Journal of Computational Physics 255 (2013) 266–292

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Numerical investigation of a modified family of centered schemes applied to multiphase equations with nonconservative sources

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ARTICLE INFO

Article history:
Received 21 January 2013
Received in revised form 17 July 2013
Accepted 1 August 2013
Available online 27 August 2013

Keywords:
Multiphase flows
Finite-volume methods
Riemann problem
Hyperbolic systems
Nonconservative sources

ABSTRACT

Systems of hyperbolic partial differential equations are frequently used to model the flow of multiphase mixtures. These equations often contain sources, referred to as nozzling terms, that cannot be posed in divergence form, and have proven to be particularly challenging in the development of finite-volume methods. Upwind schemes have recently shown promise in properly resolving the steady wave solution of the associated multiphase Riemann problem. However, these methods require a full characteristic decomposition of the system eigenstructure, which may be either unavailable or computationally expensive. Central schemes, such as the Kurganov–Tadmor (KT) family of methods, require minimal characteristic information, which makes them easily applicable to systems with an arbitrary number of phases. However, the proper implementation of nozzling terms in these schemes has been mathematically ambiguous. The primary objectives of this work are twofold: first, an extension of the KT family of schemes is proposed that formally accounts for the nonconservative nozzling sources. This modification results in a semidiscrete form that retains the simplicity of its predecessor and introduces little additional computational expense. Second, this modified method is applied to multiple, but equivalent, forms of the multiphase equations to perform a numerical study by solving several one-dimensional test problems. Both ideal and Mie–Grüneisen equations of state are used, with the results compared to an analytical solution. This study demonstrates that the magnitudes of the resulting numerical errors are sensitive to the form of the equations considered, and suggests an optimal form to minimize these errors. Finally, a separate modification of the wave propagation speeds used in the KT family is also suggested that can reduce the extent of numerical diffusion in multiphase flows.

1. Introduction

Systems of hyperbolic partial differential equations are commonly used to analyze inviscid two-phase flows [1–5]. These include the well-established Baer–Nunziato (BN) model [6], which was formulated to predict compaction-induced deflagration-to-detonation (DDT) transition in granular energetic materials. The system of equations consists of balance laws for mass, momentum, and energy for each phase, supplemented by a separate compaction equation that evolves the solid density. Neglecting the effects of interphase interactions, this system is given by:

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0021-9991/$ – see front matter
http://dx.doi.org/10.1016/j.jcp.2013.08.010

$$\frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{q}) = \mathbf{G}(\mathbf{q}) \cdot \nabla \phi_s, \tag{1}$$

where

$$\mathbf{q} = [\phi_s \rho_s,\ \phi_g \rho_g,\ \phi_s \rho_s \mathbf{u}_s,\ \phi_g \rho_g \mathbf{u}_g,\ \phi_s \rho_s E_s,\ \phi_g \rho_g E_g,\ \rho_s]^\top, \tag{2}$$

$$\mathbf{F}(\mathbf{q}) = \big[\phi_s \rho_s \mathbf{u}_s,\ \phi_g \rho_g \mathbf{u}_g,\ \phi_s \rho_s \mathbf{u}_s \mathbf{u}_s^\top + \phi_s P_s \mathcal{I},\ \phi_g \rho_g \mathbf{u}_g \mathbf{u}_g^\top + \phi_g P_g \mathcal{I},$$
$$\phi_s \rho_s \mathbf{u}_s (E_s + P_s/\rho_s),\ \phi_g \rho_g \mathbf{u}_g (E_g + P_g/\rho_g),\ \rho_s \mathbf{u}_s\big]^\top, \tag{3}$$

$$\mathbf{G}(\mathbf{q}) = [\mathbf{0},\ \mathbf{0},\ P_g \mathcal{I},\ -P_g \mathcal{I},\ P_g \mathbf{u}_s,\ -P_g \mathbf{u}_s,\ \mathbf{0}]^\top. \tag{4}$$

Here, ϕ is volume fraction; ρ is density; $\mathbf{u}$ is velocity; P is pressure; $E = e + \mathbf{u} \cdot \mathbf{u}/2$ is the total energy per unit mass and e is specific internal energy; and $\mathcal{I}$ is the identity tensor. The subscripts s and g refer to the solid and gas phases, respectively. Thus, the BN system is a two-velocity, two-pressure model, which is closed using an equation of state $e = e(\rho, P)$ for each phase, in addition to the saturation constraint $\phi_s + \phi_g = 1$. When local interphase sources accounting for mass, momentum, and energy exchange are considered, the numerical errors arising from the purely convective system (1) may be amplified substantially by the numerically stiff interphase sources. This is particularly significant for flows where detonation waves develop and very thin physical flow structures exist [7]. The presence of substantial errors arising from the convective solver can therefore make distinguishing between artificial and physical structures in these flows very difficult. This requires the convective errors to be characterized accurately before applying the modified method to systems with realistic interphase sources.

The two-phase BN model has been extended to include mixtures containing an arbitrary number of phases [8,9], such as those encountered in the dynamic compaction of metalized explosives. The resulting general form of the governing equations is similar to that given in Eq. (1):

$$\frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{q}) = \sum_{i=1}^{N} \mathbf{G}_i(\mathbf{q}) \cdot \nabla \phi_i, \tag{5}$$

where N is the number of solid phases; ϕ_i is the solid volume fraction of the i-th solid phase; and $\{\mathbf{G}_i\}_{i=1}^N$ is a sequence of rank-two source tensors. These sources, appearing in both Eqs. (1) and (5), are required to formally satisfy the Second Law of Thermodynamics [6,10], and the resulting equations cannot be posed in divergence form. The products of the sources $\mathbf{G}_i$ and the solid volume fraction gradients are referred to as nozzling terms in the literature. The use of P_g and u_s in these nozzling terms represents gas–solid interface properties based on the much higher compressibility of the gas phase relative to the solid. The resulting physical interpretation of the nozzling sources is analogous to the effects of cross-sectional area variation in single-phase, quasi-one-dimensional duct flows. Here, the solid volume fraction gradients locally accelerate the gas flow, with the porosity $1 - \phi_s$ corresponding to the duct area. Likewise, the gas–solid interface velocity is taken to be that of the solid phase u_s due to its low compressibility and its role in pore–collapse models. Other multiphase flow models utilize different interface quantities in the nozzling terms [4,11], particularly mass-averaged values useful for analyzing separated flows with a well-defined interface, rather than the dispersed flows considered here. However, the selections made in the BN model are generally well-accepted for use in gas–granular solid mixtures where gas compressibility far exceeds that of the solid.

It should be noted that a class of two-phase models has been developed by Romenski et al. [12,13] based on the theory of thermodynamically compatible systems, which allows for a fully conservative alternative formulation of the governing equations and avoids the need to consider nozzling discretizations in numerical schemes. Recently, La Spina and De' Michieli Vitturi proposed a modification to the KNP method used to solve these conservative two-phase systems [14]. However, the formulation of these alternative systems can be quite complex, and introduces additional evolution equations which increase computational expense. It is also unclear whether it is practical to obtain analogous N-phase conservative systems, particularly in specifying interphase interaction sources.

The proper discretization of nozzling sources poses a significant challenge in the development of accurate, stable numerical schemes. Many finite-volume methods are based on Godunov schemes, which require the exact or approximate solution of Riemann problems at the computational cell interfaces to compute the fluxes $\mathbf{F}(\mathbf{q})$. Upwind techniques require a full characteristic decomposition of the two-phase system (1), which was performed by Embid and Baer for the one-dimensional case to obtain simple wave solutions to the Riemann problem [15]. Although the full solution for the two-phase BN system has been obtained [16–18], this approach has several disadvantages. The correct wave structure can be difficult to determine, and the existence of non-unique solutions requires a technique to determine the physically admissible solution within the numerical scheme [16,19]. For materials that obey complex equations of state this method is prohibitively expensive. Although the exact solution of the Riemann problem for the system (5) with multiple solid phases can be obtained by extending the approach of Schwendeman et al. [17], the computational expense is significantly higher, and there is no available analogue of the two-phase approximate Riemann solver.

Consequently, the use of central schemes, which require only estimates of the local wave speeds at the cell boundaries, is particularly appealing. The family of central methods proposed by Kurganov and Tadmor [33] was originally formulated for