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A spectrally refined interface approach for simulating multiphase flows

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A B S T R A C T

This paper presents a novel approach to phase-interface transport based on pseudo-spectral sub-grid refinement of a level set function. In each flow solver grid cell, a set of quadrature points is introduced on which the value of the level set function is known. This methodology allows to define a polynomial reconstruction of the level set function in each cell. The transport is performed using a semi-Lagrangian technique, removing all constraints on the time step size. Such an approach provides sub-cell resolution of the phase-interface and leads to excellent accuracy in the transport, while a reasonable cost is obtained by pre-computing some of the metrics associated with the polynomials. To couple this approach with a flow solver, an converging curvature computation is introduced. First, a second order explicit distance to the sub-grid interface is reconstructed on the flow solver mesh. Then, a least squares approach is employed to extract the curvature from this distance function. This technique is found to combine the high accuracy and good conservation found in the particle level set method with the converging curvature usually obtained with classical high order PDE transport of the level set function. Tests are presented for both transport as well as two-phase flows, that suggest that this technique is capable of retaining the thin liquid structures that are expected in turbulent atomization of liquids.

1. Motivation and objectives

Accurately simulating complex, turbulent, multiphase flows poses several major numerical challenges. The two phases can have different material properties, such as densities in 1:1000 ratio, which renders the discretization of the Navier–Stokes equations challenging. Moreover, the curvature of the phase-interface generates a surface tension force, which acts only at the interface itself. The singular nature of this force requires specific numerical treatments. Moreover, accurately computing this force can be problematic since it requires the knowledge of the interface curvature. The interface curvature is a high order term that is obtained by taking second derivatives, and it is hence prone to amplify numerical errors. Hence, ensuring the convergence of the curvature is a major hurdle of multiphase simulations. Finally, the accuracy of the interface transport itself can lead to difficulties, since the quality of the transport for most methods deteriorates greatly when considering small-scale structures. While this may not be an issue for some applications, it can become critical for problems such as turbulent atomization, where the focus is precisely on the smallest liquid structures that are being generated by the flow. Because of all these issues, multiphase flows remain difficult to simulate with good accuracy and robustness.

Several methods have been used in the past to handle the discontinuous material properties that can be found in two-phase flows. One of the most frequently used approaches is the continuum surface force (CSF) model introduced by Brackbill et al. [1]. The idea behind this method is to smear out the discontinuities over a few grid cells in order to resolve them. While

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this enables a standard discretization of the density jump and the surface tension force, it can be expected to deteriorate the accuracy of the small-scale structures. The ghost fluid method (GFM) [2] provides an interesting alternative to CSF by expressing all discontinuities explicitly. The discretization is performed on variables that are extended by continuity in order to remove the jumps. These jumps are then explicitly added, leading to a sharp description of the interfacial terms. Additionally, GFM naturally embeds the surface tension force in the pressure equation as a pressure jump. GFM has been used recently to simulate complex problems such as the atomization of liquid diesel jets [3–5], and possible improvements to this approach have been proposed [6].

However, all these methods rely on a numerical scheme to represent and transport the phase-interface, in order to localize the jumps and to provide the interfacial curvature. Many approaches have been developed to perform these tasks, the most common being probably the volume of fluid (VOF) [7] and the level set (LS) [8,9] methods. While the first tracks the liquid volume fraction, the second tracks the phase-interface itself in the form of an iso-contour of a level set function. Other techniques exist that rely on a two-dimensional unstructured mesh in combination with Lagrangian methods to represent and transport the interface [10]. All these approaches have some strengths and shortcomings, and no method has clearly emerged as the ideal interface transport scheme.

Amongst the fundamental requirements of an interface transport scheme is the capability to compute a curvature that converges as the mesh is refined, and the capability to transport accurately small liquid structures without loosing mass. However, most of the schemes that try to improve the accuracy of the small-scale transport, either by coupling LS with VOF information [11,12] or with Lagrangian particles [13] tend to degrade the accuracy of the curvature computation, because of the use of local corrections to the LS field. Coyajee et al. [14] showed that such an approach leads to inaccurate curvatures, and that a delocalization of the corrections should be devised to avoid this problem.

Other interesting strategies have been developed to obtain a converging curvature. Sussman et al. [6] uses a version of the coupled level set/volume of fluid (CLSVOF) method where the curvature is computed directly from the volume fraction scalar instead of the taking it from the level set field, leading to a second order converging curvature. However, this approach might seem unpractical in complex problems, since large seven points-stencils are associated with the curvature computation. Herrmann [15] proposed the refined level set grid (RLSG) method to locally refine the LS mesh, in order to control the errors associated with the interfacial transport, and to retain a converging curvature. However, this method can be demanding to implement, since it requires a separate mesh for the LS field. Moreover, it is unclear how much refinement can be afforded in realistic problems, considering that an explicit time integration is used, leading to smaller time steps as the LS mesh is refined. Lagrangian-based methods that extract a converging curvature from Lagrangian particles have been developed [16]. Classical Lagrangian methods [13,10] naturally provide the strong solution rather than the weak solution to the interface transport equation, and therefore do not naturally perform curvature regularization. In the context of complex turbulent flows, Lagrangian-based methods can be challenging to employ. The complex nature of the turbulent velocity field can interfere with the ability of particle-based approaches to maintain sharp sub-grid interfacial structures, ultimately affecting the numerical accuracy and robustness of the transport.

In this work, the choice is made to improve the sub-cell representation of a level set function through a pseudo-spectral approach. In each cell, a polynomial reconstruction of the level set function is created, leading to highly improved accuracy of the transport at the smallest scales. By maintaining a Eulerian-type description of the interface, topology changes and characteristics crossings are handled automatically. Such a strategy is not new, and has been employed before [17–19]. However, all the previous work relied on a fully pseudo-spectral description of all the equations. Because of the cost associated with high order pseudo-spectral schemes, the order of the pseudo-spectral method presented by Marchandise et al. [18] remained limited. In Sussman and Hussaini [17], only level set transport tests were performed, without the coupling to the Navier–Stokes equations. Here, in a similar spirit as in the RLSG method [15], the pseudo-spectral description is used only for the LS, with the objective to introduce sub-cell interface resolution. Thanks to the potentially high order polynomial description, the frequent re-initialization step that is characteristic to level set methods becomes superfluous, since the increased accuracy handles both small and large gradients adequately. In order to allow for very fine resolution without affecting the time step size, the interface transport is performed using a semi-Lagrangian approach. Finally, a method to extract the curvature is proposed that computes a converging curvature at the scale of the flow solver grid, therefore removing all possible coupling with sub-cell fluctuations.

This paper is organized as follows: the next section presents the spectrally refined interface approach, including the transport scheme and the approach used to extract the interfacial curvature. The third section presents the coupling with the Navier–Stokes solver, as well as the methods used to solve the momentum equations. Finally, the fourth section presents numerical tests used to validate the methodology, including the numerical simulation of a turbulent two-phase shear layer.

2. Spectrally refined interface (SRI) approach

This section describes in details the pseudo-spectral, collocation-based, polynomial reconstruction of a level set function that is used to improve the quality of the interface description by introducing sub-cell resolution.

2.1. Level set methodology

In the level set approach, the interface is defined implicitly as an iso-surface G_0 of a smooth function G. Formally, any function can be used as a level set function, however a signed distance to the interface is the most commonly used function,