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Positivity-preserving moving mesh scheme for two-step reaction model in two dimensions☆

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ABSTRACT

In this paper, we have proposed a moving mesh scheme for the two-step chemical reaction model in two dimensions. This moving mesh scheme consists of two independent parts: governing equations evolution and mesh-redistribution. The second-order finite volume scheme is used in the governing equations evolution part. In the mesh-redistribution part, the mesh points are first redistributed, and then the cell averages of the conservative variables are remapped onto the new mesh in a conservative way. In addition, the positivity-preserving improvements are shown for the two parts. The positivity-preserving thresholds guarantee the average value positive, and then an improved implementation is given to make each cell value positive. Several numerical experiments are carried out to demonstrate the accuracy and effectiveness of the proposed method.

1. Introduction

Chemical reaction kinetics plays major roles in many fields of modern physics. 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. There are two main challenges in detonation simulations. One is to calculate the process of energy release in reaction flow; the other one is to capture the strong discontinuity in detonation waves. Successful solutions to above two challenges depend on the development of chemical reaction models and numerical schemes, respectively [1].

Many chemical reaction models such as the C-J model, the two-step reaction model, and the detailed chemical reaction model have been applied to numerical simulations of detonation waves. The two-step chemical reaction model can describe the chemical reaction process and does not need many resources [2,3]. Thus the two-step chemical reaction model is also studied by many scholars, which is also studied here.

To capture the strong discontinuity in detonation waves, increasing the number of mesh cells is a conventional method. However, with the increase of mesh cells, the calculating quantity rapidly grows. Mesh adaptation is an indispensable tool for use in the efficient numerical solution of this type of problem. The moving mesh method is one of the mesh adaptation methods, which relocate mesh point positions while maintaining the total number of mesh points and the mesh connectivity [4–6]. Especially, Tang and Tang proposed a moving mesh method that contained two parts: physical PDE time evolution and mesh redistribution [7]. The physical PDE time evolution and mesh redistribution was alternating, and conservative interpolation was used to transfer solutions from old mesh to new mesh. This method is shown to work well generally for hyperbolic conservation. Han, He and Tang applied this moving mesh method to two-dimensional ideal magnetohydrodynamics equations [8,9]. In this paper, we extend Tang and Tang's method to two-step chemical reaction model and focus on how to render numerical schemes stable for gaseous detonation situation. In practice, it is quite often to encounter situation in which the density or pressure of the numerical solutions become negative. For instance, highly energetic flows may contain regions with a dominant kinetic energy, and a relatively small internal energy that 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.

There are some positivity-preserving results have studied by some scholars about the numerical schemes under the fixed mesh. Einfeldt et al. started the study about the positivity-preserving one-dimensional Euler equations [10]. A general framework is established which shows the positivity of density and pressure whenever the underlying one-dimensional first-order building block based on an exact or approximate Riemann solver and the reconstruction are

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both positivity-preserving by Perthame and Shu [11]. The positivity-preserving high-order schemes are attracted attentions and many papers have been appeared in recently years [12–17]. Especially Wang et al. extended the positivity-preserving schemes to the Euler equations with an Arrhenius form of chemical reaction source term and an additional equation for the evolution of the reaction rate in two dimensions [17]. However, there are few discussions about positivity-preserving moving mesh schemes, which we focus on here. This article is organized as follows. Section 2 introduces the chemical and physical model. Section 3 presents the numerical scheme. Section 4 is devoted to the positivity-preserving analysis. Section 5 conducts several numerical experiments to demonstrate the efficiency of the proposed adaptive moving mesh method. The paper ends with a conclusion and discussion in Section 6.

2. Chemical and physical model

Instead of using many real elementary reactions, a two-step reaction model was utilized in the calculation. Two-step reaction model considers a complicated chemical reaction to be an induction reaction and an exothermic reaction. For both induction reaction and exothermic reaction, the progress parameters α and β are unity at first, then α decreases to zero, β decreases until an equilibrium state is reached. The rates ω_α and ω_β are given as follows [18]

$$\omega_\alpha = \frac{d\alpha}{dt} = -k_\alpha \rho \exp\left(-\frac{E_\alpha}{RT}\right), \tag{1}$$

$$\omega_\beta = \frac{d\beta}{dt} = \begin{cases} 0 (\alpha > 0), \\ -k_\beta p^2 \left[\beta^2 \exp\left(-\frac{E_\beta}{RT}\right) - (1-\beta)^2 \exp\left(-\frac{E_\beta + Q}{RT}\right)\right] (\alpha \le 0), \end{cases} \tag{2}$$

where ρ is the mass density, p the pressure, T the temperature, R the gas constant, Q the heat release parameter, k_α and k_β the constants of reaction rates, and E_α and E_β the activation energies.

In deriving fundamental equations, the gas is assumed to be perfect, nonviscous, and non-heat-conducting. Governing equations for a two-dimensional gaseous detonation problem, including the above chemical reaction, are

$$\frac{\partial \mathbf{w}}{\partial t} + \frac{\partial}{\partial x}\mathbf{F}(\mathbf{w}) + \frac{\partial}{\partial y}\mathbf{G}(\mathbf{w}) = \mathbf{S}(\mathbf{w}), \tag{3}$$

$$\mathbf{w} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ E \\ \rho\alpha \\ \rho\beta \end{pmatrix}, \mathbf{F}(\mathbf{w}) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (E+p)u \\ \rho\alpha u \\ \rho\beta u \end{pmatrix}, \mathbf{G}(\mathbf{w}) = \begin{pmatrix} \rho v \\ \rho v^2 + p \\ \rho uv \\ (E+p)v \\ \rho\alpha v \\ \rho\beta v \end{pmatrix},$$

$$\mathbf{S}(\mathbf{w}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \omega_a \\ \omega_\beta \end{pmatrix}.$$

where u and v are the Cartesian components of the fluid velocity in x and y direction. Total energy density E is defined as

$$E = \frac{p}{\gamma - 1} + \frac{\rho\left(u^2 + v^2\right)}{2} + \rho\beta Q. \tag{4}$$

Here γ is the specific heat ratio. We are interested in schemes for (3) producing the numerical solutions in the admissible set G. G will be given and be proven to be a convex set in Lemma 2.1.

Lemma 2.1. *Define the set of admissible states by*

$$G = \left\{ \mathbf{w} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ E \\ \rho\alpha \\ \rho\beta \end{pmatrix} \middle| \rho > 0 \text{ and } p(\mathbf{w}) \ge 0, \beta \ge 0 \right\}, \tag{5}$$

then G is a convex set.

Proof. From (4), we have

$$p(\mathbf{w}) = (\gamma - 1)\left[E - \frac{1}{2}\frac{(\rho u)^2}{\rho} - \frac{1}{2}\frac{(\rho v)^2}{\rho} - \rho\beta Q\right]. \tag{6}$$

For $0 \le s \le 1$, $\mathbf{w}_1 = (\rho_1, \rho_1 u_1, \rho_1 v_1, E_1, \rho_1\alpha_1, \rho_1\beta_1)^T$ and $\mathbf{w}_2 = (\rho_2, \rho_2 u_2, \rho_2 v_2, E_2, \rho_2\alpha_2, \rho_2\beta_2)^T$, we have the following equivalent relations,

$$\begin{aligned} &p \text{ is a concave function} \\ &\Leftrightarrow p(s\mathbf{w}_1 + (1-s)\mathbf{w}_2) \ge p(s\mathbf{w}_1) + p((1-s)\mathbf{w}_2) \\ &\Leftrightarrow \tilde{p}(s\mathbf{w}_1 + (1-s)\mathbf{w}_2) - (\gamma-1)[Q(s\rho_1\beta_1 + (1-s)\rho_2\beta_2)] \\ &\ge \tilde{p}(s\mathbf{w}_1) - (\gamma-1)Qs\rho_1\beta_1 + \tilde{p}((1-s)\mathbf{w}_2) - (\gamma-1)Q(1-s) \\ &\quad \rho_2\beta_2 \\ &\Leftrightarrow \tilde{p}(s\mathbf{w}_1 + (1-s)\mathbf{w}_2) \ge \tilde{p}(s\mathbf{w}_1) + \tilde{p}((1-s)\mathbf{w}_2) \\ &\Leftrightarrow \tilde{p} \text{ is a concave function,} \end{aligned} \tag{7}$$

where

$$\tilde{p}(\mathbf{w}) = (\gamma - 1)\left[E - \frac{1}{2}\frac{(\rho u)^2}{\rho} - \frac{1}{2}\frac{(\rho v)^2}{\rho}\right].$$

when $\rho > 0$, Zhang and Shu have claimed that $\tilde{p}$ is a concave function [12,20]. So $p(\mathbf{w})$ is a concave function of $\mathbf{w}$. In addition, G is a convex set. □

3. Numerical scheme

Our adaptive scheme is formed by two independent parts: the evolution of the governing equation and the iterative mesh redistribution.

3.1. Second-order accurate Godunov scheme on quadrilateral meshes

In the following, we begin to introduce second-order accurate Godunov scheme of (3) on quadrilateral meshes. The average on the (i,j) cell $K_{i,j}$ is $\bar{\mathbf{w}}_{i,j}$. Integrating (3) over $K_{i,j}$, we have

$$\iint_{K_{i,j}} \frac{\partial \mathbf{w}}{\partial t} d\sigma + \iint_{K_{i,j}} \left(\frac{\partial}{\partial x}\mathbf{F}(\mathbf{w}) + \frac{\partial}{\partial y}\mathbf{G}(\mathbf{w})\right) d\sigma = \iint_{K_{i,j}} \mathbf{S}(\mathbf{w}) d\sigma. \tag{8}$$

Applying the Green-Gauss's theorem and rewriting, we have

$$|K_{i,j}| \frac{\partial}{\partial t}\bar{\mathbf{w}}_{i,j} + \oint_{\partial K_{i,j}} \mathcal{F}(\mathbf{w}) \cdot \mathbf{n}_{i,j} ds = \iint_{K_{i,j}} \mathbf{S}(\mathbf{w}) d\sigma, \tag{9}$$

where $|K_{i,j}|$ is the area of the element $E_{i,j}$. $\mathbf{n}_{i,j}$ is the outward unit normal vector of the boundary $\partial K_{i,j} := \bigcup_{k=1}^{4} e_{i,j}^k$, and $\mathcal{F}(\mathbf{w}) = \langle \mathbf{F}(\mathbf{w}), \mathbf{G}(\mathbf{w}) \rangle$. The Lax–Friedrichs flux is defined by

$$\mathbf{h}(\mathbf{u}, \mathbf{v}, \mathbf{n}) = \frac{1}{2}[\mathcal{F}(\mathbf{u}) \cdot \mathbf{n} + \mathcal{F}(\mathbf{v}) \cdot \mathbf{n} - a(\mathbf{v} - \mathbf{u})], \tag{10}$$