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EDITORIAL

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The study of the flow behavior of particulate material, including solid particles, bubbles, droplets or biological cells has received a growing attention over the last decades [3,7–9,12]. It is increasingly appreciated that, in dispersed systems, microscopic details of interfacial mechanics have a dominant effect on the macroscopic behavior of the flow [11]. In addition, there is intense interest in looking beyond solid interfaces to include particle-particle or particle-wall interactions with complex (fluid, elastic or viscoelastic) interfaces [2,6,10]. In recent years, this interest has led to many efforts by the multiphase fluid mechanics community, aimed at understanding interfacial interactions by capturing their effects in simulations [4,5] or experiments [1].

By relying on our numerous exchanges with the two-phase flow community and, in particular, with colleagues working on problems involving interfacial interactions in multiphase systems, we found it timely to propose a collection dedicated to the state of the art in the modeling and simulation of interfaces in flows. In 2024, 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. All submitted manuscripts were then subject to evaluation by anonymous reviewers as per the regular publication procedure in Acta Mechanica. Altogether, 9 reviewed and revised papers are published in this collection. The papers focus on the different physical, modeling and numerical issues that emerge when interfacial mechanics become important in different flow instances (ranging from viscous to turbulent). We believe that these papers provide a vivid picture of the latest advances achieved in the prediction of interfacial effects in fluid flows. Indeed, what emerges is that numerical simulations dominated by interfacial effects, which were considered nearly impossible a few decades ago, have become almost routine, or at least within the reach of capable scientists. We see the convergence of two trends. On the one hand, some of the most critical conceptual hurdles underlying the development of numerical simulation methods for interface dominated flows (such as volume-of-fluids, level-set, immersed boundary) have been solved, so that scientists can now devote themselves to develop and implement models that represent richer interfacial physics. On the other hand, the fact that problems with relatively simple boundary conditions have been simulated for some years now shows that scientists can use resolved simulations, akin to direct numerical simulations (DNS), to explore statistical or collective properties of multiphase structures displaying more complex interfacial conditions than it was possible a few years ago. For example, state-of-the-art simulation approaches allow nowadays to analyze the effect of inter-particle friction on the dynamics of concentrated suspensions [6] as opposed to assuming that particles are perfectly slippery (which is a strong assumption!).

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The articles in this collection are examples of both trends just discussed and can be divided into two categories: articles that deal with development of numerical methods and articles that focus on the exploration of new interesting flow physics. Among the first article category, the paper by El Ouafa et al. entitled “Efficient and scalable preconditioning for large saddle point systems in multiphase flow simulations” introduces a block lower-upper triangular approximation preconditioner specifically designed to address the challenges posed by large saddle point systems in multiphase flow simulations. The development of this preconditioner is grounded in an algebraic decomposition of the linear system preconditioning resulting from the discretization of the Navier–Stokes equations. The two papers by Quirós Rodríguez et al. entitled “A levelset-based cut-cell method for interfacial flows: Part 1—Navier–Stokes equations and Rayleigh-Bénard instability with melting boundary” and “A levelset-based cut-cell method for interfacial flows: Part 2—Free-surface flows and dynamic contact angle treatment” respectively, address the challenges posed by the treatment of complex geometries in computational fluid dynamics applications that couple the dynamics of two flow fields. In the first part of the study, the authors discuss a cut-cell methodology formulates discrete operators for the solution of the incompressible Navier–Stokes equations on staggered Cartesian grids in arbitrarily shaped domains, showing that such methodology (which can be can be coupled with any interface representation method) performs well in canonical two-dimensional flow configurations at low Reynolds number compared to previous works and in the presence of moving boundaries. In the second part of the study, they extend the methodology to moving contact lines and free surfaces in two-dimensional free-surface flows, showing promising results toward its future application to three-dimensional flows. The last paper devoted to the development of new numerical methods is entitled “Boiling heat transfer by phase-field method” by Roccon. In this paper, a phase-field method tailored specifically for modeling boiling phenomena and performing large-scale simulations of phase-changing flows is proposed. The method relies on the coupled numerical solution of the Navier–Stokes equations with the conservative Allen-Cahn equation and the energy equation. To close the set of governing equations, an energy-based model is used to compute the vaporization rate. The study also features a thorough validation against different benchmarks, which reveals the potential for future application of the method to complex phase-changing flows like film boiling.

We then have five articles that belong to the second category. Among these, the power of high-resolution simulation for investigating the influence of particle-particle contact on the rheology of dense suspensions is cogently exemplified by the article of Peerbooms et al. entitled “Transient behavior and steady-state rheology of dense frictional suspensions in pressure-driven channel flow.” In this article, rheological statistics for Poiseuille flow of a concentrated suspension of low-Reynolds spheres are examined comparing frictional and non-frictional particles. The article demonstrates two of the most useful aspect of DNS simulations of disperse systems. First, such simulation approach can be used to extract new rheological models and validate existing ones. Second, it can be used to deconvolute the dissipative contributions that give rise to the particle stress, which is given by the frictional contact and hydrodynamics contribution to the suspension stress in the case examined by the present article. These benefits of DNS are particularly useful in the case of dense particle systems, which are notoriously difficult to address experimentally owing to their optical opacity. Interfaces, however, come in various forms: Density interfaces and their effect on particle settling are the subject of the paper by Abdal et al. entitled “Pairwise interaction of in-line spheroids settling in a linearly-stratified fluid.” When particle pairs cross-density interfaces, their interaction dynamics is different from that occurring in uniform density systems owing to the influence of buoyancy on wake-mediated flow interactions. While some work has been published on the subject for spherical particles, the paper of Abdal et al. sheds light into the pair dynamics at finite Reynolds number for oblate and prolate spheroids. Anisotropic particles are also the subject of the paper by Eatson et al. entitled “Capillary assembly of anisotropic nanoparticles at cylindrical fluid interfaces in the immersion regime.” In this case, the particles are embedded at a fluid interface, rather than being completely immersed in a fluid. The presence of a curved interface couples with the anisotropy of the particle, giving rise to very robust effects of capillary orientation driven by surface tension which can be exploited in materials assembly applications.

A very nice example of microscopic interfacial mechanics influencing macroscopic flow behavior is provided by the article entitled “Buoyancy driven motion of non-coalescing inertial drops: microstructure modeling with nearest particle statistics” by Fintzi et al. In this article, the term microstructure refers to the various arrangements that droplets can form within dispersed buoyant emulsions and the authors use the well-known open-source code Basilisk to quantify the microstructure properties. It is shown that droplets tend to form isotropic clusters in moderately inertial flows, whereas clusters become non-isotropic and horizontally layered in high inertial regimes, with the viscosity ratio playing a major role in determining this transition. Finally, last but not least, the article entitled “Effect of thermal fluctuations on the average shape of a graphene nanosheet suspended in a shear flow" by Gravelle et al. investigates the propensity to undergo deformation under flow of graphene and other sheet-like nanomaterials. The authors characterize numerically, by combining molecular dynamics simulations and continuum boundary integral simulations, the rheological behavior of such flexible particles. The main findings discussed in the paper suggest that the orientational and deformation statistics of graphene nanosheet can be examined relying on the statistics of the hydrodynamic load on flat rigid slip plates, at least within a certain range of sheet lengths.

The collection of papers presented in this editorial, albeit not exhaustive of all the current lines of research in this field, highlights several important advances that are currently being achieved in modeling and simulating interfacial interactions in multiphase systems. The collection deals with different numerical methods, new flow physics, and touches upon emerging practical applications. It also covers a wide range of topics, from interface-resolved simulations to particle and droplet dynamics, rheology of suspensions, boiling, capillary assembly, and nanoscale deformation, all of which bridge microscopic mechanics with macroscopic flow behavior. A key perspective emerging from the collection is that future progress will hinge on integrating advanced numerical methods with high-resolution simulations to capture increasingly complex interfacial phenomena. This will enable predictive modeling across scales, guiding applications from industrial multiphase processes to materials design and nanotechnology.

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