



Nonlinear preconditioning for efficient and accurate interface capturing in simulation of multicomponent compressible flows



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ABSTRACT

Single fluid schemes that rely on an interface function for phase identification in multicomponent compressible flows are widely used to study hydrodynamic flow phenomena in several diverse applications. Simulations based on standard numerical implementation of these schemes suffer from an artificial increase in the width of the interface function owing to the numerical dissipation introduced by an upwind discretization of the governing equations. In addition, monotonicity requirements which ensure that the sharp interface function remains bounded at all times necessitate use of low-order accurate discretization strategies. This results in a significant reduction in accuracy along with a loss of intricate flow features. In this paper we develop a nonlinear transformation based interface capturing method which achieves superior accuracy without compromising the simplicity, computational efficiency and robustness of the original flow solver. A nonlinear map from the signed distance function to the sigmoid type interface function is used to effectively couple a standard single fluid shock and interface capturing scheme with a high-order accurate constrained level set reinitialization method in a way that allows for oscillation-free transport of the sharp material interface. Imposition of a maximum principle, which ensures that the multidimensional preconditioned interface capturing method does not produce new maxima or minima even in the extreme events of interface merger or breakup, allows for an explicit determination of the interface thickness in terms of the grid spacing. A narrow band method is formulated in order to localize computations pertinent to the preconditioned interface capturing method. Numerical tests in one dimension reveal a significant improvement in accuracy and convergence; in stark contrast to the conventional scheme, the proposed method retains its accuracy and convergence characteristics in a shifted reference frame. Results from the test cases in two dimensions show that the nonlinear transformation based interface capturing method outperforms both the conventional method and an interface capturing method without nonlinear transformation in resolving intricate flow features such as sheet jetting in the shock-induced cavity collapse. The ability of the proposed method in accounting for the gravitational and surface tension forces besides compressibility is demonstrated through a model fully three-dimensional problem concerning droplet splash and formation of a crownlike feature.

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1. Introduction

The use of oscillation-free single fluid discretization schemes for numerical simulation of multiphase compressible flows is an effective and well established strategy [1–17]. These schemes use enforcement of appropriate constraints across the diffuse material interface (such as preservation of pressure and normal velocity continuity (cf. [18–20])), as the guiding principle to achieve a consistent discretization of an extended system of governing equations consisting of Euler or Navier Stokes equations for multicomponent compressible flows along with appropriate interface function equations for each of the individual species. In essence, these schemes utilize conventional discretization methods for single phase compressible flows in the respective components while invoking appropriate mixture rules to attain correct wave transmissions and reflections across the numerically diffuse material interface. Since these schemes are natural extensions of single fluid algorithms to multicomponent flows, they are simple and easy to implement, do not require phase or interface specific numerical treatment, and as a consequence have found widespread use in investigations ranging from cavitation damage in biomedical applications such as shock-wave lithotripsy [21–23] to detonation initiation in heterogeneous energetic materials [24]. A notable feature of these schemes is their natural ability to dynamically create a material interface which is indispensable in simulations that involve formation and growth of an initially nonexistent phase. This has inspired development of multiphase models for chemically reacting and cavitating flows [25–29], including relaxation methods [30–32] which are derived from the general non-equilibrium models [33–36]. These methods can also be adapted to account for the effects of gravity and surface tension [37,38] and have been extended to model two vastly different phases such as solid and gas [39].

Despite these desirable attributes schemes based on single fluid discretization of multicomponent compressible flows are often hampered by a loss of accuracy associated with an upwind discretization of the governing equations. The small but finite mesh size dependent numerical dissipation introduced by the standard shock capturing methods is necessary to ensure that accurate and convergent shock propagation speeds are recovered in simulations. This numerical dissipation, however, has a deleterious effect on the accuracy in that it leads to a growth in the width of the contact discontinuity in time. This growth persists even for high-order spatial discretizations based on WENO schemes and typically results in a convergence rate that is lower than first-order [40,41]. Ways of improving the accuracy by suppressing this numerical artifact through artificial steepening have been suggested in the literature for single component compressible flows [42–45]. Since the material interface is also a contact discontinuity, the accuracy of the numerical solution, in the vicinity of the material interface, will be limited by the accuracy of the underlying numerical method in capturing the contact wave. In case of flows with large variations in density and compressibility (water and air, for instance), the continuous increase in the width of the material interface has a severe impact on the accuracy with which shock–interface interactions are computed (see Section 7). In addition, a significantly diffuse material interface results in a loss of intricate flow features since any feature smaller than the width of the interface is not represented accurately on the computational mesh. Thus, the interface becomes increasingly less resolved in time owing to its ever increasing width. For miscible components such as gases this necessitates computationally intensive simulations on extremely fine mesh using adaptive techniques (e.g. [105–107]) or use of high-resolution schemes with grid-dependent artificial fluid properties (e.g. [108,109]). The problems that are of interest in this work involve immiscible components and any time dependent increase in the width of the material interface is completely spurious.

Our primary objective is to develop an interface capturing method which alleviates the above mentioned shortcomings of the conventional shock capturing method for simulation of multicomponent compressible flows while retaining as many of its favorable characteristics as possible. Our approach towards achieving this objective is to attribute the increasing width of the material interface to the rapid variations in the interface function. The interface function attains constant values of 1 and 0 in the interior and exterior of the associated fluid component, respectively, while undergoing a smooth but sharp transition across the material interface. On one hand, this sharp transition is necessary to ensure that the thickness of the artificial diffuse zone is kept to a minimum. On the other hand, this steep variation poses difficulties in discrete representation of the interface function on the computational mesh and has an adverse impact on the accuracy with which it can be transported or its derivatives be computed. Furthermore, monotonicity requirements which ensure that the interface function remains bounded, especially in the presence of discontinuous shocks, are of paramount importance and necessitate use of relatively low-order accurate TVD discretizations for approximation of steep gradients in the neighborhood of the interface. This exacerbates problems related to the limited accuracy with which the steep interface function can be captured on the computational mesh.

We propose to meet these challenging requirements through a novel nonlinear preconditioning technique that utilizes information on local variations of the steep interface function to define a nonlinear map to a significantly smooth transformed function. The transformed function thus obtained should be amenable to high-order discretization, be less prone to numerical errors and should allow for a more accurate computation of geometric quantities (normal and curvature) including derivatives. This technique was originally proposed in [46] to transform phase field equations for a diffuse interface model of crystalline interface motion and phase transition. Subsequently Ramirez and Beckermann [47] employed nonlinear preconditioning to simulate growth of free dendrites and advocated its use in a phase field equation based interface tracking method [48]. However, an investigation aimed at developing this technique for simulation of multicomponent compressible flows has not been undertaken to the best of the author's knowledge.

In our attempt towards development of an appropriate nonlinear preconditioning method, we are faced with two major difficulties that are specific to multicomponent compressible flows. The first complication arises from the fact that

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