Gdańsk, 20.10.2020

Abstract of doctoral dissertation

"MODELLING OF INTERFACIAL FLOWS WITH THE DIFFUSE-INTERFACE METHOD USING WEAKLY COMPRESSIBLE APPROACH"

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The present dissertation is dedicated to the mathematical modelling and computer simulation of the two-phase flows of immiscible fluids featuring interphasial surfaces (or interfaces), in particular gas-liquid systems. In the study the flow is described assuming that both phases are compressible fluids and low Mach numbers are set. This is in contrast to the traditional, truly incompressible approach that assumes no density variations in the bulk of the individual phases. In the regime of low Mach numbers the density variations are low and such way of modelling is referred to as weakly compressible. The type of model equations allows to solve them very efficiently using massively parallel computing devices, such as Graphics Processing Units (GPU) and multicore CPUs, which is problematic when the truly incompressible flow models are imposed (especially for GPUs).

In **Chapter 1**, I present a short survey on the artificially compressible and weakly compressible flow models as an alternative to the truly incompressible approach. I also make a short introduction to the one-fluid formulation of two-phase flows and to the interface capturing methods widely used to describe the dynamics of the interphasial surfaces.

The most important, original content of the thesis is given in three parts.

Chapter 2: First, I examine the feasibility of the Entropically Damped Artificial Compressibility (EDAC) model for simulation of single phase, wall-bounded turbulence. A favourable feature of EDAC is the purely parabolic type of governing equations resulting from the introduction of a damping ter m to the pressure evolution equation. This significantly reduces noise in the velocity divergence field when central schemes are applied for the spatial discretisation. The method of lines is used for the solution of the EDAC equations. A conservative finite difference method of purely 2nd- and mixed 4th/2nd-order is applied. The explicit 4th-order, six-stage low-storage Runge-Kutta method is used for time advancement. As expected, the mixed scheme is superior to the 2nd-order one in terms of both accuracy and computational efficiency. For the first time, the EDAC model is assessed for the direct numerical simulation of wall-bounded turbulent flow requiring a non-uniform mesh. As a particular test case I have chosen the channel flow at the friction Reynolds numbers Re_τ=180 and 395. A very good agreement with the reference data is obtained, as documented by the chosen one-point velocity statistics: the mean and r.m.s. profiles and the budgets of the Reynolds stresses. The use of explicit time discretisation and local (rather than compact) spatial schemes results in a solution algorithm that is easily and efficiently parallelisable. Very high computational performance has been achieved on a desktop computer when solving the EDAC equations using my in-house code dedicated for the GPU. The aspects of the GPU implementation are discussed.

Chapter 3: I present a novel mathematical model of two-phase interfacial flows. It is based on the EDAC model, coupled with a diffuse-interface (DI) variant of the so-called one-fluid formulation for interface capturing. The proposed EDAC-DI model conserves mass and momentum. I find appropriate values of the model parameters, in particular the numerical interface width, the interface mobility and the speed of sound. The EDAC-DI governing equations are of the mixed parabolic--hyperbolic type. For such models, the local spatial schemes along with an explicit time integration provide a convenient numerical handling together with a straightforward and efficient parallelisation of the solution algorithm. The weakly-compressible approach to flow modelling, although computationally advantageous, introduces some difficulties that are not present in the truly incompressible approaches to interfacial flows. These issues are covered in detail. I propose a robust numerical solution methodology which significantly limits spurious deformations of the interface and assures oscillation-free behaviour of the flow fields. The EDAC-DI solver is verified quantitatively in the case of a single, steady water droplet immersed in gas. The pressure jump across the interface is in good agreement with the theoretical prediction. Then, I performed a study of binary droplets coalescence and break-up in two chosen collision regimes. The topological changes are solved correctly without numerical side effects, such as false gas bubbles entrapment and mass diffusion. The computational cost incurred by the stiffness of the governing equations (due to the finite speed of sound and the interface diffusion term) can be overcome by a massively parallel execution of the solver. I achieved an attractively short computation time when the EDAC-DI code is executed on a single, desktop-type GPU.

Chapter 4: Based on the proof of concept of the novel EDAC-DI model, presented in Chapter 3, I further develop it along with the numerical methodology used for the discretisation. At the level of modelling, it is revealed that although the effective Mach numbers are low (0.05 or smaller) the compressible part of the viscous stress tensor should be taken into account in the governing equations since, due to the presence of the surface tension, the velocity divergence is high near the fluid-fluid interface. It is also shown that the maximal resolved speed of capillary waves should be used to define the reference velocity scale for the proper choice of the speed of sound and the mobility in the DI equation. Moreover, it was found that the mobility value should be at least two times higher than it was initially proposed in Chapter 3. The most important numerical improvements are: (i) the use of a less diffusive approximate Riemann solver of Harten -- Lax – van Leer with contact wave resolution for the hyperbolic part of the governing equations; (ii) the Mach number independent interface identification; (iii) smoothing of the chosen fluxes on the border of the interfacial region; (iv) the use of optimised 3rd-order strong stability preserving Runge-Kutta method for the time integration. The above improvements allow to reduce the magnitude of the parasitic currents and obtain convergence to the steady state, properly predict the topological changes independently of the spatial resolution, and increase the resolving power of the fine details of the flow. The proposed approach is validated both qualitatively and quantitatively in the case of two dimensional simulations of: a layered Poiseuille flow, steady droplet, droplets collision, the Rayleigh-Taylor instability and rising bubble. In general, very good agreement with the reference data is observed.

In **Chapter 5**, I summarise the findings of the investigation presented in this dissertation and propose directions of further development.