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EDITORIAL

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Special issue on finite-size particles, drops and bubbles in fluid flows: advances in modelling and simulations

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Multiphase flows laden with finite-size particles, droplets and bubbles are of fundamental importance in a huge variety of practical applications embracing environmental phenomena as well as industrial processes [3]. Over the last decade, modelling and simulation of such flows have become feasible thanks to the increase in computational power, and the subject has received growing attention within the multiphase flow community. This is proven by the appearance of dedicated sessions in all major international scientific events dedicated to multiphase flows. Among those organised in the last 5 years, and limiting the list to specialised events, we can cite Euromech colloquia (in particular the Colloquium 555 on *Small-scale numerical methods for multiphase flows*, held in August 2013 in Pessac, France, and the Colloquium 596 on *Numerical simulations of flows with particles, bubbles and droplets*, held in May 2018 in Venice, Italy); the Turbulence and Interaction international conference series (the 4th edition was held in November 2015 in Corsica, France; the 5th edition was held in June 2018 in Martinique, France) [8,9]; as well as symposia (e.g. the mini-symposia on *Modeling and Simulation of Multiphase Flow and Heat Transfer*, included in the programme of the 6th International Symposium on Advances in Computational Heat Transfer, which took place at Rutgers University, USA, in May 2015; or the IUTAM Symposium on Motile Cells in Complex Environments, held in Udine, Italy, in May 2018). The importance of the topic is also proven by the growing number of advanced courses organised for research scientists and engineers: Among others, we recall the summer schools organised by the International Centre for Mechanical Sciences (CISM) in Udine, specifically those on *Small Scale Modeling and Simulation of Turbulent Multi-phase Flows* held in May 2016 and on *Fluid Dynamics Effects on Particle Formation in Crystallization Processes* held in July 2018, and the lecture series on Industrial Computational Fluid Dynamics organised by the Von Karman Institute (VKI), with specific reference to the lecture on *Industrial multi-scale applications: Modeling and simulation of multi-phase flows with fictitious domain approaches*, held in May 2017.

Relying on our numerous exchanges with the two-phase flow community and, in particular, with colleagues working on the modelling and simulation of dispersed flow problems, we found it timely to propose a special issue dedicated to the state of the art in modelling and simulation of finite-size particles in fluid flows. In 2018, invitations were sent to several research groups with a well-established activity in the field to contribute a paper to this special issue of Acta Mechanica. To our great pleasure, almost all of the invitees were able to accept the invitation and submitted their works in late fall. All manuscripts were then subject to evaluation by anonymous reviewers as per the regular publication procedure in Acta Mechanica. Altogether, 15 reviewed and revised

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papers are published in this special issue. The papers focus on the different physical, modelling and numerical issues that emerge when the behaviour of finite-size particles in different flow instances (ranging from viscous to turbulent) is examined. We believe that this Special Issue provides a vivid picture of the latest advances achieved in the numerical prediction of deformable particle dynamics (in particular, fluid particles like drops and bubbles) as well as solid particle motion in fluid flows.

1 Models and numerical methods

When one is interested in the modelling and simulation of two-phase incompressible flows in which the dispersed phases are represented by finite-size particles, one issue of primary importance is the tracking of the interface separating the fluid inside the droplet/bubble and the fluid outside of it, or the surface separating the interior of the particle from the surrounding fluid in case of solid inclusions. Previous attempts to use approaches on unstructured (UNS) meshes can be found in the literature, see, for example, [19] for solid particles and [6] for fluid particles. However, due to the cost of the automatic mesh generation that is required as soon as the particle interface/surface is advected or deformed, the UNS discrete framework is restricted mostly to two-dimensional space problems and can account only for low interface deformations when drops/bubbles are dealt with. Generating the carrier fluid mesh around a large set of particles is very CPU-time-consuming and often impossible to achieve automatically in three dimensions. The other class of discrete methods to deal with finite-size particle simulations is structured grids. In this case, describing the time and space evolution of the interface separating a swarm of particles from the surrounding fluid is not straightforward if the mesh is not allowed to conform to the interface itself and does not evolve with it. Following the pioneering works of [12,14,15,20,27,29], this difficulty has been overcome by introducing an auxiliary phase function in the equations of motion: an Eulerian function, termed volume of fluid (VOF), level set, solid fraction or phase field depending on the specific modelling approach, is used to characterise particle advection and identify whether a given mesh cell pertains to the carrier fluid or to the dispersed phase. In this Special Issue, the majority of the contributions reports simulations that have been conducted with VOF-like methods, but simulations based on phase field methods are also presented.

Once the multiphase character of the investigated system is properly described by the phase function, the heterogeneity and multiphase character of the problem must be accounted for. In particular, when the flow is laden with solid particles, the most commonly used approaches are the immersed boundary method (IBM) [1,5,11,16,25], which consists in adding forces into the mesh cells pierced by the interface, and the incompressible Navier–Stokes equations. These approaches are widely spread and validated in the literature and do not require any modifications of the underlying numerical schemes used in the single-phase solver. However, alternative approaches are available that are also reported in the present issue: in particular, implicit viscous penalty methods [4,26] and Lattice Boltzmann methods (LBM) [21]. As far as fluid particles are concerned, two contributions [18,22] rely on the one-fluid model [15,23], which is the most widely used approach in the literature as it only requires to adapt density and viscosity at the interface without changing the numerics of the single-phase solver. In addition, one contribution [7] makes use of a Boltzmann approach, which allows an easy parallel implementation of particulate flows, while another contribution [13] exploits the IBM, to track non-deformable bubbles in a way similar to what is typically done with solid particles. One last contribution examining fluid particles [24] is based on the phase field approach, which can be understood as a diffuse VOF method based on small-scale physics of the interface, and is particularly well suited for handling capillary effects.

When the particle mass loading or even the flow regime becomes an important factor in the behaviour of the two-phase system, it is interesting to notice that the contributions of this Special Issue cover a variety of particulate flows ranging from fluidised or fixed beds to wall-bounded turbulence, from emulsions and bubble dynamics with wetting and capillary effects to spherical and non-spherical particles (both fluid and solid). The mass fraction of the dispersed phase ranges from 1 to 50%, and flows are unsteady or even turbulent. In terms of numerical approaches, time splitting or projection methods are used in all contributions (a lot of efficient parallel solvers exist on the Web and in freely available libraries), except in the penalty contributions of [4,26], where a fully coupled approach is considered based on augmented Lagrangian techniques [28].

2 Papers dealing with solid particles

The majority of the papers included in this Special Issue considers suspensions of solid particles in a variety of fluid flows (from linear shear flows to wall-bounded turbulence), and the simulations are based on the IBM. Most works focus on the case of spherical particles with different sizes and loadings.

Among the IBM-based works, Chouippe and Uhlmann [5] study the motion of large heavy particles in the presence of forced turbulence and gravity. Particle size is several times the Kolmogorov scale. Results refer to fixed density ratio and Galileo number, with values chosen on purpose to generate strong wake-induced particle clustering in the absence of turbulence. It is observed that forced turbulence decreases the level of clustering and the relative velocity otherwise observed under ambient settling. However, this decrease is not monotonic with the turbulence intensity. This is explained in terms of reduced interaction time due to particle settling through the surrounding eddy (crossing trajectories), which shifts upward the range of eddies with a time scale matching the particle characteristic time.

A similar problem is investigated in the paper by Fornari et al. [11], who used the IBM to study the settling of finite-size rigid spheres in two different flow configurations (quiescent fluid and forced homogeneous isotropic turbulence). The authors consider different solid volume fractions (up to 10%), again at fixed density ratio (just above unity to mimic sediment particles) and Galileo number. The particle diameter is in the order of ten times the Kolmogorov scale. It is found that turbulence has different effects on different observables: It decreases the mean settling speed compared to quiescent fluid, this effect being weaker at higher volume fractions, but increases particle angular velocities regardless of the volume fraction. The authors also examine the collision frequency, which is higher (resp. lower) in quiescent fluid for small (resp. high) volume fraction. The behaviour at low volume fraction is attributed to drafting–kissing–tumbling events occurring in quiescent fluid, while the behaviour at high volume fractions is explained via the increase in the relative approaching velocities.

A more fundamental study has been performed by Andersson and Jiang [1], who use the IBM to study the motion of the three-dimensional flow field around a prolate spheroid with fixed aspect ratio, fixed orientation of the particle axis with respect to the incoming flow but at varying Reynolds number. The objective of the study is to compute the drag and lift force coefficients as well as the torques and to test the existing correlations. Present results indicate that correlations are more reliable at Reynolds numbers well above unity and that the largest discrepancies occur for the moment coefficient.

One contribution, by Li et al. [16], makes use of the IBM to study of the motion of ellipsoidal (prolate and oblate) particles in shear flow and in wall-bounded turbulence. Simulations are fully resolved and based on a new formulation of the IBM, referred to as immersed boundary projection method, in which the pressure and the momentum forcing are regarded as multipliers for enforcing the divergence-free constraint of the flow field and the no-slip condition along the immersed boundary [17]. The particle Reynolds number (based on the longest axis of the particle) covers two orders of magnitude. In shear flow, the authors are able to correlate the rotational dynamics of the ellipsoidal particle with specific orientations of the longest particle axes, which lead to a large drag force. In wall-bounded turbulence, particles in the buffer region and outside of the boundary layer behave similarly.

The paper by Li et al. [16] provides a nice example of the different formulations of the IBM that have been developed over the years. Among the papers included in this Special Issue, two other formulations have been used. Tavanashad et al. [25] use the Particle-resolved Uncontaminated-fluid Reconcilable Immersed Boundary Method (PUReIBM) to investigate the motion of spherical particles in homogeneous flow driven by an imposed pressure gradient. Through this method, the authors solve for the motion of both phases over a wide range of values for the particle volume fraction and the particle-to-fluid density ratio. The study focuses on the velocity fluctuations of the fluid and the particles, which are examined by looking at the turbulent kinetic energy and the granular temperature. A dependence of these observables on the density ratio is observed, which indicates that energy extraction from mean flow to fluctuations is less efficient at low density ratios. Such dependence seems to persist over the whole range of volume fractions considered.

In the paper by Abdol Azis et al. [2], the authors use an immersed boundary method based on a new Regularised Discrete Momentum Forcing (RDMF) scheme to study the dynamics of dense particle suspensions. To extend the original RDMF scheme to high volume fractions, a modified direct-forcing formulation is proposed, which results in an offset of the imposed no-slip boundary from a moving immersed boundary. This offset is exploited in an iterative strong flow-particle coupling scheme, where the boundary forces are applied at the location of the immersed boundary known from the previous time level. A radius retraction procedure is also introduced to compensate for the diffuse representation of the smooth-interface IBM. The main advantage of the proposed method is to avoid reconstruction of the interpolation and spreading stencils at each iteration of the flow-particle coupling, therefore reducing the computational cost of the method. The method is tested considering the problems of fluidisation of heavy rigid particles and rise of closely packed light particles. Significant improvements are found in the range of low to intermediate Reynolds numbers.

Other methods that are used to perform the particle-resolved simulations are the lattice Boltzmann method, used by Peng and Wang [21], and the penalised VOF method, used by Thiam et al. [26] and by Chadil et al. [4]. More specifically, the paper by Peng and Wang [21] is devoted to the study of turbulent pipe flows laden with finite-size particles in pipes and channels. Numerical simulations are aimed at understanding the turbulence modulation induced by the particles, which exhibits similar features in pipe flow and in channel flow. Particles are found to reduce the bulk flow speed proportionally to their size, by reducing the mean velocity gradients within the buffer region and accelerating the flow very close to the walls. Particles are found to have two opposite effects on the Reynolds stress: They damp the Reynolds stress proportionally to their size, but also increase the Reynolds stress via rotation, which may induce additional ejection and sweeping events.

In the work of Thiam et al. [26] from Institut de Mécanique des Fluides de Toulouse (France) and Multiscale Modeling and Simulation (MSME) laboratory in Paris, fictitious domains, penalty methods and VOF techniques are used to simulate heat transfer in gas-solid flows by considering particle-resolved motions. In particular, a discussion is made regarding the form of the Nusselt number that has to be considered when random assemblies of motionless particles are undertaken. A model is proposed based on a connection between the ratio of two Nusselt numbers and the fluctuating velocity–temperature correlation in the mean flow direction.

The contribution of Chadil et al. [4] results from a joint collaboration between the Institut de Mécanique des Fluides de Toulouse and the Multiscale Modeling and Simulation (MSME) laboratory, and focuses on the estimate of drag forces in particle-resolved simulation of particulate flows. Their numerical method is based on fictitious domains, viscous penalty methods and Lagrangian description of particle shapes, which can be spherical or ellipsoidal. A third-order Taylor interpolation coupled with a third-order Lagrange extrapolation is proposed to calculate the drag force on each particle surface. Various detailed validations are considered with isolated particles or with networks of particles, always motionless. In all situations, numerical force estimates compare favourably to reference literature laws, experiments and body-fitted simulations.

The work by Dotto and Marchioli [10] exploits the point-particle Eulerian–Lagrangian approach to studying the dynamics of inertial flexible fibres in dilute turbulent channel flow. Simulations are not resolved at the particle level, yet fibres are considered to be of finite size because they are longer than the Kolmogorov length scale of the carrier flow. Fibres are modelled as chains of sub-Kolmogorov rods that can undergo relative rotation under the action of the fluid velocity gradients acting along the fibre, and the authors focus on their preferential concentration and wall accumulation. To highlight the effect of flexibility, statistics are compared with those obtained for rigid fibres of equal mass. The authors find that, regardless of fibre inertia and aspect ratio, flexibility enhances the tendency of inertial fibres to accumulate in the very-near-wall region under the action of turbophoresis. In such region, bending appears to depend quantitatively on fibre inertia, which modulates the response to mean shear and turbulent Reynolds stresses.

3 Papers dealing with fluid particles

Five contributions in this Special Issue have concentrated their attention on flows laden with fluid particles, namely drops or bubbles that can be either deformable or not. These works consider various flow regimes, ranging from wall-bounded turbulence to emulsions and local motions of drop on solid surfaces, and report on various improvements and developments stemming from existing models and numerical methods (LBM, phase field, spectral approaches). These new methods are validated against theoretical investigations (lubrication theory), experiments as well as other modelling approaches such as molecular dynamics.

Among the contributions that deal with drops and bubbles, Liu and Bothe [18] from the Technische Universität Darmstadt (Germany) use an incompressible simulation tool with VOF-based tracking of the deformable interfaces. A multiscale modelling approach is considered to deal with bouncing or coalescing droplets. At large scales, the interfacial motion is solved by the VOF two-phase Navier–Stokes equations, while the small-scale dynamics of the carrier gas phase comprised between two colliding droplets is solved by a subgrid-scale closure based on lubrication theory. Simulations are validated and compared with success to analytical results and DNS of droplet-laden flows in terms of pressure.

Heitkam and Fröhlich [13] from the Institute of Process Engineering and Environmental Technology and Institute of Fluid Mechanics of the Technische Universität Dresden (Germany) investigate the effect of osmotic pressure and steady and oscillatory shearing motions on a bubble cluster. Numerical simulations are based on an incompressible Navier–Stokes solver coupled with IBM, under the assumption that bubbles are light, non-deformable spheres. An explicit force model accounting for viscous and elastic effects during bubble collisions is also implemented. The simulations of infinite bubble clusters show the formation of shear bands over a certain range of simulation parameters, and the influence of these bands on rheometric measurements is discussed.

The paper by Derksen and Komrakova [7] from the University of Aberdeen (UK) and the University of Alberta (Canada) is devoted to multiscale simulations of droplets sliding on a solid substrate under shear flow forcing. A free-energy Lattice Boltzmann scheme is used and compared to molecular dynamics simulations. Low Reynolds numbers and low capillary numbers are undertaken in the simulations. The main point of the work relies on proposing a tuning-free parameter at the interfacial condition in the Lattice Boltzmann approach in order to recover the dynamics of the contact line predicted in molecular dynamics.

Rosti et al. [22], from KTH Mechanics in Stockholm (Sweden), have investigated the behaviour of an emulsion in shear flows. A VOF-based, incompressible flow solver was used to simulate a Couette flow acting on the emulsion. The main original features of the numerics are, on the one hand, the implementation of a hyperbolic tangent smoothing MTHINC of the volume fraction in order to improve the calculation of the interface curvature and of the normal to the interface, and on the other hand the use of a FFT solver when density jumps are present at the interface by formulating a specific time splitting approach. Validations of the two-phase flow solver are given, followed by a parametric study of suspensions under various volume fractions of the dispersed phase.

In the context of turbulent multiphase flows, the improvement of mass conservation in phase field methods is investigated by Soligo et al. [24] from Technische Universität Wien (Austria) and Università di Udine (Italy). This paper provides an overview and a benchmark of various existing phase field methods with specific new numerical ingredients based on profile-corrected and flux-corrected techniques. The different formulations are compared in relatively simple situations, involving bubble rise in a quiescent fluid and two droplets interacting in a shear flow, and show that the proposed corrections improve significantly mass conservation. In the last part of the paper, the motion of a swarm of large deformable droplets in wall-bounded turbulence is considered: Clear differences are reported on dispersed phase mass over time when the flux and profile corrections are activated or not.

4 Conclusions

The articles compiled in this issue are a representative collection of research activities in the area of two-phase flows, covering different methodological aspects and allowing now physical insights and technical developments. All contributions use fixed meshes, and most of them are based on numerical simulations of two-phase flows laden with finite-size objects, i.e. a dispersed phase composed of drops, bubbles or particles with an immersed interface or boundary. In all DNS-based contributions, an Eulerian approach is adopted to describe the two-phase medium with interface. All the different formulations of this approach presented in the special issue are intimately related to an Eulerian phase function, which is in fact the result of the non-conformity of the interface with the fixed and structured meshes used. We can notice that the main advantage of all these approaches is, on the one hand, to allow implementation on computer clusters for massively parallel simulations and, on the other hand, the use of parallel libraries within the solver (iterative, spectral). Compared to a decade ago, significantly larger swarms of drops, bubbles or particles can be now tracked in direct numerical simulations. Thanks to that, statistical processing and advancement of physical knowledge are therefore emerging to bridge resolved-scale simulations, large-scale quantities and models, which are useful for feeding mesoscopic Lagrangian or macroscopic Eulerian models. The collection of papers presented in this editorial, albeit not exhaustive of all the current researches in this field, demonstrates the enormous potential for thorough investigations of various aspects of finite-size particles in fluid flows and gives a new interest to DNS of two-phase flows, allowing investigation of flow configurations that become closer and closer to real-world conditions.

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