Application of Positivity-Preserving Discontinuous Galerkin Schemes for Gaseous Detonations

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1 Introduction

In numerical simulation of gas detonation propagation, the density, pressure, or chemical reaction process is sometimes negative. For example, when detonation wave passes through certain complex geometries, there appear some domains with low density and pressure in the diffraction area. Under such conditions, density and pressure may become negative in the simulation, which runs counter to the actual physical process and causes blow-ups. The traditional solution is to replace the negative values by positive ones or zero, resulting in the destruction of conservation and stability [1]. How to build positivity-preserving schemes without destroying the accuracy, conservation and stability becomes an urgent problem in the high order numerical simulation of detonation wave.

First order and second order positivity-preserving schemes were well studied in [2, 3]. High order positivity-preserving Runge-Kutta discontinuous Galerkin (RKDG) scheme for two-dimensional Euler equations with one-step chemical reaction is proposed in [1]. RKDG is an important method in numerical simulation. It has the ability to easily handle boundary conditions with complicated geometry. It is an efficient method suitable for parallel computing. In this paper, we construct high order positivity-preserving RKDG scheme in two-dimensional Euler equations with two-step chemical reaction to solve the problem of negative density or pressure in numerical simulation. The reliability of RKDG method with positivity-preserving limiter is verified by several examples of detonation diffraction.

2 Positivity-preserving discontinuous Galerkin method

We consider two-dimensional Euler equations with two-step chemical reaction

$$\frac{\partial \boldsymbol{U}}{\partial t}+\frac{\partial \boldsymbol{F}}{\partial x}+\frac{\partial \boldsymbol{G}}{\partial y}=\boldsymbol{S} \tag{1}$$

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$$\boldsymbol{U}=\begin{pmatrix}\rho\\ \rho u_x\\ \rho u_y\\ \rho E\\ \rho\alpha\\ \rho\beta\end{pmatrix},\ \boldsymbol{F}=\begin{pmatrix}\rho u_x\\ \rho u_x^2+p\\ \rho u_x u_y\\ \rho u_x(E+p/\rho)\\ \rho u_x\alpha\\ \rho u_x\beta\end{pmatrix},\ \boldsymbol{G}=\begin{pmatrix}\rho u_y\\ \rho u_x u_y\\ \rho u_y^2+p\\ \rho u_y(E+p/\rho)\\ \rho u_y\alpha\\ \rho u_y\beta\end{pmatrix},\ \boldsymbol{S}=-\begin{pmatrix}0\\ 0\\ 0\\ 0\\ \rho\omega_\alpha\\ \rho\omega_\beta\end{pmatrix},$$

$$p=\rho RT,\ E=\frac{RT}{\gamma-1}+\beta q+\frac{1}{2}(u_x^2+u_y^2),\ \omega_\alpha=\frac{\mathrm{d}\alpha}{\mathrm{d}t}=-k_1\rho\exp(-E_1/RT),$$

$$\omega_\beta=\frac{\mathrm{d}\beta}{\mathrm{d}t}=\begin{cases}0, & \alpha>0\\ -k_2p^2\left[\beta^2\exp\left(\dfrac{-E_2}{RT}\right)-(1-\beta)^2\exp\left(-\dfrac{E_2+q}{RT}\right)\right], & \alpha\le 0\end{cases}$$

where p,ρ,E,T,u_x,u_y denote pressure, density, energy, temperature, *x*-velocity and *y*-velocity; α and β denote chemical reaction process; E_1 and E_2 denote activation energy, k_1, k_2 denote chemical reaction rate constant, ω_α denote induction-reaction process rate, ω_β denote exothermic-reaction process rate.

We define the set of admissible states by

$$G=\left\{\boldsymbol{U}=\begin{pmatrix}\rho\\ \rho u_x\\ \rho u_y\\ \rho E\\ \rho\alpha\\ \rho\beta\end{pmatrix}\middle|\ \rho>0,p\ge 0\ \text{and}\ \beta\ge 0\right\}.$$

It is easy to know that *p* is a concave function of $\boldsymbol{U}$, and *G* is a convex set.

The weak formulation of DG method solving (1) is, find $\boldsymbol{U}_h\in V_h$ satisfying,

$$\frac{\mathrm{d}}{\mathrm{d}t}\iint_K \boldsymbol{U}_h v_h\,\mathrm{d}x\mathrm{d}y+\sum_{e\in\partial K}\int_e \boldsymbol{h}_{K,e}(\boldsymbol{U}_h^{int(K)},\boldsymbol{U}_h^{ext(K)},v_{e,K})v_h\,\mathrm{d}\Gamma$$
$$-\iint_K \boldsymbol{F}(\boldsymbol{U}_h)\cdot\nabla v_h\,\mathrm{d}x\mathrm{d}y=\iint_K \boldsymbol{s}(\boldsymbol{U}_h)v_h\,\mathrm{d}x\mathrm{d}y \tag{2}$$

where $\boldsymbol{F}(\boldsymbol{U}_h)=(\boldsymbol{f},\boldsymbol{g})$, $v_{e,K}$ is the outward normal vector of the edge *e* on the element *K*. We consider the Lax-Friedrichs flux,

$$\boldsymbol{h}(\boldsymbol{U},\boldsymbol{V},v_e)=\frac{1}{2}\left[\boldsymbol{F}(\boldsymbol{U})\cdot v_e+\boldsymbol{F}(\boldsymbol{V})\cdot v_e-a(\boldsymbol{V}-\boldsymbol{U})\right],\quad a=\left\|\left(\left|<u_x,u_y>\right|+c\right)\right\|_\infty.$$

To construct positivity-preserving schemes, the most important step is to achieve positivity for the cell averages. Taking the test function as $v_h=1$ in (2), we get the scheme satisfied by the cell averages in the DG method. Consider the Euler forward time discretization,

$$\frac{|K|}{\Delta t}(\bar{\boldsymbol{U}}_k^{n+1}-\bar{\boldsymbol{U}}_k^{n})+\sum_{e\in\partial K}\int_e \boldsymbol{h}\left(\boldsymbol{U}_h^{int(K)},\boldsymbol{U}_h^{ext(K)},v_e\right)\mathrm{d}\Gamma=\iint_K \boldsymbol{s}(\boldsymbol{U}_h)\,\mathrm{d}x\mathrm{d}y. \tag{3}$$

First, we consider rectangular meshes. At time level *n*, assume $\boldsymbol{q}_{ij}(x,y)$ is the DG polynomial of degree *k* on the (i,j) cell $\left[x_{i-\frac{1}{2}},x_{i+\frac{1}{2}}\right]\times\left[y_{j-\frac{1}{2}},y_{j+\frac{1}{2}}\right]$ with $\boldsymbol{U}^+_{i-\frac{1}{2},j}(y)$, $\boldsymbol{U}^-_{i+\frac{1}{2},j}(y)$, $\boldsymbol{U}^+_{i,j-\frac{1}{2}}(x)$, $\boldsymbol{U}^-_{i,j+\frac{1}{2}}(x)$ denote the traces of $\boldsymbol{q}_{ij}(x,y)$ on the four edges respectively.

We use a *L*-point Gauss quadrature for the line integral and two *L*-point Gauss quadratures for the double integral in (3) where $L \geq k+1$. Let w_k denote the Gauss quadrature weights on $\left[-\frac{1}{2},\frac{1}{2}\right]$ such that $\sum_{k=1}^{L} w_k = 1$.

Then (3) becomes

$$\bar{\boldsymbol{U}}_{ij}^{n+1} = \bar{\boldsymbol{U}}_{ij}^{n} - \lambda_1 \sum_{k=1}^{L} w_k \left[\boldsymbol{h}_1(\boldsymbol{U}^-_{i+\frac{1}{2},l}, \boldsymbol{U}^+_{i+\frac{1}{2},l}) - \boldsymbol{h}_1(\boldsymbol{U}^-_{i-\frac{1}{2},l}, \boldsymbol{U}^+_{i-\frac{1}{2},l}) \right]$$
$$-\lambda_2 \sum_{k=1}^{L} w_k \left[\boldsymbol{h}_2(\boldsymbol{U}^-_{l,j+\frac{1}{2}}, \boldsymbol{U}^+_{l,j+\frac{1}{2}}) - \boldsymbol{h}_2(\boldsymbol{U}^-_{l,j-\frac{1}{2}}, \boldsymbol{U}^+_{l,j-\frac{1}{2}}) \right] + \Delta t \sum_{m=1}^{L}\sum_{k=1}^{L} w_m w_k \boldsymbol{s}(\boldsymbol{U}(x_i^m, y_j^k)) \quad (4)$$

Theorem 2.1. $\forall a_1, a_2 > 0$ such that $a_1 + a_2 = 1$. If the DG polynomial $\boldsymbol{q}_{ij}(x,y) \in G$, then the scheme (4) is positivity-preserving, namely, $\bar{\boldsymbol{U}}_{ij}^{n+1} \in G$ under the time step restriction

$$a(\lambda_1+\lambda_2) \leq a_1 \hat{w}_1, \ \max\left\{ \Delta t \cdot k_2 p^2 \left[\beta \exp\left(\frac{-E_2}{RT}\right) - \frac{(1-\beta)^2}{\beta} \exp\left(-\frac{E_2+q}{RT}\right) \right] \right\} \leq a_2,$$

where $\hat{w}_k$ denote the Gauss-Lobatto quadrature weights on $\left[-\frac{1}{2},\frac{1}{2}\right]$ such that $\sum_{k=1}^{N} \hat{w}_k = 1$.

Second, we consider triangular mesh K. We can obtain the conclusion for triangular meshes similar as rectangular meshes. (4) becomes:

$$\bar{\boldsymbol{U}}_K^{n+1} = \bar{\boldsymbol{U}}_K^{n} - \frac{\Delta t}{|K|} \sum_{i=1}^{3}\sum_{j=1}^{L} \boldsymbol{h}\left(\boldsymbol{U}_{i,j}^{\mathrm{int}(K)}, \boldsymbol{U}_{i,j}^{\mathrm{ext}(K)}, \nu^i\right) w_j l_K^i + \Delta t \sum_{\gamma=1}^{M} \tilde{w}_\gamma \boldsymbol{s}(\boldsymbol{U}(x_K^\gamma)) \quad (5)$$

where l_K^i $(i=1,2,3)$ denote the length of triangle's edges. $\boldsymbol{\nu}^i$ $(i=1,2,3)$ denote its outward unit normal vector. Assume the line integrals in (5) are solved by the *L*-point Gauss quadrature where $L \geq k+1$, and the source integral is solved by a *M*-point quadrature on a triangle with positive weights (for example, 7-point quadrature, see [4-6] for more details).

Theorem 2.2. $\forall a_1, a_2 > 0$ such that $a_1 + a_2 = 1$. If the DG polynomial $\boldsymbol{q}_{ij}(x,y) \in G$, then the scheme (5) is positivity-preserving, namely, $\bar{\boldsymbol{U}}_{ij}^{n+1} \in G$ under the time step restriction

$$a\frac{\Delta t}{|K|}\sum_{i=1}^{3} l_K^i \leq \frac{2}{3} a_1 \hat{w}_1, \ \max\left\{ \Delta t \cdot k_2 p^2 \left[\beta \exp\left(\frac{-E_2}{RT}\right) - \frac{(1-\beta)^2}{\beta} \exp\left(-\frac{E_2+q}{RT}\right) \right] \right\} \leq a_2.$$

Then we show the steps of positivity-preserving limiter:

First, enforce the positivity of density. For each element *K*, compute

$$\hat{\rho}_K(x) = \theta_K^1 \rho_K(x) + (1-\theta_K^1)\bar{\rho}_K, \quad \theta_K^1 = \min_{x \in S_K}\left\{1, \left|\frac{\bar{\rho}_K - \varepsilon}{\bar{\rho}_K - \rho_K(x)}\right|\right\}.$$

ε is a very small positivity number for all *K* to avoid $\rho_K = 0$. We can choose $\varepsilon = 10^{-13}$.

Similarly, enforce the positivity of $\rho\beta_K$

$$\overline{\overline{\rho\beta}}_K(x) = \theta_K^2[\rho\beta_K(x) - \overline{\rho\beta}_K] + \overline{\rho\beta}_K, \quad \theta_K^2 = \min_{(x,y)\in S_K}\left\{1, \left|\frac{\overline{\rho\beta}_K}{\overline{\overline{\rho\beta}}_K - \rho\beta_K(x)}\right|\right\}.$$

Second, enforce the positivity of pressure. We should find θ_K such that

$$\tilde{\boldsymbol{U}}_K(x) = \theta_K[\hat{\boldsymbol{U}}_K(x) - \bar{\boldsymbol{U}}_K] + \bar{\boldsymbol{U}}_K \ \text{ and } \ p(\tilde{\boldsymbol{U}}_K(x)) \geq 0.$$

Notice that *p* is a concave function of $\boldsymbol{U}$, thus we have

$$p(\theta_K[\hat{\boldsymbol{U}}_K(x)-\bar{\boldsymbol{U}}_K]+\bar{\boldsymbol{U}}_K)=p(\theta_K\hat{\boldsymbol{U}}_K(x)+(1-\theta_K)\bar{\boldsymbol{U}}_K)\geq\theta_K p(\hat{\boldsymbol{U}}_K(x))+(1-\theta_K)p(\bar{\boldsymbol{U}}_K)$$

because of Jensen's inequality.

Let $\theta_K p(\hat{\boldsymbol{U}}_K(x))+(1-\theta_K)p(\bar{\boldsymbol{U}}_K)=0$, then

$$\theta_K=\frac{p(\bar{\boldsymbol{U}}_K)}{p(\bar{\boldsymbol{U}}_K)-p(\hat{\boldsymbol{U}}_K(x))}$$

satisfies that $p(\tilde{\boldsymbol{U}}_K(x))\geq 0$.

The method does not destroy the accuracy and stability. It is proved in [1,6].

3 Numerical test

In this section, we verify the reliability of RKDG method with positivity-preserving limiter by several examples of detonation diffraction. In simulations, the parameters in chemical reaction are: $\gamma=1.2$, $k_1=27.7$, $k_2=k_1/20.0$ and $q=1.71$.

Example 3.1 We simulate the propagation of the detonation wave from narrow duct into unconstraint space when corner angle is 90°. An initiation zone is set at $x\in[0,1]$, and its initial value is given as $(\rho,u_x,u_y,E,\alpha,\beta)=(11,6.18,0,970,-1,1)$. The rest region is filled with the unreacted H_2/O_2 mixture with initial condition of $(\rho,u_x,u_y,E,\alpha,\beta)=(1,0,0,55,1,1)$. The left inlet is inflow condition. The other boundaries are rigid walls.

Fig.1 presents the colored contour of density and pressure. We observe that a rarefaction zone appear at the corner after diffraction when detoantion wave propagates into the large space. The pressure and density in the zone lower sharply. In the simulation, although the pressure and density drop very low at rarefaction region, they have not been negative.

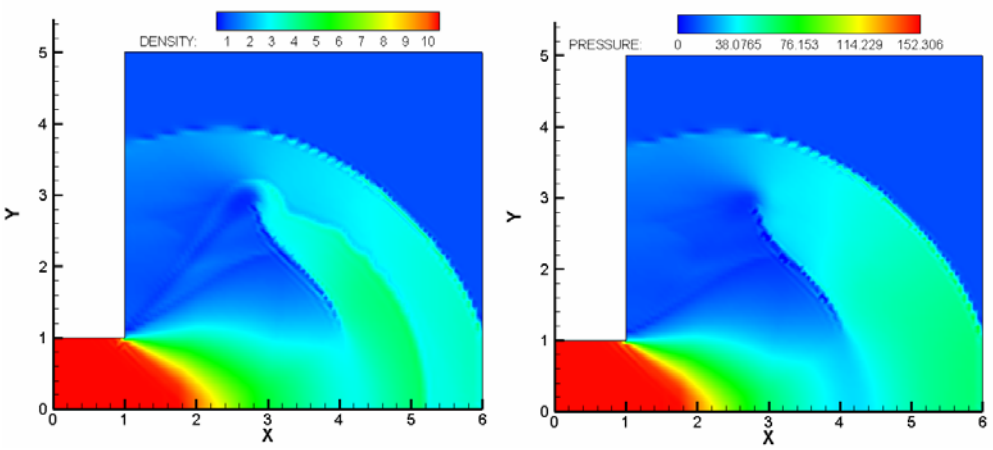

Fig. 1 Colored contour of density and pressure. Left: density. Right: pressure.

Example 3.2 This example is similar as example3.1. The simulation of gaseous detonation waves from narrow duct into unconstraint space when corner angles is 150°. An initiation zone is set at $x\in[0,2]$, and its initial value is given as $(\rho,u_x,u_y,E,\alpha,\beta)=(11,6.18,0,970,-1,1)$. The rest region is filled with the unreacted H_2/O_2 mixture with initial condition of $(\rho,u_x,u_y,E,\alpha,\beta)=(1,0,0,55,1,1)$. The left inlet is inflow condition. The other boundaries are rigid walls.

Similar as example3.1, the pressure and density drop very low at rarefaction region when detonation waves from narrrow duct into unconstraint space and they have not been negative.

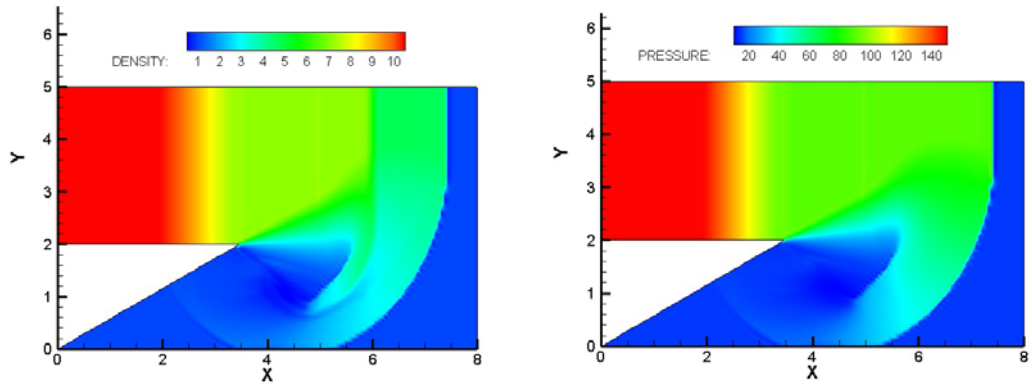

Fig. 2 Colored contour of density and presure. Left: density. Right: pressure.

Example 3.3 The simulation of gaseous detonation waves though the sawtooth geometry, as shown in fig.3. An initiation zone is set at $x \in [0,1.5]$, and its initial value is given as $(\rho, u_x, u_y, E, \alpha, \beta) = (6.14,1,0,13.782,-1,1)$; The rest region is filled with the unreacted H_2/O_2 mixture with initial condition of $(\rho, u_x, u_y, E, \alpha, \beta) = (1,0,0,0.6,1,1)$. The left inlet is inflow condition. The other boundaries are rigid walls.

Fig. 4 and fig. 5 show the colored contour of density and pressure. From the figure we can see that detonation wave becomes more complex after multiple diffraction and reflection. The pressure and density drop very low in diffraction zone and raise highly in reflection zone. Gas in pocket is rare and the reflection wave couldn't propagate here. Although the pressure and desity lower more and more and close to zero, they have not been negative. It shows that the method can simulate the detonation diffraction quite well in complex geometrical configurations.

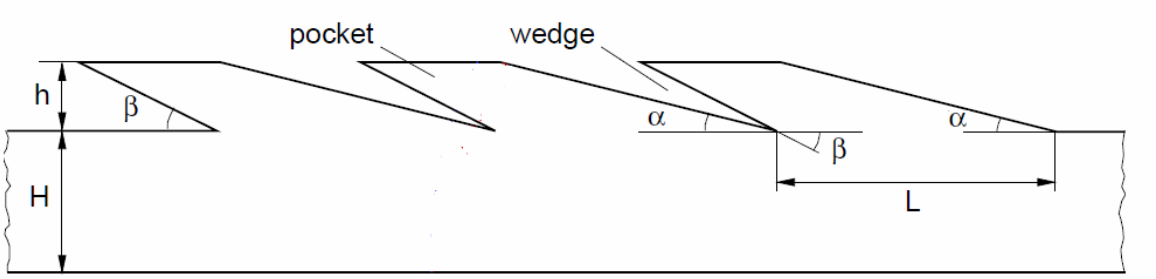

Fig. 3 Channel geometry. H=1, h=0.5, L=2, α=14°, β=27°

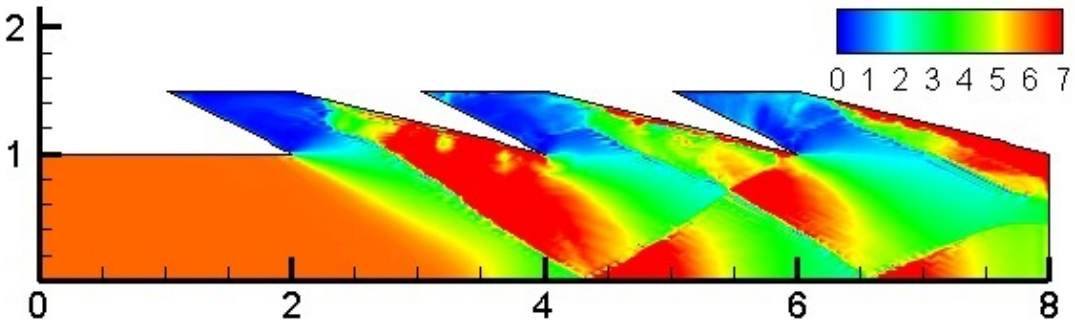

Fig. 4 Colored contour of density.

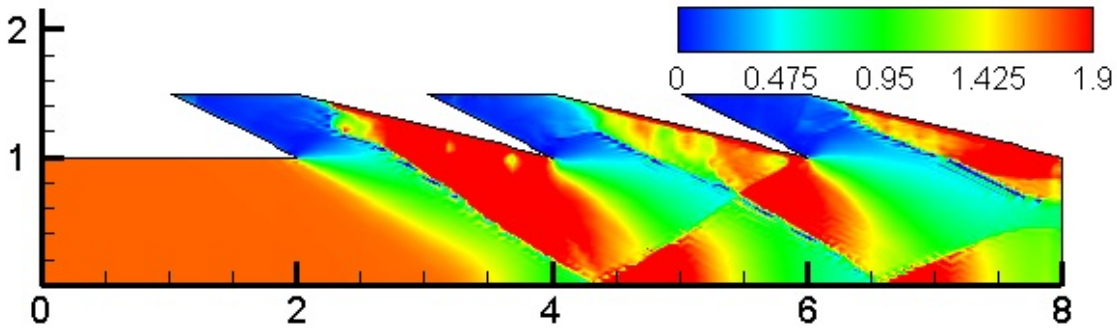

Fig. 5 Colored contour of pressure.

4 Conclusion

We discuss the positivity-preserving high order discontinuous Galerkin method for two-dimensional Euler equations with two-step chemical reaction, and show a method to solve the problem of negative density or negative pressure in high order numerical simulation. The method can keep the density and pressure positive without destroying accuracy and stability. In future work, we will use the method to carry out numerical simulation on gaseous detonation in more complex geometrical configurations and extend the method to numerical simulation of three-dimensional detonation.

Acknowledgments

This research is supported by the National Natural Science Foundation of China under grants 11221202 and 11272056, National Basic Research Program of China (Grant Nos. 2010CB832706 and 2011CB706904), and the Foundation of State Key Laboratory of Explosion Science and Technology (Grant No. ZDKT11-01).

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