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A method for compressible multimaterial flows with condensed phase explosive detonation and airblast on unstructured grids

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ABSTRACT

An efficient method for the simulation of compressible multimaterial flows with a general form of equation of state is presented for explosive detonation and airblast applications. Multimaterial flows are modeled with a volume-fraction type approach for immiscible fluids governed by the compressible Euler equations on three-dimensional unstructured grids. The five-equation quasi-conservative system is discretized in space using an edge-based finite volume approach with a second-order accurate HLLC approximate Riemann solver and temporal discretization with an explicit multistage Runge–Kutta method. The computational model is robust enough to handle flows with strong shocks, while being general enough to model materials with different equations of state and physical states. Numerical tests demonstrate the accuracy of the method for strong shock and interface interactions. A program burn method is implemented to describe the conversion of solid unreacted explosive to reacted gases in condensed phase detonations. The accuracy of the burn model is validated by comparison with published numerical results of flow profiles during detonation and for near-field airblast. Numerical simulations of hemispherical and plate-shaped explosive charge detonations are performed to investigate the influence of charge shape on airblast. The predicted pressure and impulse from simulation compare well with published experimental data.

1. Introduction

The study of compressible fluid flow with multiple materials or phases is important for a wide range of applications in astrophysics, supersonic combustion, energetic material detonations and biology. Challenging problems arise with shock-interface interactions involving bubbles, liquid droplets, or solid materials and other phenomena, such as Richtmeyer–Meshkov or Rayleigh–Taylor instabilities. The multimaterial flows considered here are a subset of multiphase flows in which the fluids are immiscible and diffusive effects, surface tension, cavitation, and phase change are neglected [1]. This includes not only flows of gases and liquids, but also solids which behave like fluids under very high pressure. Although numerical methods for resolving single phase compressible flows have reached a high level of maturity, multimaterial compressible flows present new challenges. In particular, there are difficulties in handling the interface discontinuity which may result in pressure oscillations and an unstable solution [2,3]. The development of various sharp-interface and interface-capturing methods over the last few decades has considerably advanced the study of multimaterial flows.

Sharp-interface methods, which aim to determine a precise location of the interface, include front-tracking [4,5], volume of fluid (VOF) [6–8], and level-set methods [9,10]. Front-tracking is a surface-marker method where the interface is discretized with marker points and tracked on a lower dimensional grid. Although this method offers highly accurate resolution of interfaces and detailed flow features, it has difficulties in dealing with severe interface topological changes and extension to multiple dimensions are non-trivial and expensive [5]. VOF methods [6] use a scalar volume fraction function that is advected with the flow to reconstruct an exact boundary of the material interface. Popular reconstruction procedures include the simple line interface construction (SLIC) method [7] or second-order piecewise linear methods [8]. VOF methods can resolve the interfaces sharply but present a significant computational cost for complex reconstruction algorithms. Level-set methods, introduced by Osher and Sethian [9], utilize an auxiliary function which is advected at the local flow velocity and used to recover the interface location. Level-set methods are relatively easy to implement in multiple dimensions and do not suffer from topological problems like front-tracking.

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Level-set methods are known to suffer from mass loss, but have been improved through the development of coupled level-set/VOF methods [10]. For compressible flows, Karni [2] found that a non-conservative form of the level-set equations was necessary to eliminate oscillations in pressure. The ghost fluid method [11] avoids some problems with level-sets in compressible flows by applying elements of a Lagrangian scheme. Although the ghost fluid method can naturally handle different equations of state and is relatively easy extension to higher dimensions, it is based on extrapolation of the interface state variables and has difficulties handling strong shocks and large density ratios at the interface [12].

Interface-capturing methods identify the material interface through a scalar function, such as volume or mass fraction, and allow it to numerically diffuse over several computational cells. A mixture model is utilized to determine the equation of state (EOS) for the region containing multiple components. These methods offer a simple treatment for breakup and coalescence of different fluids, but are inherently less accurate in resolving the interface. However, they remain attractive due to their ease of implementation for multiple dimensions and lower computational cost compared to sharp-interface methods [5]. Early methods for compressible multicomponent flows of perfect gases used a four-equation model with a ratio of specific heats for the mixture, γ, calculated via mass fraction weighting [13,2]. However, this method was susceptible to spurious oscillations at the interface and was later rectified by Abgrall [3] by averaging with the quantity $1/(\gamma-1)$ rather than γ in the material transport equation. Shyue [14] developed volume-fraction and γ-based models for multicomponent flows with the stiffened gas EOS. Shyue later applied this method to flows with the van der Waals EOS [15] and more complex Mie-Grüneisen EOS [16]. The number and complexity of the transport equations in the γ-based model is directly linked to the type of EOS and increases with the number of EOS parameters. In contrast, volume-fraction models require only one transport equation for the fluid mixture, independent of EOS type. Volume fraction formulations can be found for multiphase models [17,18], which include conservation equations for each phase, and various reduced models which utilize a single mixture density and energy [19]. Allaire et al. [20] proposed a five-equation model with a volume fraction transport equation and mass conservation equations for each phase, which is closer in spirit to multiphase models. Murrone [21] later derived a similar five-equation model by reduction of the Baer–Nunziato multi-phase model [22] through asymptotic analysis in the limit of zero relaxation times.

In [20], isothermal and isobaric closures of the five-equation model were investigated, and it was found that only an isobaric closure is able to avoid spurious pressure oscillations at the interface. For mathematical consistency, it is required that the EOS recovers only a single value of pressure for the calculated conserved quantities. For a truly general EOS, pressure must be found from the non-linear algebraic expression through an iterative method or a tabulated EOS [20]. However, this is costly and may not be practical for large simulations. A better solution is to develop an explicit expression for pressure of the fluid mixture for a particular EOS. Allaire et al. demonstrate this for stiffened gases, generalized van der Waals gases, and Mie-Grüneisen materials. Many EOS types can be cast into the Mie-Grüneisen form. Therefore, it is commonly used as a "general form" EOS for representing different materials [17,20,16,12,23].

The modeling of high explosive detonation and airblast is a primary subject of investigation in this work. Detonation occurs when strong shock waves propagate into an energetic material resulting in compression and heating which triggers a rapid decomposition [24]. This release of chemical energy supports the detonation wave as it continues to propagate into the unreacted material. Immediately behind the shock front, there is a thin reaction zone (<1 mm for conventional explosives such as TNT or RDX [25]) which is followed by a rarefaction wave. As the detonation wave reaches the outer surface of the explosive charge, a blast wave in the surrounding air is formed. The dense high pressure detonation product gasses accelerate outwards resulting in Rayleigh–Taylor instabilities at the contact interface [26]. In 1955, Brode [27] developed simulations of explosions using a Lagrangian method with the artificial viscosity concept of von Neumann and Richtmeyer [28]. Brode was able to represent a spherical charge of TNT explosive through an isothermal sphere initial condition and capture the complete explosion wave structure, including the evolution of the secondary shock originating from the tail of the inward traveling rarefaction wave. Much of the early work on gas-dynamics with the Euler equations utilized finite difference methods, such as the Lax-Friedrich scheme [29]. However, modern numerical methods are largely based on solutions of local Riemann problems [30] with Godunov-type methods [31] and high-order schemes.

The bursting sphere approach with TNT equivalent charge weight is a common method for modeling airblast [27,26,32]. Unfortunately, TNT equivalence values are highly subjective as they depend on standoff distance and may be obtained through a variety of methods (e.g. detonation energy, combustion energy, blast pressure, blast impulse). Additionally, the bursting sphere approach is not appropriate for scenarios where the explosive is non-spherical or near a reflective surface. For an accurate simulation of explosives, a condensed phase detonation model should be used with an EOS specifically for the detonation products, such as the Jones–Wilkins–Lee (JWL) EOS [33]. This presents a challenging problem as it requires a method which can handle very strong shocks and different material phases. In two-phase models, such as the Baer–Nunziato model [22], the solid and gas phases are not required to be in equilibrium and are described by separate sets of Euler equations and EOSs. These models can be reduced through pressure and velocity relaxation [17,18] to give a single-fluid Euler system with fluid properties that represent the mixture of reactant and products. The reaction kinetics and compaction terms (for porosity effects) are included through additional equations [34,35]. The kinetics equation includes terms related to the initiation mechanism (shock compaction, hot-spot formation) and reaction growth [24,36,34] to capture details of the detonation physics. The widely used ignition and growth models of Cochran and Chan [37] and Lee–Tarver [36] have proven valuable for modeling the shock initiation and non-ideal detonation effects. For applications that do not require such detail of the detonation process, program burn models are well established in research [38] and commercial codes [39], and provide a simplified representation of the detonation process.

In this work, we first describe the numerical model for the compressible multimaterial flows. Next, we develop a model for the condensed phase explosive detonation using a program burn approach with separate equations of state for the unreacted and reacted explosive. Then we describe the implementation within an unstructured grids framework with the positivity-preserving HLLC approximate Riemann solver and extension to second-order accuracy. We present several numerical tests for validation of the method in cases with strong shocks, different equations of state, and interface interactions. The tests include an interface advection problem, shock tube problem with complex EOS, two solid materials impact, and interaction of explosive detonation gas (modeled with JWL EOS) with a solid material. We validate the detonation model through a comparison with literature and commercial solvers for detonation and near field blast. Finally we investigate the influence of charge geometry on near field air blast. Our