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Robust high order discontinuous Galerkin schemes for two-dimensional gaseous detonations

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ABSTRACT

One of the main challenges in computational simulations of gas detonation propagation is that negative density or negative pressure may emerge during the time evolution, which will cause blow-ups. Therefore, schemes with provable positivity-preserving of density and pressure are desired. First order and second order positivity-preserving schemes were well studied, e.g., [6,10]. For high order discontinuous Galerkin (DG) method, even though the characteristicwise TVB limiter in [1,2] can kill oscillations, it is not sufficient to maintain the positivity. A simple solution for arbitrarily high order positivity-preserving schemes solving Euler equations was proposed recently in [22]. In this paper, we first discuss an extension of the technique in [22–24] to design arbitrarily high order positivity-preserving DG schemes for reactive Euler equations. We then present a simpler and more robust implementation of the positivity-preserving limiter than the one in [22]. Numerical tests, including very demanding examples in gaseous detonations, indicate that the third order DG scheme with the new positivity-preserving limiter produces satisfying results even without the TVB limiter.

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1. Introduction

Gas detonation is a supersonic flow phenomenon that consists of a precursor shock igniting a combustible mixture gas, with a thin reaction zone behind the shock. Although detonation has been studied for many years, it remains an active area of research in both theoretical studies and numerical simulations due to its practical importance. To study the gaseous detonation numerically, the governing equations could be chosen as the Euler equations describing inviscid compressible flow with the chemical reaction added. There are many difficulties in designing stable numerical schemes solving a general hyperbolic system with source terms accurately. For example, the width of reaction zone attached to the shock might be very narrow, see [3], and the source term might induce stiffness, see [9].

In this paper, we focus on how to render numerical schemes stable for gaseous detonation simulation. In practice, it is quite often to encounter situations in which the density or pressure of the numerical solutions becomes negative. For

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instance, highly energetic flows may contain regions with a dominant kinetic energy, and a relatively small internal energy which is easy to become negative in the simulation. Another example is the computational simulation of gas detonation propagation through different geometries. The shock diffraction may result in very low density and pressure. Under such conditions, it has been observed that numerical schemes may produce negative density or pressure, even for non-reactive gas flows, which can lead to blow-ups. This phenomenon tends to be amplified by the chemical activity. Crude replacement of negative values by positive ones not only destroys local and global conservation, but also often does not cure the instability. Therefore, it is strongly desirable to design schemes with a provable positivity-preserving property. Moreover, a conservative positivity-preserving scheme can be easily proved to be L^1 -stable.

First order and second order positivity-preserving schemes were well studied in the literature [6,10]. So we are mainly interested in high order positivity-preserving schemes. On the one hand, low order schemes have been used in the simulation of detonation waves [12,13], but numerical results have some deviation from the experimental results. On the other hand, some high order schemes have been developed in recent years [5,4,16,19,20]. Successful high order numerical schemes for hyperbolic conservation laws, for example, the Runge–Kutta discontinuous Galerkin (RKDG) method in [1,2], the essentially non-oscillatory (ENO) finite volume and finite difference schemes in [7,18], and the weighted ENO (WENO) finite volume and finite difference schemes in [11,8], do not automatically satisfy a strict positivity-preserving property. In fact, they may all fail for very demanding low density or low pressure test cases. Special treatments for different schemes may lead to positivity-preserving and conservation, but it is very difficult to simultaneously also maintain high order accuracy for smooth solutions with such treatments. Constructing high order schemes which automatically preserve the positivity of density and pressure is highly nontrivial. In [22,23], two of the authors proposed an arbitrarily high order positivity-preserving Runge-Kutta discontinuous Galerkin method for compressible Euler equations, which were extensions and applications of [21,15]. The main idea is to find some straightforward sufficient condition for the DG method of any spatial order of accuracy with first order Euler forward time discretization to keep positivity. A simple limiter which is easy and inexpensive to implement will enforce the sufficient condition without destroying conservation and accuracy. Strong stability preserving (SSP) high order Runge-Kutta or multi-step methods [18,17] will still keep the positivity since they are convex combinations of Euler forward. With this limiter, high order RKDG methods will be positivity-preserving of density and pressure during the time evolution.

We will show an extension of this method to Euler system with an Arrhenius form of chemical reaction source term and an additional equation for the evolution of the reaction rate, which are typical governing equations for modeling the gaseous detonation. Besides density and pressure, our scheme can also maintain the positivity of the reaction rate, which is crucial to the stability of schemes in this model. We also propose a more robust implementation of the positivity-preserving limiter. The DG scheme with this new positivity-preserving limiter is stable even for very strong shocks without the need of additional TVB limiters. Extensive numerical tests of the third order DG method are reported to demonstrate the effectiveness of our scheme.

2. Positivity-preserving high order discontinuous Galerkin method for two-dimensional reactive Euler equations

2.1. Preliminaries

We consider the dimensionless two-dimensional compressible Euler equations with a source term representing chemical reactions for the ideal gas,

$$\mathbf{w}_t + \mathbf{f}(\mathbf{w})_x + \mathbf{g}(\mathbf{w})_y = \mathbf{s}(\mathbf{w}), \quad t \ge 0, \quad (x, y) \in \mathbb{R}^2,$$

$$(2.1)$$

$$\mathbf{w} = \begin{pmatrix} \rho \\ m \\ n \\ E \\ \rho Y \end{pmatrix}, \quad \mathbf{f}(\mathbf{w}) = \begin{pmatrix} m \\ \rho u^2 + p \\ \rho uv \\ (E+p)u \\ \rho uY \end{pmatrix}, \quad \mathbf{g}(\mathbf{w}) = \begin{pmatrix} n \\ \rho uv \\ \rho v^2 + p \\ (E+p)v \\ \rho vY \end{pmatrix}, \quad \mathbf{s}(\mathbf{w}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \omega \end{pmatrix}$$
(2.2)

with

$$m = \rho u, \quad n = \rho v, \quad E = \frac{1}{2}\rho u^2 + \frac{1}{2}\rho v^2 + \frac{p}{\gamma - 1} + \rho qY,$$

where q is the heat release of reaction, γ is the specific heat ratio and Y denotes the reactant mass fraction. The source term is assumed to be in an Arrhenius form

$$\omega = -\widetilde{K}\rho Y e^{-T/T}$$

where $T = \frac{p}{\rho}$ is the temperature, \tilde{T} is the activation temperature and \tilde{K} is a constant. The eigenvalues of the Jacobian $\mathbf{f}'(\mathbf{w})$ are u - c, u, u, u, u, u + c and the eigenvalues of the Jacobian $\mathbf{g}'(\mathbf{w})$ are v - c, v, v, v, v + c, where $c = \sqrt{\gamma \frac{p}{\rho}}$.

We define the set of admissible states by

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