Phase Field/Fluctuating Hydrodynamics approach for bubble nucleation

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ABSTRACT

Vapour bubbles form in liquids by two main mechanisms: boiling, by increasing the temperature over the boiling threshold, and cavitation, by reducing the pressure below the vapour pressure threshold. The liquid can be held in these metastable states (overheating and tensile conditions, respectively) for a long time without forming bubbles. Bubble nucleation is indeed an activated process, requiring a significant amount of energy to overcome the free energy barrier and bring the liquid from the metastable conditions to the thermodynamically stable state where vapour is observed. Nowadays molecular dynamics is the unique tool to investigate such thermally activated processes. However, its computational cost limits its application to small systems (less than few tenth of nanometers) and to very short times, preventing the study of hydrodynamic interactions. In this work a continuum diffuse interface model of the two-phase fluid has been embedded with thermal fluctuations in the context of the so-called Fluctuating Hydrodynamics (FH), enabling the description of the liquid-vapour transition in extended systems and the evaluation of bubble nucleation rates in different metastable conditions by means of numerical simulations. Such an approach is expected to have a huge impact on the understanding of the nucleation dynamics since, by reducing the computational cost by orders of magnitude, it allows the unique possibility of investigating systems of realistic dimensions on macroscopic time scales.

Thin-Domain Asymptotics in Fluid Mechanics

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ABSTRACT

Failing to be able to solve the Navier-Stokes equations exactly in most situations, one must find accurate approximate solutions. The series of talks will discuss a family of asymptotic methods that depend on the slenderness of the domain The slenderness is a small parameter which can be used to develop approximations to the exact solution. Such methods will be shown to apply to solutions that are steady or unsteady, 2D or 3D, viscous or inviscid, high or low Reynolds number, and internal or external flows. A uniform approach makes all the approaches 'rational'.

Direct Numerical Simulation of Complex Turbulent Flows

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ABSTRACT

We describe the recent developments in Volume of Fluid (VOF) Interface tracking. In particular we discuss methods that are accurate for the computation of capillary forces, well-balanced with the pressure gradient, and tested in three dimensions. We also discuss momentum-conserving methods that are consistent with the VOF advection. The implementations of these methods in a massively parallel environment is a key point of the whole computationally intensive strategy.

The ultimate goal of this strategy is to allow the Direct Numerical Simulation of Interfacial and Multiphase flows. We focus on several problems of recent heightened interest, such as the atomization of jets, sheets and droplets, and the possibility in that context to perform converged simulations at least at moderate Reynolds and Weber numbers. The resulting droplet size distributions, and various turbulence statistics such as power spectra, correlation, dissipation and enstrophy integrals are used to test for convergence.

We also apply these methods to a range of other problems, such as nucleate boiling, and in that context the issue of the microscopic liquid layer that forms at the base of attached bubble. The dynamic contact angle problem is also attacked by direct numerical simulation and the dynamic contact angle singularity investigated by Huh and Scriven is compared to numerical results. A manner of mitigating the effect of this singularity on simulations is discussed and tested in the context of the Landau-Levich-Derjaguin transition form partial wetting to full wetting in the withdrawing-plate problem.

Efficient numerical schemes for gradient flows and multiphase incompressible flows

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Topics to be covered:

1. The scalar auxiliary variable (SAV) approach for gradient flows
2. Applications of SAV approach for various gradient flows
3. Phase-field models for multiphase incompressible flows
4. Efficient numerical schemes for phase-field models