.g. the notorious stationary droplet, are examined. Both - two-dimensional and three-dimensional variants - are considered. To provide insight what performance can be expected of these solvers in microfluidic applications, a characteristic length scale in the millimeter to sub-millimeter range is used and exemplary technical fluid pairings, e.g. water-air, are covered. The aim is to give researchers and engineers a reference point regarding current possibilities and limitations of these solvers through the presented benchmark data. The benchmark data for all tested solvers will be made publicly available to facilitate future direct comparisons.

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A coupled VOF-fictitious domain technique for the simulation of interfacial flows interacting with moving particles

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Multiphase flows involving the coexistence and interactions of interfacial structures and moving rigid particles occur in a variety of applications from microfluidics to large-scale chemical processes. In this study, a coupled interface capturing-fictitious domain method is presented for the interface-resolved simulation of such complex multiphase systems. While the fluid-fluid interface is simulated by a geometric volume of fluid (VOF) technique, the rigid spherical particle is accounted for as an immersed body in the computational domain. In this fictitious domain approach, the finite volume cells occupied by the solid particle are identified by a smooth particle representation algorithm, and the presence of the particle is represented by a continuous scalar field that is zero at the particle region and one elsewhere. Then, the hydrodynamic body and surface forces acting on the particle are computed separately over these particle-covered cells, and the particle moves under Newton's second law. For the momentum coupling of the fictitious domain, two different approaches are adopted: (i) direct method where a correction step is added to the pressure velocity-coupling to account for the particle's velocity at the particle-covered cells and keep the velocity field divergence-free, and (ii) continuous forcing method where a penalization term is explicitly added to the momentum equation at the particle-covered cells. Consequently, the VOF algorithm is also modified to prevent penetration of the fluid-fluid interface into the particle region and allow contact line motion. A couple of benchmark problems such as particle impact on a liquid pool as well as particle-droplet collisions at different impact and wetting conditions are simulated (as shown in Fig. 1). The results show satisfactory agreement with literature data. The present approach is developed by coupling two open-source software packages of OpenFOAM (VOF with the isoAdvector method [1]) and LIGGGHTS® (resolved CFD-DEM technique [2]), which facilitates the implementation of further sub-models and functions across physical scales and regimes.

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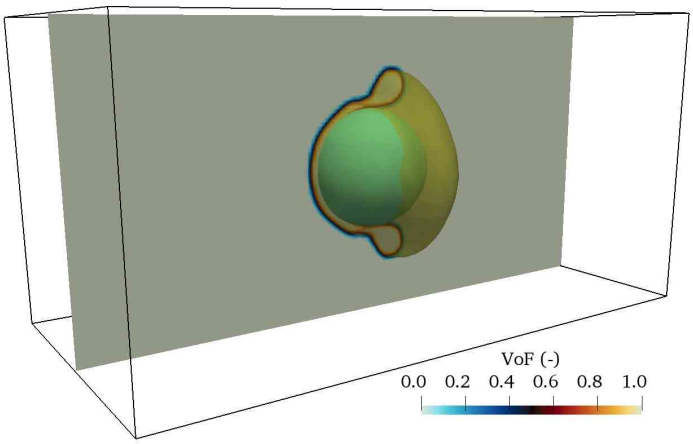

Figure 1: Head-on collision of a water droplet with a rigid spherical particle at $We = 70$.

Limitations and perspectives of phase-change modelling based on interface capturing methods for evaporation simulations

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The high-fidelity simulation of phase-change has been a growing subject of interest in the last decade with the emergence of multiple solvers dedicated to the resolution of evaporating flows [1, 2, 3]. These solvers rely on an Eulerian interface representation and incompressible phases. The numerical methods associated with phase change simulations are not as mature as the techniques developed for simulating isothermal two-phase flows.
Indeed, the literature on this subject offers a broad investigation of incompressible two-phase flows. The main challenges are well-understood, and such approaches' limitations are clearly stated. For example, surface tension modelling has caused much trouble in the early works while it has been thoroughly studied later. Thanks to the contributions of many authors all along the last 30 years, state-of-the-art methodologies manage to provide accurate and robust simulations of capillary-driven flows [4]. They include well-balanced discretization combined with accurate curvature evaluation and appropriate interpolation to the interface position when necessary.
From this observation, it is clear that applications with phase change require the same efforts to carefully state the numerical obstacles and propose new perspectives of improvement. This work details phase-change modelling in an incompressible two-phase flow solver without restricting the numerical methods to a specific interface capturing method. The two main challenges when building a phase-change procedure are the transport of temperature and species mass fraction with flux discontinuities and the reconstruction of the evaporation rate $\dot{m}$ which drives the accuracy and convergence rate of such a solver. Thus, particular attention is devoted to handling flux discontinuities at the interface and the reconstruction of gradient normal to the interface.
The thorough study presented in this work brings out the limitations and perspectives to improve the accuracy of modern two-phase flow solvers with phase change. More precisely, today's phase-change solvers are limited to first-order convergence and require important mesh resolution to provide high-fidelity simulations. These limitations could be removed by increasing the accuracy of scalar transport and using higher-order interface representations.

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An extended numerical model for the Direct Numerical Simulation of evaporating droplets : Application to Leidenfrost droplets

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Dominique Legendre‡
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In this presentation, we will present new developments on the numerical methods for the Direct Numerical Simulation of evaporating droplets with interface capturing methods. In particular, standard models as the ones proposed in Ref [1,2] are usually based on constant thermo-physical properties as density, surface tension and viscosity, whereas such variables can be subject to important variations due to the variations of the thermal field and mass fraction field around and inside the droplet. These variations do not only appear as variable coefficients in the primitive equations, they also imply new source terms for which specific numerical techniques must be employed.

For the purpose of this work, to account for density variations a low Mach number variable density solver has been developed and coupled to standard liquid-vapor phase change solvers. Surface tension variations along the interface due to the variations of the internal thermal field have been taken into account by adding a source term in the jump condition on the tangential viscous stresses. The latter term enables accounting for Marangoni convection inside the droplet, as one can observe in Fig. 1.

Several validations of the overall solver have been performed with reference benchmarks and new test-cases have been also designed. We will specifically emphasis on Leidenfrost droplets for which convincing validations against experiments [3] have been achieved, by accounting for the Marangoni convection, as it can observed in Fig. 2.

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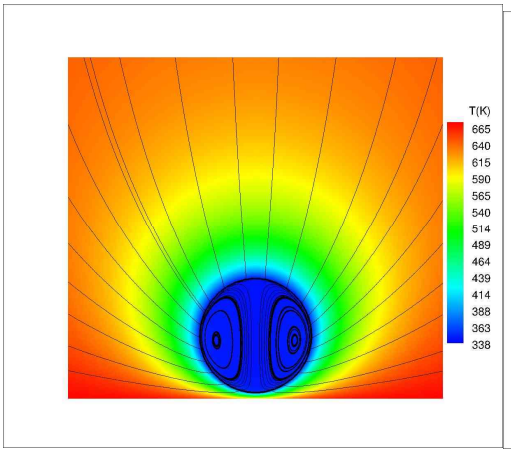

Fig.1 : Temperature field and streamlines around and inside a Leidenfrost droplet

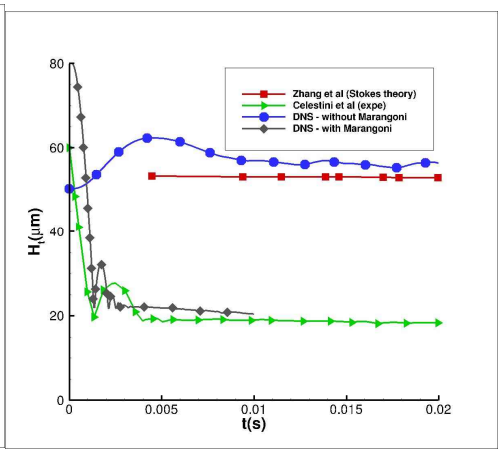

Fig. 2 : Temporal evolution of the vapor layer thickness, comparisons DNS vs experiments

A hybrid method between sectional and moment method for the description of a population of soot

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Accurate predictions of soot formation in laminar sooting flames can be computationally challenging due to the polydisperse nature of the soot particle population and the difficulties associated with the solution of the population balance equation (PBE) for soot particulate matter in terms of the particule size and morphology. Different kinds of models, like sectional, which introduces a size discretization, and moment methods, are classically developed from this purpose. However, on the one side, the sectional methods require a high computational cost, since the transport of a large number of sections is needed to guarantee a good accuracy. On the other side, the development of moment methods is quite complex due to the need for closure models and due to realizability constraints on high order moments.

Therefore, in this work, an alternative method is proposed based on the extension to soot of a recently developed two size moment (TSM) method for sprays and aerosols [1, 2]. The TSM model is an hybrid method combining sectional and moments methods, by considering a size discretization in sections and two moments per section: the number density and the volume fraction. To account for the non-spherical particle morphology, an additional size variable is introduced as well as an additional moment in each section. Moreover, adapted and accurate numerical schemes are developed, able to preserve the realizability of the moments. The integrated model is validated by comparisons with reference simulations using the Monte-Carlo method for sooting premixed and non premixed laminar flames.

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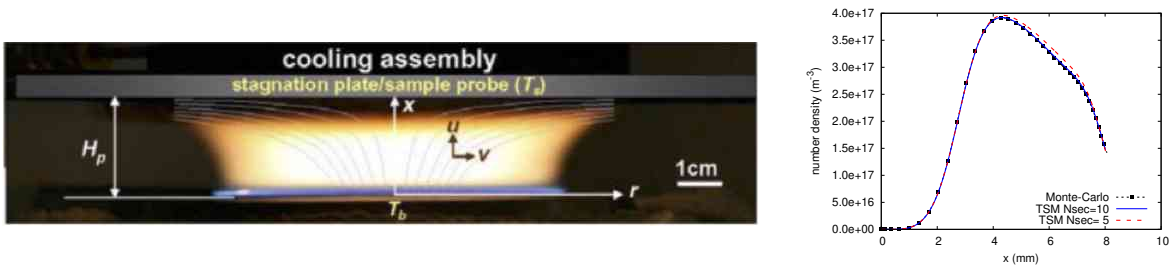

Figure 1: Premixed flame: scheme of the flame burner configuration and evolution of the number density along the centerline.

Application of a morphology adaptive multifield model towards a plunging jet considering entrainment

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The numerical simulation of gas-liquid flows is a challenging task, when dynamics of systems at industrial scales are considered. A significant contribution to this complexity arises due to the coexistence and interaction of different flow morphologies, such as bubbly and stratified flows. One of the phenomena is the entrainment of small gas bubbles into the liquid bulk at a large-scale gas-liquid interface in regions of high shear rates. In order to capture such phenomena and make reliable predictions, hybrid modelling approaches are used. One of those is the morphology adaptive multifield model developed by Meller et al. (2021), which combines an Euler-Euler method with an algebraic Volume-of-Fluid method for disperse and continuous gas structures, respectively. The interfacial drag coupling is adapted to the local grid resolution at the interface location (Meller *et al.*, 2022). In such a modelling framework, morphology changes are realised by transfers between numerical phases, which are treated differently according to the basic simulation methodologies mentioned above.

In that sense, entrainment processes are characterised by multiple numerical aspects: 1) entrapping of large-scale gas structures, which subsequently disintegrate into smaller ones and 2) direct conversion of continuous towards disperse portions of gas due to processes taking place at sub-grid scales, which are described by dedicated entrainment models, such as the one of Ma *et al.* (2011). In this work, the individual effects as well as the interplay of the aforementioned processes are assessed and validated in comparison to experimental data of a liquid plunging jet (Chanson *et al.*, 2004). This also considers the balance between the two numerical aspects mentioned above. The goal is to improve the reliability of predictions of gas entrainment with high as well as with low spatial resolution.

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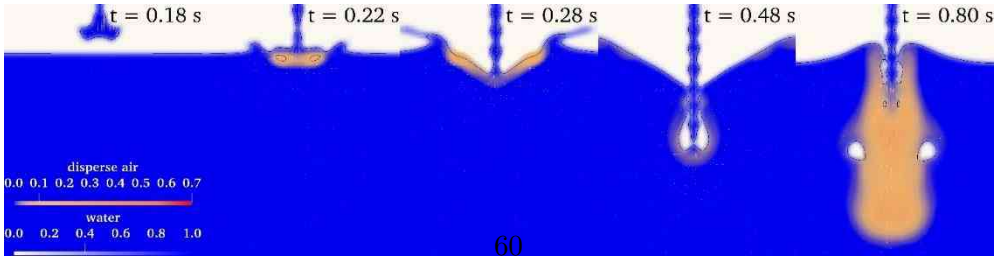

Figure 1: Simulation of plunging liquid jet with morphology adaptive multifield solver with continuous water (blue), continuous air (white) and dispersed air (orange-red).

Multi-Euler/Lagrange simulation of gas/liquid/solid multiphase flows

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Multi-phase flow simulations have been widely developed in academics as well as industrial research for several decades now. Their effectiveness to predict complex systems is widely agreed upon. In many fields of application, solid particles can be found in multiphase flows, understanding their behaviour becomes a key element when they can induce enhanced wear, device malfunction or failure. In nuclear power plants during loss of coolant accidents, solid particles may be transported to the bottom of the reactor building by a water-gas mixture, allowing for the possibility to hinder the recirculation pumps and negate the cooling of the reactor core.

This work proposes a new approach to use stochastic Lagrangian tracking for solid particles evolving in an Eulerian multi-fluid RANS simulation with neptune_cfd, a code developed by EDF, CEA, Framatome and IRSN. This code is based on the one pressure multi-fluid approach [1]. It solves separate balance equations for each phase coupled through interfacial transfer terms with a discretization according to a 3D full unstructured finite volume scheme with collocated variables.

One drawback of current stochastic Lagrangian tracking methods is that they are based on the hypothesis that only one turbulent fluid transports the particles. The main idea, assuming drag is the dominant fluid force, leads to consider its average and turbulent contribution for every Eulerian phase in the particle momentum conservation equation. The particles are then subjected to gravity and the pressure gradient force. Each Eulerian phase contributes to the total drag with an amount comparative to the volume fraction for that phase at the position of the particle. Then, in order to take into account the turbulence effects, simulated in neptune_cfd with Reynolds stress transport models, Lagrangian stochastic modelling is used to predict the local instantaneous value of all the fluid velocities seen by the particle. The models have to be consistent with the system of equations solved underneath, in neptune_cfd. Therefore, we propose a new Lagrangian stochastic system that includes interfacial transfer terms between the Eulerian phases. The reverse coupling from the solid phase to the Eulerian phases is not taken into account.

The model's results are compared with analytical results for a particle falling through a density interface, as well as with experimental and simulation results obtained with a multi-fluid Eulerian method on a slurry bubble column [2].

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Algebric momentum preserving method with a fully-coupled 3D parallel solver for the simulation of two-phase incompressible flows

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Two-phase flows with separated phases are prevalent in several industrial and environmental applications, where the conditions and regimes encountered spread wide and far. In the energy sector for example, the atomisation of liquid jets results from complex interactions between a coherent liquid jet, a gas-filled plenum and (potentially) a co-flowing gaseous jet. Breaking waves are another instance of two-phase flows, characterised by a high degree of turbulence, as are droplet impacts on liquid surfaces, nanofabrication by thermal plasma jets, to name a few.

The high density and viscosity ratios encountered in these two-phase flows couple strongly the velocity components in the interface vicinity, and often result in strong shear at these interfaces. This yields in ill-conditioned linear systems (as a result of the semi-discretisation of the two-phase incompressible Navier-stokes equations) that pose significant problems together with the treatment of the coupled velocity-pressure saddle-point system [Chorin(1968), Témam(1969), Vincent *et al.(2004)*, Vincent *et al.(2011)*, El Ouafa *et al.(2020)*, El Ouafa *et al.(2021)*]. Solving these systems remains a challenging task for mathematicians as well as engineers. In addition, it has been demonstrated that solving theses equations in a non-conservative form with high density ratios leads to incorrect velocity field or volume fraction and often a failure of numerical scheme, due to numerical error accumulation near the highly deforming interface [Bussmann *et al.(2002)*, Desjardins *et al.(2008)*, Raessi and Pitsch(2012), Le Chenadec and Pitsch(2013), Nangia *et al.(2019)*, Zuzio *et al.(2020)*].

The main objective of the present work is to further investigate the solution of the coupled system (without any time-splitting approach) by means of a preconditioned BiCGstab(2) solver [J-J. Dongarra *et al (1998)*]. We obtain high performance with a new preconditioning strategy that combines a triangular block preconditionning for the velocity block with a pressure convection diffusion (PCD) preconditionner for the Schur complement [Bootland *et al.(2019)Bootland, Bentley, Kees, and Wathen*]. To provide the stability of the numerical scheme in the presence of high density and viscosity ratios, we use an algebric momentum preserving mass and momentum transport in the conservative form of discrete equations. The consistency between mass and momentum advection is achieved by resolving a new auxiliary continuity equation, using fifth-order WENO scheme and third Runga-Kutta SSP time integrator.

Test cases such as the transport of a very-high density fluid sphere and the free fall of dense sphere are performed to validate the models, especially in the presence of strong density and viscosity ratios. Other cases, like the phase inversion, demonstrate the ability of the new fully-coupled solver to tackle problems of more than one billion cells, with excellent scalability.

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On the numerical approximation and transport of the mean curvature in Volume-of-Fluid methods

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The numerical modeling of surface tension is a central element in the simulation of capillary two-phase flows [1]. In particular, it requires the numerical approximation of the interface curvature, which is a challenging task. In the present work, we focus on curvature computations for the Volume-of-Fluid method [2] which tracks the interface location using the discrete volume fraction field. A well-established method to compute curvatures from volume fractions on Cartesian grids is the height function method, which constructs a local graph representation of the interface. In its modern form [3], the method is computationally efficient and offers formally second-order convergence. However, the convergence of the method crucially depends on the quality of the volume fraction data. As the method involves numerical double differentiation, it is subject to numerical error amplification. A fact that has not deserved much attention in the literature (with some exceptions, including [1], [4]).

We provide a rigorous error estimate for the height function method, taking into account the (unavoidable) errors in the volume fraction data [5]. In particular, it is shown that convergence for the curvature is reached only if the error in the volume fractions converges faster than second-order.
In practice, there are at least two significant sources for perturbations of the volume fractions, namely the initialization and numerical transport during advection. The importance of highly accurate initial data is shown by comparing a standard volume fraction initialization approach with an advanced method based on differential geometry [6]. Moreover, we study the errors caused by the numerical amplification of advection errors. As expected from the error analysis, convergence of the curvature transport can only be achieved with higher-order advection schemes combined with a sufficiently accurate initialization. Finally, we study the impact of regularization schemes developed in the field of inverse problem theory to stabilize the numerical approximation of the mean curvature in Volume-of-Fluid methods.

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Divergence free CutFEM for the Darcy interface problem

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We present a Cut Finite Element Method (CutFEM) for the Darcy interface problem [1] with optimal rates of convergence in the L^2-norm for velocity and pressure, optimal convergence in the L^∞-norm for the divergence, with pointwise divergence-free approximations of solenoidal velocity fields, and the resulting linear systems are well-posed. These properties hold independently of how the interface cuts through the computational mesh.

The Darcy interface problem is a model of porous two-phase liquid flow, wherein the interface models a fracture. In CutFEM, the computational mesh is unfitted with respect to the interface and possibly the external boundary as well, making the method highly suited for applications in which the construction of a fitted mesh is complicated and expensive. We start with an unfitted background mesh and appropriate standard finite element spaces on that mesh. We then define 1) two active unfitted meshes corresponding to the two subdomains occupied by the fluids and separated by the interface; 2) active finite element spaces; 3) a weak formulation, such that the proposed discretization is accurate and robust independently of the interface position relative to the background mesh. Using the active spaces we build pressure and velocity spaces with functions that are double valued on elements that are cut by the interface. Hence functions in our function spaces can be discontinuous across the interface. We glue the solutions in the two subdomains by imposing the physical interface conditions weakly. A new stabilization is introduced in the weak form that controls the condition number of the resulting system matrix without destroying the mass conservation.

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Maximum Gradient Based Compression Algorithm for Interface Capturing

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For numerical simulation of multiphase flows, one of the major research area is interface capturing between two or more fluids. Interface capturing algorithms typically fall into one of the two categories : Geometric or Algebraic. These available methods work very good as long as simulation time-step size is guided by strict Courant criteria. Stable simulation at larger time-steps than what is suggested by Courant criteria is open problem to be solved.

Maximum Gradient Based Compression Algorithm or MaxGBCA is one step in direction of simulations at higher Courant numbers. We would like to present the main idea and concepts leading upto development of MaxGBCA. We would also then like to demonstrate results from bench-marking and validation problems using MaxGBCA scheme in Wilkdatze CFD solver.

Shown in Figure [1] are results for one of the benchmark problem described in Reference [1] using MaxGBCA scheme in Wildkatze solver. As shown in Figure [1] MaxGBCA performs good even at high Courant numbers.

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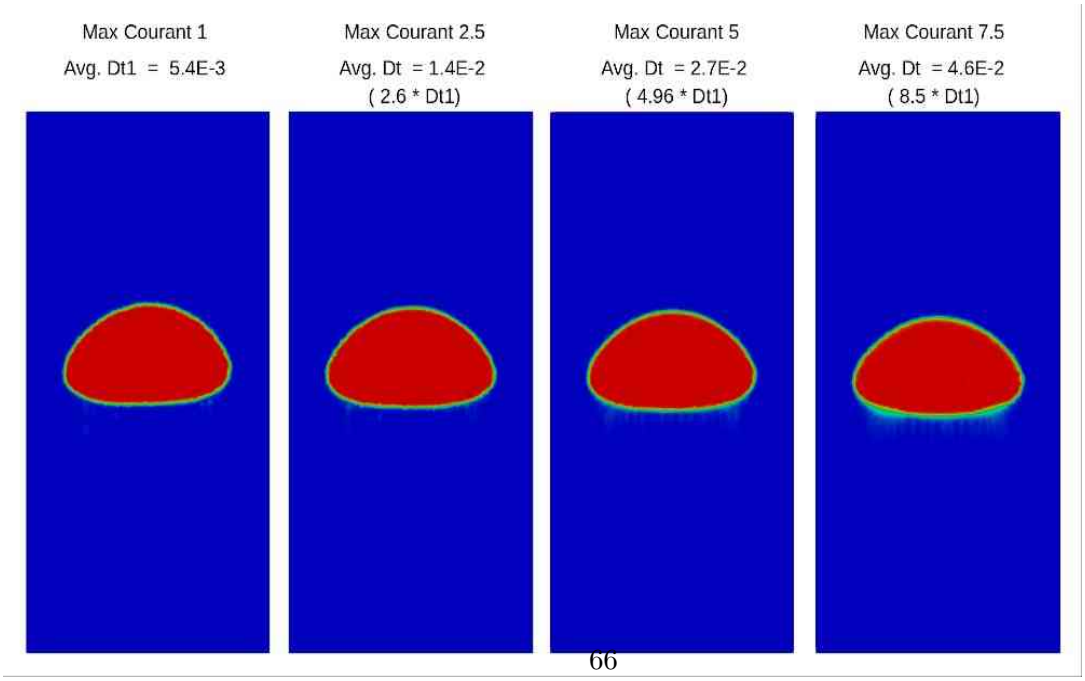

Figure 1: Results of Bubble interface capturing at various Courant numbers using MaxGBCA

Enabling accurate interface advection with isoAdvector at larger time steps

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The accuracy of geometric Volume of Fluid (VOF) methods is known to depend heavily on the interfacial Courant number value ($\boldsymbol{Co_I}$). Being able to accurately advect an interface while having $\boldsymbol{Co_I \approx 1}$ is a property that enhances the applicability of a VOF algorithm in industrial applications where large time steps are vital. Here, we present the isoAdvector, a fast and accurate geometric VOF algorithm that works on both structured and unstructured meshes with no requirements on cell shapes [1, 2]. An implementation of isoAdvector can be found in the open-source Computational Fluid Dynamics (CFD) software OpenFOAM®. The algorithm has been used in various interfacial flow simulations (e.g. pressure swirl atomizer, breaking waves and hydraulic jumps) [3, 4, 5]. As any geometric VOF algorithm, the allowable time step size with isoAdvector is naturally limited by the interfacial Courant number.

In this presentation, we initially investigate how the interface advection step of the isoAdvector algorithm is affected when interfacial Courant number approaches unity from below ($\boldsymbol{Co_I \approx 1}$). It is found that the algorithm's performance degrades in terms of shape preservation and volume conservation for $\boldsymbol{Co_I \approx 1}$. We have found that a problem with the original implementation is that it does not account for cells, that are not interface cells at the beginning of a time step, but into which the interface propagates during the time step. To solve this issue, we propose an extension of the spatial range of the advection step, including certain *downwind-to-interface* cells, for the prediction of the interface. This extension significantly improves the allowable time step while at the same time retaining the levels of accuracy (shape sharpness, shape conservation and volume fraction conservation).

We investigate the effect of the algorithm extension by comparing before and after behaviour for several canonical pure advection benchmark cases as well as industrial cases. An example of such a comparison is shown in Figure 1 for diagonal advection of a disc in a constant, uniform velocity field at $\boldsymbol{Co_I = 0.9}$. The figure shows the disc at the final time step, demonstrating a clear improvement in shape preservation.

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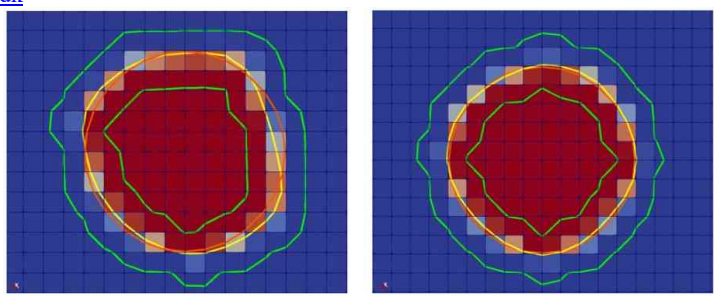

Figure 1: Volume fraction field at the last time step before (left) and after (right) the extension of the advection stencil. The true $\alpha = 0.5$ contour is illustrated in red. Simulation $\alpha = 0.5$ contour is shown in yellow, while $\alpha = 0.01$ and $\alpha = 0.99$ contours are shown in green.

Wednesday – 2022-09-28

Session IV

- **Numerical benchmarks (verification & validation) for method development**
  (Chair: B. Motta, Room: Aula Magna 1-E)
- **Progress in Eulerian-Lagrangian & Eulerian-Eulerian modeling of dispersed flow**
  (Chair: C. Marchioli, Room: Aula 1-G)
- **Phase transition & numerical modeling of interfacial heat & mass transfer**
  (Chair: H. Kuhlmann, Room: Aula 1-G)

Turbulent Poiseuille flow of two immiscible liquid layers inside a channel

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We use pseudo-spectral Direct Numerical Simulation (DNS), coupled with a Phase Field Method (PFM), to investigate the turbulent Poiseuille flow of two immiscible liquid layers inside a channel. The two liquid layers, which have the same thickness ($h_1 = h_2 = h$), are characterized by the same density ($\rho_1 = \rho_2 = \rho$) but different viscosities ($\eta_1 \neq \eta_2$). The full problem is described in terms of the following flow parameters: the shear Reynolds number (Re_τ, which quantifies the importance of inertia compared to viscous effects), the Weber number (We, which quantifies surface tension effects compared to inertia) and the viscosity ratio λ between the two fluids. In particular, we fix $Re_\tau = 300$, $We = 1$, and we consider viscosity ratios in the range $0.1 \leq \lambda = \eta_1/\eta_2 \leq 1$. We focus on the role of turbulence in initially deforming the interface and on the subsequent growth of capillary waves. Compared to a single phase flow at the same shear Reynolds number ($Re_\tau = 300$), in the two-layers case we observe a strong interaction between the turbulent flow and the deformable liquid-liquid interface. A full characterization of the interface deformation, its time evolution and the corresponding turbulence modulation will be presented and discussed.

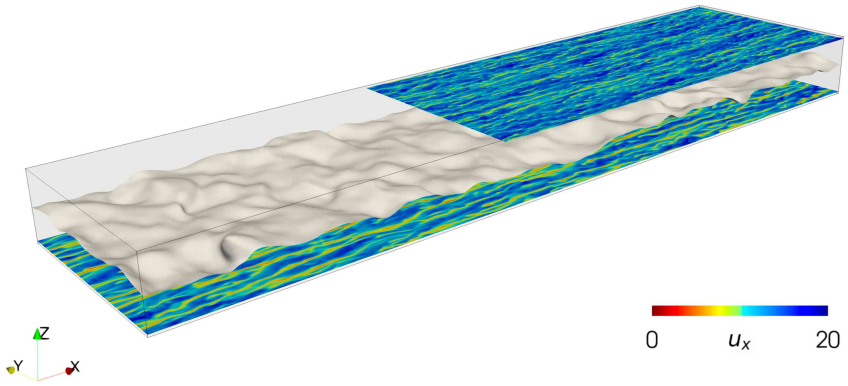

Figure 1: Channel geometry and flow topology of a two-layer turbulent flow simulation. Capillary wave formation can be seen on the interface between the two layers. The fluid in the upper half of the channel has a viscosity that is 50% lower than that of the fluid in the lower half of the channel. This fact is responsible for the difference between top and bottom near-wall turbulence structure, here made visible using the value of the streamwise component of the velocity vector (u_x)

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Droplet deformation and breakup in shear-thinning viscoelastic fluid under simple shear flow

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A three-dimensional lattice Boltzmann method, which couples the color-gradient model for two-phase fluid dynamics with a lattice diffusion-advection scheme for the elastic stress tensor, is developed to study the deformation and breakup of a Newtonian droplet in the Giesekus fluid matrix under simple shear flow (see figure 1). This method is first validated by the simulation of a single-phase Giesekus fluid in a steady shear flow and the droplet deformation in two different viscoelastic fluid systems. It is then used to investigate the effect of Deborah number De, mobility parameter α, and solvent viscosity ratio β on steady-state droplet deformation. We find for $0.025 < \alpha < 0.5$ that as De increases, the steady-state droplet deformation decreases until eventually approaching the one in the pure Newtonian case with viscosity ratio of $1/\beta$, which is attributed to the strong shear-thinning effect at high De. While for lower α, the droplet deformation exhibits a complex non-monotonic variation with De. Under a constant De, the droplet deformation decreases monotonically with α but increases with β. Force analysis in figure 2 shows that De modifies the droplet deformation by altering the normal viscous and elastic stresses at both poles and equators of the droplet. Finally, we explore the roles of De and α on the critical capillary number Ca_{cr} of droplet breakup. By establishing both Ca - De and Ca - α phase diagrams, we find that the critical capillary number increases with De or α except that a plateau critical capillary number is observed in Ca - De phase diagram.

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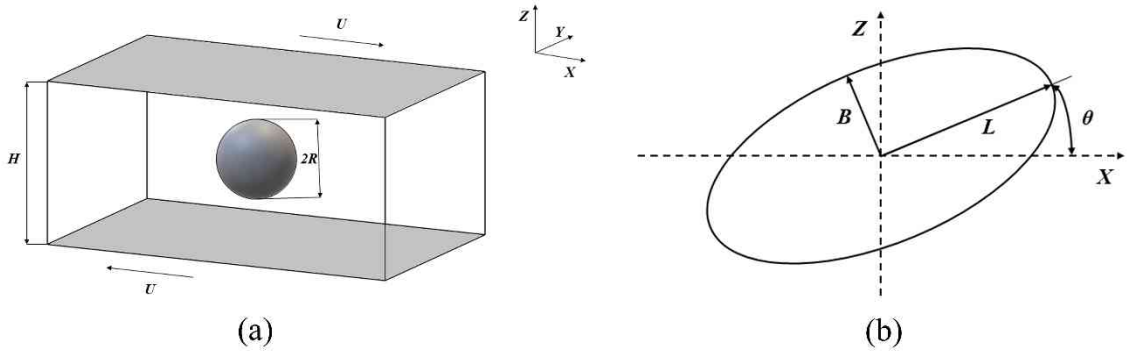

Figure 1 Schematics of (a) a spherical droplet under simple shear flow and (b) measurements of droplet deformation D and inclination angle θ.

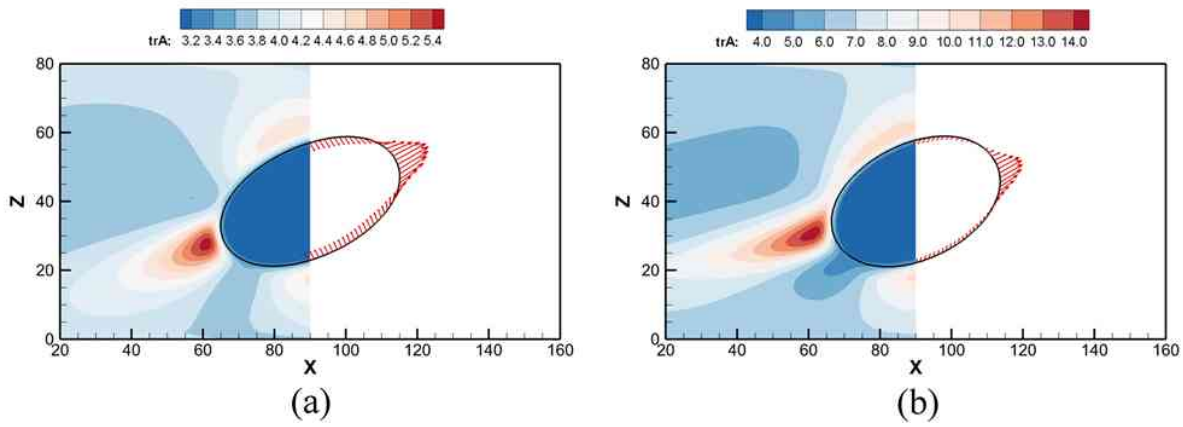

Figure 2 The contours of the trace of conformation tensor (left half) and the vectors of the elastic force (right half) at the two-phase interface for (a) $De = 1.0$ and (b) $De = 4.0$.

Analysis of the dynamics of an isolated cavitating vortex

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Cavitation is a well-known and widely studied phenomenon as it is responsible for various, often negative, effects which, for elements such as pumps or propellers, are related to loss of performance, erosion, damage, vibrations, and noise. At the same time, cavitation is also characterized by temporal and spatial scales that make it impossible to carry out accurate simulations from an industrial point of view. Now there is growing interest in the noise generated by marine propellers both to increase the comfort of staff and passengers on board, such as in cruise ships, and to minimize the negative effects on the marine environment. Various studies, including [1,2], have noticed that one of the main sources of noise is associated with the cavitating tip vortex produced by the propeller blades, and in particular, the noise source is associated with the variation of the volume of the cavity [3], and more generally to the dynamics of the cavitation.

Here the dynamics of a vapor cavity in an isolated vortex have been studied numerically by using the hypothesis of homogeneous mixture with the approach with the transport equation for the volumetric vapor fraction. The vortex was generated by imposing an initial velocity field according to the formulation of the Burnham-Hallock vortex [4] and by imposing a far-field pressure value such that the vortex core was in a cavitation regime. The dynamic of the cavity was studied considering both a two-dimensional and three-dimensional domain. The results obtained were then compared with the analytical and experimental results of the literature; during the comparison, particular attention was paid regard to the shape of the cavity and the oscillation frequency of the simulated cavity compared with the first resonance modes found analytically by Pennings [5].

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Finite Volume Computation of Journal Bearing Cavitation

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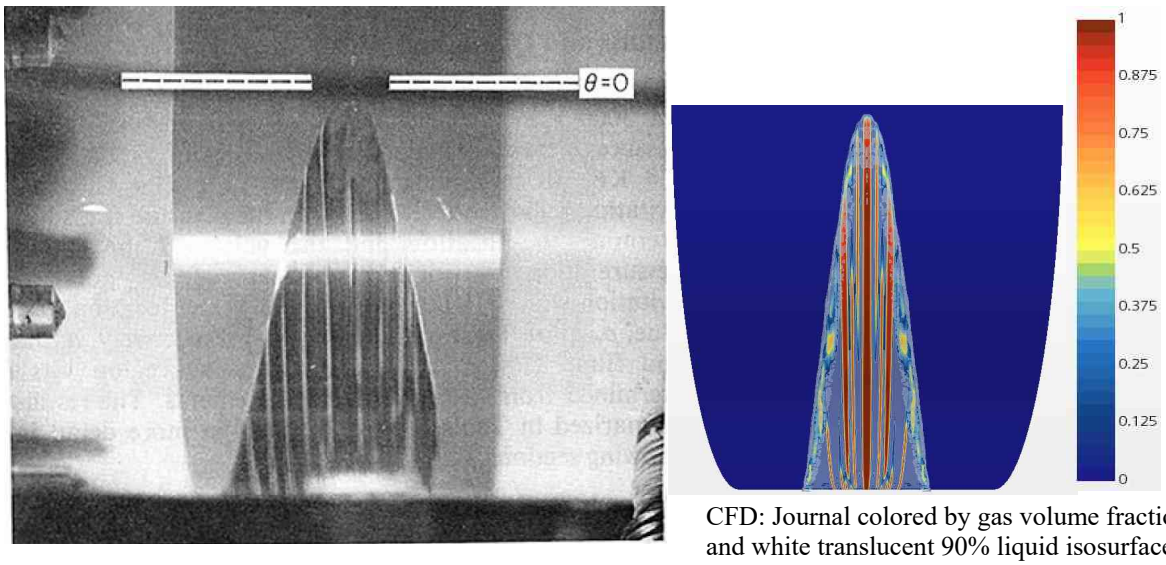
Journal bearing cavitation has been a topic of scholarly interest for more than 50 years [1]. Cavitation occurs in nearly all practical journal bearing applications. However, a few particulars common to the typical journal bearing cavity have not been supported by a detailed, physics-based numerical model. In particular, the observations have been made (e.g. [1],[2],[3]), that in the ruptured, cavity region, a significant fraction of both liquid and gas are present, and the fluids are largely segregated radially; any liquid within the cavity region remains attached to the journal (moving) surface and the bearing (stationary) surface is relatively dry. Further, the cavity region is interspersed with distinct *streamers*. The *streamers* are liquid streaks attached to the journal. They are apparently *two-dimensional* droplets, stretching lengthwise along the cavity, parallel to the journal motion. Although the pressure within the cavity region is nearly constant (relative to the outer film flow), the liquid inside each streamer, within the cavity, due to interfacial surface tension, is contained at a slightly higher pressure than the surrounding gas cavity. This is roughly at the film rupture (i.e. cavitation) pressure.

To support this work, numerical solutions of the Navier-Stokes equations, including key modeling elements, a mixture multiphase, volume of fluid formulation, a cavitation model [4] and a surface tension model [5], implemented using the finite volume method [6] are presented. The solutions demonstrate the phenomenon of journal bearing flow cavitation. The cavitation solutions, based on reasonable, first-principal numerical physics, exhibit the characteristic liquid attachment to the journal (relative moving) surface with gas filling the remaining volume of the cavity. Figure 1 contains an image from Etsion and Ludwig [3] alongside a CFD visualization. In the photographic image, streamers appear as light streaks in the darker cavity. In the preliminary CFD result, the streamers appear as red streaks. Red indicates areas where the journal is dry. Note that in the final presentation, discrepancies in absolute cavity dimensions will be addressed.

Preliminary results evidently capture the tendency of the liquid in the cavity region to adhere to the journal as well as the streamer phenomenon itself. In the final presentation, conclusions based on numerical results will relate the governing dynamics to these phenomena. Additionally, in the final presentation, a review of numerical and physical sensitivity based on significant parameters such as the capillary number will be included.



CFD: Journal colored by gas volume fraction and white translucent 90% liquid isosurface.

Figure 1: Photographic image [3] and CFD visualization. Journal running at 1840 RPM with a back pressure of 40.8kPa(g). Cavitating flow in journal bearing.

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A multi-fluid Large-Eddy Simulation framework based on the Conservative Level Set approach for predicting two-phase heat transfer

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15^{th} March 2022

Heat transfer in liquid-gas flows is ubiquitous in industrial applications such as droplet evaporation in combustion chambers, or sloshing in cryogenic tanks. Unsteady simulations of these configurations are challenging because they involve a large range of scales and transported properties are discontinuous across the interface. This work presents a new framework to perform Large-Eddy Simulation (LES) on unstructured meshes with transported scalars that are discontinuous across an interface. In LES, the profile of the filtered phase indicator or of the liquid volume fraction depends on the LES filter kernel. Assuming a flat interface, this profile corresponds to a filtered Heaviside function, which can be resolved on the LES mesh. In the proposed work, the considered filtered phase indicators are i) an hyperbolic tangent profile as in conservative level set approaches [2], and ii) the error function. The corresponding filter kernels are used to filter the scalar transport equations in each phase. Similarly to multi-fluids approaches [1], the proposed method consists in transporting discontinuous scalars considering as many equations as phases and one equation for the phase indicator. The main challenge lies in the consistency of all the transport equations. Indeed, the filtered phase indicator is advected according to the level-set method [4] and reinitialized with a mapping function [3]. To ensure consistency with the phase indicator, the discontinuous scalars also have to be reinitialized with a proper reinitialization equation that takes into account the interface flux. Two different flux models which both consider sub-grid scale distributions, are derived and assessed on numerical experiments of increasing complexity. Fig. 1 illustrates the evolution of the temperature field in a heated and convected droplet computed with this new method.

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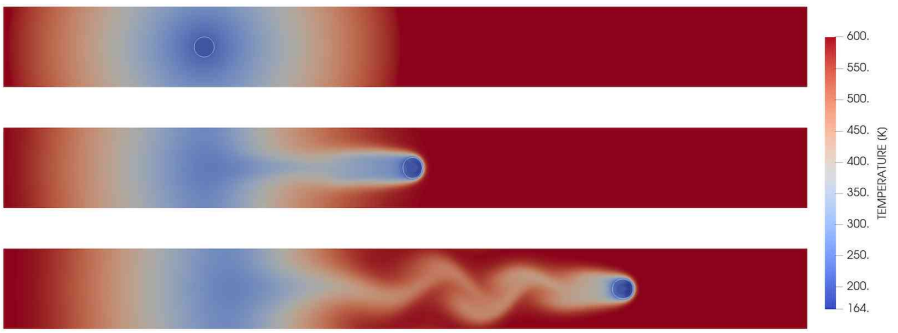

Figure 1: Temperature of a moving water droplet of diameter $d = 0.5\,\mathrm{mm}$ and $u = 3\,\mathrm{m/s}$ in air at rest, after $1.8\,\mathrm{ms}$ and after $3.6\,\mathrm{ms}$. Triangular mesh resolution is $d/\Delta x = 42$

Numerical simulation of spraying systems using the Euler/Lagrangian method with an advanced stochastic droplet collision model

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The Euler/Lagrangian approach is very powerful for predicting polydisperse turbulent two-phase flows. Important applications of such flows are spraying systems used in many areas of process technology and also pharmaceutics. In this contribution the effect of inter-droplet collisions and their proper modelling on the spray spreading and the resulting droplet size distributions is analyzed in detail. The flow is computed by solving the usual Eulerian equations combined with the k-ε turbulence model (i.e. RANS approach). The spray is simulated by the Lagrangian parcel concept. Here, representative droplets are tracked accounting for turbulent dispersion according to Sgrott and Sommerfeld [1] and considering 2-way-coupling. The considered spray systems are generated by using measurement results from phase Doppler anemometry (PDA) at planes located below the nozzle exit where breakup was completed. Therefore, the primary breakup process of liquid jets is not considered, which still has many open issues and is not yet well established. The droplet collision model is based on the fully stochastic droplet collision approach from Sommerfeld [2], also considering the influence of impact efficiency from Ho and Sommerfeld [3]. This effect may remarkably reduce collision rates for a wide droplet size spectrum. The collision outcomes (bouncing, coalescence, stretching and reflexive separation) are determined so-called droplet collision maps (the non-dimensional impact parameter B plotted versus collision Weber number; B = f(We)) with theory-based boundary lines recently developed which also take into account droplet size ratio effects. In the collision map, the droplet collision boundary line for coalescence-stretching separation is taken from Sommerfeld and Pasternak [4], the bouncing boundary line including dissipation is based on Sui et al. [5], and the reflexive separation boundary line is based on the correlation of Ashgriz and Poo [6]. For validating the collision model and the spray creation procedure implemented in OpenFOAM®, first a simple hollow cone spray is considered based on the measurements of Rüger et al.[7]. The second applications concerns a complex multi-fluid nozzle (liquid jet plus a number of steering air jets) which is, among others, applied in the pharmaceutical industry for tablet coating. Several measurements downstream of the injection plane allow analyzing the spray dispersion for different model assumptions.

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Numerical Simulation of Gas Atomization Process for Metal Powder Production

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The emerging technological field of Additive Manufacturing (AM) typically needs specifically tailored materials and particles, especially metal powders with precisely optimized size, shape, and morphology. At present fine powders for metal AM are produced primarily by the gas atomization technology. Hence, a CFD-based numerical modeling approach is built to consider both the primary breakup of the melt stream from the gas atomization nozzle and the secondary breakup of the primary melt droplets in the spray chamber. For the modeling of the primary breakup modeling, a VOF based two-phase flow model in OpenFoam is applied to track the dynamic deformation of the gas-melts interface. The generation of melt primary droplets is recorded with the information of droplet size, position, and velocity. For the secondary breakup, a Lagrangian-Eulerian multiphase flow model based on Ansys Fluent DPM (Discrete Phase Method) is adopted to track the secondary breakup of the primary melt droplets under the effects of the high-speed compressible gas flow. The final particles at the spray chamber outlet are sampled and analyzed statistically. The particle size distribution are then obtained.

The process of gas atomization will be affected by many factors such as the geometry of the atomization nozzle, operating conditions (melt flow rate and gas pressure) and material properties (melt viscosity and surface tension). The quality of final particles produced by the gas atomization process is affected by the combination of all these factors. The goal of the numerical modeling is to, with the flow physics involved in the gas atomization process, investigate the effects of different operating conditions on the particle quality, and optimize the operating conditions to produce powders with the required quality.

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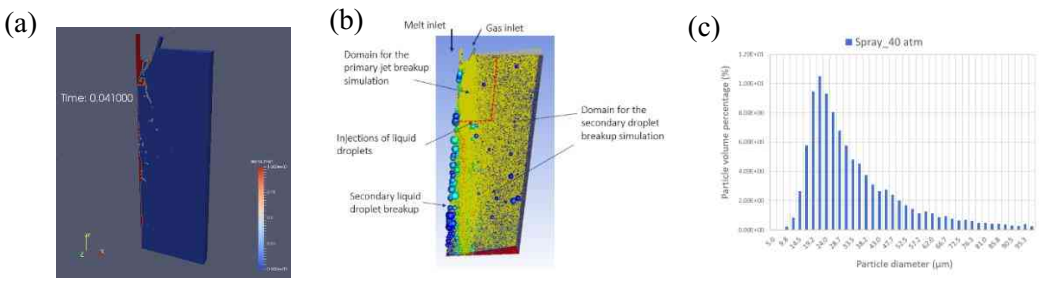

Figure 1: (a) Model for the primary break of melt stream; (b) Model for the secondary breakup of the primary melt droplets; (c) Simulation predicted particle size distribution under gas operation pressure 40 atm.

Stochastic sprays in the under-resolved turbulence

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The recent DNS studies of the high Reynolds number statistically stationary box turbulence (see Buaria et al. 2019, for example) show the strongly intermittent local flow structures. These structures give rise to extreme local accelerations. With increasing the Reynolds number, the PDFs of those accelerations expose heavier tails. Concerning the multiphase flows, such effects of intense small-scale dynamics may have a strong impact on the interface formation, its motion and evaporation. However the resolution of those effects is a too difficult task even in one-phase flows. In our talk, we will discuss on how the traditional approach, such as LES-VOF, may be successfully completed by stochastic processes on residual scales for the interface curvature and the interface normal direction. These stochastic models are developped coherently with the recent knowledge from the experimental and numerical observations. Namely, both models are linked to the acceleration of the fluid particle ("stochastically seen" on subgrid scales), with accounting in the same time for the influence of the surface tension effects. As illustration of simulated extra-structures of the interface are seen in Fig.1 in comparisson with standard LES approach. We are going also present the recently developped stochastic models for droplets breakup, motion and evaporation. To this end, the new motion equations, as well as the evaporation and breakup rate expressions, are linked to the orientation and the intensity of strained flow structures to be modeled on residual scales. The analysis is supported by DNS. The droplet motion and evaporation models are described partly in (Gorokhovski and Zamansky 2018, Barge and Gorokhovski 2020, Gorokhovski and Oruganti 2022).

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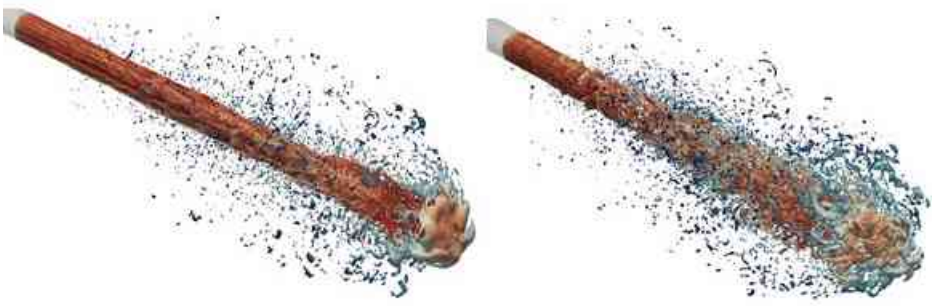

Figure 1: Iso-surface of liquid volume fraction for time instance 5.0μs. On the left-hand side standard LES-VOF; the right-hand side LES-VOF with interface stochastic SGS model.

Volume-of-Fluid method with phase change applied to water jet cooling

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Liquid jet cooling is frequently used in applications that require high amounts of thermal energy to be removed, for example, metals and glasses process industries, cooling of turbine components and many others. Phase change is one of the most important heat transfer mechanisms involved in the impinging jet cooling process and must not be ignored when seeking for accurate results. Numerical simulations capable of tracking the interface between two fluids and take into consideration phase change are still in the early days [1]. The volume-of-fluid (VOF) and level-set methods are well stablished methods for reconstructing and locating fluid-fluid interfaces. The VOF method is preferred due to its inherent mass-conservation property, which is an important feature when dealing with phase changes [2]. Closure formulations for phase change, either condensation or evaporation, have been proposed in the literature [3][4] and were validated for specific cases. Their implementation together with the VOF method is usually not publicly available and needs therefore to be implemented. In this work, a VOF solver already present in OpenFOAM is extended with a phase change model [5] and conjugate heat transfer (CHT) in order to simulate a metal plate cooled by an impinging water jet. The phase change model used here is based on the original approach from Hardt and Wondra [3], but with modifications that allow the use of coarser meshes without losing accuracy. Experiments are also carried out in a testbench that consists of an induction heating system used to heat the metal plate, an infrared camera used to obtain the temperature field at the rear face of the plate and high-speed cameras to record the hydrodynamic behavior of the jet. The transient temperature field of the rear face of the plate and the transient mean heat flux between jet and metal are used as parameters to compare simulation and experiments. By combining experimental and numerical analyses, this paper ought to contribute to the understanding of the complex phenomena involved in processes with interfaces and phase change.

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Large-eddy simulation of cavitating tip leakage vortex

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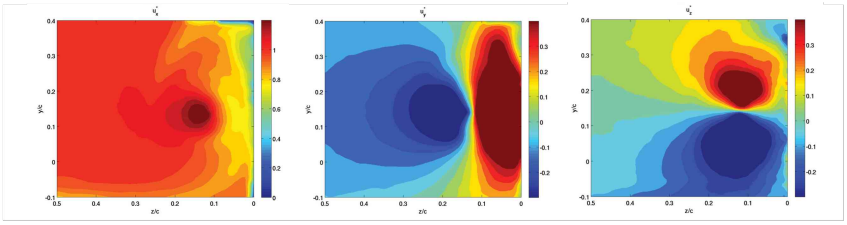
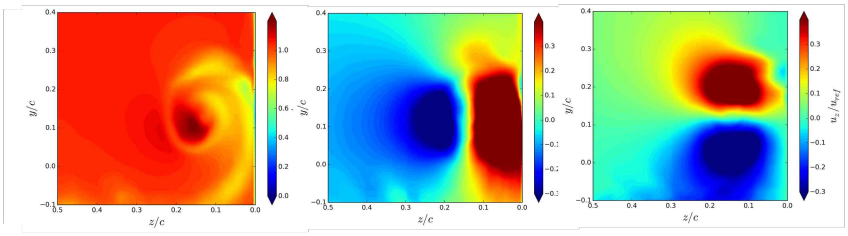
Tip Leakage Vortices (TLV) are very common in axial turbomachines. This type of vortex forms as the result of an interaction between the leakage flow, a flow from the pressure side of a blade to its suction side, and the upstream flow. In hydraulic machines, the high rotation in TLVs can cause a significant pressure drop at the core of the vortex leading to formation of cavitating structures. Previous experimental studies have shown that the formation of these cavitating structures is responsible for many adverse effects such as cavitation breakdown and a high level of noise and vibration [1, 2, 3]. To avoid such adverse effects, a better understanding of the flow dynamics in TLVs is needed. Numerical simulations can be a useful tool for this purpose as they provide a complete access to the flow field, especially near the cavitating regions where it is difficult to get optical access in the experiments.

In this study, we numerically investigate non-cavitating and cavitating TLVs around a NACA0009 foil using a large-eddy simulation approach. The results of the non-cavitating simulation are validated against the experimental data provided in Dreyer et al. [4]. This comparison, shown in Fig. 1, indicates that the simulation can capture the main features of the flow field. Furthermore, a cavitating condition is simulated and the effect of cavitation on the structure of the TLV is discussed in detail.



(a) Exp.



(b) Num.

Figure 1: Comparison between the velocity field in the TLV in the simulation and the experiment, a) Experimental data by [4] and b) numerical simulation results.

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Multicomponent Droplet Evaporation in a Geometric Volume of Fluid Framework

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Abstract

The vaporization of multicomponent droplets is a complex and multidisciplinary problem which has been studied for years with different levels of detail. Recent advances in CFD modeling of gas-liquid systems allow the detailed description of non-spherical deforming droplets to be combined with the detailed characterization of the vaporization process.
This work presents a numerical model for solving the incompressible Navier-Stokes equations in multicomponent gas-liquid systems with phase change. The proposed model accounts for the expansion term at the interface due to the phase change phenomena (Stefan flow) and it extends state-of-the-art models for the simulation of pure evaporating droplets via a novel approach for the solution of multiple chemical species in the liquid phase, which can participate in the vaporization process.
The final model has been implemented in the open-source code Basilisk, and it includes:

- Two different approaches to obtain a liquid velocity that is divergence-free and that can be used to advect the liquid volume fraction field.
- The introduction of a phase change velocity which shrinks the droplet.
- The solution of the non-linear interface jump condition to quantify the vaporization rate for each chemical species.
- A two-field approach to solving the transport of the scalar quantities, accounting for the interface jump conditions.

The resulting model was tested against literature benchmark simulations and analytical solutions to quantify the error, the mass conservation, and the order of accuracy of the implemented numerical methods.
The importance of this work is two-fold: first, it improves the numerical models for the simulation of phase change in a VOF framework; second, it paves the way for the simulation of realistic multicomponent fuel droplets, which is fundamental for the characterization of complex systems like sprays.

Modeling of droplet condensation on walls based on the adaptation of the Ranz-Marshall correlation for twophase turbulent flow with CFD approach

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This work is dedicated to the wall condensation of steam in the presence of noncondensable gases for a turbulent two-phase flow with the aim of dealing with a large scale geometry such as the containment of a nuclear reactor. The heat and mass transfer taking place on the containment walls represents mass and energy sinks allowing the limitation of the pressure increase caused by the huge amount of steam released in the case of a hypothetical loss of coolant accident.

In this scope, the use of the CFD approach for calculating turbulent flow in large-scale geometries can be very expensive when detailed boundary layer resolution for velocity, temperature, and concentration is adopted. This computational cost can be significantly reduced by using wall functions and even more so when heat and mass transfer on walls is predicted with correlations such as those based on the heat and mass transfer analogy [1],[2].

In the present work, a heat and mass transfer model for droplet condensation on wall based on an adaptation of the Ranz-Marshall correlation initially developed for droplet evaporation [3] is proposed. The multicomponent flow is governed by the conservation equations of the mass, momentum and energy of the dispersed liquid phase and of the gaseous mixture considered as the continuous phase [4]. The standard k-ϵ model is used for the gaseous mixture turbulent flow. These equations are solved by using a pressure-based numerical scheme and a finite volume method for the space discretization. The model is validated on separate effect condensation experiments of wall condensation in steady state flow and also on coupled effect experiments with wall condensation occurring during a transient of steam injection within an enclosure in presence of noncondensable gases. These tests involve different gas mixture composition and are ranging from natural convection to forced convection regimes. The obtained results show great improvements of the heat and mass transfer rate predictions and also of the flow field variable distribution. The sensible heat transfer modeling is shown to be of great influence on the temperature field and on the condensation transfer rate.

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Thursday – 2022-09-29

Session I

- **Advanced Computational and Numerical Method Developments**
  (Chair: V. Moureau, Room: Auditorium)
- **Simulation of complex multiphase flows – Applications**
  (Chair: F. Denner, Room: Aula Magna 1-E)

A numerical model for two-phase liquid-vapor flows with arbitrary-rate heat and mass transfer

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We describe liquid-vapor flows by a single-velocity six-equation two-phase compressible flow model [1], which is composed of the phasic mass and total energy equations, one volume fraction equation, and the mixture momentum equation. The model contains relaxation source terms accounting for volume, heat and mass transfer. The system of equations is numerically solved by a classical fractional step algorithm, where we alternate between the solution of the homogeneous hyperbolic portion of the model system via a HLLC-type finite volume scheme, and the solution of a sequence of systems of ordinary differential equations for the relaxation source terms driving the flow toward mechanical, thermal and chemical equilibrium. For an accurate description of the thermodynamic processes involved in transient liquid-vapor flow problems it is often important to be able to simulate both instantaneous and finite-rate relaxation processes. For instance, in some phenomena such as fast depressurizations the delay of vaporization and the appearance of metastable states are key features in the flow dynamics [2]. In the present work we present new numerical relaxation procedures to integrate interphase transfer terms with two significant properties: the capability to describe heat and mass transfer processes with arbitrary relaxation time, and the applicability to a general equation of state. The main idea of the novel numerical relaxation procedures is to describe relaxation processes by systems of ordinary differential equations that admit analytical semi-exact exponential solutions [3]. Several numerical tests are presented to show the effectiveness of the proposed numerical techniques, including simulations of depressurizations leading to metastable superheated liquid, and the simulation of a two-dimensional fuel injector. Some results of the latter test are shown in Figure 1.

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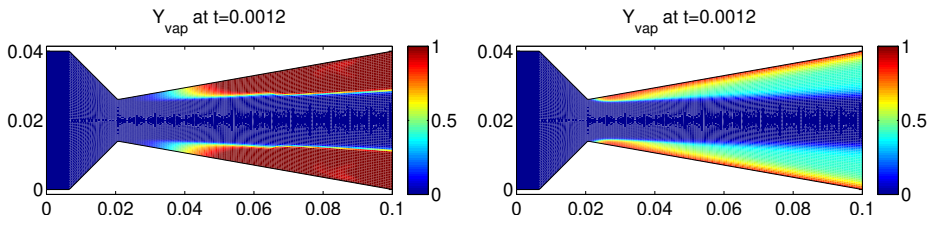

Figure 1: High-pressure fuel injector. Liquid dodecane is injected from a high-pressure tank to a chamber filled with dodecane vapor at atmospheric pressure. Computed vapor mass fraction Y_{vap} at time $t = 0.0012\,\mathrm{s}$ for the case of slow finite-rate mass transfer (left) and instantaneous mass transfer (right). Grid: 200×80 cells.

A Discontinuous Galerkin Method for Compressible Gas/Liquid Interfacial Flows

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Simulating compressible gas/liquid interfacial flows efficiently and with high accuracy is a challenging multi-physics problem due to large gradients, variable material properties, and disparate time and length scales. To address these challenges, we develop a discontinuous Galerkin method to solve the compressible Navier-Stokes equations using the five-equations multiphase model. [1]. The temporal scheme is explicit (Runge-Kutta) and the spatial scheme relies on a discontinuity sensor to identify regions where high-order limiting is applied, i.e., at interfaces and shock waves. The limiting is performed so as to prevent the generation of spurious oscillations at material interfaces by appropriately reconstructing the density, velocity, and pressure in a conservative fashion. Viscous effects and heat transfer are included and different kinds of meshes can be implemented while still maintaining arbitrarily high orders of accuracy. We demonstrate the viability of our method through a variety of one- and multi-dimensional compressible gas/liquid interfacial problems, including high-speed impact of a liquid droplet onto a rigid wall (Figure 1).

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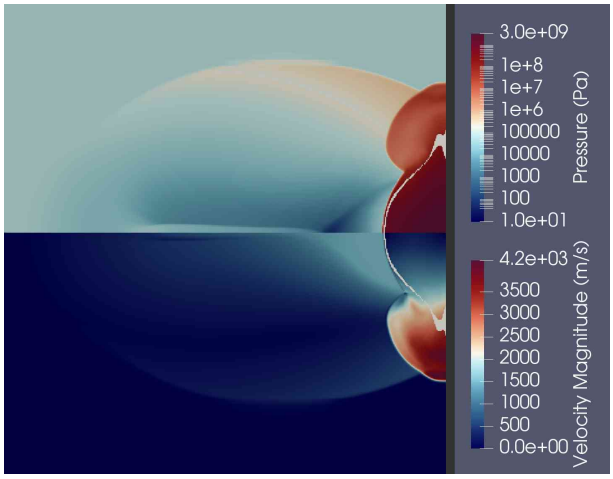

Figure 1: Numerical simulation of a Mach 6 water droplet in air impinging upon a rigid wall. Droplet outline is overlaid in white.

An analytical wall function for turbulent wall condensation in the presence of noncondensable gas with buoyancy, suction and interdiffusion convection

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The use of CFD for simulations of turbulent flow in industrial applications often requires using wall functions in order to reduce the computational cost. When wall condensation occurs, it creates density variations in the boundary layer that can lead to significant buoyancy effect. The aim of this work is to propose wall functions for velocity, temperature and steam mass fraction that can be applied for all convection regimes. The new model is an extension of the analytical wall function developed by Craft & al. [1]. This method also allows to account for the influence of suction and interdiffusion convection within wall functions. The suction effect describes the mass transfer normal to the wall induced by the steam condensation. Both suction and interdiffusion could have significant effect when high heat and mass transfer is considered.

In forced convection regime, the new wall functions have shown good agreement with the standard wall functions based on the Prandtl mixing length. For mixed and natural convection, the influence of buoyancy, suction au interdiffusion convection can be observed. The comparison between results from simulations and experimental data show that the implemented wall functions give a better estimation of the condensation heat flux than the standard wall functions, especially for mixed and natural convection.

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A Unified Multiphysics Framework for Multi-Region Coupling and its Application to ALE Interface-Tracking

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We have developed a novel unified solver framework for "multiphysics" of multi-region coupling type, i.e. transport processes coupled across region boundaries/interfaces. The code is implemented as C++ library in FOAM-extend 4.1 for computational continuum physics and follows the principles of object-oriented programming. A versatile and physics-guided code structure is tailored to flexibly incorporate user-defined types of regions representing regions of specific physics in the form of a set of transport equations. The coupling and communication between regions is realised in a likewise modular fashion where interface-specific physics as well as interpolation/mapping methods are accessible in boundary conditions. Moreover, for each region, a (sub-)set of transport equations can be coupled across the region boundaries, either utilising an explicit (partitioned) or implicit (monolithic) coupling method. The implementation is readily parallelised for all medium and large scale computations in domain decomposition mode for runs on distributed-memory parallel computer architectures – see also [1]. The suggested unified framework could lay ground for a variety of multiphysics applications, such as Conjugate Heat Transfer (CHT), multi-material Arbitrary Lagrangian Eulerian (ALE) methods, Fluid-Structure-Interactions (FSI), battery and fuel cells models.
The focus of the presentation will be on demonstrating the framework capability to implement an enhanced moving mesh ALE interface-tracking method originally developed by Tuković and Jasak [2]. The code for the mesh and interface motion is refactored to support multiply regions and multiple moving surface patches per region (multi-material ALE), relying on the introduced multi-region coupling strategy. For illustration, we detail on incompressible flows of Newtonian fluids separated by sharp capillary interfaces. The governing Navier-Stokes equations are solved for each region separately using a collocated finite volume method (FVM) on unstructured meshes of general topology. Coupling between regions is accomplished in an iterative manner using the PIMPLE-C (combination of PISO and SIMPLE-C) algorithm for pressure-velocity coupling where a Dirichlet-Neumann scheme is deployed to consistently enforce the momentum jump and transmission conditions at the interface. For a stable and convergent procedure, coupled boundary conditions are devised deploying the finite area method (FAM), by means of which the local area force density due to surface tension is calculated using a force-balanced numerical discretisation of second order accuracy [2]. An enhanced backward differencing (BDF) scheme is employed to ensure time consistency for moving meshes [3]. Skewness errors of the significantly deformed meshes and interfaces are corrected with second order accuracy. For heat and species transfer both partitioned and monolithic coupling are available and tested. The solver is verified and validated for a selection of multiphase flow simulations / benchmark test cases.

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A particle-center-averaged Euler-Euler model for bubbly flow simulations

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An inconsistency exists in bubble force models used in the standard Euler-Euler simulations. The bubble force models are typically developed by assuming that the forces act on the bubbles' centers of mass. However, in the standard Euler-Euler model, each bubble force is a function of the local gas volume fraction because the phase-averaging method is used. This inconsistency can lead to gas over-concentration in the center or near the wall of a channel when the bubble diameter is larger than the computational cell size[1-2]. Besides, a mesh-independent solution may not exist in such cases. In addition, the bubble dimension is not fully considered in the standard Euler-Euler model.

In the present study, a particle-center-averaging method is used to represent the bubble forces as forces that act on the bubbles' centers of mass. A particle-center-averaged Euler-Euler approach for bubbly flow simulations is developed by combining the particle-center-averaged Euler-Euler framework with a Gaussian convolution method. The convolution method is used to convert the phase-averaged and the particle-center-averaged quantities. The test results illustrate that the particle-center-averaging method alleviates the over-prediction of the gas volume fraction peak in the channel center and provides a mesh-independent solution (Fig. 1). In the particle-center-averaged Euler-Euler model, the bubble dimension is fully considered and bubble deformation can be considered by using anisotropic diffusion in quantities conversion. The test results for the gas volume fraction of a spherical and an oblate ellipsoidal bubble are presented in Fig. 2.

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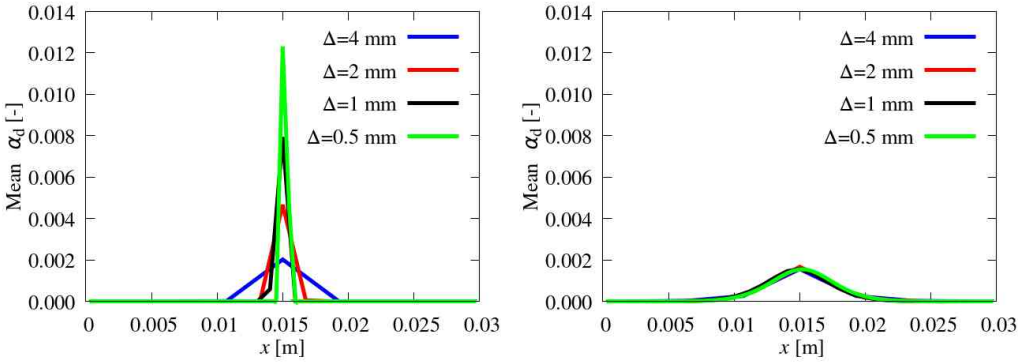

Figure 1: Mesh sensitivity results for standard (left) and particle-center-averaged Euler-Euler model (right)

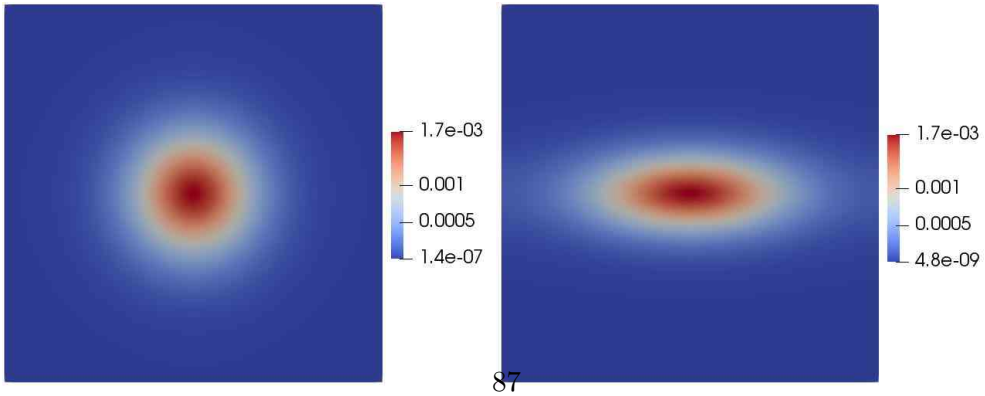

Figure 2: Gas volume fraction distribution for a spherical bubble (left) and an oblate ellipsoidal bubble (right)

On the effect of in-plane solidity on the different regimes of canopy flows

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We have carried out highly resolved Large Eddy Simulations (LES) of an incompressible, turbulent, open channel flows bound by a canopy of rigid filaments that are flush mounted, slender, normal to an impermeable wall. The Immersed Boundary (IBM) formulation [1] that is adopted allows the computation to tackle the region occupied by the canopy directly by imposing the zero-velocity condition on every single stem. In the current investigation, we have considered six canopy configurations that differ only in the solidity (λ) obtained by varying the in plane solid fraction (obtained by increasing the stems number density) with the same canopy height. The selected solidity nominally falls in the so called 'transition-dense' canopy flow configurations [2] (i.e., $\lambda \in [0.05, 0.6]$). While the above regime was investigated recently [3] by altering the canopy height alone, the variation of the in-plane solid fraction (ΔS^2) and its effect on the overlying turbulent flow have not been explored. The former discriminates the scales of the outer flow that can penetrate the canopy and control the overall interactions of the inner and outer flows. All the mean velocity profiles exhibit two inflection points [3], one located at the top of the canopy and the other closer to the bottom wall. While the origin of the inner flow corresponds to the solid wall, the origin for the outer layer can be identified by a virtual location below the tip of the canopy, similar to the one adopted in describing turbulent flows over rough walls. While the coarsest and the transitional scenarios share some features with the flows sharing the same solidity, obtained by changing the canopy depth, the densest case features a radically different behaviour with an almost complete decoupling of the interaction between the outer and the intra canopy flows. This suggests the existence of a new quantitative measure that characterises the transition beyond the value of λ.

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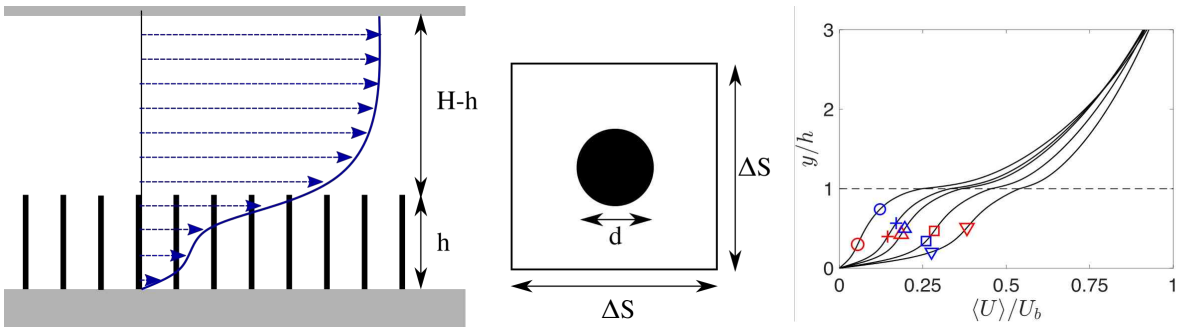

Figure 1: Geometrical parameters that govern canopy flows (left and middle). Mean velocity profile on the right, with the location of the virtual origin (red) and internal inflection point (blue). Horizontal dashed line represents the canopy height.

Numerical assessment of cavitation erosion in a high-pressure fuel injector

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Numerical cavitation erosion assessment of industrial high-pressure fuel injectors is still challenging as it requires computationally expensive simulation of flows with a wide range of time and length scales. This study aims to provide a numerical methodology for experimentally available high-pressure (2200 bar) Woodward L'Orange fuel injector. The experiment had been carried out with two separate, fixed, high and low lift needle positions. Same conditions are numerically investigated to provide comparison to that experiment.

A periodic single hole geometry is simulated with a pressure-based finite volume solver in the commercial Ansys Fluent software. Cavitation erosion assessment is examined with the collapse detector algorithm method, previously applied by Mouvanal [1].

Unsteady Reynolds-averaged Navier-Stokes (URANS) turbulence modelling is employed with k-Omega SST [2]. Here, the turbulence viscosity is retreated with Reboud's correction [3]. Besides the URANS approach, scale-resolving simulations are also carried out. Assuming a homogeneous mixture, cavitation is modelled via the mass transfer approach. Hence, the Zwart-Gerber-Belamri cavitation modelling is used with altered model coefficients.

Below, the figure on the left, shows the photograph taken at the end of experiment. Here, the geometry is filled with an epoxy material, which fills gaps of the eroded material. On the right, numerical result from the URANS solution is presented. Here, the maximum collapse pressure on the injector nozzle wall during the simulation period is recorded and presented with a contour plot.

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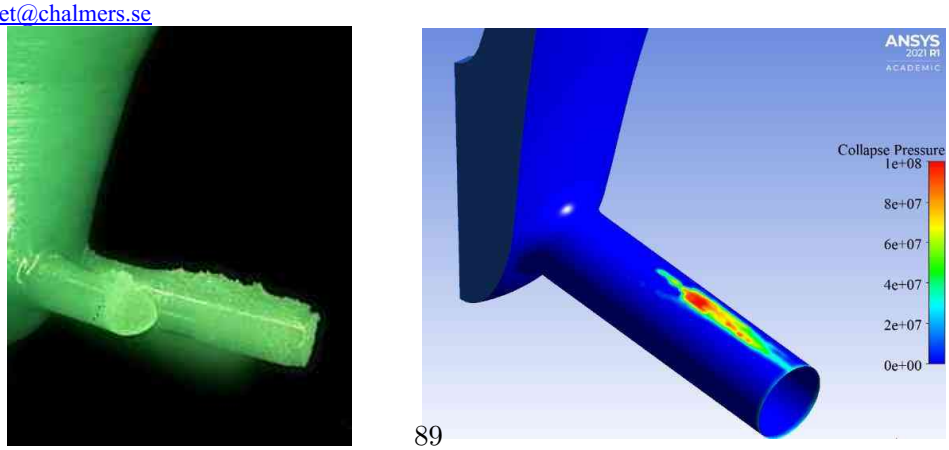

Figure 1: Comparison of the experimental (left) and numerical result (right) for high lift condition

An Investigation of Rain Droplet Interaction for Reentry Vehicles

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As vehicles enter the atmosphere at hypersonic speeds, as seen with the Orion spacecraft, the potential interaction with rain remains a possibility. A rain droplet can apply a load of up to 40 kN to a small area. Thus, to understand the necessary structure to withstand these loadings, the state the droplet is in as it passes through the preceding bow shock is necessary. The proposed effort presents the multiphysics phenomena relating to the droplet loading that includes droplet deformation, evaporation/boiling, and cavitation via interaction with a shock which will lead to droplet breakup to relieve the load. The effort will explore this using a multiscale, multiphysics simulation to estimate the loadings of an entry vehicle to understand such events.

Within this system, there are two scales at which physics acts: a macro-scale of the reentry vehicle and a micro-scale of the droplet. The issue with a conventional approach to this is that the disparity in sizes of the two scales will cause one scale to not be accurately captured. This paper presents a novel method to model this scenario using a Multiscale approach. This approach uses compressible, fully coupled computational fluid dynamics to simulate the gas motion around the vehicle. The flow is coupled to a model of trajectory predictions for various droplet sizes relevant to rain to quantify the direct, or unbroken impact speed. This model is then coupled to a secondary model of a domain attached to the droplet itself to directly resolve the breakup mechanism using a direct simulation, volume-of-fluid method that tracks the droplet evolution, evaporation, and cavitation processes. This approach will sufficiently capture the vehicle and droplet scales without requiring excessive meshing or computational power.

The proposed results of the paper are a predictive model which implements the multiscale approach above. The results involve several components. Firstly, a steady-state solution for the launch vehicle is reached. Then, the droplet is introduced in the flow in an implicitly unsteady solver. Results will produce fluid mass flux and relative speed data at each timestep. Graphical representation will be created at specified intervals to observe and characterize physical phenomena such as cavitation and breakup. The proposed solutions explore multiple relevant reentry scenarios where rain can be present such as water rain on earth, methane rain on Titan, and sulfuric acid rain on Venus. These atmospheric predictions lend novel data to the ever-expending push towards other planets.

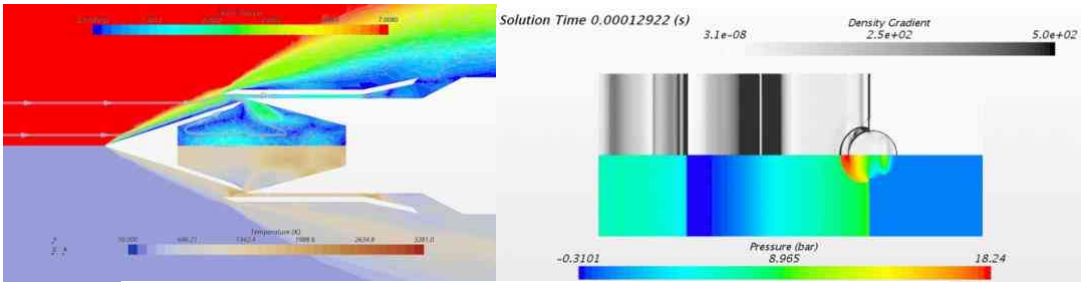

Figure 1: Macro flow domain with droplet streamlines (left) and micro flow domain interacting with shock wave (right).

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Direct Numerical Simulation of CMAS Particles and Their Deposition on Aircraft Components

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The ingestion of CMAS (Calcium-Magnesium-Alumino-Silicate) particles into aircraft engines is an issue for both the safety and resilience of aircraft. One incident occurred on British Airways Flight 9 in 1982, where all four engines on a Boeing 747 failed during flight through a cloud of volcanic ash (composed of CMAS). In this scenario, the CMAS particles melt due to high temperatures within the engine and resolidify on coolant lines. This process can erode compressor blades, erode/infiltration thermal barrier coatings, and causes overheating and stall. This work aims to study the details of CMAS infiltration at a detailed level. The effort specifically aims to directly modeling the melting and deposition processes in the context of coupling to the fluid-dynamic processes.

This work presents a novel approach to exploring CMAS dynamics in the context of a melting particle. The methodology was accomplished by resolving a single CMAS particle in a DNS approach, using the volume-of-fluid method in Eulerian multiphase physics. The effort will involve a single, spherical, CMAS particle simulation exposed to variable thermal conditions. The methodology/framework is developed within the commercial CFD tool, Star-CCM+. The slip Reynolds numbers of interest lead to transitional regimes better suited to DNS. To account for thermal properties of the flow and particle, the melting-solidification modeling was implemented. The particle was initialized at a stagnant condition with a temperature under its solidus temperature. The flow around the particle was initialized at turbine relevant conditions, including high velocities and temperatures above the particle's liquidus temperature. Transient conditions were explored in context of non-dimensional numbers (including slip Reynold's Number, Weber number, and Ohnesorge number), as well as several ratios ($\rho s/\rho g$ and $Ts/T\infty$). For validation, sensitivity to mesh, as well as experimental comparisons were examined. The experimental comparison benchmarked the temperature ratio of particles at varying thermal Stokes numbers against the experimental correlation shown in Bojdo et al. [1].

FIGURE 1: Shows the evolution of the CMAS particle's melting layers in the flow field

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An eXtended Discontinuous Galerkin Method for three-dimensional two-phase flows: Application to viscous droplet oscillations

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Florian Kummer TU Darmstadt
Günter Brenn TU Graz
Martin Oberlack TU Darmstadt

We are going to present a high-order eXtended Discontinuous Galerkin (XDG) method for transient two-phase flow problems within a three-dimensional setting. The XDG method adapts the local ansatz functions to conform to the position of the interface and provides separate degrees of freedom for each fluid phase in cells which are cut by the interface [1]. This allows a sub-cell accurate approximation of the incompressible Navier-Stokes equations in their sharp-interface formulation. The interface is described as the zero-set of a signed-distance level-set function and is discretized by a standard DG method. For the interface, resp. level-set, evolution, an XDG adapted marching algorithm for the construction of an extension velocity field was presented in [2] for the 2D case. For the 3D case, we present the construction of a divergence-free extension velocity field by solving the two-phase Stokes equations with the XDG approach. Furthermore, we discuss some issues regarding the extension to 3D problems, such as the continuity projection of the interface by a patch-wise approach and the agglomeration of cells cut by the interface.

The numerical investigations will focus on nonlinear axisymmetric shape oscillations of a Newtonian drop in a near dynamically inert ambient phase. The initial drop shape is given by a Legendre polynomial of degree m. We compare the numerical results with the theoretical results of the weakly nonlinear analysis presented in [3]. The analysis is based on series expansions of the flow field variables and the drop shape with respect to a deformation parameter. The weakly nonlinear approach is carried out to third order and accounts for the coupling of different oscillation modes. Modes of initial deformation up to $m = 4$ are addressed. The properties to be compared include the droplet aspect ratio over time with corresponding period times and damping rates, and mode decomposition of the droplet shape into Legendre polynomials. Further, we present the kinetic and surface energy over time for the numerical simulations.

Acknowledgements

Funding of this joint project of the two reporting partner groups (TU Darmstadt and TU Graz) by the German Research Foundation (DFG - project number 330615302) together with the Austrian Science Fund (FWF - project number I 3326-N32) in the DACH framework is gratefully acknowledged. The work by M. Smuda is in part funded by the Federal Ministry of Education and Research (BMBF) and the state of Hesse as part of the NHR Program.

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Thursday – 2022-09-29

Session II

- **Numerical multiphysics modeling of surfactants & interfacial transport**
  (Chair: V. Le Chenadec, Room: Auditorium)
- **Machine-learning and data-driven techniques for multiphase flow simulations**
  (Chair: S. Sasic, Room: Aula Magna 1-E)

Coupled level-Set Volume-of-fluid solver for Thermocapillary applications

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Jorge Cesar Brändle de Motta‡
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Surface tension is modified by temperature and concentrations of surfacic active agents or impurities. This phenomenon plays an important role in applications where heat transfer processes are involved such as cooling methods, inking or painting. Accurate numerical approaches to tackle variable surface tension are necessary to study 3D complex and practical problems. Models should have many ingredients such as good curvature estimation or well-balanced and stable schemes [1].

In this communication, a coupled Level-set Volume-of-fluid method [2] is used to numerically study the effects of the interfacial forces driven by in-homogeneous surface tension. Continuum surface force and ghost fluid methods are both tested to accounts for the pressure jump. The computation of the surface tension surfacic gradient is needed to implement the Marangoni force. The knowledge of both, Level-set and VoF is used to propose different implementations of this term.

The new scheme of the surface operators is detailed and validated against analytical solutions. The study of a planar interface submitted to a temperature gradient is studied [3] [See Fig. 1]. Also, the study of the thermocapillary motion on a 2D and 3D single droplet due to a temperature gradient is considered [4] [See Fig. 2]. To test the implementation in a complex situation referenced in a previous study, the thermocapillary schemes are applied on a case of a homogeneous isotropic turbulence flow [2].

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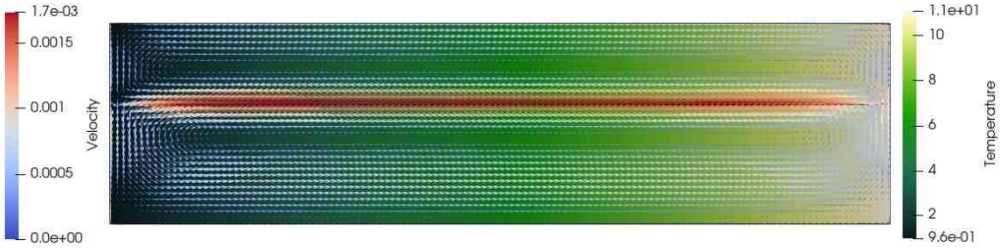

Figure 1: Two layered flows submitted to a temperature gradient in horizontal axis.

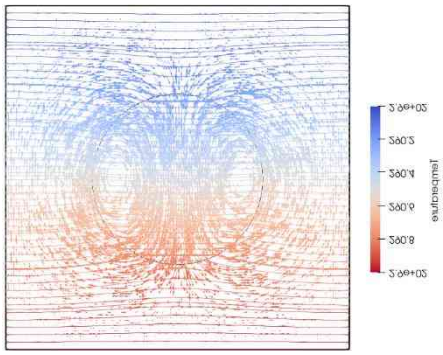

Figure 2: Droplet migration due to a vertical temperature gradient.

A 2D hybrid method for interfacial transport of passive scalars

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In this article, we propose a hybrid method to simulate the evolution of the passive scalar transport on the interface. The evolution of the interface is tracked by level set method [1] with 5^{th} order WENO scheme in Eulerian framework, while the passive scalar transport is resolved by the total Lagrangian Smoothed Particle Hydrodynamics (SPH) method [2]. When the particle distribution exhibits irregularity, such as clamping or void region, the particles will be regenerated with proper mass to recover the regularity. In order to minimize the induced error adaptively, based on classical remeshing process [3], we generalize the remeshing algorithm to redistribute the mass to the new particles. Taking the advantages from both Lagrangian and Eulerian descriptions, the mass conservation is achieved. Since the particles are only located on the reduced-order surface and the remeshing process can be done adaptively, the introduced computational effort is acceptable.

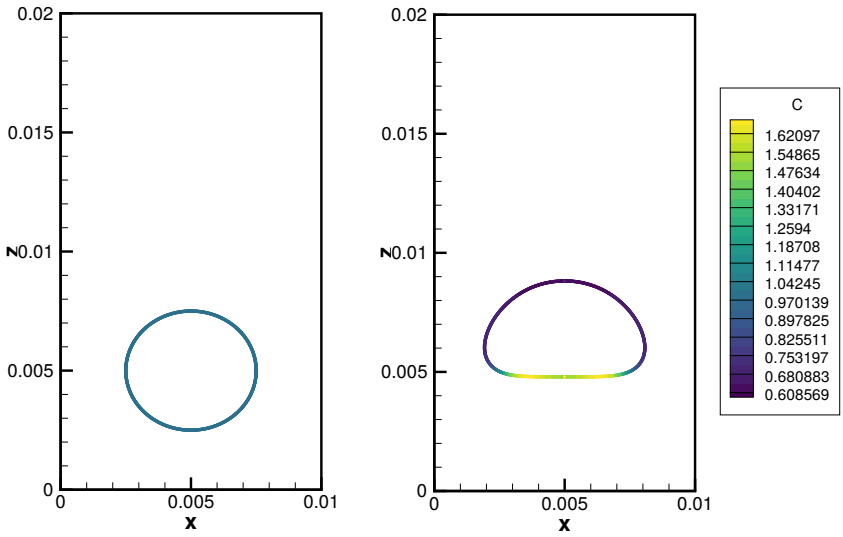

Figure 1: The concentration variation of rising bubble. Initial concentration field on the bubble interface (left panel); concentration field at $t = 0.25$ (right panel).

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Quadratic interface reconstruction from volume fractions on arbitrary polyhedral meshes

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In order to simulate interfacial two-phase flows, geometric volume-of-fluid methods require the construction of local piecewise approximations of the interface from the knowledge of the discrete volume fractions. So far, and with a few notable exceptions (e.g., [1, 2, 3]), piecewise-linear interface approximations have commonly been used, resulting in a second-order accurate solution of the interface's evolution. Attempts at high(er)-order solutions are either not discretely conservative [1], or limited to two-dimensional problems [2, 3].

In this work, with the aim to increase the order of accuracy of three-dimensional geometric volume-of-fluid methods while retaining their discrete conservation properties, we present a framework for exactly computing the volume of any arbitrary simple polyhedron clipped by a paraboloidal interface and, inversely, for reconstructing such a quadratic interface approximation from the knowledge of the discrete volume fractions. The proposed tools rely upon consecutive applications the divergence theorem so as to transform the integral over the clipped volume into a sum of integrals over two-dimensional line segments and conic section arcs. We derive analytical expressions for these curve integrals, making for a remarkably fast execution. Moreover, rounding errors due to the limited floating-point arithmetic can be comprehensively mitigated with a judicious choice of curve parametrization and a careful implementation. The proposed computational tools are implemented in the Interface Reconstruction Library [4]. We present their extensive and detailed testing over a wide range of arbitrary polyhedra and paraboloidal interfaces.

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`https://github.com/robert-chiodi/interface-reconstruction-library`

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Fully-coupled algorithm for viscoelastic interfacial flows

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Viscoelastic *interfacial* flows exhibit complex and often counterintuitive phenomena. Robust numerical methods to predict these flows reliably can facilitate progress for a broad variety of multiphase flow applications, ranging from inkjet printing of polymer inks to the airborne transmission of viral diseases. Yet, it has proven difficult to solve viscoelastic flows robustly and efficiently, even for single-phase flows. The presence of geometric singularities and locally exponential stress growth when elasticity becomes sufficiently large has hampered progress in modelling viscoelastic flows and still poses substantial challenges for state-of-the-art numerical algorithms [1]. Fernandes et al. [2] recently proposed an algorithm for viscoelastic flows in which the governing and constitutive equations are solved implicitly in a coupled system of equations, demonstrating a substantial speed-up compared to segregated algorithms.

Building upon the work of Fernandes et al. [2] on viscoelastic flows and our own work on Newtonian flows [3], in this contribution, we present a fully-coupled pressure-based algorithm for viscoelastic interfacial flows. The viscoelasticity of the flow is described using an upper-convected Maxwell formulation, considering the Oldroyd-B and Phan-Thien-Tanner constitutive models [1]. The discretized continuity and momentum equations, as well as the viscoelastic constitutive model are implicitly coupled and solved simultaneously in a single linear system of equations for pressure, velocity and the viscoelastic stress tensor. This new algorithm is tested using canonical test-cases, such as the droplet in a shear flow shown in Figure 1, considering both Volume-of-Fluid and front tracking methods. Particular attention is dedicated to the linearization and implicit treatment of the governing equations as well as the stress-velocity coupling, with respect to the stability and performance of the algorithm.

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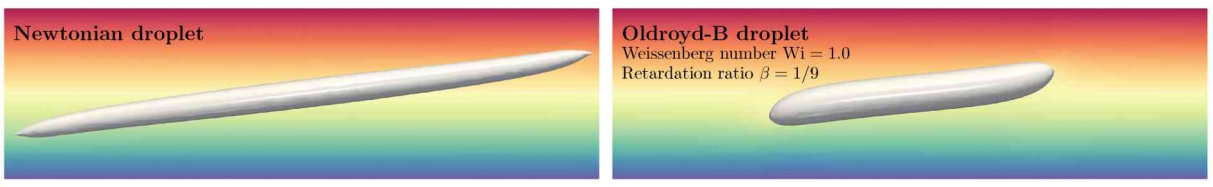

Figure 1: Newtonian and viscoelastic droplets in a Newtonian fluid subject to a shear flow with Reynolds number $\mathrm{Re} = 1.0$ and capillary number $\mathrm{Ca} = 1.0$. The colour contours depict the horizontal velocity.

Nano- and microscale simulations of water boiling on heterogeneous surfaces

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Despite the extensive use of water in industrial applications and the number of studies examining it, the heterogeneous nucleate boiling mechanism controlling evaporation and condensation is still not sufficiently understood. This is particularly important within the fuel assembly systems of nuclear reactors (both boiling and pressurized), where the boiling on the surface leads to the buildup of crud.

To investigate the boiling behavior near the fuel cladding, a molecular dynamics (MD) approach investigating the effect of the different possible crystallographic orientations of zirconia (ZrO2) was pursued [1]. The molecular mechanism of water boiling has been deciphered and it has been shown that the locations of the boiling nucleation site are strongly dependent on the solid surface hydrophobicity. Moreover, the contact angles have been measured (see Fig. 1).

The MD results have been incorporated in a two-relaxation-time Lattice-Boltzmann (LB) scheme [2] and multiple simulations investigating the behavior of a bubble lying on a surface have been carried out, for both flat and rough surfaces. The effect of the contact angle has also been investigated for bubble nucleation and dynamics. Figure 2 shows the effect on bubble generation, while Figs. 3 and 4 show bubble coalescence and nucleation above rough surfaces respectively. The results show that bubble waiting periods are reduced with the increase of the heating rate and bubble departure occurs faster in hydrophilic surfaces.

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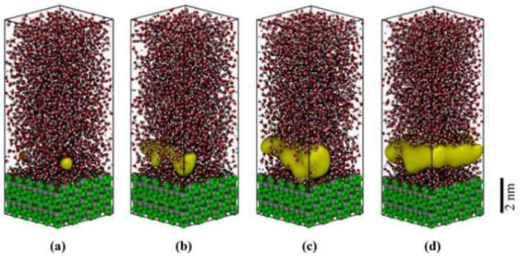

Figure 1: Representation of the initial stage of heterogeneous water nucleate boiling in contact with the hydrophilic (−111) interface of mZrO2. [1]

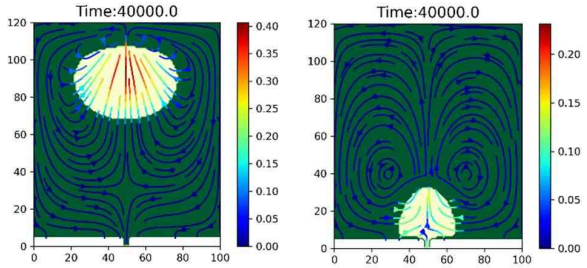

Figure 2:Bubble generation for different ZrO_2 contact angles obtained from MD simulation– hydrophilic (left) and hydrophobic (right)

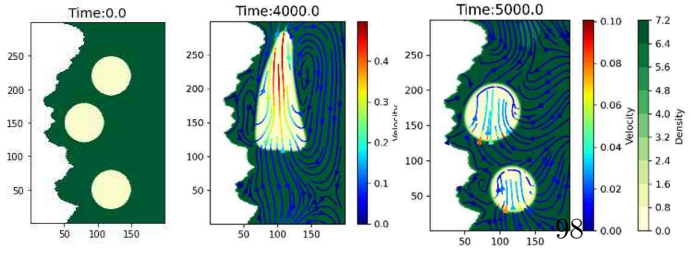

Figure 3:Bubble behaviour above a rough surface for different flow velocities – 0.5ms^{-1} (middle) and 0.1ms^{-1} (right)

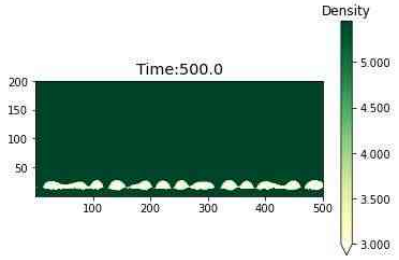

Figure 4:Bubble nucleation above a rough surface

Direct numerical simulation of the gas-liquid mass transfer around a rising bubble in the presence of surfactants

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Gas-liquid mass transfer is a topic of interest for industrial processes using bubble columns or chemical reactors. The corresponding dispersed two-phase flows are generally contaminated: surrounding impurities or surfactants adsorb to the interfaces and affect the surface tension. The Marangoni effect, resulting from surface tension gradients along the interface, was shown to decrease the rising velocity. Regarding the mass transfer, surfactant effects are generally not considered, whereas significant transfer decrease of a bubble was observed in experiments. Here, numerical investigation about the mass transfer rate around rising bubbles in the presence of surfactants is carried out.

The Direct Numerical Simulations (DNS) are performed with the in-house code DIVA based on the Level-Set and the Ghost Fluid methods, which are respectively used to capture the interface motion and the discontinuities across the interface. Besides the resolution of the Navier-Stokes equations, the transport equation of adsorbed surfactants Γ is solved along the interface with a surface advection-diffusion equation, and the Marangoni effect is considered through a jump condition on the tangential viscous stress across the interface. The transport of surfactant concentration in the liquid phase C_t (figure a)) is solved with an advection-diffusion equation coupled with a Robin boundary condition at the interface, in order to take into account the adsorption/desorption flux of surfactants between the bulk and the interface, which are modelled by a Langmuir kinetics. Finally, the transfer of a solute of concentration C is computed by an advection-diffusion equation, considering that resistance to transfer only lies in the liquid phase. Simulations are performed by varying the Reynolds, Marangoni and Schmidt numbers in a large range to deduce relevant scaling laws.

First, for a spherical bubble, the local mass transfer rate at the front of a bubble is higher than at the rear, covered by surfactants, because the thickness of the mass boundary layer scales differently between the case of slip or no-slip interfacial velocity (figure b)). However, it is shown that the transfer rate at the front part is lower than for a clean bubble at same Reynolds number, because the tangential velocity of the fluid has decreased, even in the front part. As the latter parameter is found to be relevant to describe mass transfer, a prediction of the dimensionless maximum interfacial velocity is proposed as a function of the contamination angle θ_{cap} formed by the advected surfactants at the bubble rear, which is then used to correlate the Sherwood number in addition to both the Reynolds and the Schmidt numbers (figure (c)). Then, a parametric study is carried out for deformed bubbles to investigate on the effect of the aspect ratio. It is found that the previous correlation, established for spherical bubbles, enables to predict Sh even when the bubble is deformed (figure b)).

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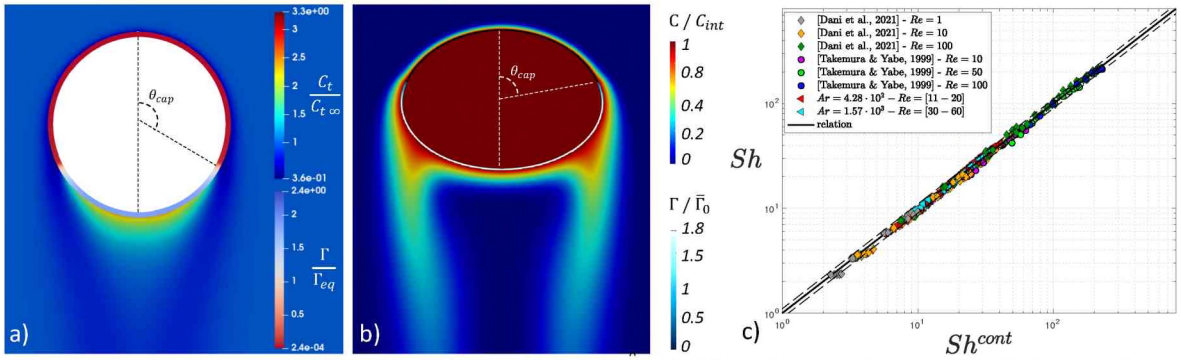

Figure 1: DNS of mass transfer around a rising contaminated bubble: a) concentration of surfactants in the bulk phase and at the interface, b) concentration of the dissolved solute, c) scaling law to predict Sh.

Data-assisted simulations of recurrent multiphase flows: the benefits and the drawbacks of simplicity

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Many fluid-mechanical systems show a wide range of spatial and temporal scales. While filtering approaches allow to systematically handle the former, the simultaneous presence of fast and slow degrees of freedom poses a massive problem for any method solving the underlying equations of motion: Highly dynamic flows require small time steps which prevent long-term studies of slow processes.

With recurrence CFD (rCFD) [1], we have introduced a data-assisted simulation technique suitable for any type of problem exhibiting recurrent, characteristic patterns (e.g. eddies in turbulent flows, bubbles in fluidized beds). Using simple nearest-neighbor identification within a database of previously recorded flow fields, an approximation to the evolution of the dynamics for arbitrarily long durations is constructed with little numerical costs. This allows for the study of slow processes like heat transfer [2, 3] or chemical conversion [1].

In stark contrast to our conceptually very simple method, sophisticated machine-learning (ML) techniques such as convolutional neural networks in combination with autoencoders [4] or reservoir computing [5] have also been employed to predict the evolution of complex, dynamic systems. In this talk, we discuss the benefits of rCFD (stability with regards to both numerical long-term behavior and to sensitivity of noisy input data [6]) and its disadvantages (lack of flexibility to model transients) compared to powerful ML methods. Finally, we address possible future developments to overcome current limitations.

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Parametric high-fidelity data generation for multi-particle flow systems using physics-informed operator networks[§]

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The potential of Euler-Lagrange (EL) methodology to closely replicate true dynamics (particle-resolved direct numerical simulation, PR-DNS) depends heavily on the accuracy of closure models for hydrodynamic force and torque on the involved particles. Recent efforts [1, 2] indicate that there is a need for systematic N-body interaction models that go beyond pairwise interaction to achieve this ambitious goal. Deep Learning (DL) methods can act as efficient tools for the development of these higher-order interaction models. Developing forefront closure models for particle laden flows using DL relies greatly on the availability of abundant PR-DNS data among other factors. Generating this high-fidelity data using a computational fluid dynamics (CFD) solver over a desired range of parameters such as particle arrangement, particle volume fraction, macroscale flow direction, and Reynolds number is an extremely compute intensive task.

Hence, we present a DL methodology that possesses the ability to perform these simulations in the parametric space on a significantly accelerated timeframe [3]. This work leverages physics-informed neural networks (PINNs [4]) approach to satisfy governing equations and boundary conditions, which enables the presented methodology to be free of training data. The idea of operator networks [5] is implemented to achieve better generalization of the trained neural network. Performance of the network is evaluated through analysis and validation of network produced data for canonical structures like Simple Cubic, Face Centered Cubic, and Body Centered Cubic. Extension of the methodology to more complex scenarios such as random particle configurations will also be discussed.

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[§]We kindly request the organizers to place this talk after the talk titled **"Universal Closure Models of Drag, Lift, Torque, and Pseudo Turbulence Using Physics-Guided Deep Learning"** by S. Balachandar, and B. Siddani.

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Universal Closure Models of Drag, Lift, Torque, and Pseudo Turbulence Using Physics-Guided Deep Learning

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One of the fundamental quest in particle laden flows is to be able to accurately and efficiently predict the fluid-dynamic force and torque on a particle from the knowledge of the mesoscale (averaged) flow around the particle along with the position, translational and rotational motion of its neighbors. The quest also extends to accurate and efficient modeling of pseudo turbulence generated by the particle, which can be important component of the Reynolds stress closure of the continuous phase. With such universal models of the microscale physics, an Euler-Lagrange simulation can be made to reliably shadow the true dynamics (as computed in a particle-resolved simulation).

A number of recent efforts have addressed these modeling quests in the context of a frozen random array of particles using deep-learning neural networks [1-4]. The accuracy of these models has been limited since they had to employ pairwise approximation and going beyond pairwise interaction in a generalizable way required vast amount particle-resolved training data, which was beyond current reach. This talk will present a systematic deep-learning approach to going beyond the pairwise approximation. The enabling features are a rigorous N-body interaction framework, imposition of rotational and reflectional symmetries, and assimilation of data from many different sources. Extensions of the universal closure models to non-frozen systems where particle are allowed to freely move will also be discussed.

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Two-phase flow reduced-order model : a two-scale model of polydisperse oscillating droplets

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Samuel Kokh CEA Saclay
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In the context of two-phase compressible flows involving both separated and dispersed phases i.e. spray of droplets, Direct Numerical Simulations (DNS) using an interface-tracking method are not tractable for industrial applications because of the multi-scale nature of the flow. Two-scale multi-fluid models with diffuse interface, amenable to realistic computational time, can be predictive for atomization, as long as they rely on the proper modeling of the small-scale interfacial dynamics below a given threshold.

From given large- and small-scale potential and kinetic energies, the Stationary Action Principle (SAP) and the second principle of thermodynamics [1, 2] provide a framework to derive two-scale models with coherent momentum and energy equations. Several works (see e.g. [3, 4]) also indicate that geometrical quantities such as interfacial area density or surface average of mean and Gauss curvatures are relevant to describe small-scale phenomena. Among them, the well-studied oscillation dynamics of droplets is strongly linked to these geometrical variables, and it is then a natural starting point for our model.

In [5] we design a two-scale flow model with geometrical variables, extending [4, 6]. First, we assess the relevance of a new set of geometrical variables through differential geometry and DNS with geometrical post-processing. Second, we describe the small-scale as a spray of oscillating droplets with a statistical distribution, and we interpret the geometrical variables as moments of this distribution. Third, monodisperse and polydisperse closures are proposed for the dynamics of the small-scale. Finally, we construct the corresponding small-scale energies, and we derive a two-scale model with the SAP and second principle of thermodynamics.

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Simplified erosion modeling in gas dominant flow with enhanced learning from CFD models

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Entrainment in multiphase flows changes solid particle trajectories and near wall characteristics. While experiments can unveil the ultimate impacts of entrainment and liquid on solid particle distribution and erosion, only limited information can be obtained to visualize and model the process. With the advancement of computational power, fine meshes can be applied for the purpose of resolving entrainment in pipes and elbows. In the paper, VOF model is used to model the multiphase flow. The model is first validated with experimental data in predicting average void fraction and entrainment. The resulting phase distribution on the cross sections of the pipe and liquid droplet/lump size and slippage are examined and tested for simplified erosion modeling. Particle tracking utilizing mixture velocities is conducted to predict erosion and results are compared to the data collected at E/CRC to verify the confidence of the models. Particle data within the domain is then extracted to investigate particle trajectories, particle distribution, impact speed and angle on the elbow. The information is also used to generalize a characteristic liquid film for simplified film particle tracking for predicting erosion in gas dominant flow. The results from the present study is to further improve and develop simplified and accurate approaches for predicting erosion in multiphase flows.

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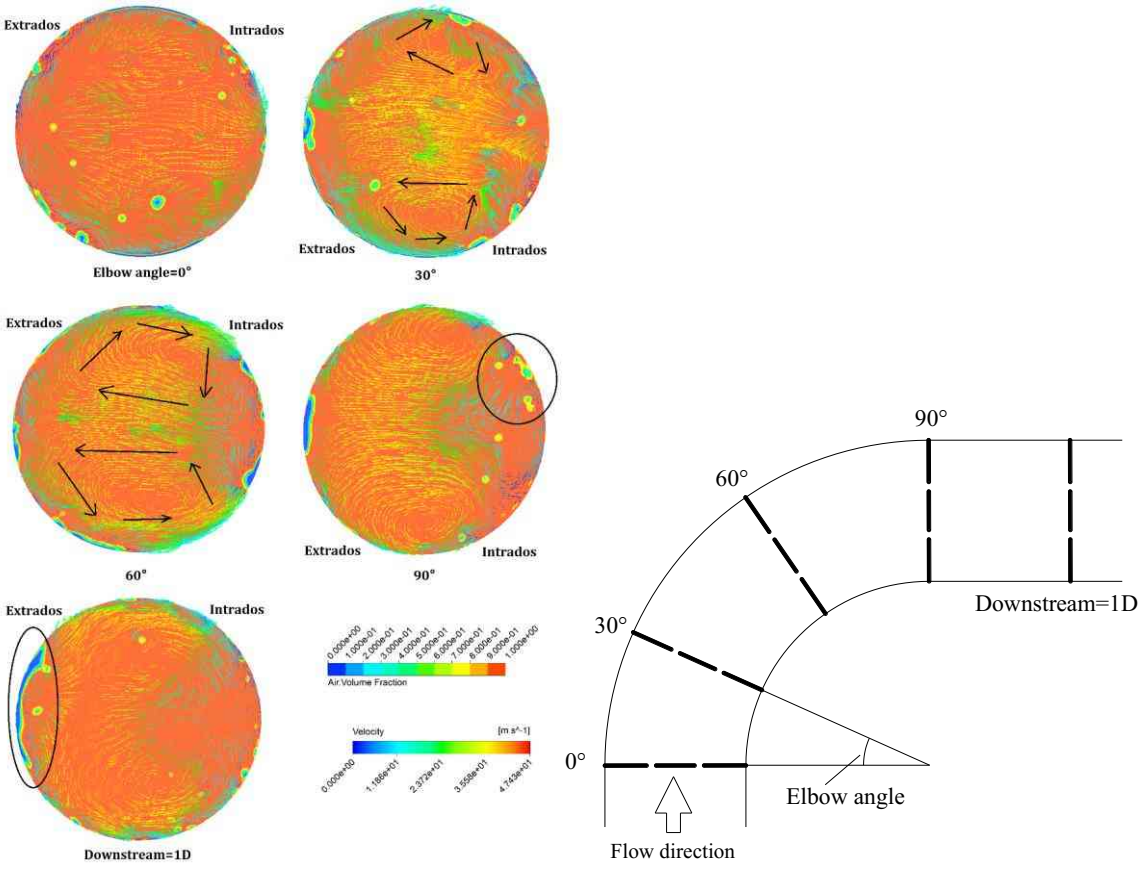

Figure 1: Phase and velocity distribution in elbow at different angles

Development of an automated framework for data-based modeling of filtered drag for coarse-grained simulations of fluidized beds based on Artificial Neural Networks and Bayesian optimization

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Multiphase chemical reactors such as fluidized beds are used for applications requiring an enhanced level of mixing between the gas and solid phases, but having two separate flow phases entails complex hydrodynamic phenomena such as the formation of clusters, streamers, and bubbles. Euler-Euler and Euler-Lagrange simulations capture well the complex physics of these systems, but they come with associated computational costs (for the fine grids and the high number of particles that are required, respectively), making their use impractical for industrial applications [1]. Therefore, computational simulations of large-scale fluidized beds are usually accomplished by coarse-graining and taking into account sub-filter scale fluctuations with a correction factor to the gas-particle drag. Data-based approaches relying on Artificial Neural Networks (ANN) prediction have recently been proposed to model the drag correction factor in coarse simulations, showing an excellent agreement with the physics especially compared to the simulations employing analytical models [2, 3, 4]. Nevertheless, ANNs accuracy is largely influenced by the chosen architecture and hyperparameters (activation functions, number of epochs, learning rate etc.), and no defined rule is available for the user to set these *a priori*. Therefore, the prediction accuracy becomes largely dependent on the user expertise in hand-tuning hyperparameters via grid searches or random searches.

In this work, an automated framework to train ANN-based models for the correction coefficient of gas-particle drag is proposed and validated *a posteriori*. A probabilistic model is first constructed via Bayesian optimization to converge, in an unsupervised fashion, to the optimal settings for the ANN regression in terms of architecture and model's hyperparameters [5]. Subsequently, the optimized machine learning model for the drag is included in the flow solver, and beds with different coarse-graining ratios are simulated. Finally, three different acquisition functions for the design space exploration are tested (i.e., probability of improvement, expected improvement, and lower-confidence bound), and their influence on the networks' size and accuracy of the simulations is assessed.

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Thursday – 2022-09-29

Session III

- **Advanced Computational and Numerical Method Developments**
  (Chair: O. Simonin, Room: Auditorium)
- **DNS/LES of two-phase flows**
  (Chair: J. Capecelatro, Room: Aula Magna 1-E)

Effect of gravity term discretisation on spurious velocities at the fluid interface

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It is a well-known problem that interfacial flow simulation with large density ratio may be prone to velocity errors at the fluid interface, not only for surface tension dominated flows, but also when only gravity acts on the surface[1]. In our development and usage of the geometric VoF method, isoAdvector[2], we have experienced how this problem may be exacerbated by the sharper interface obtained compared with algebraic VoF methods. Characteristic velocity spikes are shown in Fig. 1. The occurrence of such spikes can reduce stability and accuracy and increase calculation times.

The problem is intimately linked to the details of the gravity term discretization in the momentum equation. In OpenFOAM's inter(Iso)Foam solvers a term, $-\rho g z$, is absorbed in the pressure, and we are left with a source term, $-gz\nabla\rho$, to evaluate on the mesh faces. In the standard solvers, the height, z, is evaluated as the face centre height. But with geometric interface data available from isoAdvector, we can give a better estimate of the interface height at mesh faces. Implementing this leads to the reduced spurious velocities observed in Fig. 2 (note difference in colour maps).

In the presentation, we will elaborate on these results and discuss further improvements.

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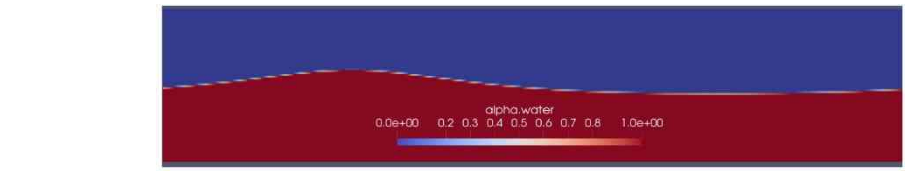
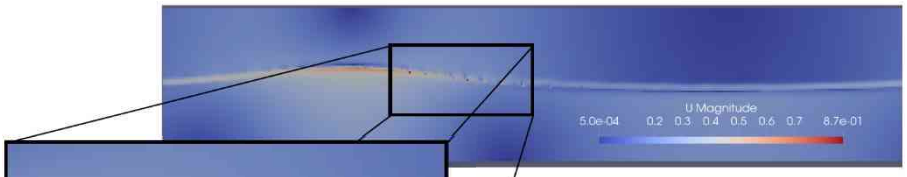
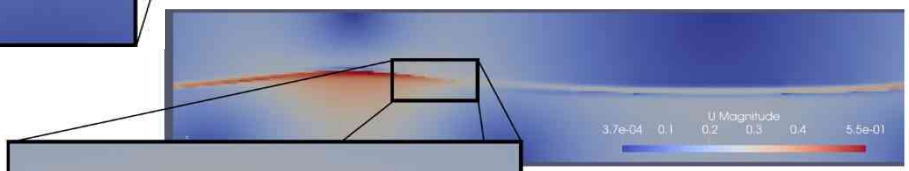




← Figure 1. Stream function wave simulation with OpenFOAM's interIsoFoam solver. Large spurious velocities at air-water interface shown in zoom.



↑ Figure 2. Same as Fig. 1 but with improved discretization using interface height data from geometric VoF method. Zoom shows reduced spurious velocities.

A microstructure-based model to predict fluid-particle forces and heat fluxes in random particle arrays

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Belgium

A recent challenge in the modeling of fluid-particle flows is to build microstructure-informed models to overcome the average description of the drag force provided by the correlations currently used in the Euler-Lagrange and Euler-Euler models. To that end, we study through particle-resolved direct numerical simulations (PR-DNS) the flow past random arrays of monodisperse spherical particles for a range of particle Reynolds numbers and solid volume fractions (see Figure 1). Our results are then used to characterize in details the statistics of the force distribution in such arrays. The microstructure formed by the solid phase is described using a limited number of quantities inspired from the "fabric" tensor used in granular media. First, the distribution of those microstructure-based quantities is investigated. Then, significant correlations are identified between the force experienced by any particle in the array and a few key quantities characterizing the anisotropy of its neighborhood. A microstructure-based deterministic multi-linear model is subsequently proposed and validated against independent test cases (see Figure 2). The model is seen to perform better in the viscous and dense regimes. We also show that the addition of a stochastic contribution to the deterministic model allows to recover the correct level of force fluctuations; yet at the cost of a lower correlation between the model and the data. Finally, we investigate the distribution of the fluid-particle heat flux in the flow past random arrays with non-isothermal particles. The impact of the thermal saturation on the distribution of the fluid-particle heat flux is discussed and it is shown that the Nusselt number based on the local bulk temperature constitutes a better candidate to recover the distribution of the heat flux from the local microstructure.

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Hardy, B., Simonin, O., De Wilde, J., & Winckelmans, G. (2022). Simulation of the flow past random arrays of spherical particles: Microstructure-based tensor quantities as a tool to predict fluid-particle forces. *International Journal of Multiphase Flow*, 103970.

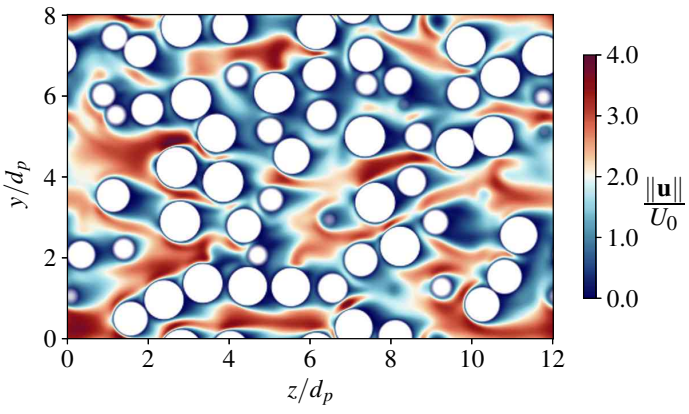

Figure 1: PR-DNS of the flow past a random array of spherical particles: velocity field magnitude ($Re_p = 50$, solid volume fraction 0.30)

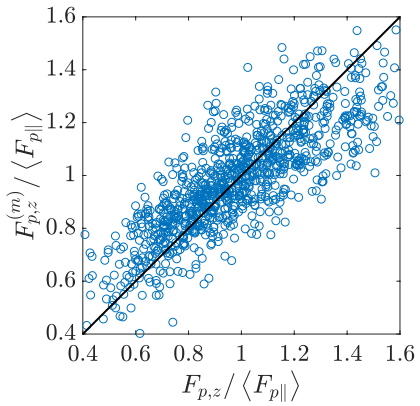

Figure 2: Regression plot between the streamwise component of the force predicted by the microstructure-based model and the PR-DNS data ($Re_p = 50$, solid volume fraction 0.30)

Splitting schemes for phase-field models

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Vladimir Puzyrev [‡] Curtin University

In this presentation we consider several splitting schemes for unsteady problems for the most common phase-field models: Allen-Cahn, Cahn-Hilliard, Swift-Hohenberg , and Phase-field Crystal Model . The fully implicit discretization of such problems would yield at each time step a nonlinear problem that involves second or higher order spatial operators. We propose a new approach for the derivation of factorized schemes that linearize the equations and split the higher order operators in a product of second order operators that can be further split direction-wise. We prove the unconditional stability of the first-order schemes in the case of constant mobility. If the spatial discretization uses Cartesian grids, the most efficient schemes are Locally One Dimensional (LOD). The results of the theoretical analysis are illustrated on 2D numerical examples. For more information the reader is referred to [1].

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Neuroevolution-enabled adaptation of the Jacobi method for Poisson's equation with density discontinuities

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Consider the following homogeneous Poisson equation and its discretization on a 1D domain

$$\nabla \cdot \left(\frac{1}{\rho}\nabla p\right) = 0, \quad \frac{\frac{1}{\rho_{i+\frac{1}{2}}}\frac{P_{i+1}-P_i}{\Delta x} - \frac{1}{\rho_{i-\frac{1}{2}}}\frac{P_i - P_{i-1}}{\Delta x}}{\Delta x} = 0, \tag{1}$$

where ρ is the density, p is the pressure, the subscript i is the index of the x grid, and Δx is the grid spacing. Discontinuities in the density, which are often present in multiphase flows, give rise to numerical difficulties to iterative solvers. Lacking labeled examples of working numerical strategies, adapting an iterative solver to accommodate a numerical issue is non-trivial and usually involves a lot of trial and error.

Here, we resort to evolutionary neural network (ENN). Figure 1 (left panel) is a sketch of ENN. An ENN observes the outcome of an action and adapts its strategy accordingly. The process requires no labeled data but only a measure of a network's performance. We apply neuro-evolution and adapt the Jacobi iterative method for the Poisson equation in 1D, 2D, and 3D spaces and various types of density discontinuities. We show that the adapted Jacobi method is able to accommodate density discontinuities. Figure 1 (right panel) shows the convergence rate of the Jacobi method, and we see significant acceleration. Further details of the work can be found in Ref. [1].

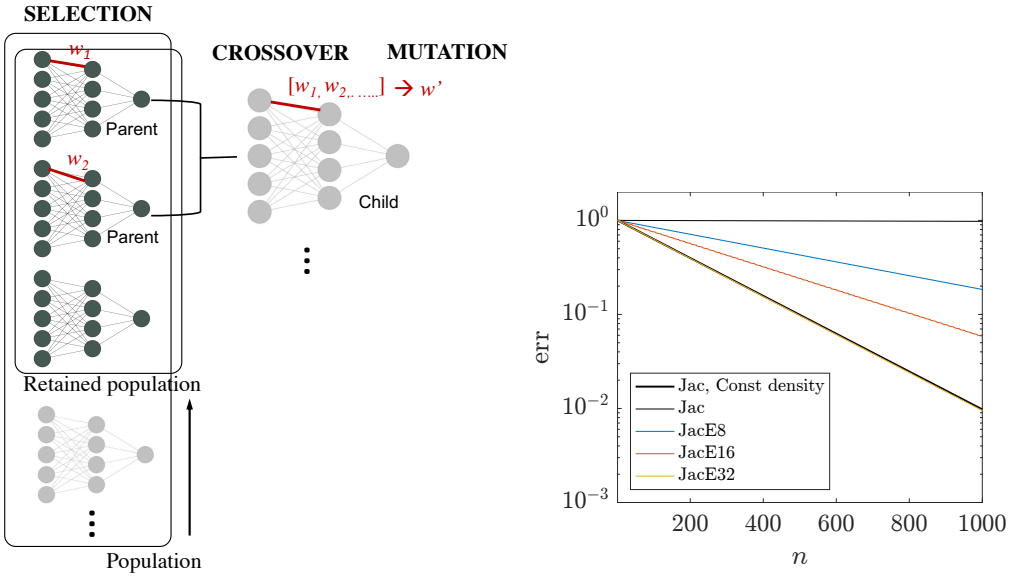

Figure 1: Left: A sketch of evolutionary neural network. Right: Convergence history for Jacobi method. There are discontinuities in the density fields except for "Const density". E8, E16, and E32 are results of different ENNs.

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Drop impact onto a thin liquid film: extension from two to three phase scenarios using phase-field method

Milad Bagheri[*], Martin Wörner[†], Holger Marschall[‡]

While the drop impact process onto thin liquid film for identical liquids has been extensively studied both experimentally and numerically, the impact process for non-identical liquids has received much less attention. For the case when the film liquid is different from that of the drop the immiscibility and miscibility of the liquids play an important factor and can result in a completely different spectrum of topological changes that the system undergoes.

In this talk we detail on the extension of our numerical methodology from $N = 2$ to $N > 2$ immiscible, incompressible and isothermal phases for numerical simulation of drop impact onto a thin liquid film. We are also working on the extension of our numerical framework to miscible systems. Our methodology is based on a diffuse interface phase-field interface capturing method, which we implemented in OpenFOAM (FOAM-extend 4.1). The phase-field method is an energetic variational formulation originally based on the work of Cahn and Hilliard [1] where the interface is composed of a region of finite thickness resembling realistic interfaces.

In this talk, we present numerical simulation results of drop impacts onto thin films of two different liquids. This is considered a direct continuation of our recently published work [2]. Figure 1 depicts preliminary results of interface-resolved Direct Numerical Simulation of a three-phase immiscible fluid system compared to in-house experimental results. In this system, a silicone oil drop of diameter 1.44 mm impacts a stagnant water film of 0.5 mm thickness at 2 m/s while the ambient phase is air.

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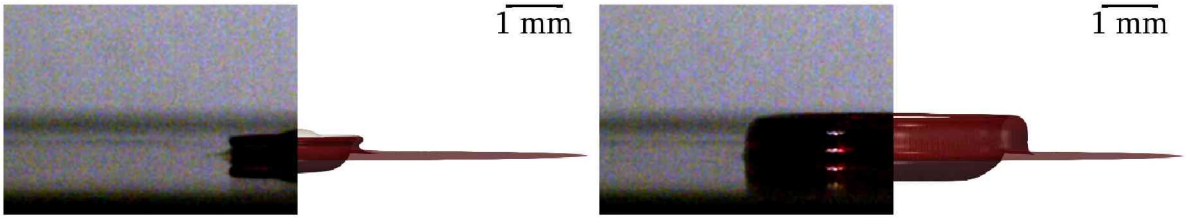

(a) $t = 0.5$ ms (b) $t = 3$ ms

Figure 1: Recordings from the experiments (left) and simulations results (right). Water film is colored maroon and the oil drop is gray.

Water droplet impact on thin oil film and bubble entrapment: Three phases simulation

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Alidad AMIRFAZLI† York University
Christophe JOSSERAND‡ Ecole Polytechnique

Bubble entrapment is seen when a drop impacts onto a dry surface or one that is covered by a thin liquid film. The bubble is formed due to an air layer trapped between the drop and the surface during the impact process [1, 2]. However, to date it is not clear how presence of a liquid film may change the process of bubble entrapment. Numerical simulations (an adaptation of the Volume of Fluid method for two fluids in the *Basilisk* software [3]) is used to investigate the bubble entrapment dynamics when the drop impacts a thin immiscible film. We characterise the entrapped bubble by varying the impact parameters and liquid properties, starting by the oil viscosity. The effect of the thin liquid film on the bubble entrapment, is discussed by comparing it with the impact on a solid substrate or on the same a miscible liquid thin film.

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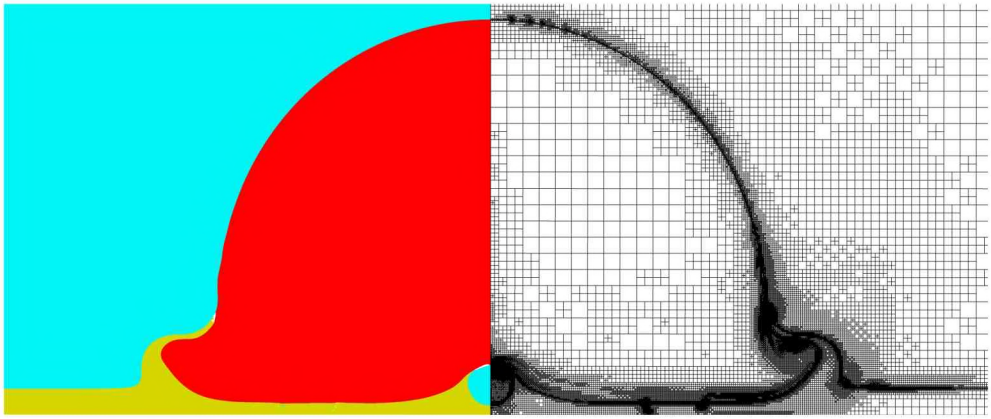

Figure 1: Water droplet (Red) impacts a thin oil film (Yellow) and a small gas bubble is trapped (Blue).

The mechanisms behind a shear-induced lift force on deformable bubbles - a DNS study

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Chalmers University of Technology, Gothenburg, Sweden

Bubbles rising in a shear flow experience a shear-induced lift force in a direction perpendicular to its relative motion. This lift force governs the spatial distribution of bubbles in many common applications such as bubbly pipe flows. Depending on the bubble properties and the flow conditions, the lift force may either push the bubbles towards the pipe walls or the pipe centre. To predict the correct spatial distribution of the bubbles, it is thus essential to have accurate lift force models, and, to develop such models, it is crucial to understand the physical mechanisms behind the highly non-linear behaviour of the lift force. Previous studies have identified four different lift force mechanisms, and we show, using a theoretical framework supported by our efficient 3D multiphase DNS framework [1], how the characteristic bubble-induced vorticity can explain these mechanisms. In the numerical framework, we use the open-source code Basilisk [2] and implement a PID-controlled moving reference frame technique to efficiently follow the motion of the fast-rising bubbles over relatively long spatiotemporal scales. We use our numerical framework to examine how the lift force coefficient C_L scales with the shear rate in conditions governed by the different mechanisms. Our findings show that C_L scales differently and changes its sign depending on the governing lift force mechanism and the shear rate. Our results increase our understanding of the physical mechanisms generating lift and identify under what conditions the shear rate should be considered when developing new and improved lift force correlations.

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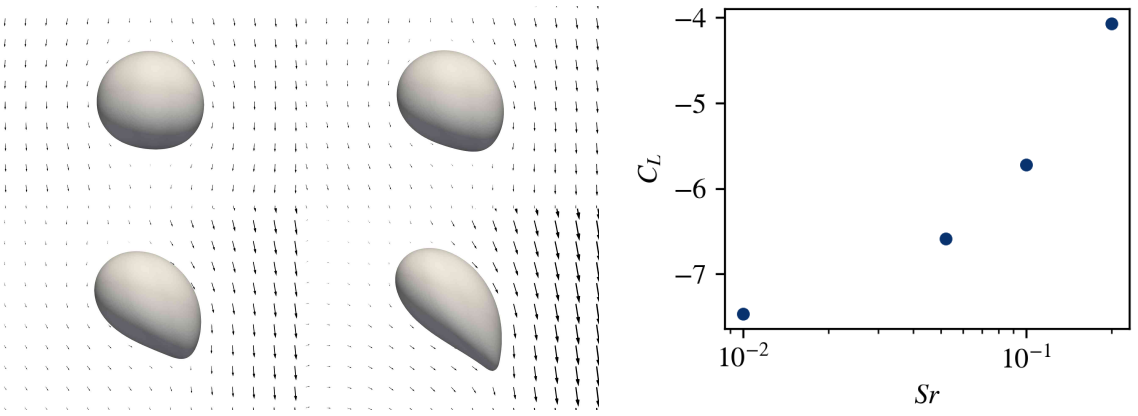

(a) (b)

Figure 1: (a) Bubble shapes at increasing non-dimensional shear rate Sr in low Re-number conditions with relatively weak surface tension (high Eötvös number). (b) Corresponding lift force coefficient against Sr.

Direct Numerical Simulation of the collapse of a bubble in contact with a wall

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In this work we explore the capabilities of the all-Mach solver presented in [1] to simulate the collapse of a bubble in contact with a wall. This solver is shown to be suitable for the DNS of bubble dynamics processes with a wide range of flow velocities and time scales of the process, from slow dynamics at the beginning of the collapse stage, to very small times and high velocities during the last instants of the collapse stage.

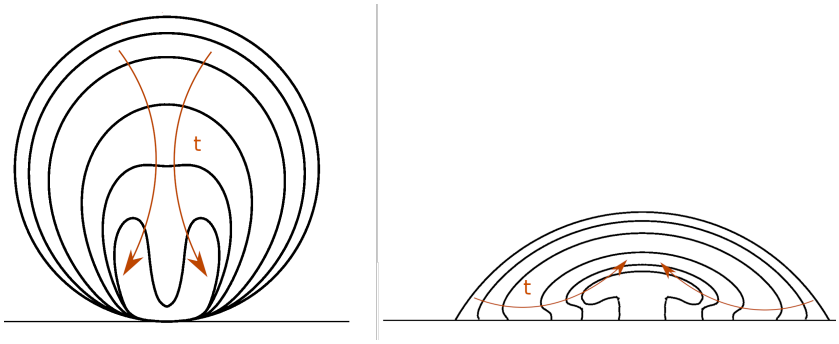

Figure 1: Results of the DNS of the bubble interface evolution of a collapsing bubble in contact with a wall with an initial contact angle (left) $\alpha = 0$ and (right) $\alpha = 120^o$.

Simulation results reveal that the solution of the problem is shown to be sensitive to the contact angle at the instant of maximum radius. In particular we reveal the existance of a singularity on the solution at the initial time when the initial contact angle is larger than 90 degrees. The physical response during the overall collapse process and the consequences of it are makedly different depending on wether this angle is smaller or larger than 90 degrees. While in the former case a classical jet directed towards the wall is observed, a re-entrant jet is generated when the angle is larger than 90 degrees (see figure 1). Under some circumstances this jet is shown to generate a vortex dipole propagating upwards that eventually leads to long-range interactions with the surroundings. The influence of viscosity, surface tension and pressure difference on the peak pressures and temperatures reached during the collapse of the bubble will be dicussed numerically and compared to some theoretical predictions available for the Rayleigh collapse problem for both, spherical and non-spherical bubbles.

We acknowledge the European Union (EU) support of this work under the MSCA-ITN grant agreement number 813766. Part of this work was part of the PROBALCAV program supported by The French National Research Agency (ANR) and cofunded by DGA (French Minisitry of Defense Procurment Agency) under reference Projet ANR-21-ASM1-0005 PROBALCAV.

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Thursday – 2022-09-29

Session IV

- **Simulation of complex multiphase flows – Applications**
  (Chair: D. Lucas, Room: Auditorium)
- **DNS/LES of two-phase flows**
  (Chair: A. Vié, Room: Aula Magna 1-E)

A three-phase cavitation solver for the simulation of ventilated cavitating flow in OpenFOAM

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Abstract Cavitation occurs when submerged vehicle moves fast underwater. Liquid water will undergo phase change into vapor at low pressure region. Traditionally, the natural cavitation flow can be simulated by two-phase (water and vapor) solver with phase change model. However, the two-phase solver cannot simulate artificially ventilated cavitation flows where a third air phase must be considered. In this paper, a OpenFOAM solver is developed for simulating the ventilated cavitating flow over high-speed underwater vehicle. The proposed solver is capable of calculating the three-phase (air, water and vapor) cavitation flow and considering the miscibility of the air and vapor phases inside the cavity. It uses the Volume of Fluid method to capture the interphases between the phases and Kunz cavitation model to calculate the mass transfer rate. Three benchmark cases with air ventilated into the cavitating flow are conducted in this paper. The simulation results agree well the experimental data, which verify the accuracy of the numerical method and boundary conditions.

Keywords: three-phase, cavitation, ventilation, VOF, OpenFOAM

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Simulation of oil-water core-annular flow through an inclined pipe

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The present work reports a Volume of Fluid (VOF) multiphase flow simulation of oil-water core-annular flow through an inclined pipe (15° downward inclination angle with respect to the horizontal). Three different geometries of the flow entry and initial mixing region (i.e., nozzle part) have been sketched for the simulations: (1) a "simplified" geometry, in which water and oil are injected and mixed at the inlet section of the main pipe without any nozzle part; (2) a "branch" geometry, in which water and oil are injected through a branch then mixed in the nozzle, (3) an "extended" geometry, in which water and oil are injected through an extended pipe then mixed in the nozzle. A structured hexahedral grid has been created for each geometry [1]. In all the cases, water is injected circumferentially, whereas oil is injected annularly.

Simulated results with respect to each geometry were compared with experimental results [2]. The simulations were run for 8 flow conditions with oil superficial velocity ranging from 0.56 to 1.06 [m/s] and with water superficial velocity ranging from 0.66 to 1.33 [m/s]. The turbulence model was set realizable k-ε for steady state pseudo-transient simulations and standard k-ε for transient simulations [3]. The "extended" geometry (Figure 1) shows the trend closest to the experimental results. The average oil holdup obtained from simulations is consistent with the experimental data with a maximum deviation error of 13%.

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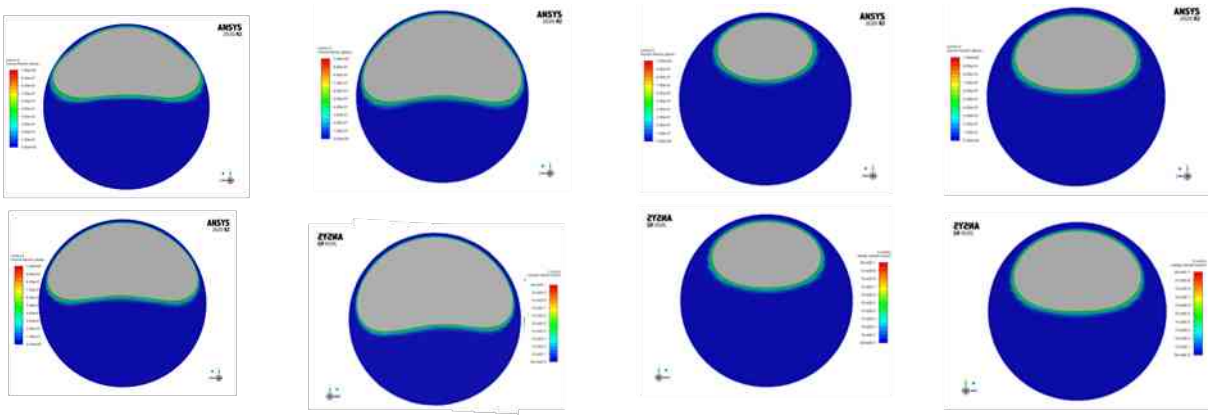

(a) (b)

Figure 1: VOF contours for the "extended" geometry; minimum (a) and maximum (b) water superficial velocity.

On the effect of Dean vortices on particle focusing in microfluidic applications

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In the context of multiphase flows in microchannels, inertial effects can be exploited to generate secondary flows and particle migration, so that desired particle focusing can be achieved without the need for external forces acting on the system. An interesting review of the inertial microfluidics and its effects is provided by Zhang et al. [1]. Particles moving in such configurations migrate laterally to different equilibrium positions due to the counteraction of two inertial effects: the shear gradient lift force due to the curvature of the fluid velocity profile, and the wall lift force as result of the interaction with the adjacent walls. Secondary flow can also appear in curved channels, where two counter-rotating Dean vortices can develop due to the pressure distribution in the radial direction. This generates an additional force on particles that changes the equilibrium position and allows differential particle size-dependent focusing, based on the the ratio of inertial lift force to the secondary flow resistance.

The effects of inertial forces, centripetal forces and viscous forces lead to different flow regimes and different strength of Dean vortices; these effects are described by the Dean number, whose definition includes the Reynolds number and the curvature ratio.

With the aim of providing an accurate investigation of the physical mechanism of inertial particle focusing in curved microchannels, we present a parametric study carried out by using a numerical solver based on Lattice-Boltzmann method [2], well suited for particle-resolved simulations in inertial microfluidics flow regimes. The study is performed in spiral microchannels with a rectangular cross section. First, the numerical solver is validated comparing results with experimental data by Guan et al. [3]. Then, several simulations are performed increasing the Dean number, in order to span the effects of vortex intensity without exceeding the inertial microfluidic regime. Different equilibrium positions and different particle separation are obtained as consequence of the balance of the involved forces.

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Numerical simulation of dust deposition on fixed-tilt solar arrays in a desert environment

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Deposition of dust particles over the surface of PhotoVoltaic (PV) modules can strongly affect their energy yield [1]. This phenomenon is called soiling and it poses challenges particularly in regions where the airborne dust concentration is significant. Understanding the process of dust deposition and predicting its rate on PV modules would enable an optimized field operations. In this study, we investigated the influence of wind speed and particle size on deposition through numerical simulations. The Euler-Lagrange formalism and the Reynolds-Averaged Navier-Stokes $k-\epsilon$ turbulence model were adopted to simulate a neutral Atmospheric Boundary Layer (ABL), dust transport, and deposition behavior on a set of PV arrays. These numerical simulations are performed using the open source CFD toolbox OpenFOAM®*v2006* on High Performance Clusters (HPC). An Eddy-Life-Time stochastic model is applied for particle dispersion due to turbulence. A stochastic deposition model [2] is employed at the wall cell to account for the coarse description of the boundary layer when using industrial scale mesh size namely with a $y^+ \gg 1$. The deposition model is revisited and its predictions are validated corresponding to both vertical and horizontal channel flow. The effect of the ABL wind speed and dust particle size on deposition are investigated with a range of $30 < y^+ < 100$ at the PV arrays wall cell centroid. Figures (1a-1b) show respectively the macroscopic Eulerian field of mean wind speed U in the computational domain and the mean deposition velocity of the downstream arrays $\bar{v}_d^+$ adimensionalized by the upstream conditions. It was found that the first two PV arrays experience a pecular behaviour in hydrodynamics and deposition. With the range of particle size and wind speed considered in the study, it was found that dust particle deposition mechanism is governed by both turbulence and gravity. Further investigations will be conducted to study the influence of wind direction and modelling turbulence by Large Eddy Simulation (LES) on deposition.

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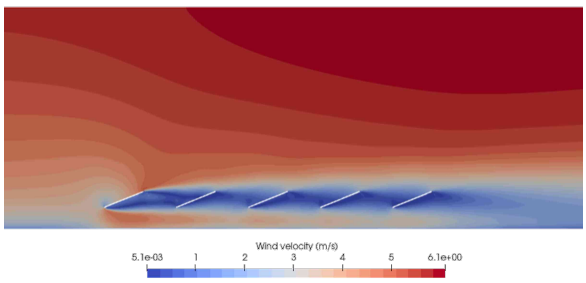
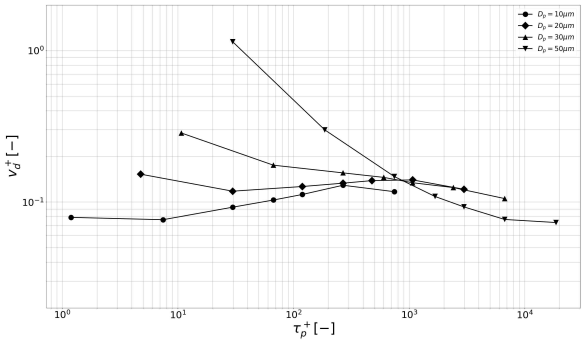


(a)



(b)

Figure 1: (a) : Wind speed fields around the PV arrays; (b) : Mean deposition velocity $\bar{v}_d^+$ as a function of the dimensionless particle relaxation time τ_p^+ adimensionalized by the upstream conditions (particle concentration C_{ref} and friction velocity u^* of the ABL) for different particle diameters

The velocity jump discontinuity for single bubbles rising in a viscoelastic fluid – insights from direct numerical simulations

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It has been known for about 60 years [1] that bubbles rising in viscoelastic liquids may exhibit a jump discontinuity of the rise velocity as a critical bubble volume is exceeded. However, a convincing physical explanation of the mechanism behind this jump phenomenon has only recently been given [2]. 3D DNS of the transient rise of single bubbles can provide detailed insight into the flow kinematics and polymer relaxation in the flow around the bubble by a local analysis of the polymer conformation tensor, which proves to be reasonable for understanding the occurrence of the velocity jump. Indeed, the local conformation tensor analysis shows that polymer molecules traveling along the upper bubble hemisphere are stretched in the circumferential direction, due to the flow kinematics. The stored elastic energy is associated with the formation of a hoop stress, which is unloaded as the polymer molecules travel along the bubble interface. Depending on the polymer relaxation time and the time scale of the transport of polymer molecules along the bubble contour, the hoop stress can be completely released above the bubble's equator, slowing down the bubble. On the other hand, the relaxation of the hoop stress can take place essentially below the bubble's equator, accelerating the bubble, which leads to a self-amplification of the effect and thus causes the bubble rise velocity to jump to a higher level.

This talk presents the extended VOF method [3] that was used for the DNS of the bubbles rising in a viscoelastic fluid and the local polymer conformation tensor analysis. For modeling viscoelastic flow behavior, the numerical framework includes numerous constitutive equations of the rate type and stabilization methods for high Weissenberg numbers [4]. The bubble rise velocity jump and further characteristic flow phenomena of bubbles rising in viscoelastic liquids are accurately captured with respect to experiments [5] and recent findings are reported.

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Energy balance in lubricated drag-reduced turbulent channel flow

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We use direct numerical simulation (DNS) to study the problem of drag reduction in a lubricated channel, a flow instance in which two thin layers of a lubricating fluid (density ρ_1, viscosity η_1, thickness h_1) are injected in the near-wall region of a plane channel, so to favor the transportation of a primary fluid (density ρ_2, viscosity η_2, thickness h_2). In the present configuration, the two fluids have equal densities but different viscosity, so that a viscosity ratio $\lambda = \eta_1/\eta_2$ can be defined. To cover a meaningful range of possible oil/water configurations, we consider two different viscosity ratios in the range $0.1 \leq \lambda \leq 0.01$. All DNSs are run using the constant power input (CPI) approach, which prescribes that the flow-rate is adjusted according to actual pressure gradient so to keep constant the power injected into the flow. The CPI approach has been purposely extended here to the case of multiphase flows. A phase-field method (PFM) is used to describe the dynamics of the liquid-liquid interface. We unambiguously show that a significant drag reduction (DR) can be achieved for both the viscosity ratios considered (up to $\simeq 100\%$). Upon a detailed analysis of the mean kinetic and turbulent kinetic energy budgets, we are able to characterize the effects of the surface tension forces and viscosity contrast on the production and dissipation of mean and turbulent kinetic energy in the two phases.

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Numerical investigation of the in-nozzle flow dynamics in pressure-swirl atomizers

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Liquid injection systems play a key role in a wide range of industrial applications. Among the variety of existing technologies, swirl simplex atomizer is one of the most commonly used for its good atomization performances in a large range of operating conditions. In this technology, the liquid is injected in a swirl chamber through a number of tangential channels. The swirling liquid thus creates an air core that extends from the discharge orifice throughout the whole swirl chamber and, consequently, emerges from the discharge orifice as an annular sheet which spreads radially outward and disintegrates into a hollow conical spray. Even if the destabilisation process of the liquid sheet has been widely investigated [1, 2], the role of the inner flow, in particular of the air core instability in liquid sheet disintegration dynamics is not fully understood. This is due to the limited optical access that makes the experimental investigation complicated. The present work thus proposes an in-deep analysis of this mechanism through the high-fidelity Large-Eddy Simulation of the well-documented commercial swirl simplex atomizer used in the CORIA Rouen Spray Burner (CRSB) experiment (see TCS 6 and 7 at http://www.tcs-workshop.org/). This type of simulation is very challenging as it has to involve robust and accurate numerical methods to deal with interface dynamics as well as a fine discretization to resolve the physical phenomena occurring at the interface. To tackle this challenge and perform a full atomizer geometry simulation including the in-nozzle flow, the present work combines the Conservative Level-Set sharp interface method of Janodet et al. [3] with dynamic mesh refinement of unstructured grids to describe accurately and characterize precisely the liquid flow disintegration dynamics. The results presented in Fig. 1 show the type of air core instability that can be captured with the present methodology.

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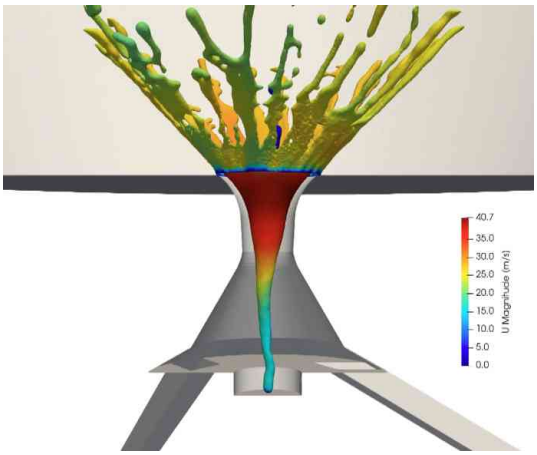

Figure 1: Simulation of the in-nozzle flow dynamics in the CRSB atomizer.

Dynamics and wakes of a fixed and freely moving tetrahedron in an inertial flow

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As a result of its importance in many physical and engineering applications such as particulate air pollution and ocean dynamics, there has been a sustained research activity on flows past a 3D bluff body [1]. Various numerical studies consider a Newtonian flow past a sphere, a spheroid or a cube in a bounded domain, and reveal the complexity of vortex interactions in the particle wake region. However, some aspects of the influence of the particle angularity on the flow regime transitions still remain unclear.

We first examine the unbounded inertial flow of a Newtonian fluid past a fixed tetrahedron with three different angular positions: face facing the flow, edge facing the flow and vertex facing the flow at Reynolds number $10 < Re < 500$. Then we consider a heavier or lighter freely moving tetrahedron in an unbounded domain filled with an otherwise quiescent Newtonian fluid at Galileo numbers $10 < Ga < 400$. Computations are performed by a DEM-DLM/FD approach implemented in Basilisk on octree adaptive grids where a parent cube cell can be recursively divided into 8 sub-cubes to achieve local mesh refinement of the areas of interest [2].

In the fixed tetrahedron case, we discuss the effects of the particle angular positions on the drag and lift coefficients, the wake symmetry and the vortex structures. We analyze and determine the two well known regime transitions: loss of symmetry of the wake and loss of stationarity of the flow, as a function of the Reynolds number Re. A symmetric double hairpin vortex shedding is noted for the first time in the edge facing the flow case. In the moving tetrahedron cases, we analyze the variation of the drag coefficients in connection with the vortex structures and the regime transitions in the wake region for different Galileo numbers Ga and solid-fluid density ratios.

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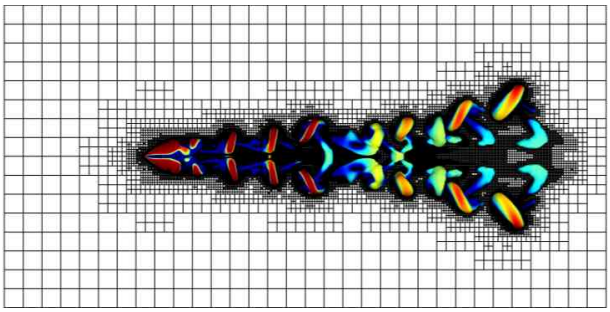

Figure 1: Wake past a tetrahedron computed on an octree grid in l_2 criteria isosurface.

Friday – 2022-09-30

Session I

- **Mini-Symposium: Dynamic wetting and numerical treatment of moving contact lines**
  (Chair: D. Bothe, Room: Aula Magna 1-E)
- **High Performance Computing and parallel computing methods, techniques for large-scale simulations of multiphase systems**
  (Chair: O. Tammisola, Room: Aula 1-G)

Volume-of-Fluid based simulation of dynamic wetting processes based on the generalized Navier boundary condition

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Mathis Fricke† TU Darmstadt
Tomas Fullana‡ Sorbonne University
Stephane Zaleski§ Sorbonnne University

The (static or dynamic) contact angle boundary condition is the classical approach to model the wettability of the solid surface in a sharp interface two-phase flow model of dynamic wetting. It prescribes the orientation of the interface normal at the contact line, i.e. the line of intersection between the moving interface and the solid boundary. Consequently, the prescribed contact angle is usually also used as a boundary condition for the interface reconstruction in numerical methods such as the geometrical Volume-of-Fluid (VOF) method considered in this work. Moreover, in the classical model, the wettability is treated separately from the standard Navier slip boundary condition at the solid boundary which is frequently used to regularize the force singularity in moving contact line. The "generalized Navier boundary condition" (GNBC), introduced by Qian et al. [1],[2] in a diffuse interface formulation, combines the modeling of both effects into one single boundary condition for the fluid velocity at the solid boundary. The uncompensated Young stress enters the force balance between friction and viscous stress at the contact line leading to a qualitative change of the velocity field close to the moving contact line. Hence, the geometric boundary condition for the contact angle is dropped and the GNBC leads to a relaxation of the contact angle. Interestingly, using the kinematic evolution equation for the dynamic contact angle [3], unlike the standard Navier slip, one finds a functional dependence between contact angle and capillary number in steady state

$$Ca = \frac{\lambda}{\varepsilon}(\cos\theta - \cos\theta_{eq}).$$

Using the geometrical VOF solver Basilisk [5], we develop a second-order accurate interface reconstruction method at the boundary in three dimensions (see [3] for 2D). This allows to reconstruct the interface and hence the dynamic contact angle with high accuracy from the local volume fraction field. This local reconstruction of the contact angle forms the basis of the discetization of the GNBC in our VOF framework.

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Improvement of VOF two-phase flow method in a collocated Finite Volume framework

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Keyworks: Well-balanced PISO algorithm, Height Function, Spurious currents, Dynamic contact angle

The development of a solver to simulate the direct liquid cooling of the stator end-windings of an electric motor is challenging since its geometry is naturally complex. In this study, an accurate two-phase flow Volume Of Fluid (VOF) solver coupling with a dynamic contact angle model is implemented to take into account this complex geometry over which the liquid film flows. The accuracy of the dynamic contact angle model is directly related to the local velocity calculated near the contact line. The parasitic currents encountered by the classical VOF method make the use of the dynamic contact model inaccurate.

To reduce the spurious currents, a well-balanced formulation [1,2] coupled with an accurate curvature estimation based on the Height Function method [3] is then implemented. In a collocated finite volume framework, the Rhie Chow / PISO algorithm is modified to properly balance the pressure gradient and capillary force terms in the momentum equation. The Height Function method is used to calculate the curvature and is applied for implementing the dynamic contact angle model of Cox [4].

. Finally, the experiments of Roisman [5] are used to validate the implementations (Figure 1).

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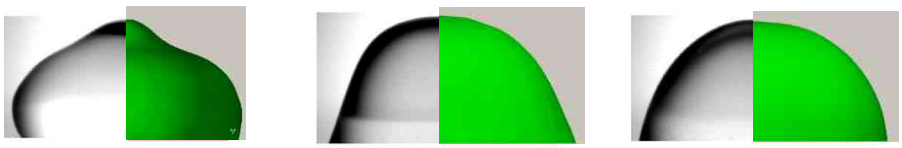

Figure 1: Numerical results of spreading droplet (right half, green) and experimental results (left half). The contour is the C = 0.5 iso-surface.

A coupling VOF/embedded boundary to model arbitrary contact angles on solid surfaces

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Two-phase flows in presence of solid boundaries are present in numerous natural environment and industrial applications. In the past decades, a lot of experimental and numerical[1] studies have been carried out to deal with the dynamics of the contact angles at the triple point between the two fluids and the solid. From a numerical point of view, there is still a remaining challenge for the triple point computation depending on the tracking interface method (VOF, level-set, front-tracking...) used and how the solid surface is taken into account (boundary conditions, IBM...)[2] for the contact angle imposition. A numerical methodology is presented here for simulating contact angles on solid surfaces of arbitrary shape. We use the Basilisk solver where a 2nd order conservative Cartesian embedded boundary method is used to tackle with solid geometries.The fluid-fluid interface is tracked by a conservative volume of fluid VOF method. In our method, an apparent contact angle θ_s is implicitly imposed by setting the right conditions in ghost fluid cells in the embedded solid. The developed methodology is validated in different test cases with several geometry shapes such as the spreading droplet on an embedded horizontal solid. The results obtained show that the present method works well and stay robust in a wide range of contact angle as shown in Fig. 1 where the numerical maximum height and radius droplet are compared to the analytical solutions. Finally, an application to a phase change problems, the solidification of a droplet on a cold substrate, is also studied.

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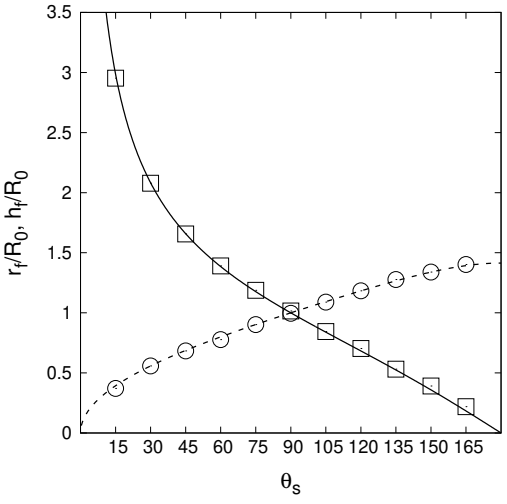

Figure 1: Dimensionless droplet height h_f/R_0 and radius r_f/R_0 evolution as a function of θ_s

A thermodynamically consistent phase-field model for moving contact line problems and its application in vesicle motions

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Under a thermodynamically consistent phase-field modeling framework[1] for the binary incompressible (quasi-incompressible) fluid, which allows for the different properties (densities, viscosities and heat conductivities) of each fluid component, we will first show how to derive such a model for a variable density moving contact line problem[2]. Then we will apply the idea to model vesicle (e.g. red blood cell) motions, deformations and vesicle-vesicle and vesicle-channel wall interactions. Mass conserving and energy law preserving finite element schemes will be designed for these models. A few computational examples including multi-vesicle interactions and red blood cells through the narrowed vessel wall will also be presented.

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Numerical study of particle suspensions in elastoviscoplastic (EVP) duct flows

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Elastoviscoplastic (EVP) fluids are ubiquitous in nature and industries, from biological fluids, food products such as chocolate and mayonnaise, slurries and drilling fluids, building materials, to pharmaceuticals and 3D printing. EVP fluids are often mixed with particles, which either move with the flow or be trapped in fouling regions; the interaction between EVP fluids and particles has not been well characterized. Here, we perform interface-resolved 3D direct numerical simulations (DNS) to study particle suspensions in a pressure-driven EVP duct flow. In particular, we investigate the effects of plasticity (Bingham number), elasticity (Weissenberg number), inertia (Reynolds number), and shear-thinning (flow index) on the particle migration and the unyielded regions of the suspending fluid. The numerical code enjoys a direct forcing immersed boundary method to simulate the dispersed phase as moving Lagrangian grids, while the carrier fluid is discretized on a fixed Eulerian frame, in which the Saramito-Herschel-Bulkley constitutive equation is applied to account for elastoviscoplastic stresses. A soft-sphere collision model with lubrication correction is also employed to model the close-range particle-particle/wall interactions [1]. EVP fluids behave like soft solids where the imposed stress on them is small (unyielded regions, below yield stress), and flow like viscoelastic fluids in regions where the imposed stress is large (above yield stress). We observe that different types of unyielded regions appear in the single-phase flow: a moving “plug” at the center and four static fouling regions at the corners of the duct. Unsteady structures, including secondary flows and re-circulation regions, are present, and their intensity increases with inertia and elasticity of the fluid. Furthermore, we observe particle migration depending on the particle inertia: particles with low inertia concentrate at the corners, while a uniform distribution of particles around the plug region is observed when increasing the particle inertia. Particles trapped in the unyielded regions do not migrate, and instead move with the same velocity as the plug region, as observed in our previous study of a single particle [2]. A certain combination of elasticity and plasticity parameters are observed to facilitate particle deposition into the core plug region.

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Subgrid-scale modeling of droplet bag breakup

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The acceleration of liquid droplets by a fast-moving gas stream causes their deformation and possible breakup into small liquid fragments, where the breakup mechanism depends on the droplet Weber number, We. In the bag breakup regime, which occurs at low to moderate We, the droplet flattens and forms a liquid sheet that inflates into a bag shape that subsequently bursts. Accurate prediction of the droplet size distribution from bag breakup and related sheet fragmentation events in numerical simulations of liquid-gas flow can facilitate the design optimization of processes such as air-blast atomization. However, the liquid sheet and resulting droplets can have characteristic dimensions of a few microns, and their resolution by typical two-phase Navier-Stokes simulations requires the use of micron-scale meshes that may inhibit their use in turbulent large-eddy simulations (LES) of full-scale atomization, even with the use of adaptive mesh refinement.

To enable the accurate prediction of drop size statistics in full-scale simulations, we present a subgrid-scale modeling strategy for the bag breakup of droplets within an volume-of-fluid framework. A two-plane reconstruction is used to maintain liquid sheets below the grid size, while a Lagrangian identification method tracks the evolution of liquid sheets within the domain. Upon satisfaction of a specified breakup criterion, a film-to-droplet conversion model transfers the liquid volume in the droplet bag from the Eulerian volume fraction field to Lagrangian point particles with specified diameter. A structure classification method then identifies the remaining rim structure as a ligament, and a ligament-to-droplet conversion model performs a Eulerian-to-Lagrangian liquid volume transfer. We perform mesh convergence studies to establish the robustness of our method and then compare the predicted droplet size statistics with those from experiments. Finally, we demonstrate the ability of our breakup model to accurately predict the droplet size statistics of a full-scale LES of air-blast atomization.

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A fast and highly scalable Direction splitting algorithm to solve momentum and heat transfer in flow laden with non-spherical rigid bodies

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We present an accurate and scalable solver for non-spherical rigid particle-laden flows implemented on *PacIFiC*, an in-house C/C++ parallel library to solve Partial Differential Equations. The solver uses a direction splitting algorithm [1] which transforms all three-dimensional Poisson problems (and in particular the pressure Poisson problem) into a sequence of three one-dimensional Poisson sub-problems, thus improving its scalability up to multiple thousands of cores. We employ this algorithm to solve mass, momentum and energy conservation equations in flows laden with non-spherical particles and spatially homogeneous particle temperature. We account for the presence of non-spherical particles on the (uniform or non-uniform) Cartesian fluid grid by modifying the diffusion and divergence stencils near the rigid body boundary using the Dirichlet boundary conditions for the velocity and temperature field on the particle boundary. Compared to [1], we use a higher-order interpolation scheme for the temperature and velocity fields to maintain a second-order heat flux and stress estimation, respectively, on the particle boundary, resulting in more accurate dimensionless coefficients such as drag (C_D), lift (C_L) and Nusselt number (Nu). We also correct the interpolation scheme due to the presence of any nearby particle to avoid any loss of accuracy, making the solver robust even when particles are densely packed in a subregion of the computational domain. We present classical validation tests involving single or multiple, fixed or freely moving particles and assess the robustness, accuracy and scalability of the solver. Finally, we discuss results related to the large-scale computation of the flow through a random array of multiple thousands of three-dimensional finite length circular cylinders with heat transfer.

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High performance computing of the collapse of a bubble array near a wall

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The investigation of the pressure loads developed by collapsing cavitation bubbles leading to erosion is of primary interest for hydraulic and marine applications. In order to find effective preventive measures, the detailed mechanism of a bubble collapse and the physical phenomena involved in the process need to be carefully investigated. In the present work, the flow field resulting from the interaction between a planar incident shock wave and multiple gas bubbles is numerically investigated. The study of collective effects and the potential amplification of the pressure peaks on the wall in comparison with a single-bubble collapse is proposed.

The numerical simulations are carried out using an in-house massively parallel multiphase code solving a one- fluid compressible system. The model consists in three conservation laws for mixture quantities (mass, momentum and total energy) and an additional equation for the void fraction. The PDE system is discretized through the finite-volume method. Numerical fluxes are computed with a HLLC scheme combined with the predictor-corrector Hancock approach in order to obtain the second order in both time and space. The software is designed for high performance computing (HPC) and is parallelized with a hybrid paradigm using the MPI, OpenMP, and openACC programing models. It has been validated on various two-phase cases involving shock waves and has computed 3D well-resolved bubble collapse leading to grids composed by 5 billion nodes [1,2].

The interdependence of bubbles and the possible intensification of the peak pressure has been discussed by different author [3]. Yet 3-D simulations of bubble arrays are very scarce in the literature due to the large computational cost [4]. The dynamics of such configurations are significantly different from those in two dimensions. In the present study, we investigate configurations involving five gas bubbles of equal size, with different relative position. The distance to the wall is fixed. Bubbles are immersed in a water pool at rest and collapsed by a normal shock wave moving at the Mach number 1.71. Exploiting the symmetry of the problem, only a quarter of the configuration is computed (see Figure 1 on the top). First results indicate that the amplification of the maximum wall pressure can reach a factor of 2 in comparison with the single-bubble case, which can induce significant material damage.

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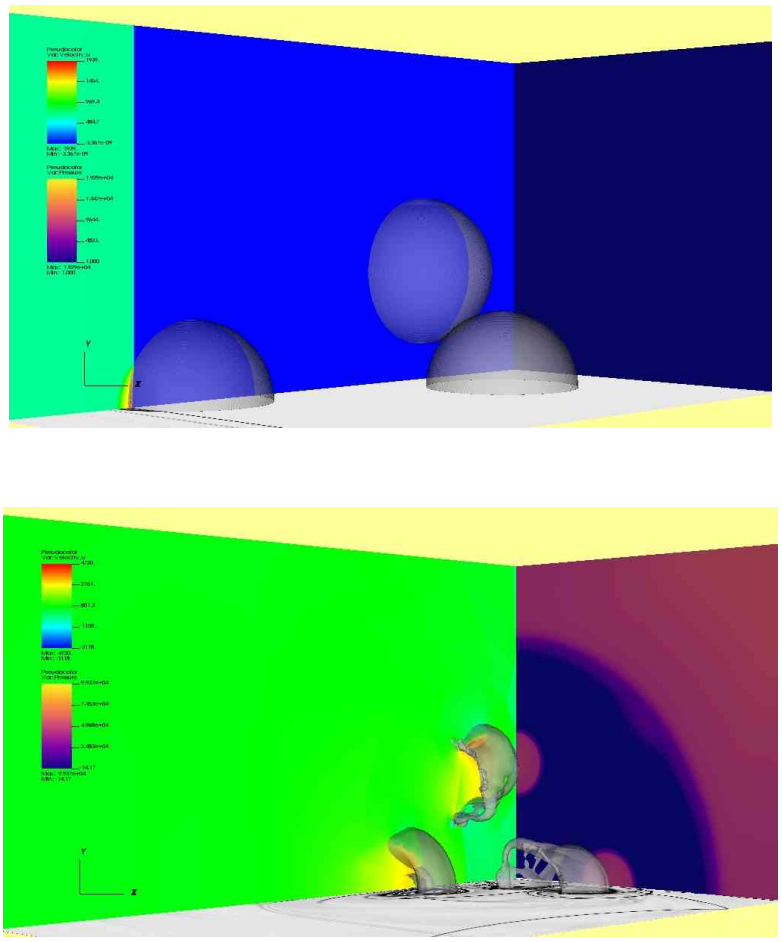

Figure 1Visualization of the collapse of a bubble array : pressure field on the wall, longitudinal velocity component and iso-surface of void fraction.

Friday – 2022-09-30

Session I

- **Mini-Symposium: Dynamic wetting and numerical treatment of moving contact lines**
  (Chair: H. Marschall, Room: Aula Magna 1-E)
- **Advanced algorithms and solution techniques for coupled multiphase systems**
  (Chair: C.M. Casciola, Room: Aula 1-G)

Simulating wetting of geometrically complex surfaces using the plicRDF-isoAdvector unstructured Volume-of-Fluid method

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Mathis Fricke TU Darmstadt
Dieter Bothe TU Darmstadt
Tomislav Maric TU Darmstadt

In this work, we benchmark the plicRDF-isoAdvector [1] unstructured Volume-of-Fluid (VOF) method (see [2] for a recent review) with the curvature approximated by a parabolic fit [3], for wetting problems. The verification is done using the advected contact angle verification case introduced in [4]. The effect of the contact angle boundary condition and Bond number ($Bo = \frac{\rho g R^2}{\sigma}$) is investigated using droplet spreading over a flat or solid spherical surface and the capillary rise as validation test cases. Furthermore, we investigate the droplet sliding across heterogeneous surfaces (Fig. 1) bearing physical and chemical heterogeneity. This allows us to study the contact angle hysteresis and pinning phenomena for a sliding droplet. The numerical results of these test cases are compared against analytical and experimental results.

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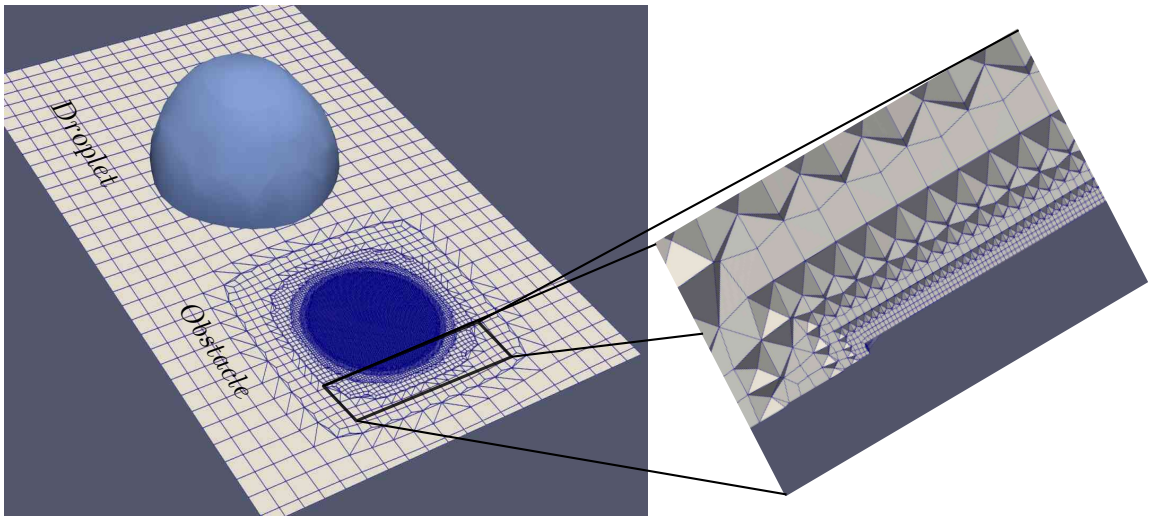

Figure 1: Sliding droplet over an obstacle, with mesh refined around the obstacle

Adhesion in coalescence-induced jumping droplets – relevant or not?

Konstantinos Kontantindis* Chalmers Univ. of Technology

Johan Göhl Fraunfoher-Chalmers Centre

Andreas Mark Fraunfoher-Chalmers Centre

Srdjan Sasic Chalmers Univ. of Technology

Significant number of studies have uncovered details related to the jumping droplets phenomenon upon coalescence on superhydrophobic surfaces. Such surfaces have attracted interest for industrial applications such as self-cleaning, improved drop-wise condensation and anti-icing[1]. To broaden our understanding on how important adhesion is for the jumping process, a thorough numerical investigation has been undertaken that performs a series of simulations with surfaces of different hysteresis, dynamic contact angle models and different droplets radii. We use a previously developed combined immersed boundary – Volume-of-fluid method with a slip boundary condition and different contact angle models[2], in order to observe the sensitivity of jumping to dynamic contact angles models and the wetting area expansion. The framework is validated by good qualitative and quantitative agreements to previous experimental studies[3] (see Fig. 1).

The jumping is driven by strong capillary forces while the droplet resulting from coalescence of two or more smaller droplets is attached to a low-adhesion surface[4]. Therefore, the contact line dissipation becomes a crucial factor, yet unexplored numerically to our best knowledge. Our results predict how the surface boundary treatment affects the final kinetic energy available for jumping. The extension of the framework to an immersed boundary method promises a variety of new implementations that can model randomized geometry in surfaces, or even solid particles removal. Finally, we present examples how dynamic contact angles capture adhesion effects in jumping droplets with radii as small as a few microns.

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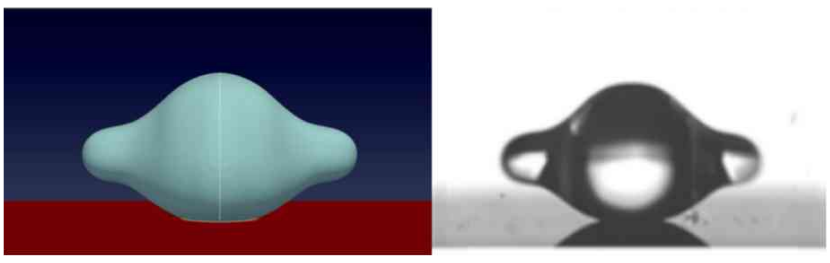

Figure 1: Example of validating the framework to experimental data of Yan et al[3].

To coalesce or not to coalesce
Understanding sessile droplets subject to surface tension gradients

Stefan Zitz* Roskilde University

Johan Roenby† Roskilde University

Droplets play an important part in many applications, e.g. in heat transport via spray cooling and crop protection by dispersion of pesticides [1, 2]. One use case that has attracted particular interest during the years is inkjet printing [3]. Printing a well–resolved structure on a penetrable substrate is a challenging task since ink droplet coalescence must be avoided to prevent degrading resolution.

Two sessile droplets of miscible liquids will typically coalesce immediately when brought into contact. As shown by Karpitschka and Riegler, a remarkable exception can occur for liquids of different surface tension [4]. We study this phenomenon in Lattice Boltzmann simulations, imposing a varying surface tension, $\gamma(x)$ (see Fig.1, left). In agreement with [4], sharp surface tension gradients result in non-coalescence (see Fig.1, right). We repeat the simulation with different gradients of the surface tension profile. Interestingly, we find a sharpness threshold below which coalescence reoccurs.

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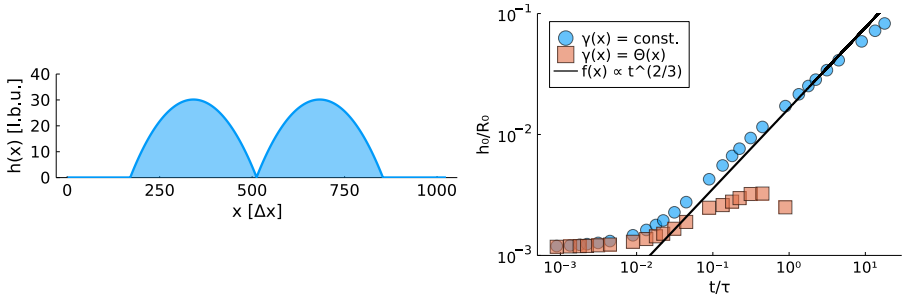

Figure 1: Left: Initial interface shape for the droplet coalescence simulation. The aspect ratio is 1/7 and the droplets have a contact angle of $\theta = 20°$. Right: Evolution of the bridge height h_0 normalized by the droplet radius, $R0$, with time normalized by inertio-capillary time, τ. Blue bullets and orange boxes are for constant surface tension and Heaviside shaped ($\Theta(x)$) surface tension profile, respectively. Black curve shows power law with exponent 2/3 [5].

Wettability pattern mediated trapped bubble removal from an immiscible liquid-liquid interface

Imdad Uddin Chowdhury[a], Pallab Sinha Mahapatra[a], Ashis Kumar Sen[a]

The passage of a bubble through an immiscible horizontal liquid-liquid interface has a wide range of applications, from chemical processes to microfluidic devices. Buoyancy governs this passage of the bubble, and at the liquid-liquid interface, the bubble encounters a downward pulling force due to surface tension. Depending on the volume of the bubble, it may pass through or become trapped at the interface. In this study, for the first time, we proposed the idea of trapped bubble removal from a liquid-liquid interface with the aid of a wettability-patterned cone. The bubble detachment dynamic is investigated using numerical results and theoretical analysis. The effect of fluid properties and cone parameters on bubble detachment has been extensively studied. It is found that density contrast (ρ_r) and viscosity contrast (μ_r) of both the liquids, surface tension ratio (σ_r), bubble diameter (d_0), wettability of the cone (θ) and cone angle (α) play a crucial role in bubble detachment. Here, we studied the effect of each parameter on the bubble detachment and, based on that, identified two distinct regimes e.g., Detached Regime and Non-detached Regime. The regime map is represented by two non-dimensional groups β and ψ which are functions of Bond number (Bo), Ohnesorge number (Oh), α and θ. Furthermore, the transport characteristics of the bubble on the cone after the detachment indicate that the bubble velocity decreased as it moved from the narrower to the wider section of the cone.

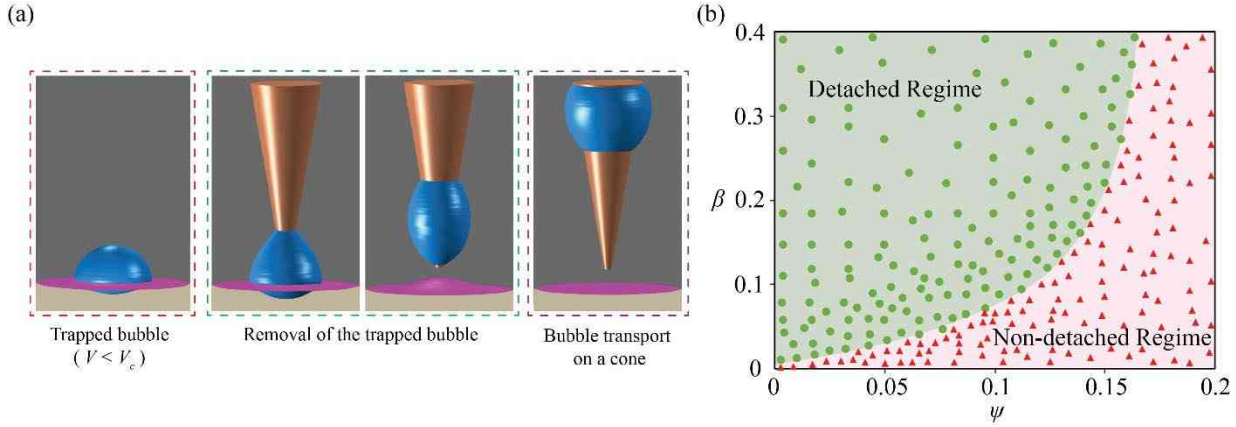

Figure 1: (a) Demonstration of the problem. A bubble of diameter D = 2 mm trapped at the liquid-liquid interface. A cone of length h = 1 cm with varying cone angle ($\alpha = 1^0 \, to \, 90^0$) and wettability ($\theta = 1^0 \, to \, 90^0$) is used to remove the trapped bubble. (b) Two distinct regimes are proposed through two non-dimensional groups β and ψ

A trapped bubble on a liquid-liquid interface in small-scale chemical industries is not favorable. Thus, the removal of the trapped bubble is essential. In this work, a technique for the removal of a trapped bubble from an initially horizontal liquid-liquid interface is proposed. We used a cone with varying wettability and a cone angle to remove the bubble (refer Fig. 1(a)). A detailed numerical analysis of bubble detachment for a wide range of flow configurations is performed. For the numerical modeling, the Cahn-Hilliard model with Navier-Stokes equations is used. The dynamics of the bubble detachment are analyzed through the numerical results and are supported by a force balance analysis. Two distinct regimes e.g., Detached Regime and Non-detached Regime, based on the liquid properties, cone parameters, and bubble diameters, have been identified (refer Fig. 1(b)). The findings of the present work are helpful for the experimentalist to understand the critical parameters required to remove a bubble from a horizontal liquid-liquid interface using a wettability-patterned cone. This technique of trapped bubble removal could be very useful in small-scale chemical industries.

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Time-implicit multilayer modelling of gravity and capillary waves

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A very large number of practical applications involve the flow of small-scale liquid films in which surface tension plays a key role. Probably one of the best known example of such flows is the formation of Kaptiza waves [1] at the surface of a liquid film flowing down an inclined plane (Figure 1.a). When the dynamics are dominated by viscous dissipation, the lubrication approximation makes some of these problems tractable analytically.

In many cases however, the lubrication approximation is not verified and inertial effects must be taken into account, which often requires a numerical approximation. Using a time-explicit discretisation of surface tension, as is most commonly done, leads to drastic stability restrictions which severely limits the practical interest of these numerical methods for a wide range of problems.

At the other hand of the spatial spectrum, one may be interested in the large-scale oceanic balance between gravity, Coriolis acceleration and surface wind stress, as demonstrated for example when looking at the free-surface elevation due to the Gulf Stream (Figure 1.b). From a numerical perspective, it is now the explicit treatment of barotropic gravity waves, which propagate several orders of magnitude faster than other modes, which drastically restricts the computational efficiency.

In this presentation, I will show how both issues can be addressed using a generic time-implicit discretisation of interfacial terms, applicable to surface tension, gravity and other terms, while retaining accurate dispersion relations for the associated waves.

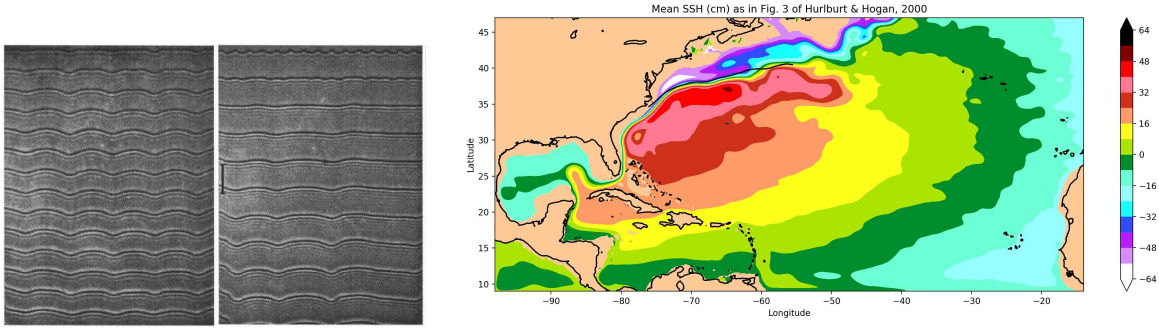

Figure 1: (a) Kapitza waves. (b) Time-averaged free-surface elevation in the North Atlantic [3].

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Front-Tracking approaches for the modelling of breakup and coalescence

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In this work two-phase flows are modelled by a multi-scale approach involving dedicated meshes, one for the interface, mobile and deformable, for the Front-Tracking [1] and called Lagrangian, and the other Eulerian and fixed for the conservation equations of mass and momentum.

These multi-scale models are difficult to achieve numerically because they require managing dynamically in time and space the mesh of the interface (made up of connected triangles). In exchange for this complexity, they offer an explicit description of the interface even in the presence of strong curvatures and a better control of topological changes (coalescence and breakup). The models and algorithms must run in parallel on distributed memory computers to conduct convergence studies, validate academic cases and then tackle more complex configurations.

In order to describe efficiently the thin features of the interface, we implemented an adaptive remeshing procedure with local surface reconstruction. Topological changes are handled geometrically. The volume fraction is calculated with a geometric method: the Ray-Casting with local refinement.

Experimental and numerical configurations from the literature will be used to verify the models and numerical methods. Among them, we can mention the collision of two drops [2].

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Front tracking with surface normal propagation restriction

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The modelling of interfacial flows with the front tracking method comes along with potential computational expenses and difficulties. One of the main computational expenses, and a source of numerical error is the remeshing of the front mesh due to its distortion and compaction during the advection of the front vertices. Classical remeshing operations are error-prone and do not strictly conserve the volume of the interacting bulk phases or preserve the shape of the interface. Mitigating or eliminating these inaccuracies requires additional and potentially computationally expensive methods.
The aim of the presented method is to overcome tangential front vertex movement and vertex clustering in order to prevent, or at least reduce or postpone front remeshing. For the proposed front tracking method, the suppression of vertex movement tangential to the front is achieved by a reformulation of the surface velocity vector at each discrete front vertex position. The front vertices are no longer moved with the interpolated fluid velocity as in the classical front tracking advection, but the new velocity vector is composed of the sum of the center-of-mass velocity of the body enclosed by the front mesh plus a vertex velocity relative to the center of mass velocity. This velocity relative to the center of mass velocity is decomposed into a surface tangential and surface normal component from which only the surface normal velocity component is used for front vertex advection to cancel tangential vertex movement. This new front tracking method is tested using canonical test-cases, such as a rising bubble in an otherwise quiescent flow, shown in Figure 1, or a droplet in shear flow, focusing on mass conservation, shape preservation and the computational costs.

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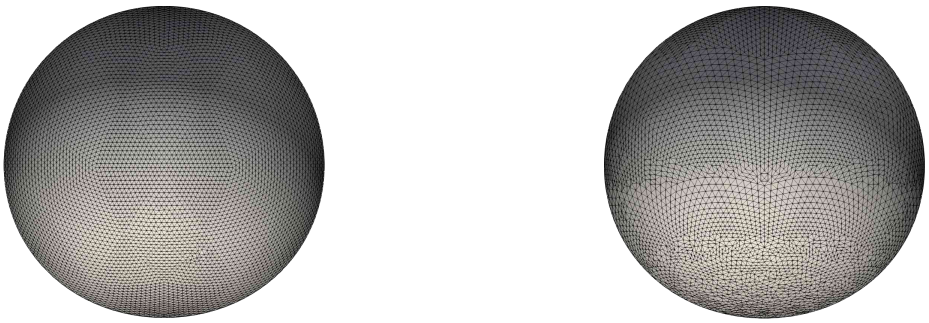

(a) Proposed front tracking method without remeshing (b) Classic front tracking method with remeshing

Figure 1: Comparison of the proposed and the classic front tracking methods for a rising bubble shown here at terminal velocity in the Stokes regime ($\mathrm{Bo} = 17.7$, $\mathrm{Mo} = 711$).

FastRK3P*: a fast and stable pressure-correction method for two-fluid incompressible homogeneous shear turbulence

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Direct numerical simulation (DNS) of droplet-laden homogeneous shear turbulence (DLHST) presents computational challenges as a result of the time-integration method. The second order Adams-Bashforth (AB2) scheme is weakly unstable when simulating HST on fine grid resolutions [4, 5]. In order to address this issue, we have developed a new numerical method called FastRK3P* for accurately simulating immiscible two-fluid incompressible flows. FastRK3P* is the result of combining FastRK3 of [1] and FastP* of [3] with the VoF method of [2] and a newly developed mass-conserving algorithm for applying shear-periodic boundary conditions with the VoF method. FastRK3P* is stable and requires solving the Poisson equation for pressure only once per time step instead of three times as required by the iterative Crank-Nicholson scheme adopted in [5] or standard RK3 methodologies. Figure 1 shows that AB2 exhibits unphysical oscillations in the spectrum of turbulence kinetic energy at high wavenumbers, whereas FastRK3 does not. We have applied FastRK3P* to perform DNS of DLHST for different values of shear number, Sh, and Weber number, We, and, we will discuss the physical mechanisms responsible for the modulation of TKE in DLHST.

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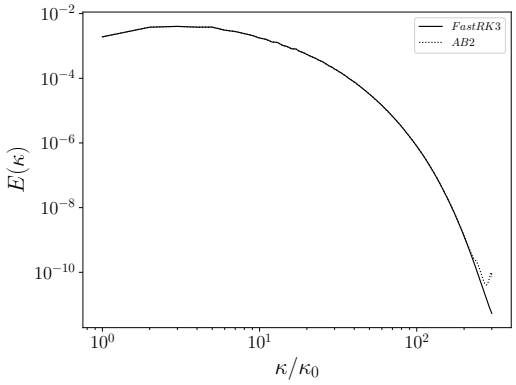

Figure 1: Comparison of spectra between AB2 and FastRK3. AB2 exhibits unphysical oscillations at higher wavenumbers, whereas FastRK3 does not.

An eXtended Discontinuous Galerkin Method for three-dimensional two-phase flows: Application to viscous droplet oscillations

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Dino Zrnić TU Graz
Florian Kummer TU Darmstadt
Günter Brenn TU Graz
Martin Oberlack TU Darmstadt

We are going to present a high-order eXtended Discontinuous Galerkin (XDG) method for transient two-phase flow problems within a three-dimensional setting. The XDG method adapts the local ansatz functions to conform to the position of the interface and provides separate degrees of freedom for each fluid phase in cells which are cut by the interface [1]. This allows a sub-cell accurate approximation of the incompressible Navier-Stokes equations in their sharp-interface formulation. The interface is described as the zero-set of a signed-distance level-set function and is discretized by a standard DG method. For the interface, resp. level-set, evolution, an XDG adapted marching algorithm for the construction of an extension velocity field was presented in [2] for the 2D case. For the 3D case, we present the construction of a divergence-free extension velocity field by solving the two-phase Stokes equations with the XDG approach. Furthermore, we discuss some issues regarding the extension to 3D problems, such as the continuity projection of the interface by a patch-wise approach and the agglomeration of cells cut by the interface.

The numerical investigations will focus on nonlinear axisymmetric shape oscillations of a Newtonian drop in a near dynamically inert ambient phase. The initial drop shape is given by a Legendre polynomial of degree m. We compare the numerical results with the theoretical results of the weakly nonlinear analysis presented in [3]. The analysis is based on series expansions of the flow field variables and the drop shape with respect to a deformation parameter. The weakly nonlinear approach is carried out to third order and accounts for the coupling of different oscillation modes. Modes of initial deformation up to $m = 4$ are addressed. The properties to be compared include the droplet aspect ratio over time with corresponding period times and damping rates, and mode decomposition of the droplet shape into Legendre polynomials. Further, we present the kinetic and surface energy over time for the numerical simulations.

Acknowledgements

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Algebric momentum preserving method with a fully-coupled 3D parallel solver for the simulation of two-phase incompressible flows

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Two-phase flows with separated phases are prevalent in several industrial and environmental applications, where the conditions and regimes encountered spread wide and far. In the energy sector for example, the atomisation of liquid jets results from complex interactions between a coherent liquid jet, a gas-filled plenum and (potentially) a co-flowing gaseous jet. Breaking waves are another instance of two-phase flows, characterised by a high degree of turbulence, as are droplet impacts on liquid surfaces, nanofabrication by thermal plasma jets, to name a few.

The high density and viscosity ratios encountered in these two-phase flows couple strongly the velocity components in the interface vicinity, and often result in strong shear at these interfaces. This yields in ill-conditioned linear systems (as a result of the semi-discretisation of the two-phase incompressible Navier-stokes equations) that pose significant problems together with the treatment of the coupled velocity-pressure saddle-point system [Chorin(1968), Témam(1969), Vincent *et al.(2004)*, Vincent *et al.(2011)*, El Ouafa *et al.(2020)*, El Ouafa *et al.(2021)*]. Solving these systems remains a challenging task for mathematicians as well as engineers. In addition, it has been demonstrated that solving theses equations in a non-conservative form with high density ratios leads to incorrect velocity field or volume fraction and often a failure of numerical scheme, due to numerical error accumulation near the highly deforming interface [Bussmann *et al.(2002)*, Desjardins *et al.(2008)*, Raessi and Pitsch(2012), Le Chenadec and Pitsch(2013), Nangia *et al.(2019)*, Zuzio *et al.(2020)*].

The main objective of the present work is to further investigate the solution of the coupled system (without any time-splitting approach) by means of a preconditioned BiCGstab(2) solver [J-J. Dongarra *et al (1998)*]. We obtain high performance with a new preconditioning strategy that combines a triangular block preconditionning for the velocity block with a pressure convection diffusion (PCD) preconditionner for the Schur complement [Bootland *et al.(2019)Bootland, Bentley, Kees, and Wathen*]. To provide the stability of the numerical scheme in the presence of high density and viscosity ratios, we use an algebric momentum preserving mass and momentum transport in the conservative form of discrete equations. The consistency between mass and momentum advection is achieved by resolving a new auxiliary continuity equation, using fifth-order WENO scheme and third Runga-Kutta SSP time integrator.

Test cases such as the transport of a very-high density fluid sphere and the free fall of dense sphere are performed to validate the models, especially in the presence of strong density and viscosity ratios. Other cases, like the phase inversion, demonstrate the ability of the new fully-coupled solver to tackle problems of more than one billion cells, with excellent scalability.

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Direct Numerical Simulation of Bubble Formation and Dynamics in Water Electrolysis Using a Phase-Field Method

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The efficient generation of hydrogen (H_2) bubbles in electrolyzers requires understanding the fundamental interaction of the coupled physico-chemical processes, which govern the detachment of H_2 bubbles from electrodes under real operating conditions, and how that influences the efficiency of electrolyzers [1].

We have extended our diffuse-interface phase-field solver `phaseFieldFoam` (FOAM-extend4.1) by thermal Marangoni effects [2], taking into account temperature-driven local variations in interfacial energy. To include solutal and ohmic Marangoni effects, we have developed and implemented a model framework for the transport of multi-component species mixtures, which to this end incorporates recent open-source community development work such as [3]. With our modular approach, we now aim to flexibly cope with different types of mixtures (individual thermodynamical properties) in a generic framework – here, considering electrolytes (charged species mixtures). The charged species transport in electrolyte mixtures is incorporated solving the coupled Navier-Stokes Nernst-Planck-Poisson (NS-NPP) equations.

In our contribution, we will discuss the current state of method development. We will further elaborate both on advanced modeling aspects and on the modular structure of the code framework that supports the deployment of our model library for multiple types of mixtures of chemical species. In addition, we will discuss some of the fundamental test cases that benchmark our new library for multicomponent transport in mixtures.

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Non-Coaxially Rotating Motion in Casson Martial along with Temperature and Concentration Gradients via First-Order Chemical Reaction

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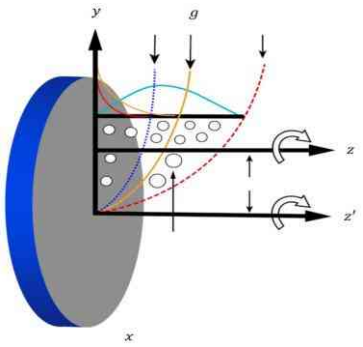
The effect of non-coaxial rotation on the transport of mass subjected to first-order chemical rea ction is studied analytically. The effects of thermal radiation, buoyancy, constructive and des tructive chemical reactions along with Casson fluid in rotating frame are discussed. Time evol ution of primary and secondary velocities, energy and solute particles are analyzed. The behavio r of flow under the variation of intensity of magnetic field is also investigated. Evoluti onary behavior of primary velocity is opposite to the evolutionary behavior of secondary velocit y. The impact of buoyant force on primary velocity is opposite to the role of buoyant force on th e secondary velocity. The evolutionary behavior of temperature is also examined and a remarka ble enhancement in temperature is noticed. Thermal radiation causes the fluid to be cooled do wn as heat energy is escaped by thermal radiation. Evolutionary behavior of concentration is also analyzed and an increasing of concentration versus time is noted. Destructive ch emical reaction results a remarkable reduction in the concentration and vice versa for gene rative chemical reaction.



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Simulation of binary-phase-fluids and wettable-rigid-bodies interactions

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Interactions among solids, liquid and drops are ever-present in nature (raindrops falling into the sand) and in the industry (flotation froth, spray scrubbing, emulsion stabilisation process) at different scales. In this ongoing investigation, we aim to develop a numerical tool that allows the study of such three-phase flow considering the immersed solid phase properties, the type of drops and the characteristics of the carrier fluid in which they interact, as controlling parameters. To simulate numerically these interactions, we employ a Eulerian-Lagrangian methodology where direct numerical simulation of the Navier-Stokes equations is performed using a pseudo-spectral method for the carrier fluid. The drop phase is modelled by the Phase Field Method (PFM) and the solid objects are coupled using the Direct Forcing Immersed Boundary approach (DFIB) which accounts with a virtual force acting in the region accupied by the rigid-solid, and it is added to the Navier-Stokes equation [1, 2]. The solid-fluid sharp-interface is replaced by a continuous hyperbolic function resulting in a smooth transition of the properties between both phases. The binary-fluid-phase system is extended to a ternary system adopting the approach proposed by Shinto [3], where the free-energy density functional is modified in order to account for a solid phase and where we can prescribe the wettability in the solid surface. In this poster we present some study cases such as a fluid flow around a sphere, a solid sphere interaction with an interface (Fig. 1), sedimentation of a circular disk in a quiescent fluid; and the validation cases of the contact angle of stationary circular cylinders (Fig. 2) [4, 5] and a single sphere settling in a vertical tank at different Reynolds numbers [6] (Fig. 3).

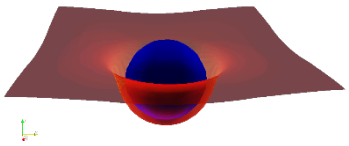

Fig. 1 Stationary cylinder (ca=60°)

Fig. 2 Solid-interface interaction

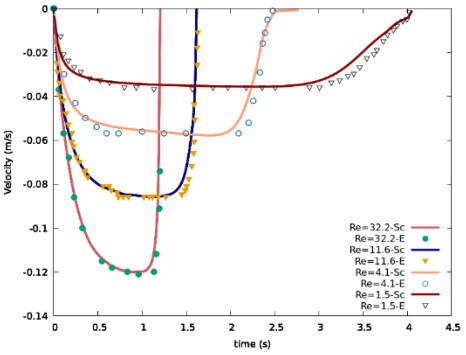

Fig.3 Settling sphere in a tank

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