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An accurate conservative level set/ghost fluid method for simulating turbulent atomization

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ABSTRACT

This paper presents a novel methodology for simulating incompressible two-phase flows by combining an improved version of the conservative level set technique introduced in [E. Olsson, G. Kreiss, A conservative level set method for two phase flow, J. Comput. Phys. 210 (2005) 225–246] with a ghost fluid approach. By employing a hyperbolic tangent level set function that is transported and re-initialized using fully conservative numerical schemes, mass conservation issues that are known to affect level set methods are greatly reduced. In order to improve the accuracy of the conservative level set method, high order numerical schemes are used. The overall robustness of the numerical approach is increased by computing the interface normals from a signed distance function reconstructed from the hyperbolic tangent level set by a fast marching method. The convergence of the curvature calculation is ensured by using a least squares reconstruction. The ghost fluid technique provides a way of handling the interfacial forces and large density jumps associated with two-phase flows with good accuracy, while avoiding artificial spreading of the interface. Since the proposed approach relies on partial differential equations, its implementation is straightforward in all coordinate systems, and it benefits from high parallel efficiency. The robustness and efficiency of the approach is further improved by using implicit schemes for the interface transport and re-initialization equations, as well as for the momentum solver. The performance of the method is assessed through both classical level set transport tests and simple two-phase flow examples including topology changes. It is then applied to simulate turbulent atomization of a liquid Diesel jet at $Re = 3000$. The conservation errors associated with the accurate conservative level set technique are shown to remain small even for this complex case.

1. Motivation and objectives

In most propulsion devices, the fuel is introduced in liquid form in a combustion chamber, where it undergoes atomization, evaporation, mixing with air, and chemical reactions in the combustion process. Since the atomization process governs the liquid droplet diameter distribution, it strongly affects both the subsequent evaporation and combustion. Consequently, full predictive capabilities for numerical tools will only be achieved once the atomization is accurately modeled. However, no satisfying models exist to this date, mostly because of the high complexity of the physics involved. Surface instabilities, ligament formation, ligament stretching and fragmentation, and droplet coalescence, all interact with turbulence to transform large scale coherent liquid structures into small scale droplets. Such a problem has scarcely been studied numerically, because it poses several great challenges.

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The first challenge lies in the fact that the material properties, such as density and viscosity, are different in the two phases. Hence, a flow solver needs to be capable of handling large density ratios, of the order of 40 for Diesel engines, up to several hundreds for aircraft engines. Second, one of the characteristics of liquid–gas flows is the presence of a surface tension force, which exists only at the interface between the liquid and the gas. The singular nature of this force leads to a difficult discretization. High robustness is therefore required from the flow solver. A third challenge lies in the interface localization and transport. While many approaches have been developed, they all suffer from various limitations, so that no clear gold standard exists today. Prerequisites for such methods include high accuracy, robustness, and the capability of accurately extracting the interface normals and curvature. Moreover, in the case of incompressible flows, the interface transport and localization should ensure that the volume of each phase is exactly conserved. Another challenge comes from the small scales that the atomization process produces. The formation of always smaller liquid structures leads to a multi-scale problem that requires high resolution to tackle, and that will generally generate liquid structures at the limit of numerical resolution.

Among the available strategies to numerically transport an interface, the volume-of-fluid (VOF) method [1] is one of the most popular. Because it relies on a liquid volume fraction scalar to represent the interface, this method ensures discrete mass conservation. However, since the VOF scalar is discontinuous across the interface, a specific geometric advection scheme is required, which puts constraints on both the accuracy of the method and the time step size. Additionally, accessing quantities such as the interface normals or curvature can prove challenging.

The front-tracking approach was introduced by Unverdi and Tryggvason [2]. It consists of discretizing the interface using an unstructured moving mesh that is transported in a Lagrangian fashion. While enjoying the benefit of a purely Lagrangian transport, this method requires frequent mesh rearrangements that affect the conservation of the liquid volume. Moreover, the parallelization of such a method is very challenging. The main limitation of this approach is the lack of automatic topology modification. Any interface merging or break-up events have to be handled manually, which can be a complex procedure, especially for three-dimensional simulations. Since topology changes are extremely frequent in primary atomization, front-tracking methods seem unadapted.

The level set method [3,4] aims at representing the interface implicitly by an iso-level of a smooth function. This smooth function is preserved with a re-initialization process. Simple Eulerian scalar transport schemes can be used to transport this function, and therefore highly accurate methods are available. Moreover, parallelization is straightforward and highly efficient, and the smoothness of the level set function makes the interface normals and curvature readily available. However, level set methods are typically plagued by mass conservation issues, for no inherent conservation property of the level set function exists. This represents a severe drawback to level set methods, considering that inaccuracies in the liquid mass of fuel in a reactive simulation could lead to large errors in quantities such as temperature, or pollutant mass fractions.

In order to improve the mass conservation property of the level set method, several hybrid approaches have been proposed. Enright et al. [5] proposed a particle level set method (PLS), where Lagrangian markers are employed to correct the front location predicted by Eulerian transport. Sussman et al. [6] proposed to couple a level set method with the VOF technique (CLSVOF), hence benefiting from both the good mass conservation property of the VOF approach and the smooth interface description of the level set method. While both these methods have been quite successful, they suffer from additional problems. Their cost is typically much greater than the cost of a simple level set method, because many particles per cell are required for an accurate solution for the PLS approach, and because of the time step size restrictions for the geometric transport of the VOF scalar for the CLSVOF method. Moreover, the complexity of these techniques is significantly greater than that of a classical level set method.

Another attempt to alleviate the mass conservation issue of level set methods has been to refine the mesh locally in order to decrease the numerical errors associated with level set transport and re-initialization. This refinement can be used for the level set equation only, such as in the case of the refined level set grid (RLSG) method of Herrmann [7], or it can be a standard arbitrary mesh refinement (AMR) approach, where the Navier–Stokes equations are also solved on the refined mesh [8]. While this approach ensures a good resolution of all structures, it remains both challenging to implement on parallel systems and significantly more expensive than classical methods. Moreover, the time step size in the case of strong local refinement is likely to be extremely restrictive.

Recently, Olsson and Kreiss [9] and Olsson et al. [10] proposed a simple modification to the level set method in order to reduce mass conservation errors while retaining the simplicity of the original method. By replacing the usual signed distance function of the classical level set approach by a hyperbolic tangent profile that is transported and re-initialized using conservative equations, they showed in Olsson and Kreiss [9] that the mass conservation errors could be reduced by an order of magnitude in comparison with the results obtained with a signed distance function. In Olsson et al. [10], they improved their re-initialization equation, and further studied their approach in the context of finite elements. The work presented here is based on the conservative level set method with the improved re-initialization equation from Olsson et al. [10]. However, the choice was made to remain in the context of finite difference methods. Starting from the observation that the conservative level set approach is difficult to use in the context of complex turbulent flows, several key modifications to this approach are introduced, resulting in both improved accuracy and robustness.

Different strategies have been developed to handle the large density ratio and the surface tension force in a flow solver. The continuum surface force approach (CSF) [11] spreads out both the density jump and the surface tension force over a few cells surrounding the interface in order to facilitate the numerical discretization. Consequently, this approach tends to misrepresent the smallest front structures. In the context of finite differences, the ghost fluid method (GFM) [12] provides a very